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Doctor's Dissertation

**An Investigation of the Vibrational
Spectra of Glucose, Galactose, and Mannose**

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AN INVESTIGATION OF THE VIBRATIONAL
SPECTRA OF GLUCOSE, GALACTOSE, AND MANNOSE

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SUMMARY

Vibrational spectra have been obtained for the following compounds: α glucose-1-d, α glucose-6,6-d₂, α glucose-O-d₅, β glucose, β glucose-6,6-d₂, β glucose-O-d₅, α galactose, β galactose, α mannose, and β mannose. Many of these spectra were better resolved than in previous reports due to the use of low sample temperatures. The data base was completed by the addition of several literature reports for other deuterated variations of these three sugars.

A 46-parameter modified valence force field has been constructed, based primarily on the Snyder-Zerbi force field for aliphatic ethers but supplemented by values from other fields for hydrocarbons, alcohols, and ethers. This field was adjusted by means of the Fletcher-Powell algorithm to produce a least squares fit of the assigned to calculated frequencies for the glucose data sets. This refinement converged at an average error of 6.37 cm⁻¹ for 306 assigned frequencies. Although intermolecular effects are clearly evident in several spectral regions, the good fit achieved suggested that most of the vibrational motion could be understood in terms of the single, isolated molecule used in the calculations. The refined force field and calculated potential energy distributions were consistent with the results of others except with respect to the hydroxyl deformations.

The refined force field predicted the mannose and galactose spectra satisfactorily with an average error of 7.47 cm⁻¹ for 248 assigned frequencies. The normal modes predicted for all three sugars were compared to the calculations and group frequency assignments of others in some detail. Particular emphasis was placed on hydroxymethylene modes, the controversial modes found near 1150 cm⁻¹, and the Barker-Stacey "anomeric" correlations.

The refined field was also used to calculate spectra for each of the three possible staggered hydroxymethylene rotamers of both anomers of the three sugars. For five of these six anomers, the agreement between observed and calculated frequencies definitely favored one rotamer over the others as the most likely structure. These choices agreed with the crystal structure for both glucose anomers. For alpha mannose, the data argued for the presence of two of the three conformations. These calculations demonstrated the potential for hydroxymethylene conformational analysis in systems where crystallographic data are more ambiguous.

A series of normal coordinate calculations for methanol and ethanol are included as an appendix. These were undertaken primarily to provide better initial estimates of some of the constants in the carbohydrate field, but they also shed light on some alcohol assignment and conformation problems.

CHAPTER I

DEVELOPMENT OF A MODIFIED VALENCE FORCE FIELD FOR GLUCOSE

INTRODUCTION

A number of normal coordinate calculations for carbohydrates have appeared in the literature in recent years (1-9). Some of the workers involved have concentrated on calculations for glucose and its polymers using force fields transferred from noncarbohydrate systems (1-5), while others have stressed development of force constants specifically tailored to carbohydrates, using simpler systems such as the pentoses or the 1,5-anhydropentitols (6-9). These two courses of investigation converge in the present study, in which a modified valence force field is developed for glucose (Fig. 1).

Glucose, fortuitously, is both a very important and interesting sugar for detailed study and is a very promising system in experimental and computational terms. The biological and commercial importance of glucose is obvious, particularly as the monomer of cellulose and starch. Much of the information developed in understanding the vibrational dynamics of glucose can presumably provide a basis for understanding the polyglucans as well. The primary advantage of glucose as an experimental system is the commercial availability of carbon deuterated glucoses. Two such deuterated products were included in this study, and data for another have been reported in the literature (1,2). Since each distinct carbon deuterated glucose can give four sets of spectral data corresponding to the combinations of anomers and D₂O exchange, there is potential for a much broader data base than those employed in previous carbohydrate studies. This in turn implies a more reliable determination of the force constants. The glucose system is also favored by a high degree of prior physical characterization. The crystal structures of both anomers are known in detail, and extensive standards of purity have been published (10-14).

Figure 1. Structures of Alpha and Beta Glucose

Our intentions in this study have been threefold. The first and most basic was development and refinement of a force field for glucose, demonstrating in the process the applicability of the Fletcher-Powell (15) refinement procedure to the largest such problem ever attempted. The second aim was to assign, interpret, and place in historical perspective the spectra of glucose and perhaps those of other hexoses. The third was to provide a force field which could serve as a basis for investigations of higher saccharides. The first two objectives have been achieved to a satisfactory degree, and studies currently in progress have suggested that the third may also have been accomplished (16).

EXPERIMENTAL

SAMPLES

SOURCE

Alpha and beta glucose were usable as received from Phanstiehl Inc. Alpha glucose-1-d and -6,6-d₂ were purchased from Merck, Sharp, and Dohme of Canada Ltd. These were suitable for infrared spectroscopy as received but were too yellow to be stable in the laser beam of the Raman spectrometer. The necessary decolorization was done with activated carbon followed by recrystallization from ethanol. Beta anomers were prepared by both pyridine (17) and water-acetone (18) recrystallization. The former gave the pure beta anomer more easily, but the latter gave whiter material more suitable for Raman spectroscopy.

DEUTERATION

Oxygen deuterated samples of the alpha anomer were prepared by repeatedly wetting but not dissolving samples with D₂O in a drybox. The liquid was removed on each cycle in a 50°C vacuum oven contained within the drybox. Anomerically mixed samples could be prepared by allowing the sugar to dissolve completely and then to crystallize from the sirup.

CHARACTERIZATION

The ordinary alpha and beta glucose samples were characterized by comparison of their room temperature infrared spectra to those published by the National Bureau of Standards (13) in the range 4000-250 cm⁻¹. They were also compared to other published spectra as discussed below. The room temperature spectra of the alpha anomers of the two carbon deuterated glucoses have also been published (1, 19). The beta anomers prepared from them could be identified by their low

temperature spectra in the hydroxyl stretch region and below 500 cm^{-1} , since they are nearly identical to the "light" or ordinary compound in these ranges.

Both the anomeric form and the degree of deuteration of the D_2O exchanged materials could be determined by examination of the shapes and relative intensities of the $-\text{OD}$ and residual $-\text{OH}$ stretching bands at low temperature. The percent exchange should be regarded as approximate due to both the normal difficulties in making quantitative measurements with mulls and the probable nonlinearity of the concentration-intensity relationship in such mixed crystals.

MEASUREMENTS

SAMPLE PREPARATION

Infrared samples were prepared as mulls with fluorolube as the immersion medium from 4000 to 1325 cm^{-1} and Nujol from 1400 to 200 cm^{-1} . Hydroxyl deuterated samples were mulled under nitrogen in a drybox and sealed in an evacuated cell before removal. Raman samples were pressed into pure pellets and were preconditioned to the laser beam to reduce background "fluorescence" when necessary.

INSTRUMENTAL

Infrared and Raman spectra were recorded at room temperature for comparability to published room temperature data, and at liquid nitrogen temperature for increased resolution. The instrumentation consisted of a Spex 1401 Raman spectrometer, excited with a Coherent 52 argon laser and equipped with a Harney-Miller (20) cryostat, and of a Perkin-Elmer 621 infrared spectrophotometer equipped with a cryostat similar to that reported by Katon, *et al.* (21). Operating conditions were optimized according to Potts and Smith (22) and generally guided by Coblentz Class II specifications (23). A more detailed description of the instrumental conditions is given in Table I.

TABLE I
INSTRUMENTAL PARAMETERS

Infrared

Instrument: Perkin-Elmer Model 621 grating spectrophotometer

Control settings:

Scan speed	20 $\text{cm}^{-1}/\text{min}$	(setting: 10 x 16)
Resolution	2-3 cm^{-1}	(setting: 1000)
Gain		(setting: 5)
Time constant	1 sec	(setting: 1350)
Speed suppression		(setting: 5)
Source current	0.8 amp	

Optics: 4000-1350 cm^{-1} - CaF_2
1350-200 cm^{-1} - CsI

Temperature measurement: None

Calibration: Polystyrene frequencies after IUPAC standard (1961)

Raman

Instrument: Spex Model 1401 grating spectrophotometer

Control settings:

Scan speed	25 $\text{cm}^{-1}/\text{min}$	(setting: 2-E)
Resolution	$\sim 3 \text{ cm}^{-1}$	(setting: 150 μm)
Gain	20,000 cps scale	
Time constant	0.25 sec	

Excitation: 0.7-1.0 w at 5145 A or 4880 A

Sample geometry: Pressed pellets,
room temperature - 180° scattering
low temperature - 90° scattering

Temperature measurement: Bailey Cryo Thermometer

Calibration: Liquid benzene-carbon tetrachloride mixture,
frequencies after G. Herzberg. Infrared and Raman
spectra of polyatomic molecules. Van Nostrand, NY, 1945

EXPERIMENTAL RESULTS

SPECTRA

The vibrational spectra are reproduced in Fig. 2-10, and the band positions are tabulated in Tables II-X. Additional data for the refinements were obtained from the literature. This data included Vasko's (1,19) infrared spectrum of alpha glucose-1,2-d₂ and Barker's (24) infrared spectrum of beta glucose-1-d.

COMPARISON TO PREVIOUSLY PUBLISHED DATA

The room and low temperature infrared spectra of alpha glucose have been published many times, and these curves are in qualitative agreement with our data. Only Vasko (1,19) provides tabulated band positions determined with a modern spectrometer, but Katon's (21) curves are reproduced with sufficient resolution to qualify them as a second source of such data. Our data are in good agreement with both of these sources. We should note that the weak band found near 890 cm⁻¹ in our spectra and in many of those in the literature seems to show considerable variation in intensity between samples and is thus not positively associated with glucose.

The Raman spectrum of alpha glucose has been published three times, twice accompanied by tabulated frequencies (1,2,25,26). Our data agree with these except for bands reported at 897, 748, and 704 cm⁻¹ by Vasko (1,2). These weak features are not reported by Spedding (25) and are not visible in Hendra's (26) spectrum. We also have copies, from several laboratories, of unpublished spectra, recorded with different samples and spectrometers, which show no trace of the three bands. One possible partial explanation of the discrepancy could be found in an anomeric impurity, since the beta anomer has bands at 898 and 714 cm⁻¹.

Figure 2. Infrared Spectra of Alpha Glucose

Figure 3a. Raman Spectra of Alpha Glucose

Figure 3b. Raman Spectra of Alpha Glucose

TABLE II

SPECTRAL DATA — ALPHA GLUCOSE

Infrared, cm^{-1}		Raman, cm^{-1}	
Low Temperature	Room Temperature	Low Temperature	Room Temperature
1463			
1457	1459	1456	1458
1449	1447	1438	
1431	1427		1430
1413	1407	1414	1404
1385	1381	1384	
1376Sh ^a		1377	
1372	1371	1371	1369
1363		1361	
1350	1345Sh		1343
1342	1339	1344	
1331	1331	1329	1328
1300	1298	1299	1295
1288	1282		
1272Sh	1272	1271	1273
1268			
1261Sh			
1226	1224	1222	1220
1204	1203	1203	1205
1168Sh			
1151	1149	1152	1152
			1141Sh
1130	1128Sh	1130	
1121	1117Sh	1123	1123
1113	1111	1113	1113
1107	1103	1105	
1088Sh			
1081	1078	1076	1076
1075			
1065		1068	1068Sh
1059	1057Sh	1059	
1050	1050	1054	1045
1048Sh			
1033Sh		1033	
1024	1023	1023	1024
1015	1014Sh	1016	
1005	1000	1001	1004
998	994	995	
917	915	915	914
890			
837	837	841	842
778	775	774	772
768			
747		750	
722	725		
660			
657	646	659	652

TABLE II (Continued)

SPECTRAL DATA — ALPHA GLUCOSE

Infrared, cm^{-1}		Raman, cm^{-1}	
Low Temperature	Room Temperature	Low Temperature	Room Temperature
632	620	647	
600		616	
590		604	606
560	557	589	
545	545	558	556
540	538	540	540
526			
436	434	442	438
421	420	424	422
410	405	410	404
		401	
392	390	393	394
377	375	369	
			360
353	345		
331	325		
310Sh			
302	300Sh		302
289	285		286
266	270		269
248	255		
239Sh			
230			228
213	219		

^aSh = shoulder.

Figure 4. Infrared Spectra of Beta Glucose

Figure 5a. Raman Spectra of Beta Glucose

Figure 5b. Raman Spectra of Beta Glucose

TABLE III

SPECTRAL DATA — BETA GLUCOSE

Infrared, cm^{-1}		Raman, cm^{-1}	
Low Temperature	Room Temperature	Low Temperature	Room Temperature
1500Sh ^a	1480Sh		1475Sh
1468	1465Sh		
1449	1449	1450	1449
1415	1410	1413	
1401Sh		1402	1405
1380Sh			
1375		1387	1382Sh
1370	1373Sh	1375	
1360	1368	1364Sh	1369
1351Sh	1358	1354	1355Sh
1343Sh		1345Sh	
1310	1308	1310	1308
		1283	1278
1274	1270	1267	1263
1250	1252	1249	1250Sh
1225			
1220	1222	1225	1222
1210			
1199	1200	1205	1202
1156	1152	1157	1152
1129	1126	1130	1128
1117	1115Sh	1116	1114
1111	1110		
		1101	1097
1081	1080	1082	1079
1075		1069	
1064	1059	1065Sh	1065Sh
1049	1048Sh	1051	1050
1038		1038Sh	
1032	1033	1031	
1027			1024Sh
1018			
1015	1015	1012	
1002		1004	1006
914	912	917	913
903	899	902	898
859Sh			
764			
748	732		737Sh
718	710	717	714
656			
637	637	640	632
594	593		
588			
573	575Sh	577	574
557	555		
540Sh			

TABLE III (Continued)
SPECTRAL DATA — BETA GLUCOSE

Infrared, cm^{-1}		Raman, cm^{-1}	
Low Temperature	Room Temperature	Low Temperature	Room Temperature
520	517	522	519
		512	
464	459	460	454
427	425Sh	426	425
422	419		
402	400	401	401
385Sh	387		
		354	347
327	317	322	
314		312	309Sh
		219	
271	271	272	274
263			
249	250	247	247
			227
			206
			185
			166

^aSh = shoulder.

Figure 6. Infrared Spectra of Alpha Glucose-6,6-d₂

Figure 7. Infrared Spectra of Beta Glucose-6,6-d₂

Figure 8a. Raman Spectra of Alpha Glucose-6,6-d₂ and Beta Glucose-6,6-d₂.
Dashed Regions Obscured by Alpha Anomer Impurity

Figure 8b. Raman Spectra of Alpha Glucose-6,6-d₂ and Beta Glucose-6,6-d₂.
Dashed Regions Obscured by Alpha Anomer Impurity

TABLE IV

SPECTRAL DATA FOR ALPHA GLUCOSE-6,6-d₂

Infrared, cm ⁻¹		Raman, cm ⁻¹
Room Temperature	Low Temperature	Room Temperature
	1462	
1450Sh ^a	1450	1450Sh
1443	1443Sh	
		1425
1408	1415	
		1400Sh
1377 } _d	1382 } _d	
1372 } _d	1379 } _d	
1360	1373	1374
	1362	
	1357Sh	1354
		1343
1326	1326	1324
1298	1302	1293
1283	1286	1276
1240	1242	1238
1210	1213	1206
1156	1159	
1147	1149	1146
	1125Sh	
1117	1121	1122
	1112Sh	1110
	1096 } _d	
1092	1093 } _d	1092
1074	1077	
1062Sh	1063	1065
1050	1051	
1040	1041	1044
1020Sh	1021	
	1014	1013
1010 } _d	1011	
1003 } _d	1004	1000Sh
	996	
980	982 } _d	
	979 } _d	978
964	966	963
	957Sh	
	937	
917 } _d	920 } _d	915Sh
911 } _d	913 } _d	
770	773	
	764	
	754	
745	745	745
632	642	631
623	627	
	599	600

TABLE IV (Continued)

SPECTRAL DATA FOR ALPHA GLUCOSE-6,6-d₂

Infrared, cm ⁻¹		Raman, cm ⁻¹
Room Temperature	Low Temperature	Room Temperature
	587Sh	
556	559	555Sh
543	541 } ^a	
	536 } ^a	537
	525	
	487	487
465	467	
450	452	
	443Sh	439
424	426	425
	420	
400	405	399
390	394	
	389Sh	
367	368	
		358
340	348	
	329	
	310	
	297	
290	289	
270	270	274
		265
	255	250
	242	
		231
	224	
	210	210

^aSh = shoulder.

TABLE V

SPECTRAL DATA FOR BETA GLUCOSE-6,6-d₂

Raman, cm ⁻¹ ^b	Infrared, cm ⁻¹	
	Room Temperature	Low Temperature
	1475	1490
	1462	1471
	1450	1458
		1411
1405	1405	1402
	1375Sh ^a	1376
1371		1370Sh
1359	1359	1362
		1352
		1339
		1322
1305	1307	1308
1280	1272	1275
1251	1254	1257 } ^d
		1251 } ^d
1229	1230	1232
1206	1205	1207
1193	1192	1196
1150	1151	1155
1117	1118	1124
	1110	1112
	1084	1086
1080		1078
	1065Sh	1069Sh
1055	1057	1059
	1028Sh	1033
1016	1018	1024
1007	1005Sh	1003
		977 } ^d
972	973	975 } ^d
		959
		951
915	917	920
		895
872		872Sh } ^d
	866	868 } ^d
803	803	808
		763
	725	742
694	692	698
		673
	627	631
	592	594
		585Sh
575	575Sh	575Sh
555Sh		
	537	540

TABLE V (Continued)

SPECTRAL DATA FOR BETA GLUCOSE-6,6-d₂

<u>Raman, cm⁻¹^b</u>	<u>Infrared, cm⁻¹</u>	
	Room Temperature	Low Temperature
		530Sh
513	510	513
454	458	463
424	418	421
398	397	399
		385Sh
	318	326
		312
		284
	268	269
	250	250
		240
		225

^aSh = shoulder.

^bRaman spectrum partially obscured by alpha anomer impurity.

Figure 9. Infrared Spectra of Alpha Glucose-1-d

TABLE VI

INFRARED DATA FOR ALPHA GLUCOSE-1-d (cm^{-1})

Room Temperature	Low Temperature	Room Temperature	Low Temperature
	1470Sh ^a		917VW
1460	1459		878Sh) ^d
	1445Sh	875	876) ^d
1425	1433		837VW
1410Sh	1413	810	810S
	1385VW	761	765S
	1373		753
	1365		744
1348	1352		659Sh
	1345Sh	637	644
	1337,8	621	628
1328	1328,9		599
1292	1294	575Sh	591
	1277		558
1270) ^d	1272) ^d	552	552
1265) ^d	1269) ^d		540Sh
1231	1234	532	535
1207	1208	463VW	466
1167	1169	450	452
1132	1137		442
	1129	433	435
1119	1122	418W	420
1106	1110		415
1095	1098	404	408S
	1076Sh) ^d	389	391
	1074) ^d	375	377
1070) ^d	1067	345	353
1063) ^d	1060	325	331
1042VS	1043VS	300	302
1020VS	1023VS	290	289
1001	1005	269	267
994	997		247
981Sh	982		228
	967) ^d	218	211
963	964) ^d		
	955		

^aSh = shoulder; S = strong; W = weak; V = very.

TABLE VII
SPECTRAL DATA FOR BETA GLUCOSE-1-d^a

Cm^{-1}
1466 M ^b
1450 S
1440 W
1420 M
1413 S
1363 S
1350 S
1332 M
1270 S
1255 W
1240 S
1208 S
1178 VS
1130 M
1115 S
1085 VS
1072 S
1050 M
1032 VS
1020 VS
1010 S
{ 972 S
{ 965 S
900 S
875 W
835 VW
730 M
700 M

^aFrom Stacey, et al. (24).

^bM = medium; S = strong;
W = weak; V = very.

Figure 10. Infrared Spectra of Alpha Glucose-O-d₅

TABLE VIII

INFRARED DATA FOR ALPHA GLUCOSE-O-d₅^a (CM⁻¹)

Room Temperature	Low Temperature	Room Temperature	Low Temperature
1457	1456		958Sh
1440	1448Sh ^b	937Sh	943
	1411Sh		930
1404	1406		915
	1400Sh	894	898
1380	1381		874
1373	1373	863	868
	1367Sh		849
	1360Sh	835	835
	1350Sh		788
1339	1342		768Sh
	1337Sh	754	757
	1330Sh	705	707
1320	1323		658
	1315Sh	630	632
1297	1299		627
1281	1284	603	600
	1273	589	592
1260		557	564
1229	1231		533
	1203 ^b	512	517
1197	1199 ^d		500
	1185Sh	480	480
1167	1170		465
1153Sh	1156	424	432
1145	1148	410	419
	1131		397
1105Sh	1108		382Sh
1097	1098		371
	1085	362	360
1061	1065		343
1035	1040		329
	1030	295	299
1018	1020	271	275
1007	1009		
	979Sh		
968Sh	968		

^aApproximately 85% -OD.

^bSh = shoulder.

TABLE IX

PARTIAL INFRARED DATA — BETA GLUCOSE-C-d₅^a

Cm⁻¹

1449

1420

1409

1395

1272

1223

1186

1157

1140

890

870

721

^aDetermined by comparison of
alpha and mixed alpha-beta
samples.

TABLE X
INFRARED DATA FOR ALPHA GLUCOSE-1,2-d₂^a

Cm ⁻¹
1457 S ^b
1447 M
1421 S
1370 M
1341
1329 W
1294 Sh
1268 S
1220 VW
1206 Sh
1179 M
1163 W
1143 S
1106 S(Sh)
1088 S
1065
1053 Sh
1032 S
1003 M
987 S(Sh)
961 M
954 M
924 W
896 W
876 W
849 W
812 S
800 W
761 M
724 M-Br
640 Sh
624 M-Br
552 M
533 W
451 VW
427 W
403 W

^aFrom Vasko (1).

^bS = strong; M = medium;
W = weak; Sh = shoulder;
V = very; Br = broad.

The infrared spectrum of beta glucose has been widely reported, but modern data is restricted to Cael's (3) tabulation and Katon's (21) curves. Our data agree with these except for the weak band found by Cael at 1425 cm^{-1} . The Raman spectrum has been tabulated twice, and these results largely agree with our own. We do not, however, detect the weak bands reported at 1430 , 1421 , 1174 , 982 , and 589 cm^{-1} by Cael (3), at 870 and 825 cm^{-1} by Spedding (25), and near 1330 cm^{-1} by both authors. Both of these sources also report weak bands at 941 cm^{-1} . These are not visible in our room temperature spectrum, but our low temperature spectrum does have a very slight inflection at this location.

Barker (24) has published infrared data for alpha and beta glucose-1-d. Vasko (1) and Vasko, et al. (19) have also published the alpha glucose-1-d data and have added data for alpha glucose-6,6-d₂. After allowance for Barker's rock-salt prism instrument and for the relatively poor band definition in Vasko's spectra, we find no major discrepancies between these data and our own.

COMPUTATIONS

GENERAL

The vibrational problem was analyzed in the traditional way, using Wilson, et al. GF formalism (27). The unfamiliar reader can find this approach discussed at various lengths in many textbooks (27-30) or in brief outline form in Appendix VI. The construction of the geometric and potential models is discussed below with details and computer input given in the appendices. The potential assumed was a valence force field augmented with selected off-diagonal terms. Such fields are often designated "modified valence force fields" (31). The field was refined to a least squares fit with the experimental data using the Fletcher-Powell algorithm (15).

SOFTWARE

Our software package was derived from that published by Schachtschneider (32). The major modification was made by Pitzner (6), who substituted the nonlinear Fletcher-Powell method (FPM) algorithm for the traditional linear least squares (LLS) routine in the force constant refinement program. Other minor modifications have been made to accommodate core limitations, to facilitate data transfer between programs, and to display the output in the most useful formats. Our version of the software package as well as the earlier Pitzner version have been deposited on magnetic tape at the computer center of The Institute of Paper Chemistry. Pitzner's discussions in combination with the programs' internal documentation are adequate for their use.

GEOMETRY

One of the two major matrices required to form the secular equation, G , is constructed from known or assumed information about the masses and equilibrium positions of the nuclei. Since our computational strategem is to hold the G matrix elements fixed while seeking corrections to the F matrix, it is clearly desirable that the initial G elements be as accurate as possible. The atomic masses are not a problem, since they are known with great accuracy. For glucose, the atomic positions are also known with considerable accuracy. Crystallographic studies of alpha glucose with neutron diffraction by Brown and Levy (10) and of beta glucose with x-ray diffraction by Chu and Jeffrey (11) both produced excellent final agreement factors, less than 0.04. These two structures are in good mutual agreement on the pyranose ring geometry, but the C-H, O-H and C-O bond lengths show the systematic differences normally expected from the different scattering properties of the two types of beams (33,34). Neutron diffraction provides better estimates of nuclear positions and is thus the favored source

of information, but it still systematically underestimates bond lengths if one of the bonded atoms has a large vibrational amplitude (35). Fortunately, Brown and Levy (33) have recently published vibrational motion corrections applicable to the O-H and C-H bond lengths in their previously published alpha glucose structure (10).

The geometric model chosen for use in the calculations was a synthesis of the diffraction results and the known corrections. The ring atoms for both anomers were placed at the relative positions found for alpha glucose while all C-H, O-H and nonanomeric hydroxyl C-O bonds were set at averaged values of 1.110, 0.986, and 1.420 Å, respectively. The anomeric C-O bond was set at 1.389 Å, again the alpha value, and all COH angles were taken as tetrahedral. All other dihedrals were as found in the respective crystal structures. Although the averaging of C-O lengths and COH angles was less necessary for alpha glucose than for beta glucose, it served to put the models for the two anomers on a more equivalent basis. Use of the alpha coordinates for the beta ring simplified the calculations considerably, since it eliminated the need to average the ring bond lengths. The bond lengths for the isotopic compounds were taken as identical to their ordinary analogs. In our experience, geometric changes comparable to the greatest uncertainties in this model (0.01 Å) do not produce significant changes in the calculated spectra.

The internal coordinates were derived according to the prescription of Decius (36,37), as supplemented by Hilderbrandt (38) with respect to the torsions. This results in a 78-member coordinate set corresponding to the 66 (3N-6) internal degrees of freedom and twelve redundancies. Since six of these redundancies result from the ring structure, they cannot be eliminated by any transformation short of full diagonalization. We must thus be aware of the linearly dependent

nature of the coordinate set and the impossibility of determining unique, independent values for the force constants (39).

The geometric information, internal coordinates, and input for the various computer programs required to construct the G matrices for alpha and beta glucose and their isotopic variants are collected in Appendix I.

INITIAL FORCE FIELD

In view of the close relationship of the two systems, the natural source for an initial glucose force field was the field developed for the pentose sugars (9). We thus began by constructing trial fields from the pentose constants augmented with some hydroxymethylene values developed for the pentitols (8). This eventually led to an 83-parameter field which reproduced the frequency data well after refinement and was consistent with the trends of the earlier carbohydrate studies. After some consideration, however, we came to question several of the assumptions underlying this solution and decided to explore other possibilities for construction of an initial field.

The most unsatisfactory feature of our 83-parameter solution was its incompatibility with the group frequency literature for hydroxyl deformations. The COH deformations were calculated primarily in the 1250-1100 cm^{-1} range, while the literature suggested that a more appropriate range would be 1500-1350 cm^{-1} (40,41). A further review of the literature revealed that the hydroxyl bending constant which had evolved through the previous studies (1-8) was of the same order as found for gaseous methanol (42,43) and 20% below that found for hydrogen bonded hydroxyls in crystalline methanol (44). Since, as previously mentioned, the various constants are not independent, the presence of one apparently spurious constant can influence the values of the others. To estimate

these effects and to aid in the construction of a better trial field for glucose, we undertook a normal coordinate study of methanol and ethanol in both the free and hydrogen bonded states. The results of this study, described in Appendix III, indicated that the deformation could be raised to an appropriate hydrogen bonded value without greatly disturbing the rest of the constants.

Although the results of the alcohol study could have been taken as justification of a corrected 83-parameter field, the process of carrying out these studies provided insight which argued for construction of a much simpler trial field. Much of this insight was derived from the use of linear refinement procedures with the small molecules and examination of the more extensive statistical information available in such refinements. These statistical tests suggested that there were several classes of interaction constants in the alcohol fields which were so highly correlated with diagonal constants that attempts to assign them independent values were nearly meaningless. These classes of constants were eliminated from the glucose field.*

We also noted that some subdivisions of the field based on differing chemical environments did not seem to be statistically justified. As an example, the 83-parameter field distinguished separate C-O stretch constants for the ring oxygen, anomeric hydroxyl, and other hydroxyls, but the range of the three refined values was comparable to the standard error estimated for such constants in the alcohol study. If the subdivisions of the field do not, on refinement, yield values which are significantly different, then the primary effects of the subdivision are the negative ones resulting from the decrease in degrees of freedom. These include increased uncertainty in the constants, greater sensitivity to initial misassignments, and decreased significance of a given level of average error.

*

The types of constants eliminated are summarized in Table XXXV, Appendix III.

Since the difficulty in estimating a constant has an inverse relationship to the number of times it appears in the $F_{\mu\nu}$ matrix, it is particularly difficult to estimate a constant corresponding to a unique location in a molecule, unless the constant gives rise to an uncoupled mode in an isolated spectral region.

In light of our discomfort with the assumptions underlying them, we decided largely to ignore the previously refined carbohydrate fields and to construct a simpler 46-parameter initial field based on the Schachtschneider and Snyder hydrocarbon field (45), on the Snyder and Zerbi aliphatic ether field (46), and on our own alcohol fields. This simpler 46-parameter field is summarized in Table XI (p. 47). The only distinctions based on chemical environment are the separate constants for deformation of free and hydrogen bonded hydroxyl groups. The choice of off-diagonal terms paralleled that for ethanol. These selections do not constitute a claim that the ideal $F_{\mu\nu}$ matrix elements are independent of chemical environment but rather an admission that we did not expect to determine them with sufficient accuracy to resolve the environmental differences. The standard errors estimated for the final glucose constants tended to support these assumptions.

Several of the environmental differences ignored in the calculations are worthy of further comment. The hydroxyl groups in alpha and beta glucose are known to be involved in hydrogen bonds which vary considerably in strength (10, 11). If the methanol data may be taken as an indication (42-44), maximal agreement with experiment might require ten distinct hydroxyl deformation constants spanning a 20-30% range of values, rather than the two we have used. Likewise, the C-O bond lengths of the anomeric hydroxyls are about 3% shorter than the rest of the C-O bonds (10,11), corresponding to about 20% double bond character (47) and seemingly requiring a separate constant. We have not made these distinctions in deference to the difficulties of estimating constants that appear

only once in the Z matrix. Since it seems unlikely that sufficient isotopic data will be available in the near future to evaluate such constants, perhaps other short term solutions should be sought to allow progress in assignments and force field precision. One possibility for this would be the use of scaling functions based on external sources of bond order information, which would recognize major environmental differences without decreasing the degrees of freedom.

REFINEMENT STRATEGY

Hardware Limitations

The overall strategy for refining the field was derived both from hardware limitations and predispositions concerning the desirable form of the final solutions. The most basic limitation was the 128K core of the IBM 360/44 computer used for most of the work. This restricted refinements to secular equations of 75×75 or less when using the Pitzner software package (6). The 78×78 glucose problem was approached by elimination of the hydroxyl stretching coordinates, which reduced the problem to 73×73 and is equivalent to setting the corresponding force constant to infinity. This has been shown to have little effect on the calculated frequencies below 1500 cm^{-1} (48).

The second basic limitation was the speed of the processor. Since, with all the data, glucose refinements taken to convergence required thirty or forty hours of execution time, they were difficult to schedule, and only five were ever carried out. All preliminary refinements were thus run either with partial data sets or were terminated short of convergence. As a result of this limitation, far fewer permutations of assignments and initial force fields were explored than has been typical in this series (6-9). While it is unlikely that further computation would have much effect on the overall form of the solutions unless a drastically different initial force field were chosen, it is likely that small improvements could be effected by exploring more permutations on the present assignments.

Late in these studies, some time was available on an IBM 370/158 computer with a 2M hard core and 14M virtual core. This disposed of the size restrictions on the secular equation for all practical purposes. While some calculations were made possible which would not have been so on the 360, such as linear refinement of the 73 x 73 problem, we saw no real value in restoration of the hydroxyl stretch coordinates at this stage. No net advantage was gained in available refinement time, since the fourfold increase in processing speed was more than offset by the heavier usage rate of the 370.

Software Limitations - Fixing of Constants

The third key computational restriction derives from the form of the secular equation rather than from the hardware configuration. The large number of redundancies implies a highly correlated force field and therefore a very nearly singular $\underline{JZ}$ matrix. In such cases, several courses are possible to obtain corrections to the force constants. The classical LLS minimization procedure requires computation of the inverse $\underline{JZ}$ matrix and is thus unstable unless the matrix can be made less singular. The concept of degrees of singularity, which may seem strange from a classical viewpoint, arises from the computational methods. Due to round-off error in the computer, the truly singular matrix with zero determinant is rarely seen. The practical measure of singularity is the value of the determinant, and a matrix may be regarded as nonsingular if the determinant has a large enough value that the inversion process is not ill-conditioned.

The normal method for reducing the degree of singularity to an acceptable level is to hold some parameters fixed, resulting in the elimination of rows and columns from the $\underline{JZ}$ matrix (31). This approach was tried with the 1,5-anhydropentitols, a simpler carbohydrate system than our own, but it failed (6). An alternative, less used method is the nonlinear Fletcher-Powell algorithm (15), which does not require the inverse $\underline{JZ}$ matrix. The linear method is much faster

computationally, but the identification of those constants which must be held fixed is arbitrary and tedious, and generally requires time consuming trial refinements. We have therefore chosen the slower Fletcher-Powell method for the simplicity provided by its superior convergence properties.

Exclusion of Constants from Refinement

Although with the FPM none of the constants had to be fixed to allow convergence, several were withheld from refinement because of doubts that they could be estimated from the experimental data. These included both cases where the parameter appeared only once in the $\underline{F}$ matrix and cases where the initial estimates did not seem sufficiently reliable to assume good assignments.

In both ethanol and diethyl ether the oxymethylene "scissors" mode near 1480 cm^{-1} is invariant with change of state or deuteration at adjacent positions (49, 50). This suggests that the HCH bending coordinate is nearly a normal coordinate and that the HCH bending force constant will influence only this frequency. In both of these studies (49, 50) the inclusion of isotopic data sets in which the scissors mode was isolated from other bands permitted a reasonable estimation of the bending force constant. The calculations (49, 50) confirmed the uncoupled nature of the scissors mode and gave values for the bending constant similar to those found for the aliphatic hydrocarbons (45). Snyder and Zerbi, however, in a study of aliphatic ethers involving less isotopic data, found a lower value for the oxymethylene bending constant and calculated a much more coupled scissors mode (46).

In glucose, the pattern and isotopic substitution behavior of the methylene bands is similar to ethanol, suggesting similar normal modes. The bending constant, however, appears only once in a much larger $\underline{F}$ matrix, and the scissors mode is much less isolated, even in the most favorable isotopic data sets. This would be expected to make the bending constant difficult to estimate,

and in fact trial refinements showed the constant drifting toward lower values with an increase in coupling for the scissors mode. To maintain normal modes similar to those found for ethanol, the methylene bending constant was fixed at 0.52, a value high enough to result in a pure scissors mode, and was excluded from refinement. We might note that Snyder and Zerbi's (46) lower value of 0.47 has been transferred more widely to carbohydrate systems (1-4,6-9) than any other value, accounting for some of the differences between our descriptions of the methylene modes and those of others.

The COH deformation constants were held fixed in recognition of the previously discussed limitations of the model and the resulting low probability of accurate initial assignments for the hydroxyl modes. The values chosen for these deformation constants were selected so that the calculated COH deformation frequencies for beta glucose-d₇ would correspond to the average of the frequencies observed experimentally for beta arabinose-d₆ (9). The primary intent of such a COH model is not to calculate the COH deformations accurately but to allow calculation of modes with lower COH contributions and to provide insight into the general form of the coupling between the hydroxyl deformations and other motions.

No attempt was made to refine the torsional constants for several reasons. First, there has been considerable variation in the conventions used for defining the torsional coordinates in earlier studies. Since the various conventions can lead to substantial variations in the resulting force constants and since the exact convention employed is not always clearly reported, it is difficult to establish consensus values from the literature for these force constants. We accept the arguments of Hilderbrandt (38) concerning the definition of torsional coordinates and have followed his conventions. This has limited our data available for initial estimates to his reported values for ethane and isobutane (38) and our values for methanol and ethanol. The C-C and hydroxyl C-O constants

were set near the values found for ethanol, and the ring C-O value was set between these two. These constants are of the same order of magnitude as those determined for various six-membered rings by Pickett and Strauss (51), but the two sets are not directly comparable since they correspond to different types of potential functions.

In addition to the uncertainty in the initial values of the constants, there is another factor arguing against attempts to refine them. Below 350 cm^{-1} , considerably more bands are observed than calculated. Although one could attempt to develop criteria for recognition of the purely internal fundamentals in this region based on such factors as relative intensities, band widths, and pressure or temperature response, such an effort would be highly speculative and unprecedented for molecules of this type. Without such recognition criteria the assignments must be regarded with caution, and it is better to postpone refinement of the torsional constants.

The OH stretching constants could not be defined, of course, since the corresponding coordinates were omitted in formulating the problem. Examination of the various isotopic data sets in the C-H stretch region suggested problems with Fermi resonance, a fairly common difficulty in this frequency range. The C-H constants were thus left at the values found for methanol and ethanol, and no attempts were made to make assignments in this region. In all, this made eight out of a total of 47 constants frozen during refinement. Since constant 47 is a dummy parameter, this left 38 variable parameters in the final refinements.

Band Assignments

While the choice of the initial force field is undoubtedly the most crucial step in the refinement process, the assignment of observed to calculated

frequencies also has considerable influence on the course of the refinement. A calculated mode is generally assigned to the nearest experimental band and unless the initial field is good enough to allow making most of the assignments on this basis, a successful refinement is unlikely. There are, however, other criteria to strengthen assignments, to guide choices in ambiguous cases, and to suggest exceptions to the minimum error rule. Some of these relate to the potential energy distributions of the calculated modes and will be discussed in connection with the evaluation of solutions, but others are specific to the assignment stage and will be discussed here.

One of the most vexing problems in the assignment process for large molecules is the recognition of the fundamental modes in the experimental spectra. We have whenever possible assigned only bands which are visible in the Raman spectrum, since overtone and combination bands are expected to be much weaker in the Raman than in the infrared spectrum in the absence of Fermi resonance (52). The 900 to 400 cm^{-1} region contains the so-called hydroxyl out-of-plane deformations. These modes, which are very intense in the infrared, apparently involve intermolecular coordinates (44) and thus do not correspond to modes calculated with the isolated molecule approximation. Since most of the amplitude for such motions is apparently associated with the hydroxyl proton, they are expected and observed to have very low Raman intensity. This makes the criterion of Raman observability even more useful.

We have used room temperature frequencies in the refinements, despite the superior resolution of the low temperature spectra, in order to utilize a number of room temperature data sets from the literature (1,19,24). The low temperature data were examined to reveal which room temperature bands were actually unresolved multiplets. Since most of the bands shift only slightly between 100 and 300°K, this convention is probably of only minor importance.

CALCULATIONS

G and Z matrices were constructed using the potential and geometric models described above. The secular equation was then solved and the potential energy distributions obtained. After assignment of the experimental spectra the average error was about 13 cm^{-1} , and the pattern of correspondence between observed and calculated frequencies was encouraging enough to suggest refinement of the force field. The constants were improved in a series of three FPM refinements involving 10, 15 and 13 cycles of nonlinear least squares adjustment. As the field evolved, assignments were adjusted between refinements to maintain the minimum error criterion. The refinement was terminated after the ratio of the sums of squared errors on successive cycles had been greater than 0.995 six times. Further details of the refinement and the convergence conditions have been given by Pitzner (6). The final field was used as the starting point for a single cycle damped LLS refinement, primarily to estimate certain statistical parameters not available with the nonlinear program.

The refined force field is listed in Table XI along with uncertainties for the constants estimated in both the linear and nonlinear refinements. Neither of the error figures should be regarded as true standard errors, but rather as very rough figures for purposes of internal comparison. The estimates from the LLS refinement are tainted by both the correlation in the force field and the damping and scaling used in the refinement. The figures developed for the nonlinear refinement are subject to both of these objections and to the fact that they are good approximations only if the number of cycles in the final refinement approaches the number of variable parameters (7). The correlation matrix determined in the linear refinement is included in Appendix II.

TABLE XI
MODIFIED VALENCE FORCE FIELD FOR GLUCOSE

Description ^a	Code ^b	Final	Initial	Change	Error ^c	Error ^d	Reported Range ^e
Bond Stretching							
1. OH	OH	(5.50) ^f	(5.50)	-	-	-	6.28 - 6.21
2. CH	CH	(4.65)	(4.65)	-	-	-	4.72 - 4.59
3. CO	CO	5.13	5.07	0.06	0.012	0.069	5.17 - 4.96
4. CC	CC	4.21	4.25	-0.04	0.013	0.122	4.43 - 4.18
Bond Angle Bending							
5. COH (free)	COH	(0.77)	(0.77)	-	-	0.016	0.80 - 0.77
6. COH (bonded)	BCOH	(0.95)	(0.95)	-	-	0.003	0.96 - 0.86
7. OCH	OCH	0.87	0.91	-0.04	0.009	0.017	0.98 - 0.85
8. HCH	HCH	(0.52)	(0.52)	-	-	0.103	0.57 - 0.45
9. CCH	CCH	0.66	0.63	0.03	0.007	0.015	0.79 - 0.62
10. CCC	CCC	1.02	1.07	-0.05	0.013	0.098	1.11 - 1.05
11. OCO	OCO	1.11	1.09	0.02	0.013	0.159	1.24 ^g
12. CCO	CCO	1.34	1.25	0.09	0.012	0.048	1.32 - 1.17
13. COC	COC	1.26	1.20	0.06	0.013	0.189	1.89 - 1.31
Torsions							
14. C-O (hydroxyl)	T-OH	(0.03)	(0.03)	-	-	0.006	0.06 - 0.02
15. C-C	T-CC	(0.10)	(0.10)	-	-	0.045	0.10 - 0.01
16. C-O (ring)	T-CO	(0.05)	(0.05)	-	-	0.060	0.07 - 0.01
Stretch - Stretch Interaction							
17. C-C-C	SS17	0.11	0.10	0.01	0.010	0.049	0.12 - 0.10
18. C-C-O	SS18	0.31	0.13	0.18	0.013	0.028	0.24 - 0.10
19. O-C-O	SS19	0.12	0.15	-0.03	0.013	0.080	0.38 ^g
20. C-O-C	SS20	0.16	0.21	-0.05	0.013	0.080	0.32 - 0.28
Stretch - Bend Interactions							
21. CC, CCC	SB21	0.48	0.41	0.07	0.012	0.049	0.48 - 0.27
22. CC, CCO	SB22	0.44	0.37	0.07	0.012	0.046	0.41 - 0.05
23. CO, COC	SB23	0.37	0.48	-0.11	0.013	0.100	0.74 - 0.48
24. CO, OCO	SB24	0.51	0.55	-0.04	0.012	0.077	0.52 - 0.24
25. CC, CCO	SB25	0.51	0.62	-0.11	0.014	0.043	0.74 - 0.62
26. CC, CCH	SB26	0.34	0.32	0.02	0.013	0.019	0.52 - 0.24
27. CC, OCH	SB27	0.52	0.48	0.04	0.009	0.018	0.48 - 0.30
28. CC, COH	SB28	0.42	0.41	0.01	0.012	0.023	0.42 - 0.24
Bend - Bend Interaction							
29. H-C-C-H (t)	BB29	0.16	0.07	0.09	0.001	0.005	0.12 - 0.04
30. H-C-C-H (g)	BB30	-0.02	0.0	-0.02	0.011	0.007	0.01 - (-0.02)
31. H-C-C-C (t)	BB31	0.02	0.05	-0.03	0.013	0.040	0.07 - (-0.15)
32. H-C-C-C (g)	BB32	0.02	-0.05	0.07	0.008	0.018	(-0.18) - (-0.05)
33. H-C-C-O (t)	BB33	0.12	0.07	0.05	0.015	0.032	0.16 - (-0.04)
34. H-C-C-O (g)	BB34	-0.19	-0.12	-0.07	0.002	0.016	(-0.24) - (-0.12)
35. H-O-C-C (t)	BB35	-0.09	0.0	-0.09	0.014	0.019	0.10 - (-0.01)
36. H-O-C-C (g)	BB36	-0.17	-0.05	-0.12	0.015	0.015	0.02 - (-0.01)
37. H-C-O-C (t)	BB37	0.18	0.05	0.13	0.017	0.047	(-0.24) - (-0.10)
38. H-C-O-C (g)	BB38	0.02	-0.10	0.12	0.012	0.048	0.03 - (-0.37)
39. H-O-C-H (g)	BB39	0.04	0.0	0.04	0.005	0.005	.12 - 0.00
40. X-X-X-X (t)	BB40	-0.01	-0.01	0.00	0.013	0.052	0.04 - (-0.09)
41. X-X-X-X (g)	BB41	0.04	0.01	0.03	0.005	0.032	0.07 - (-0.11)
42. X-(X-X)-X	BB42	0.08	-0.04	0.12	0.012	0.025	0.05 - (-0.10)
43. H-(X-X)-X	BB43	-0.08	-0.03	-0.05	0.007	0.013	0.03 - (-0.31)
44. H-(X-X)-H	BB44	0.00	-0.02	0.02	0.007	0.008	0.08 - (-0.03)
45. X-(X-H)-X	BB45	0.03	0.01	0.02	0.009	0.016	0.01 - 0.00
46. X-(X-H)-H	BB46	0.00	0.0	0.00	0.002	0.056	0.23 - 0.00

TABLE XI (Continued)

^aThe only special convention employed for interacting coordinates is in the form A-(B-C)-D which refers to the bend-bend interaction of the coordinates A-B-C and D-B-C.

^bThese codes identify the corresponding force constants when they appear in the potential energy distributions.

^cError estimated by Program FLPO at termination of glucose refinement. See Pitzner (6) for details.

^dError estimated from linear refinement Program FADJ on a single cycle refinement starting from the final glucose field.

^eValues from References 1-4,6-9,45,46,49,70,101, and Table XXXXI, Appendix III.

^fValues in parentheses were not refined.

^gOnly one literature value (9).

^hUnits for force constants:

Stretch and stretch-stretch — mdyn./A

Bend and bend-bend — mdyn.A/(rad.)²

Torsion and stretch-bend — mdyn./rad.

The statistics of the fit are included in Table XII, and the correspondence between observed and calculated energy levels is shown graphically in Fig. 11-19. In these figures, the absence of experimental bands corresponding to some of the calculated frequencies may be due to any of the following: unobservability due to band overlap, unobservability due to the limited frequency range of the spectrometer, unobservability due to low intensity, or erroneous frequency calculation due to weakness of the model. The first two situations are obvious from examination of the spectra, but the last two may be very difficult to separate. Appendix II gives the details of this fit in tabular form as well as condensed potential energy distributions for the normal modes both in terms of the force constants and the internal coordinates. The full potential energy distributions and Cartesian displacement coordinates were placed on magnetic tape for permanent retention at The Institute of Paper Chemistry.

EVALUATION OF SOLUTIONS

GENERAL

Use of the Fletcher-Powell refinement procedure has effectively eliminated convergence problems in our studies, but the mere fact of finding a solution to the least squares minimization problem does not guarantee insight into the vibrational dynamics of the system. Such a solution has no claim to uniqueness, but many investigators feel that it may provide a useful model for discussion of the vibrational problem if viewed in the proper perspective and if certain tests of validity are satisfied.

AVERAGE ERROR AND RELATED TESTS

The most basic test of a solution is a low average error between observed and calculated frequencies. Most studies claiming successful refinements have

TABLE XII
SUMMARY OF HEXOSE RESULTS

	Error, cm ⁻¹	Number of Frequencies
(1) Alpha glucose	5.74	40
(2) Alpha glucose- <u>O</u> -d ₅	7.12	44
(3) Alpha glucose-1,2-d ₂	7.70	32
(4) Alpha glucose-1-d	5.40	38
(5) Alpha glucose-6,6-d ₂	5.75	36
(6) Beta glucose	6.54	43
(7) Beta glucose- <u>O</u> -d ₅	5.09	12
(8) Beta glucose-1-d	6.33	23
(9) Beta glucose-6,6-d ₂	<u>6.81</u>	<u>38</u>
Glucose total	Average = 6.37	Total = 306
(10) Alpha galactose	7.24	40
(11) Alpha galactose-1-d	8.97	29
(12) Beta galactose	8.15	35
(13) Alpha mannose	6.05	47
(14) Alpha mannose-1-d	7.13	30
(15) Beta mannose	7.39	40
(16) Beta mannose-1-d	<u>8.28</u>	<u>27</u>
Hexose total	Average = 7.47	Total = 248
Grand total	Average = 6.86	Total = 554

ALPHA GLUCOSE

CALCULATED

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM. -1)

Figure 11. Assigned and Calculated Frequencies for Alpha Glucose

ALPHA GLUCOSE-6,6-D2

CALCULATED

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM.-1)

Figure 12. Assigned and Calculated Frequencies for Alpha Glucose-6,6-d₂

ALPHA GLUCOSE-1-D

CALCULATED

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM.-1)

Figure 13. Assigned and Calculated Frequencies for Alpha Glucose-1-d

ALPHA GLUCOSE-0-D5

CALCULATED

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM.-1)

Figure 14. Assigned and Calculated Frequencies for Alpha Glucose-0-d5

ALPHA GLUCOSE-1, 2-D2

CALCULATED

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM. -1)

Figure 15. Assigned and Calculated Frequencies for Alpha Glucose-1,2-d₂

BETA GLUCOSE

CALCULATED

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM.-1)

Figure 16. Assigned and Calculated Frequencies for Beta Glucose

BETA GLUCOSE-6, 6-D2

CALCULATED

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM.-1)

Figure 17. Assigned and Calculated Frequencies for Beta Glucose-6,6-d₂

BETA GLUCOSE-1-D

CALCULATED

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM. -1)

Figure 18. Assigned and Calculated Frequencies for Beta Glucose-1-d

BETA GLUCOSE-0-D5

CALCULATED

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM.-1)

Figure 19. Assigned and Calculated Frequencies for Beta Glucose-0-d₅

reported average errors in the 5-10 cm^{-1} range (7-9,42-46,49). Our average error after the final refinement of 6.37 cm^{-1} for 306 frequencies is thus fairly low by literature standards. While low average error is a necessary condition, it is not sufficient. Acceptability of a solution requires a more detailed error analysis as well as certain characteristics in the force field and potential energy distributions. One of the most important aspects of the error analysis is consideration of the distribution of errors, particularly for the isolated bands. Our error distribution, summarized in Table XIII, is roughly Gaussian and shows no evidence of multimodal character. A large difference between the overall average error and the errors of the isolated bands could suggest that a low overall error is the result of fortuitous misassignments in the more crowded spectral regions. Our errors for the isolated bands are higher than the overall figures, but not drastically so. Unfortunately, these statistics are hard to interpret in the present case since most of the isolated bands are found in the 1000-500 cm^{-1} region, and this region also contains the previously discussed hydroxyl out-of-plane bands. The increased error for these bands might thus reflect either misassignments elsewhere or a lower validity of the isolated molecule approximation in this region.

The extreme case of error, the unassignable mode, deserves particular attention. As evident from Fig. 11, almost all of the calculated modes fall near experimental bands. The largest group of unassignable calculated bands are COH deformations near 1400 cm^{-1} . This difficulty is not unexpected in view of the previously discussed limitations of the COH model. Bands are calculated but not observed near 940 cm^{-1} for both alpha and beta glucose. As previously discussed, two earlier authors have reported a weak Raman band at 941 cm^{-1} for beta glucose (3,25). We do not observe it and are uncertain if it represents an artifact in the previous work or an oversight in our own. The calculated

bands are primarily heavy atom stretching motions whose positions are relatively insensitive to the force field. It is thus likely that they would remain unassigned unless the initial force field were changed rather drastically.

TABLE XIII
ERROR DISTRIBUTION — GLUCOSE REFINEMENT

Range, cm ⁻¹	Positive Errors	Negative Errors	Total
0-4	73	66	139
4-8	44	37	81
8-12	26	24	50
12-16	13	9	22
16-20	5	4	9
>20	2	3	5
>30 cm ⁻¹ errors	0	0	0

Observed Number ^a	Observed, %	Predicted % (Gaussian)
21>2σ	6.7	4.6
102>σ	32.4	31.7

^aStandard deviation approximated by the average of the absolute values of the errors.

The only serious case of an apparent experimental fundamental which does not correspond to a calculated mode is the 705 cm⁻¹ band in the alpha glucose-0-d₅ infrared spectrum. The intense, isolated, temperature insensitive nature of the band nominates it as a fundamental, but the nearest calculated bands are over 50 cm⁻¹ away in either direction, and they are more readily assignable to other experimental bands. In this oxygen deuterated compound, interference from hydroxyl out-of-plane modes should be minimal at 700 cm⁻¹, but the source of the difficulty could still be the weakness of the isolated molecule approximation in this region. The composition of our data base has weighted the refinements

heavily toward the assumption that the bands assigned in the $800\text{--}500\text{ cm}^{-1}$ region for the COH compounds are pure internal modes, uninfluenced by intermolecular coupling. Any breakdown of these assumptions would be expected to manifest itself in an inability to calculate the COD spectra in the same region.

FORCE FIELD

The error analysis described above is primarily a test of the internal consistency of a solution. An external frame of reference can be established by comparison of the final field and potential energy distribution to relevant studies in the literature. Table XI summarizes the initial and final force fields as well as the ranges of values reported for other related systems. Most of the constants, particularly the crucial diagonals, showed only small changes on refinement, and the final values fall in or near the previously reported ranges. This, however, is only a very rough test, since all the fields included in the comparison were obtained using redundant internal coordinates. Although the redundancy conditions have not been expressed in exact form for any large molecules, it is highly probable that there is no unique set of force constants corresponding to a given set of eigenvalues. It is thus possible for two sets of constants to be quite dissimilar numerically yet to give the same $\underset{w}{F}$ matrix and thus to represent the same potential energy model. In practice, due to the common genealogy of many of the published fields and the use of damped refinement techniques, there is considerable similarity in the constants evaluated for similar structures. In this context a large discrepancy between a refined value and the literature range for the same constant can be regarded as a hint of trouble. We do not consider any of our constants to be an unreasonable distance from reported values.

The relatively wide ranges reported for many of the constants seem to contradict the much smaller limits of error quoted for them by various authors

and perhaps even create the false impression that there is wide latitude in the choice of an initial force field. A likely origin of these wide ranges is the correlation within the fields. Since this correlation is largely a function of the coordinate redundancies, it will differ between systems with different coordinate sets. For this reason, transfer of constants between systems with the same coordinate set and thus the same set of linear constraints defining acceptable solutions tends to be much more successful than transfer between dissimilar systems. Likewise, refinements which involve more than one type of coordinate set tend to achieve poorer fits.

Since the correlation problem limits the usefulness of direct numerical comparison in determining whether several force fields correspond to similar physical models, other tests must be applied. It is quite reasonable to expect that comparison of properties such as potential energy distributions, which, being derived from the eigenvectors, are independent of the indeterminacy in the force field, would be more meaningful than comparison of the force constants themselves. Detailed discussion of our potential energy distributions will be deferred to the next chapter, but in general they are compatible both with previously published normal coordinate studies and with the group frequency literature.

Another test of the generality of a solution which bypasses the redundancy problem is transfer of the field to other stereoisomers of the compounds studied. Since stereoisomers can be described with a common set of internal coordinates, the difficulties encountered in transferring correlated fields are avoided, and isomers not included in the refinements can provide an independent test of the field. Toward this purpose calculations were performed for both anomers of galactose and mannose as well as for some of their -1-d derivatives. These calculations, described in greater detail in the following chapter, indicated that the

galactose and mannose data could be reproduced with nearly the same degree of accuracy (248 frequencies, average error: 7.47 cm^{-1}) developed for glucose.

The stability of the least squares minimum found for glucose was demonstrated by further refinement with the glucose, galactose, and mannose data together and then by refinement for the galactose and mannose data alone. These refinements produced only small changes in the fields (maximum changes — diagonal constants: 0.01, off-diagonal: 0.03) and minimal changes in the potential energy distributions. The agreement for the galactose and mannose data sets and the effects of including them in the refinement are summarized in Table XII (page 50).

CHAPTER II

THE SOLID STATE VIBRATIONAL SPECTRA OF GLUCOSE, GALACTOSE, AND MANNOSE

INTRODUCTION

In the previous chapter we have described the development of a modified valence force field for glucose. In this chapter we will discuss the transferability of this force field to mannose and galactose, two other aldohexoses. We will then discuss in general terms the potential energy distributions calculated for all three sugars and place them in perspective relative to the older literature.

EXPERIMENTAL

SAMPLES

Alpha galactose was usable as received from Matheson, Coleman and Bell, and the beta anomer was prepared from it by the method of Hudson and Yanovsky (53). Alpha mannose from Eastman Organic Chemicals was decolorized with carbon and recrystallized twice from ethanol before use. A beta mannose sample of unknown origin was on hand and was used as found. The characterization procedures were essentially as described for glucose, with primary reliance being placed upon the National Bureau of Standards infrared collection (13).

MEASUREMENTS

The sample preparation procedures and instrumentation were as described for glucose. The spectra are presented in Fig. 20-27, and the data are summarized in Tables XIV-XX. The data for galactose and mannose-1-d were taken from Barker, et al. (24).

Figure 20. Infrared Spectra of Alpha Galactose

Figure 21a. Raman Spectra of Alpha Galactose

Figure 2lb. Raman Spectra of Alpha Galactose

TABLE XIV

SPECTRAL DATA — ALPHA GALACTOSE

Infrared, cm^{-1}		Raman, cm^{-1}	
Low Temperature	Room Temperature	Low Temperature	Room Temperature
1501	1495	1497	1492
1492	1488Sh ^a	1488	1486
1458	1456	1452	1453
1446	1443	1445	
1437		1436	1433
1424	1419		
1402	1402	1404	1403
1391	1387	1387	1381
1378	1375	1373	1375
1359	1357	1356	1358
1341	1336	1335Sh	
		1331}	1332
1328	1325	1325}	1328Sh
1306	1311	1308	1304
1299	1299	1302Sh	
1285	1282	1280Sh	
1268		1271	1273Sh
1261	1261Sh	1261Sh	1259Sh
1243	1247	1245	1246
	1237		
1233	1230Sh	1233	1230Sh
1187	1181Sh		
1153	1150	1153	1151
1137	1137	1139Sh	
		1134	1136
1120Sh		11119Sh	
		1110	1109}
1103	1102	1102	1103}
1094			
1080	1077	1078	1078
		1069}	1069}
1067	1065	1062}	1064}
1053	1052	1050	1052
1045	1044	1044Sh	
1040Sh		1038	1040
1030Sh			
1013			
1008	1009Sh		
996	994	995	997
989			
976	973	976Sh	
968Sh		969	970
957	955	956	955
928			
895			
888	886	885	887
846	835	820	828

TABLE XIV (Continued)

SPECTRAL DATA — ALPHA GALACTOSE

Infrared, cm^{-1}		Raman, cm^{-1}	
Low Temperature	Room Temperature	Low Temperature	Room Temperature
807	810Sh 791	803	
		780	787
766	764	762	763
		738	
708	705	700	702
678		677	
659	658	656	658
633		637	
619	617		
612	606	611	612
589		585	
		573Sh	575
535	532	533) ^a	
		528) ^a	529
		517	
508	500	505	
500		497	496Sh
		489	489
458		460Sh	
		440Sh	441Sh
426		423	
420	416	413	414
408	406	407Sh	406Sh
396		402	
	387	389	387
		370Sh	
		356	358
354	350	351	351Sh
344	343	341	344
336	331	334	331
327		323	323Sh
313		311	
301	298	299	299
291	288	286Sh	
270	265	268Sh	268
		260Sh	
250		255Sh	254
236	232Sh		230
228			
221			
201			
			193
			183
			174

^aSh = shoulder.

TABLE XV
SPECTRAL DATA FOR ALPHA GALACTOSE-1-d^a

Cm^{-1}
1498 S ^b
1458 S
1442 S
1424 S
1405 M
1394 W
1380 VW
1340 W
1322 S
1290 S
1282 M
1255 S
1240 S
1194 VS
1148 W
1132 S
1110 S
1090 S
1080 VS
1064 VS
1050 S
1036 M
995 S
976 S
933 S
873 W
864 S
822 S
788 S
760 S
695 M
648 M

^aFrom Stacey, et al. (24).

^bS = strong; M = medium;
W = weak; V = very.

Figure 22. Infrared Spectra of Beta Galactose

Figure 23a. Raman Spectra of Beta Galactose

Figure 23b. Raman Spectra of Beta Galactose

TABLE XVI

SPECTRAL DATA — BETA GALACTOSE

Infrared, cm^{-1}		Raman, cm^{-1}	
Low Temperature	Room Temperature	Low Temperature	Room Temperature
1512	1502	1512	1504
1466	1464	1465	1465
1452			
1439	1433	1440	1425
1414	1412		
1387	1396	1391Sh ^a	
1380		1381	1378
1370			
1365	1366	1363Sh	
1341	1338	1340	1340
1326			
1312	1313		
1307	1305	1306	1304
1303Sh	1299		
1273	1272	1273	1272
1241	1242	1245	1245
1220Sh		1218	1218
1215	1214		
1170	1168	1166	1165
1163	1160		
		1141 ^a	
1137	1136	1138 ^a	1138
1125	1124	1124	1120
1120			
1105	1108	1112	1110
1094	1091	1095	1094
1079	1078	1086	1086Sh
1067		1069	1068Sh
1058	1056	1057	1055
1049Sh			
1042Sh		1043	
1037	1035	1038	1037
1022	1021	1021	1020
949 ^a		948	948
947 ^a	946		
914		915	
904	902	905	904
889		890	888
864	840		
825Sh		833	830
784	782	786	785
710		708	
	700	703	700
677	655		
646		643	
622	619	619	623

TABLE XVI (Continued)

SPECTRAL DATA — BETA GALACTOSE

Infrared, cm^{-1}		Raman, cm^{-1}	
Low Temperature	Room Temperature	Low Temperature	Room Temperature
592			
569	570Sh	572	
560Sh		559	559
555	552		
536Sh		535	535
533	530		
477		478	477
467	468	468	
439	434	439) ^d	
		434)	434
430	427		
412Sh			
400		401	398
393	388	394	
		380	
369Sh	365) ^d	365	362
364	358)		
346			
340	335	339	
320	315	325	328
300	297	310	310
		292	292
283			
272	272	273	272
267Sh			
258		262	
251	246		
238			
221		225	225
205		202	208

^aSh = shoulder.

Figure 24. Infrared Spectra of Alpha Mannose

Figure 25a. Raman Spectra of Alpha Mannose

Figure 25b. Raman Spectra of Alpha Mannose

TABLE XVII

SPECTRAL DATA — ALPHA MANNOSE

Infrared, cm^{-1}		Raman, cm^{-1}	
Low Temperature	Room Temperature	Low Temperature	Room Temperature
1486			
1460	1460	1461	1458
1448	1452	1452	
1443Sh ^a			
1425	1420	1427	1420
1395	1395	1400	1400
			1391
1386	1383	1382	1378Sh
1373	1368	1373	1370
1357	1354	1360	1355) ^d
			1344)
1343		1348	
1334		1338	
1327	1327	1330Sh	1333Sh
1313	1312	1312	1313
1299	1293	1293	
1282		1281	1280
1272	1274	1273Sh	
			1258Sh
1254	1251	1255	1253
1237	1237	1240	1238
1222	1222	1228	1227
1216	1215	1219	
1205	1206	1208	1210
1193	1193	1195Sh	
1169			
1138Sh		1143	1138
1130	1125	1128	
1112	1108	1117	1114
1102	1103	1106	1103
1092Sh		1094	
1085		1083	1083) ^d
			1079)
1080			
1072) ^d	1070		
1066)			
	1064	1067	
		1055	1052
1040	1038	1046	1043
1026Sh	1025Sh	1027	
1022) ^d	1017	1018	1018
1015)			
971	968	972	
959	957	961	969) ^d
			958)
932			
912	912	915	914

TABLE XVII (Continued)

SPECTRAL DATA — ALPHA MANNOSE

Infrared, cm^{-1}		Raman, cm^{-1}	
Low Temperature	Room Temperature	Low Temperature	Room Temperature
886			
883	882	885	881
		864	
844	843	848	844
829		833	830
828Sh	828		
813		818	813
807	809		
	800		
		778	780Sh
738		745	
725		720	720Sh
698	707		
679	679	688	684
671			
667	662	667	663
651			
626	637		
624Sh	622Sh		
602	607	610	605) 602) ^d
572		575	575
565	567		
	547	550Sh	
535		526	529
523	518		
515Sh	513Sh		
	508		
499	495	502	503
487			
483Sh			
473		476	474
466	467	465	
457		459Sh	
449Sh	453	450	449
		425Sh	
405		408Sh	
399	402	400	397
391	388	392	
376	373	377	
362	355	365	358
322		325Sh	
312	313	316	
301	301	307	307
291	293	294	
284			
277		277	273

TABLE XVII (Continued)

SPECTRAL DATA — ALPHA MANNOSE

Infrared, cm^{-1}		Raman, cm^{-1}	
Low Temperature	Room Temperature	Low Temperature	Room Temperature
266	264	267	
252	248	250	248
		234	235
222		220Sh	
		208	207
		185	195

^aSh = shoulder.

TABLE XVIII

SPECTRAL DATA FOR ALPHA MANNOSE-1-d^a

Cm^{-1}	Cm^{-1}
1456 M ^b	1080 S
1435 W	1065 S
1422 S	1045 VS
1395 M	1025 S
1380 S	1000 S
1358 M	973 M
1330 M	966 M
1318 M	945 VW
1305 M	930 S
1288 S	912 M
1255 S	(864 S
1226 W	(854 S
1212 S	830 W
1200 W	818 S
1170 W	790 S
1155 M	765 VW
1130 M	705 M
1110 S	670 M
1090 VS	

^aFrom Stacey, et al. (24).

^bM = medium; W = weak; S = strong;
V = very.

Figure 26. Infrared Spectra of Beta Mannose

Figure 27a. Raman Spectra of Beta Mannose

Figure 27b. Raman Spectra of Beta Mannose

TABLE XIX

SPECTRAL DATA — BETA MANNOSE

Infrared, cm^{-1}		Raman, cm^{-1}	
Low Temperature	Room Temperature	Low Temperature	Room Temperature
1483	1478	1483	1477
1467		1465	1462
	1454		1445Sh ^a
1440Sh			
1435	1428		
1422	1419	1422) ^d	1415
		1412)	
1410) ^d			
1407) ^d	1406		
1380			
1372	1368	1372	1369
1364Sh	1363Sh	1363Sh	1362Sh
		1351	1350
1338	1334	1336	1330
1322	1320	1320	1316
1309	1307		
1292	1292	1292	1288
1282	1278		1275Sh
1261	1261	1263	1258
1253			
1239	1238	1240	1237
1233	1235Sh		
1212	1212	1213	1211
1171	1167		
1147		1159	1154
1135Sh			
1127			
1121	1124	1123	
1119Sh	1118	1117) ^d	1119
		1115)	
1116	1113		
1111	1108Sh	1111) ^d	
1103		1107)	1104
1092Sh			
1088	1086	1089	1085
1083	1081Sh	1077	
1072	1070	1074Sh	1072
1059	1057		1059Sh
1044	1041		
1035	1032	1035	1029
1010		1012Sh	
1007Sh	1007		
998		1001	1001
973Sh			
942Sh			
934	933	935	932
899	896	989) ^d	
892		893) ^d	893

TABLE XIX (Continued)

SPECTRAL DATA — BETA MANNOSE

Infrared, cm^{-1}		Raman, cm^{-1}	
Low Temperature	Room Temperature	Low Temperature	Room Temperature
862 ^a	859 ^a	864	858
855 ^a	853 ^a		
821Sh	819		
809Sh	805Sh		
771	769	771	767
735	730	735	727
721			
708		709	
688	689	685	688
653Sh			
624	621	623	
616			618
603	602	604	599
		581	
556		547	
	538		
513		516 ^a	525Sh
		512 ^a	
496	493	494	492
482Sh			
452			
449	448	446	444
430			
425Sh	424	427	423
408	405	408	403Sh
388		399	394
		376	370
361	359		
330	327	331 ^a	326
		326 ^a	
321	317	319Sh	
299			
287		293	288
280	281	279	273
264		265	258
252	249	247 ^a	
		240 ^a	
241			239
236			
228	228		
216		217	
200		200	193
		177	167
		156Sh	
		137Sh	
		125Sh	

^aSh = shoulder.

TABLE XX

SPECTRAL DATA FOR BETA MANNOSE-1-d^a

Cm⁻¹

1480 W^b
 1452 M
 1430 W
 1420 S
 1405 M
 1373 M
 1348 W
 1339 M
 1318 M
 1300 W
 1278 S
 1242 S
 1235 W
 1216 S
 1130 W
 1125 S
 1120 W
 1106 S
 1090 VS
 1080 VS
 1066 VS
 1055 VS
 1033 S
 985 W
 969 S
 930 M
 911 S
 885 M
 856 M
 828 S
 790 M
 758 S
 725 S
 675 S

^aFrom Stacey, et al. (24).

^bW = weak; M = medium;
 S = strong; V = very.

COMPUTATIONS

VIBRATIONAL MODEL

All assumed structures were based on the corrected alpha glucose structure described in the previous chapter, with the necessary interchanges of axial and equatorial groups. In each case, the hydroxymethylene group was placed in the fully staggered conformation which gave the best overall agreement with experiment, as discussed in the following chapter. This is a less exact model than that used for glucose, since the orientations of the hydroxyl groups in galactose and mannose would be expected to differ from those in alpha glucose, and since the hydroxymethylene groups could easily be 10-15° from one of the fully staggered minima. The potential energy model used was that developed for glucose in the preceding chapter.

CALCULATIONS

When the secular equation had been solved and assignments made as previously described for glucose, the agreement between experimental and calculated frequencies was found to be nearly as good for galactose and mannose as it had been for glucose. This agreement is summarized in Table XII (page 50) and is shown graphically in Fig. 28-34. The detailed assignments and condensed potential energy distributions are given in Appendix II. The calculated Cartesian displacements, together with those obtained previously for glucose, were used to prepare computer drawn displacement diagrams of selected normal modes. As in the glucose case, the full potential energy distributions and complete Cartesian displacement coordinates were placed on magnetic tape for permanent retention.

ALPHA GALACTOSE

CALCULATED

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM. -1)

Figure 28. Assigned and Calculated Frequencies for Alpha Galactose

ALPHA GALACTOSE-1-D

CALCULATED

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM. -1)

Figure 29. Assigned and Calculated Frequencies for Alpha Galactose-1-d

BETA GALACTOSE

CALCULATED

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM. -1)

Figure 30. Assigned and Calculated Frequencies for Beta Galactose

ALPHA MANNOSE

CALCULATED

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM. -1)

Figure 31. Assigned and Calculated Frequencies for Alpha Mannose

ALPHA MANNØSE-1-D

CALCULATED

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM.-1)

Figure 32. Assigned and Calculated Frequencies for Alpha Mannose-1-d

BETA MANNØSE

CALCULATED

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM.-1)

Figure 33. Assigned and Calculated Frequencies for Beta Mannose

BETA MANNOSE-1-D

CALCULATED

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM.-1)

Figure 34. Assigned and Calculated Frequencies for Beta Mannose-1-d

DISCUSSION OF THE NORMAL MODES

GENERAL ASSIGNMENTS

Figure 35 provides a graphical summary of the potential energy distributions for the nonisotopically substituted molecules. The upper portion of the figure shows the primary ranges of influence of the various diagonal force constants, and the lower area describes the normal modes in the more conventional group frequency terminology. These ranges are in general agreement with the group frequency literature (40,54,55), and, with one exception, they agree with previously published carbohydrate calculations (1-4,6-9). This exception is the COH deformation range which, as discussed in the previous chapter, is calculated higher than in the earlier work.

For purposes of discussion, the spectra can be divided into a number of more or less distinct regions. At the highest frequencies, the O-H and C-H stretching modes are set off a considerable distance above the rest of the fundamentals. The hydroxyl stretches, which are not calculated in our model, are intense infrared and weak Raman bands lying in the range $3550-3050\text{ cm}^{-1}$. The C-H stretching modes, which are both calculated and observed in the $3000-2850\text{ cm}^{-1}$ range, are quite strong in the Raman spectrum and of weak to medium intensity in the infrared. Between 2850 and 1500 cm^{-1} are found a number of very weak infrared bands, but these are generally assigned as overtones and combinations (56). No fundamentals are calculated in this range.

Below 1500 cm^{-1} five spectral regions can be recognized. Between 1500 and 1200 cm^{-1} closely spaced bands of medium intensity are found in both types of spectra. These modes are calculated to be primarily coupled deformations of the various proton containing functions such as hydroxyl, methylene, and methine. After a short transparent region, a closely spaced group of bands

with considerably higher intensity is observed in both spectra between 1150 and 1000 cm^{-1} . The potential energy distributions show these modes to be primarily coupled heavy atom stretching motions involving both the ring and the hydroxyl groups. Between 1000 and 600 cm^{-1} the bands are more widely spaced, having medium to high Raman intensity and low to medium infrared intensity. Their potential energy distributions are among the most complex in the entire spectrum, involving mixtures of heavy atom stretching and deformations of both proton containing and heavy atom groupings. The 800-500 cm^{-1} region also contains a group of intense infrared bands normally assigned as hydroxyl out-of-plane deformations (40). Recent calculations for crystalline methanol indicate that these are not pure internal modes (44), and thus one would not expect corresponding calculated frequencies when using the isolated molecule approximation. The presence of these bands complicates the assignment process in the region, since it makes identification of the purely internal fundamentals more difficult.

A more closely spaced group of bands having very high Raman intensity and low infrared intensity is found between 600 and 350 cm^{-1} . These modes are dominated by heavy atom bending coordinates and may be described as deformations of the ring. Below 350 cm^{-1} there are few strong bands in either spectrum. Modes in this region are calculated as primarily mixtures of heavy atom bending and torsional coordinates, but an assortment of external and mixed modes not calculated under the isolated molecule approximations are also expected here. Accordingly, one finds considerably more experimental bands than calculated frequencies. Each of these regions will be discussed in greater detail in the following sections.

SPECIFIC ASSIGNMENTS AND DISCUSSION

Hydroxyl Stretch

Our vibrational model omits the hydroxyl stretch coordinates, and thus the corresponding stretch modes are not calculated. This limitation is not serious from an interpretive viewpoint, since Michell (56) has offered evidence that the hydroxyl stretch patterns in the solid state are largely determined by intermolecular coupling. This, in combination with the variations in strength of the individual hydrogen bonds, places interpretation of this region beyond the reach of our isolated molecule approximation. Accordingly, neither we nor any of the previous investigators have attempted detailed assignments of the hydroxyl stretching region.

Experimentally, the hydroxyl stretching bands are found in the $3550\text{--}3050\text{ cm}^{-1}$ range. They are very broad and intense in the infrared and very weak in the Raman. Although the Raman bands require relatively wide slits to allow their observation, their inherently narrower band widths at any given temperature make the Raman spectrum the preferred approach to resolving the hydroxyl stretch region (57). This difference in inherent band widths is adequately demonstrated by the spectra presented in this chapter and the previous one. The infrared bands do become quite sharp if the hydroxyls are uncoupled from the crystal lattice by matrix isolation or isotopic dilution. This effect is illustrated in the spectrum of alpha glucose-O-d₅ (Fig. 10). The residual OH bands are sharper than the OH bands in alpha glucose, and the pattern has changed, confirming Michell's (56) intermolecular coupling hypothesis.

CH Stretch

Our calculations place the CH stretching modes in the $2960\text{--}2880\text{ cm}^{-1}$ range. The coupled methylene modes are found at the extremes, while the methine modes, coupled among themselves but not with the methylenes, tend toward the center of the range. We have not attempted to assign specific bands here or to refine the force constants in recognition of the possible occurrence of Fermi resonance.

This possibility is indicated by the fact that C-D substitution does not always lead to a simple disappearance of bands near 2900 cm^{-1} or to the appearance of the proper number of bands at lower frequency.

COH Deformations

Our model calculates the greatest contribution from the COH bending coordinates to fall in the $1460\text{--}1350\text{ cm}^{-1}$ range when the hydroxyl groups are hydrogen bonded and about 100 cm^{-1} lower when the groups are free. Most of these contributions are found in relatively pure COH modes above 1370 cm^{-1} , but lesser contributions are found coupled with methylene and methine deformations down to about 1300 cm^{-1} . The only free hydroxyl included in our calculations, that at O(4) in beta glucose, is not a major contributor to any single band but is a minor component of a number of bands in the 1300 cm^{-1} region. On deuteration, a number of new bands are predicted to appear in the $1000\text{--}900\text{ cm}^{-1}$ range. These COD deformations tend to be more coupled and less pure than the corresponding COH modes.

These observations are in qualitative agreement with experiment, since there are a number of bands in the $1380\text{--}1500\text{ cm}^{-1}$ region displaying the characteristics expected of COH modes. They are relatively broad with little or no Raman intensity, are quite temperature sensitive, and are removed by hydroxyl deuteration. Quantitatively, however, the use of a single deformation force constant for all the hydrogen bonded hydroxyls precludes accurate prediction of the band positions. The calculated bands tend to cluster near 1400 cm^{-1} , while the experimental bands cover the $1400\text{--}1500\text{ cm}^{-1}$ range, resulting in a number of unassigned bands. The new bands in the $1000\text{--}900\text{ cm}^{-1}$ range are calculated with greater precision, presumably due to their greater coupling with nonhydroxyl motions.

Our results are in good agreement with the alcohol group frequency literature (40) and with the recent calculations for crystalline methanol (44). They do not agree with the calculations of Vasko (1,2), Pitzner (6), Pitzner and Atalla (7), Cael, et al. (3,4), or Watson (8). All of these authors found the COH deformations centered in the $1200-1100\text{ cm}^{-1}$ region and strongly coupled with both C-H and heavy atom deformations. This disagreement has its origin in our differing choices of initial COH force constants as discussed in the previous chapter. A crucial test of these two contrasting force constant preferences is found in the spectrum of beta arabinose-d₆, reported by Edwards (9). This spectrum shows a group of bands centered near 1400 cm^{-1} which meet the experimental criteria for COH deformations. Adequate prediction of this spectrum requires a considerable increase in the COH deformation constant derived from the earlier studies to a value nearer the one we have chosen (9). Edwards' calculations for the unsubstituted pentoses using this raised constant gave potential energy distributions for the hydroxyl deformations roughly similar to our own (9). Comparison of our results to earlier prenormal coordinate deuteration studies for carbohydrates is more difficult, since most such studies were done with polymeric materials which tend to have relatively diffuse spectra. Even so, the consensus of these studies suggests that the greatest intensity reduction on hydroxyl deuteration is found near 1400 cm^{-1} (58).

Methylene Modes

Our calculations show modes for the hydroxymethylene group similar to those expected for the methylene group in hydrocarbons (59) and, in particular, very similar to those found for oxymethylene groups in diethyl ether (49) and in our study of ethanol. The scissors and twist modes are relatively pure motions, found at 1450 and 1300 cm^{-1} , respectively. These motions are illustrated in Fig. 36 and 37. The wagging mode is coupled, primarily with hydroxyl deformation,

Figure 36. Methylene Scissors Motion. The 1450 cm^{-1} Mode of Beta Glucose

Figure 37. Methylene Twisting Motion. The 1291 cm⁻¹ Mode of Beta Glucose

and contributes to a number of bands in the 1420-1320 cm^{-1} range. The rocking mode is coupled in a more complex manner and contributes to bands in the 900-700 cm^{-1} range.

The experimental results mesh fairly well with the calculations, particularly with respect to the basic coupling patterns predicted. The scissors mode is easily recognized, being the sharpest and most intense Raman band in the 1500-1400 cm^{-1} region. It is cleanly removed by deuteration of the methylene group, and its insensitivity to deuteration elsewhere in the molecule is consistent with a motion isolated at the methylene group. While all the calculated scissors modes fall near 1450 cm^{-1} , the experimental bands for alpha galactose and beta mannose are found at 1490 and 1480 cm^{-1} , respectively. Unfortunately, since structural data for these two sugars are unavailable, it is impossible to determine whether the fault lies in our geometric or potential energy approximations.

The twist mode is calculated near 1300 cm^{-1} , somewhat higher than the 1270 cm^{-1} band removed by methylene deuteration in both glucose anomers. The corresponding $-\text{CD}_2-$ twist, which appears as a new band near 920 cm^{-1} , is calculated almost exactly. The changes produced in the 1420-1320 cm^{-1} region by isotopic substitution are consistent with the calculated coupling between the methylene wag and the primary hydroxyl deformation. Methylene deuteration produces a fairly complex pattern of shifts in this region rather than the removal of any single band. Likewise, hydroxyl deuteration produces a complex shift pattern, moving some of the same bands shifted by methylene deuteration. It is also worth noting that there is no recognizable similarity between the methylene deuteration shift patterns of the two glucose anomers in the 1420-1320 cm^{-1} region. This is most easily rationalized by invoking coupling of the wagging modes with the hydroxyl deformations, which reflect the differing hydrogen bonding patterns of the two molecules. A typical wagging mode is illustrated

in Fig. 38. The behavior of the methylene rocking modes on isotopic substitution is adequately predicted, but we will defer their discussion to the section on "anomeric" modes.

As previously mentioned, the calculated methylene modes for glucose, galactose, and mannose are quite similar to those calculated for ethanol and diethyl ether. Snyder and Zerbi (46), in their study of ten aliphatic ethers, arrived at a different set of force constants and a different description of the methylene modes. Their solution is distinguished primarily by a lower value for the HCH bending constant. This results in greater coupling of the scissors and wagging modes, to the extent that it is no longer appropriate to assign bands to either type of motion separately. As discussed in the previous chapter, we feel that the more extensive isotopic data employed in the ethanol and ethyl ether studies make their higher estimate of the scissors constant the more reliable one. All three of these studies concur on a relatively pure methylene twist mode, although Snyder and Zerbi (46) calculate it at a slightly lower frequency. The ranges of the rocking modes are in general agreement, but in all cases these modes are so highly coupled that strict comparisons cannot readily be made.

The carbohydrate calculations of Vasko (1,2) and Cael, et al. (3,4) indicate coupling patterns which reflect both their use of the Snyder-Zerbi ether field and their choice of a hydroxyl bending constant value. As in the Snyder-Zerbi calculations (46), the methylene scissors and wag are heavily coupled, contributing to a number of bands in the $1450\text{--}1300\text{ cm}^{-1}$ region. Because of their relatively low choice for the COH deformation constant, the primary hydroxyl deformation and the methylene wag are less coupled than in our study. Detailed comparisons for the other modes are difficult, since they have published their potential energy distributions only in terms of the contributing force constants and not in terms of the internal or Cartesian coordinates. They have, however,

Figure 38. Methylene Wagging Motion. The 1346 cm⁻¹ Mode of Beta Glucose

published a number of normal mode displacement drawings, and these can serve as a basis for further comparison. Cael, et al. (3) show highly coupled modes involving methylene twist at 1335 and 1259 cm^{-1} for alpha glucose. This corresponds well to our calculated frequency range, but our calculation shows the twisting mode as much less coupled. This discrepancy is not readily explained, particularly since Snyder and Zerbi (46) do not calculate coupled twist modes, but the low COH deformation constant is an immediate suspect. A number of lower frequency methylene rocking modes are also drawn, but these will be discussed in a later section.

Since under our approximations for setting up the secular equation the methylene modes calculated for glucose are essentially identical to those which would be calculated for a cellulose structure with the same hydroxymethylene conformation, it is appropriate to comment on some earlier assignments for cellulose. Forziati and Rowan (60) assigned the 1430 cm^{-1} band in the infrared spectrum of cellulose to the methylene scissors mode. Later workers (61-65) tended to accept this assignment, since the band was the most intense in the 1500-1400 cm^{-1} range and seemed insensitive to hydroxyl deuteration. Liang and Marchessault (62) used this assignment as the basis of a complex assignment scheme for the rest of the cellulose spectrum based on band polarizations, and its accuracy is crucial to their arguments. Based on the Raman intensity in both the cellulose I and II spectra near 1450 cm^{-1} and on our calculations, we would suggest assignment of the scissors to either or both the 1480 and 1455 cm^{-1} bands in cellulose I and to the 1450 cm^{-1} band in cellulose II. In all the sugar anomers included in our study, the scissors frequencies, both calculated and observed, were at least as high as 1450 cm^{-1} .

Liang and Marchessault's placement of the cellulose I and II methylene wagging modes near 1320 cm^{-1} is more reasonable on a frequency basis than

Tsuboi's 1250 cm^{-1} value (61), but their choice was partly motivated by the band's insensitivity to hydroxyl deuteration. The coupling pattern we calculate would tend to nominate either or both the 1360 and 1335 cm^{-1} bands, which do show deuteration sensitivity. This calculated coupling would also tend to undermine the dichroism arguments used by Liang and Marchessault in this assignment. The only methylene twist assignment reported for cellulose, Blackwell, *et al.* (65) 1293 cm^{-1} frequency, is quite reasonable in view of our results. We find Liang and Marchessault's (62) assignments of the methylene rock near 750 cm^{-1} unlikely both in terms of the calculations and because of the band's lack of Raman intensity. Again, the calculated heavy coupling tends to cast doubt on their dichroism arguments. We will not discuss Cael, *et al.* (4) normal coordinate calculations for cellulose at any length, since the calculated methylene modes seem very similar to those from their glucose calculation (3), which we have already discussed.

Methine Deformations

Our calculations show methine deformations contributing significantly to bands in the 1420 - 1200 and 950 - 400 cm^{-1} ranges. They tend to be highly coupled, both among themselves and with every other type of internal coordinate except the proton stretches and the torsions. Examination of Fig. 38, previously used to illustrate the methylene wagging, will also reveal displacement of all the methine protons. The other extreme, found only in a few modes near 1400 cm^{-1} , is illustrated in Fig. 39. This mode, at 1386 cm^{-1} in the alpha glucose spectrum, is about 50% C(1)-H deformation and represents the approximate upper limit of such contributions.

Although a number of authors have assigned bands in polysaccharide spectra to methine deformations (61-66), these usually represented only bands in the 1500 - 1200 cm^{-1} range which could not be assigned to anything else, since the

Figure 39. Anomeric Proton Deformation. The 1386 cm⁻¹ Mode of Alpha Glucose

group frequency literature for methine vibrations was relatively sparse (54). Our calculations can be taken as support for some methine contribution in any mode within this range, but would argue against the occurrence of pure methine modes.

The only carbohydrate methine assignments supported by definite evidence are the studies by Stacey, et al. (24) and Vasko (1,19) of -l-d sugars. Stacey, et al. (24) reported that deuteration at C(1) typically removed two bands from sugar spectra in the 1400-1275 cm^{-1} range. The higher band was found in the narrow range 1387-1363 cm^{-1} for either anomer of glucose, galactose, or mannose. The lower band was found in the range 1315-1275 cm^{-1} for alpha anomers and in the 1340-1312 cm^{-1} range for beta anomers. Vasko (1,19) also reported the spectrum of alpha glucose-l-d. Although his data agreed fairly well with Stacey's he made substantially different assignments. Five bands between 1142 and 836 cm^{-1} which shifted by C(1) deuteration were assigned to C(1)-H deformation, likewise ten bands between 1419 and 810 cm^{-1} which seemed to appear on deuteration were assigned to C(1)-d deformation. Group frequency considerations would suggest that the upper limit of the quoted C-H range is rather low, while the upper limit of his C-d range is rather high.

Our spectrum of alpha glucose-l-d at liquid nitrogen temperature shows a rather complex pattern of shifts relative to alpha glucose. The only band which seems to be shifted cleanly out of its original spectral region is near 1385 cm^{-1} , in good agreement with the high C(1)-H contribution calculated here. The most prominent new band in the deuterated spectrum is at 960 cm^{-1} , which has a large C(1)-D contribution in the calculated potential energy distribution. The other shifts, which involve smaller C(1)-H contributions, are also calculated in a satisfactory manner. We will defer discussion of the proton

deformations below 900 cm^{-1} , since these are very much involved in the "anomeric" modes to be discussed below.

Ring Modes

Before describing the spectral region below 1200 cm^{-1} , which contains the heavy atom stretches and deformations, some background discussion of earlier assignments is appropriate. It was realized quite early that many ring molecules had highly coupled, delocalized normal modes, which could not be described adequately in group frequency terms. This did not pose a serious problem for highly symmetric rings such as benzene and cyclohexane, since the form of the normal modes could be inferred by group theoretical methods without recourse to calculations. Burkert and Badger (67) attempted to assign the less symmetric oxanes, tetrahydropyran, and 1,4-dioxane by assuming that their normal modes were quite similar to those of cyclohexane.

Several of the early efforts in carbohydrate assignments (62,68) aimed at development of schemes where pendant groups attached to the ring were assumed to undergo localized group frequency type motions and the rings themselves to give rise to delocalized modes which could be correlated with the cyclohexane motions by an extension of the Burkert-Badger scheme. This approach gained acceptance to the point where more attention was devoted to exact assignment of these cyclohexane type ring modes in carbohydrate spectra than to consideration of whether they represented a reasonable approximation of the coupling patterns in sugars (66,69). The correlations were made quite directly, with minimal frequency shifts assumed between a given normal mode in tetrahydropyran and in the carbohydrates.

Our calculations do not show any normal modes for alpha or beta glucose in which the pattern of ring atom motion resembles any of the cyclohexane modes

drawn by Burkert and Badger (67). This lack of correlation with the cyclohexane modes can be better understood by considering an alternative correlation path from glucose to cyclohexane, the inositols (70). For illustrative purposes, we shall follow the correlation for the A_{1g} symmetric ring breathing mode. This mode is found at 802 cm^{-1} in cyclohexane, and bands with similar intensity and polarization properties are found only slightly shifted from this frequency in p-dioxane and tetrahydropyran. Modes of this nature have been assigned in the $800\text{--}750\text{ cm}^{-1}$ region for carbohydrates (62,68), but in scyllo-inositol, the only carbohydrate with the same point group as cyclohexane, the A_{1g} ring breathing mode is actually found at 456 cm^{-1} . The shift is due primarily to the mass added by the oxygens. In scyllo-inositol, the ring breathing mode is actually a pure heavy atom stretching mode, but as the spectra of progressively less symmetric members of the inositol series are examined, the breathing mode is found to correlate to modes with increasing heavy atom bending contributions. By the time this extrapolation is extended to glucose no modes in the $500\text{--}400\text{ cm}^{-1}$ region have more than a 10% stretching component, and the thread of correlation is lost.

From this consideration of the inositol and hexose normal modes, we conclude that the combined effects of chemical substitution and removal of symmetry restrictions are so great that the normal modes of cyclohexane do not provide a useful basis for discussion of carbohydrate spectra. Thus, in the next few sections such cyclohexane type prior assignments will be mentioned where appropriate, but they will not be discussed in any detail.

Heavy Atom Stretching

The proton deformation modes extend down to about 1200 cm^{-1} in our compounds, and the region between 1200 and 1150 cm^{-1} is usually clear. From 1150 cm^{-1} to just below 1000 cm^{-1} is found a fairly closely spaced group of bands which have

high intensity in both the infrared and Raman. The potential energy distributions show these modes to be dominated by C-C and C-O stretching. Although some coupling occurs, many of the modes are fairly localized, with 50% or more of the potential energy concentrated in a single bond stretch.

These calculations are in good agreement with the group frequency literature, since heavy atom stretching modes have generally been assigned in this region (40,54). The C-O stretching modes are expected to give high intensity bands in both infrared and Raman spectra while most of the intensity from C-C stretching modes is to be expected in the Raman spectrum. More recent studies (49,50,71) which have considered the possibility of coupling between neighboring C-O and C-C bonds have reclassified the modes which were listed in earlier tables as C-O stretching and generally regard them as upper or antisymmetric members of coupled multiplets. The lower, or "symmetric," stretching modes in such groups are found as low as 800 cm^{-1} . This suggests that heavy atom stretching contributions should also be found in some of the isolated bands below 1000 cm^{-1} . This matter will be discussed further in the following section.

Many mono- and higher saccharides, including cellulose and most of the hexoses studied here, mark the transition from proton deformations to heavy atom stretches with a band of intermediate intensity near 1150 cm^{-1} . This band is usually isolated by a 50 cm^{-1} wide transparent region on the high frequency side and is typically $20\text{-}30\text{ cm}^{-1}$ above the next lower band. The striking insensitivity of this band to conformation or chemical substitution attracted the notice of the earliest workers, and many attempts have been made to assign it (60,61,64,65,72). The intervening thirty years have not produced a consensus, however. Figure 40 shows a typical mode of this type as pictured by our calculations. In this mode, most of the potential energy is in a coupled heavy atom stretching mode involving O(5), C(1), C(2), and C(3), and some contribution from proton

Figure 40. The 1158 cm^{-1} Mode of Beta Mannose

deformation is visible at C(1), C(2), and C(3). In some of the other compounds, the stretching mode involves C(5), O(5), C(1), and C(2), so the O(5), C(1), and C(2) grouping is the common factor in all of them. None involve noticeable hydroxyl deformation, and the mode is calculated as essentially unshifted in alpha and beta glucose-O-d₅. We observed no shift of the band in the alpha glucose-O-d₅ spectrum.

Previous normal coordinate calculations for various model systems have not produced a unified interpretation for these bands near 1150 cm⁻¹. Vasko (1,2), Cael, et al. (3,4), Pitzner (6), and Pitzner and Atalla (7), all using relatively low hydroxyl deformation constants, pictured these modes as primarily heavy atom stretching, coupled with both C-H and O-H deformation. Cael, et al. (3) found the 1150 cm⁻¹ mode for beta glucose to be somewhat similar to our Fig. 40, but he showed a different pattern for the corresponding alpha glucose mode. He also suggested that the 1150 cm⁻¹ band in cellulose might represent two overlapped modes, one with substantial ring COC stretch and the other dominated by the COC stretch of the glycosidic bridge. These interpretations encompassed most of the earlier suggestions concerning the character of the mode, which had previously been assigned to a ring mode (73), C-O stretch coupled with COH deformation (64,66), COC antisymmetric stretching of the glycosidic bridge (62,63), methylene rocking (74), or some complex combination of all of these (72).

One would expect that repetition of these calculations with a COH deformation constant more typical of hydrogen bonded systems would produce modes which were more purely heavy atom stretches, but it is not possible to know in advance exactly how the coupling patterns would change. The one published carbohydrate calculation with a higher deformation constant, Edwards' (9) pentose study, showed little COH contribution at 1150 cm⁻¹ and gave a fairly uniform assignment for all three compounds studied. In the spectra of beta arabinose, beta lyxose,

and alpha xylose, the 1150 cm^{-1} mode is the highest calculated heavy atom stretching mode, and motion is localized in the C(3), C(4), O(4), C(5) grouping. This agrees with our results in the sense that it provides a common assignment for a seemingly structure invariant band, but it places the motion on the other side of the ring. It is not obvious if this difference reflects the geometric differences between the pentoses and hexoses or the different assumptions used in constructing the two force fields.

At this stage it is impossible to decide whether the ubiquity of the 1150 cm^{-1} band in carbohydrates is an extended coincidence or a reflection of some structure invariant normal mode, although our calculations and those of Edwards' (9) hint at the second alternative. The calculations do discount those assignments which argue for hydroxyl deformation (64,66,72) or methylene rock (74) contributions and suggest that such modes will be so highly coupled as to limit the validity of assignments based on qualitative use of dichroism data (62,63).

A number of other assignments have been made by various workers for the $1150\text{-}1000\text{ cm}^{-1}$ region, but most of these involve analogies to the cyclohexane ring modes discussed in the previous section (69). For this reason, we will not discuss these assignments further. In any event, the bands between 1125 and 1000 cm^{-1} tend to be so closely spaced that the calculations are better viewed as an indication of the types of motion occurring in the region rather than as specific assignments for individual bands. Many of these bands might still be assigned if extensive C^{13} and O^{18} data become available, since many of the calculated modes seem to be fairly localized.

"Anomeric" Modes

Between 1000 and 600 cm^{-1} the bands are widely spaced, often being $50\text{-}100\text{ cm}^{-1}$ apart. The calculations, which fit the data well, indicate that these

modes are a complex mixture of methine bending, methylene rocking, heavy atom stretching, and heavy atom deformation. In view of the wide spacing and good fit, we may have considerable confidence in most cases that the calculated modes are a good representation of the molecular motion.

Encouraged by the relatively simple spectral patterns in this region and their seemingly high sensitivity to structure, Stacey, et al. undertook a classic series of studies in the early 1950's. In a series of publications (24,68,75-77) they established correlations between band patterns in this region and the conformation and configuration of an assortment of carbohydrates. The most widely publicized correlation concerned the relation of the spectra to the configuration at the anomeric carbon of reducing sugars and their derivatives. The assignment scheme for aldopyranoses, summarized in Table XXI, might be regarded as speculative, and the weaknesses of the cyclohexane type ring assignments have already been discussed. Still, the solid statistical basis of the correlations suggests that they might reflect common motions somehow involving the structures proposed.

TABLE XXI
BIRMINGHAM ANOMERIC CORRELATIONS

Aldopyranoses (<u>74-76</u>)		
Band Designation	Assignment	Frequency, cm^{-1}
1	Antisymmetric ring stretching	917 ± 13
2a ^a	Equatorial anomeric C-H deformation	833 ± 15
2b ^a	Axial anomeric C-H deformation	890 ± 10
2c	Axial nonanomeric C-H deformation	873 ± 10
3	Symmetric ring stretch	760 ± 20

^aType 2 bands were later reassigned to a general motion of anomeric end of ring (24).

To further explore this possibility, all modes between 950 and 700 cm^{-1} were drawn for the six hexose anomers studied, and these were examined in an attempt to discover the basis of the correlations. All the modes in this range are rather delocalized, but upon careful examination two "group" motions were found to be responsible for most of the modes in this region. Figure 41 illustrates the 837 cm^{-1} mode for alpha glucose. This motion, which will be designated Type X1, involves displacement of the four heavy atoms in the trans grouping C(6)-C(5)-O(5)-C(1) and their associated protons. The Type X2 motion is similar but of much lower amplitude about C(1). The second major type, designated Y and illustrated in Fig. 42, is a motion of a trans C-C-C-H grouping. It seems to occur when either the C(1)-C(2)-C(3) or C(2)-C(3)-C(4) grouping has an equatorial proton on either end. Table XXII summarizes the relation of the Barker-Stacey correlations and the normal modes calculated for glucose, galactose, and mannose.

The Type IIc modes shown by galactose and mannose are Y type motions. The original assignment to the deformation of nonanomeric equatorial protons is correct in the sense that such a proton is a prerequisite to the motion, but most of the potential energy is in the heavy atom coordinates. Type IIa modes are relatively pure X1 motions in alpha glucose and alpha mannose, but the 833 cm^{-1} mode in alpha galactose is a complex mixture of X, Y, and other motions. The Type IIb band in beta glucose also corresponds to a relatively pure X1 motion, but in beta mannose and beta galactose, where the Y motion is also possible, the modes assigned as IIb are a mixture of the X and Y motions. The revised assignments of the Type IIa and IIb modes as motions of the anomeric end of the ring (24) are qualitatively acceptable, although the substantial methylene rocking component was not appreciated prior to the first normal coordinate calculations.

Figure 41. Typical X Motion: The 837 cm^{-1} Mode for Alpha Glucose

Figure 42. Typical Y Motion: The 881 cm⁻¹ Mode for Alpha Galactose

TABLE XXII

RELATION OF TYPE X AND Y GROUP MOTION
TO BIRMINGHAM ANOMERIC CORRELATIONS

Barker Designation	1	2b	2c	2a
Alpha glucose	914(Y)			837(X1)
Beta glucose	909(X2)	896(X1)		
Alpha galactose	937(Y)		888(Y)	833(X+Y)
Beta galactose	955(X2)	897(X2+Y)	881(Y)	
Alpha mannose	958(Y)		883(Y)	825(X1)
Beta mannose	938(Y)	896(X1+Y)	861(X2+Y)	

The Type I modes do not represent either type of motion exclusively. In beta glucose and beta galactose they are primarily X2 motions, while in alpha glucose, alpha mannose, and beta mannose they are primarily Y type motions. The calculated modes do not resemble the cyclohexane type ring modes proposed in the original assignments. The calculations do not readily reveal the basis for the correlation of the Type III modes. They generally involve heavy atom motion in the O(5)-C(1)-C(2)-C(3)-C(4) area, but the specific motions seem to be more unique to the individual structures than was the case with Types I or II bands. Heavy atom bending increases sharply in the Type III modes relative to those at higher frequency, which may be the key to the relatively constant frequency. The beta glucose Type III band, lying at a lower frequency than the rest, has more methine deformation than the others. Comparison with Edwards' (9) calculation for beta xylose, however, does not confirm this as the reason why sugars without axial hydroxyl groups fail to show Type III absorption (78).

Comparison of our calculations to those reported by Cael, et al. (3) for the Types I and II bands of alpha and beta glucose show considerable agreement

except for the presence of hydroxyl deformations in the latter work. This would suggest that our conclusions concerning the Types X and Y motions are not extremely sensitive to the exact form of the force field.

Examination of Table XXII provides some insight into both the successes and failures of the Barker-Stacey anomeric correlations. The usefulness of the Types IIa and IIb bands reflects the fact that the X motion is usually found at higher frequency in the beta anomers. The Type IIc bands reflect a fairly constant frequency for the Y motion in molecules with a nonanomeric equatorial proton. Some of the difficulties encountered may be traced to overlap in the frequency ranges of the X and Y motions, mixing of these motions to differing degrees in different molecules, and cases such as mannose, where the X motion is at the same frequency for both anomers. Further difficulties with the hexoses can be attributed to intrusion of hydroxyl out-of-plane modes (discussed in the next section) into this frequency region for strongly hydrogen bonded systems and to multiple bands as a result of rotational isomerism at C(6) (discussed in the following chapter). The major difficulties encountered in applying the correlations to the pentoses are readily explained by the nature of the X motion, which is impossible for pentoses due to the large methylene rocking contribution. On the whole, the earlier conclusion (79) that these correlations are indicative but not conclusive proof of structure still stands.

Hydroxyl Out-of-plane Modes

All condensed alcohols show a broad, intense infrared band near 650 cm^{-1} (40). In higher molecular weight, polyhydroxy materials such as carbohydrates, the absorption is usually multiple and may cover a wider range of frequencies. Even when overlapped by other types of modes, the broad, intense band envelope in this region is still characteristic. This band is eliminated upon dilution or vaporization and shifts lower by a factor of about $1/\sqrt{2}$ on deuteration,

identifying it as a relatively pure OH proton motion. The usual terms for such bands is OH out-of-plane deformation, and such assignments have been made for carbohydrates (62,63,65). Previous carbohydrate normal coordinate calculations, however, have shown only slight COH involvement in this region (1-4, 6-9). This inconsistency has recently been criticized by Michell (80).

Dempster and Zerbi's (44) recent line group approximation calculations for crystalline methanol have shown that the 650 cm^{-1} mode for that compound involves primarily intermolecular coordinates (coordinates with their component atoms spanning more than one molecular unit). Since such coordinates are not included in the "isolated molecule" calculations, no description of these out-of-plane modes is possible with them. Much of the earlier assignment difficulty in this region probably relates to confusion in identification of the internal modes. Once recognized, however, the assignment situation is not necessarily hopeless. The size of the deuteration shift suggests relatively little coupling between the hydroxyl and internal modes, so the problem reduces to one of recognition. In our study, only bands with minimal temperature sensitivity and significant Raman intensity have been assigned as internal fundamentals. This has resulted in a reasonable correspondence between observed and calculated bands, although a few discrepancies, such as in alpha glucose- O-d_5 , remain.

Low Frequency Skeletal Motions

Most carbohydrates show strong Raman bands in the $550\text{-}350\text{ cm}^{-1}$ region, often among the most intense in the spectrum. Our calculated normal modes show primarily heavy atom, skeletal type motions. Since much of this motion is normal to the ring mean plane, these modes might be described as ring out-of-plane deformation or twisting modes. Figure 43 illustrates a typical case, the 447 cm^{-1} mode for alpha glucose. There is fairly general agreement between our results and most of the previous reported calculations (1-4,6-9) concerning the

Figure 43. Typical Low Frequency Motion. The 447 cm⁻¹ Mode of Alpha Glucose

general form of these modes. Comparison of our calculated frequencies to those of Vasko (1), Vasko, et al. (2), and Cael, et al. (3) suggests that the frequencies and by implication the form of the modes are not too sensitive to the exact values of the force constants. Since this region lies below the range of rock salt spectrometers, there is little in the older literature concerning these modes which requires discussion.

Below 300 cm^{-1} the calculated modes show coupling of heavy atom bending and torsional motion. Since there are many more experimental bands than calculated fundamentals, those assignments which we have made below 300 cm^{-1} should be regarded with caution. The excess of experimental bands is probably due to the presence of lattice modes, overtone and combination bands, and "hot" bands. While the internal fundamentals, if uncoupled from the lattice modes, may in principle be recognized by their insensitivity to temperature, there are in fact no well established guidelines for their recognition in carbohydrates. A second caution is mandated by the previously discussed ambiguities in the torsional force constants.

CONCLUSIONS

Our calculations certainly do not provide an absolute set of vibrational assignments for glucose, galactose, or mannose, and the complexity of this problem seems to preclude its complete solution in the near future. Still, our degree of agreement between experiment and calculation seems significant and suggests that our model, while limited, may still provide considerable insight. Individual band assignments may be suspect unless the band is very isolated or involved in a large isotopic shift, but the model may be considerably more reliable with respect to the frequency regions appropriate to particular types of motion and with respect to the general nature of coupling

patterns. These two constraints are sufficient to void many of the assignments in the older literature.

Perhaps the greatest importance of our calculations and similar ones is the fact that transition from a qualitative to a quantitative model has now been made. The very existence of such a model provides both a case for future improvement and a framework for the interpretation of future data. Equally important, it provides a more restrictive framework within which differences of opinion must be resolved. We shall illustrate one important application of such a model, conformational analysis, in the next chapter. Many other applications, such as the calculation of improved vibrational partition functions, are now open for exploration.

CHAPTER III

AN INVESTIGATION OF THE HYDROXYMETHYLENE
CONFORMATIONS IN GLUCOSE, GALACTOSE, AND
MANNOSE BY VIBRATIONAL SPECTROSCOPY

INTRODUCTION

The possibility of rotational isomerism about the C(5)-C(6) bond in glucopyranose structures has been the source of considerable speculation and controversy in both crystallographic and spectroscopic studies. In view of the past successes of normal coordinate calculations in conformational analysis (45,49), and in view of the ambiguous and sometimes conflicting interpretations of carbohydrate hydroxymethylene orientation produced by other methods (81), this provides an excellent opportunity to test the predictive utility of our glucose force field.

The various staggered hydroxymethylene rotamers have frequently been described in terms of a notation proposed by Sundaralingam (82). This system, illustrated in Fig. 44, is based on the relationship of O(6) to C(4) and O(5). Thus, the conformation with O(6) gauche to O(5) and trans to C(4) is designated GT (gauche-trans). One of the three conformations is expected to be energetically unfavorable due to the short distance between O(6) and O(4). In glucose and mannose, with O(4) equatorial, TG is the unfavorable form, while the axial O(4) in galactose makes GG the high energy form. X-ray investigations of glucopyranose structures have found the GT conformation in about two-thirds of the studied cases, GG in about one-third, and TG in none (82). No comparable compilation has appeared for galactose derivatives. Although simultaneous presence of two or more hydroxymethylene conformations in the same crystal has not been reported for glucopyranose structures, such a situation has been established for alpha sorbose (83).

Figure 44. Sundaralingam Notion for Hydroxymethylene Conformations

Most of the interest in C(6) conformations in carbohydrates has focused on the crystal structure of cellulose I. The data from x-ray diffraction studies have been sufficient to fix approximately the positions of the chains in the unit cell and the backbone conformations of these chains. The limited hydrogen bonding possibilities at O(3) and O(2) combined with various nonbonded interaction considerations further restrict the backbone conformation. Unfortunately, neither x-ray intensities nor packing considerations have been able to fix the hydroxymethylene conformation unambiguously, although there has been a tendency for crystallographic studies to favor the TG conformation as agreeing best with the intensity data (84,85).

Two different spectroscopic approaches have also been applied to this problem. Marchessault and Liang believed that the GT conformation was the most likely, based on a combination of infrared dichroism data and steric considerations (62). Blackwell and Marchessault (86) reaffirmed this conclusion after inclusion of calculated dichroic ratios and Sundaralingam's (82) crystallographic survey in their considerations. Zhbakov, *et al.* (87) cited the temperature sensitivity of a number of bands in the 1500-1400 cm^{-1} region as evidence of multiple hydroxymethylene conformations in cellulose I at room temperature.

None of these approaches can fix the hydroxymethylene conformation unambiguously at present, and thus the crucial question of the nature of the hydrogen bonding network in native cellulose remains open. Any new approach to this problem is thus potentially valuable. Such an approach is available through normal coordinate calculations. Several authors have demonstrated in recent years that when good geometric and potential models are available, calculations can often distinguish conformational possibilities based solely upon the presence or absence of bands in a particular frequency region (6,7,45,46,49). We have

thus undertaken calculations to explore the applicability of our glucose force field to the hydroxymethylene conformation problem, using glucose, galactose, and mannose as model systems.

EXPERIMENTAL

The vibrational spectra and tabulated frequencies for the anomers of glucose, galactose, and mannose have been presented in the previous chapters. In addition, a Raman spectrum of alpha sorbose was obtained under the previously described experimental conditions. The sample was used as received from Pierce Chemical Company, and the spectrum is included as Fig. 51 (page 146).

CALCULATIONS

Spectra were calculated for all three rotamers of each anomer using the software package described previously. The potential energy model was the force field developed for glucose in Chapter I. The geometric model was based on the alpha glucose structure described in the first chapter, with the appropriate interchanges of axial and equatorial groups. The hydroxymethylene groups were placed in each of the three fully staggered conformations. The crystallographic structures used for alpha and beta glucose in the development of the force field deviate about 10° from the fully staggered GT and GG conformations, respectively, but this difference has very little effect on the calculated frequencies. The results of these calculations are shown graphically in Fig. 45-50 and in tabular form in Tables XXIII-XXVIII. Complete results and potential energy distributions may be found in Appendix II.

ALPHA GLUCOSE CALCULATED TG

CALCULATED GG

CALCULATED GT

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM.-1)

Figure 45. Assigned and Calculated Frequencies for Rotamers of Alpha Glucose

BETA GLUCOSE
CALCULATED TG

CALCULATED GG

CALCULATED GT

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM.-1)

Figure 46. Assigned and Calculated Frequencies for Rotamers of Beta Glucose

ALPHA GALACTOSE CALCULATED TG

CALCULATED GG

CALCULATED GT

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM.-1)

Figure 47. Assigned and Calculated Frequencies for Rotamers of Alpha Galactose

BETA GALACTOSE CALCULATED TG

CALCULATED GG

CALCULATED GT

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM.-1)

Figure 48. Assigned and Calculated Frequencies for Rotamers of Beta Galactose

ALPHA MANNOSE
CALCULATED TG

CALCULATED GG

CALCULATED GT

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM.-1)

Figure 49. Assigned and Calculated Frequencies for Rotamers of Alpha Mannose

BETA MANNOSE
CALCULATED TG

CALCULATED GG

CALCULATED GT

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM.-1)

Figure 50. Assigned and Calculated Frequencies for Rotamers of Beta Mannose

TABLE XXIII

ALPHA GLUCOSE

Summary of Rotamer Calculations

Mode	GT	Δ	GG	Δ	TG	Δ	Experimental
36	962	(0)	918	(0)	974	(0)	--
37	904	10.9	903	11.0	901	13.8	915
38	835	1.6	847	10.4	851	13.6	837
39	760	14.8	758	16.8	762	12.8	775
40	632	12.1	717	96.7	634	13.9	620
41	624	19.3	594	10.9	572	33.2	605
42	556	0.3	541	15.4	555	0.9	556
43	533	5.7	530	8.5	527	12.5	539
44	453	14.2	511	71.6	484	45.1	439
45	426	4.3	432	9.6	439	17.6	422
46	388	15.5	400	3.7	391	12.8	404
47	369	8.2	355	5.8	365	3.7	361
48	322	4.4	319	7.4	331	3.8	327
49	313	3.2	312	3.6	315	0.7	316
50	304	2.3	276	26.2	302	0.2	302
Error, 36→46		9.9		25.5		17.6	
Error, total		5.5 cm^{-1}		11.4		8.4	

TABLE XXIV

BETA GLUCOSE

Summary of Rotamer Calculations

Mode	GT	Δ	GG	Δ	TG	Δ	Experimental
36	973	20.5	967	15.0	978	25.6	952
37	951	38.3	905	8.5	942	29.1	913
38	875	23.5	891	6.7	850	48.1	898
39	650	64.4	723	9.0	678	35.6	714
40	641	8.6	623	8.9	624	8.4	632
41	600	6.9	600	7.4	604	10.6	593
42	580	6.3	583	8.5	561	12.7	574
43	504	15.5	524	5.1	501	18.5	519
44	436	17.9	460	5.5	452	2.3	454
45	412	13.2	414	10.6	408	17.1	425
46	407	5.5	389	12.4	402	0.7	401
47	353	5.6	347	0.2	353	5.6	347
48	329	2.0	333	6.4	336	8.5	327
49	312	3.2	314	4.7	319	9.5	309
50	304	15.1	298	8.6	303	13.5	289
Error, 36→46		20.1		8.26		18.30	
Error, total		10.19 cm^{-1}		6.39		11.28	

TABLE XXV

ALPHA GALACTOSE

Summary of Rotamer Calculations

Mode	GT	Δ	GG	Δ	TG	Δ	Experimental
36	922	33.1	909	45.9	938	17.5	955
37	863	23.1	875	11.0	881	5.0	886
38	817	10.7	849	20.9	839	11.1	828
39	801	36.2	792	26.5	768	3.0	765
40	719	16.7	753	50.9	708	6.4	702
41	695	35.4	702	41.7	669	9.0	660
42	622	10.0	613	0.6	612	0.0	612
43	504	25.8	544	13.9	532	2.2	530
44	491	0.8	486	3.9	482	7.7	490
45	416	0.9	422	4.9	437	19.7	417
46	392	15.0	399	8.1	403	3.8	407
47	350	8.2	335	23.2	349	9.2	358
48	324	17.1	318	12.9	320	10.9	331
49	308	9.3	299	0.1	310	11.1	299
50	286	17.7	281	12.8	265	3.1	268
Error, 36→46		18.85		20.7		7.76	
Error, total		11.06 cm^{-1}		12.85		7.24	

TABLE XXVI

BETA GALACTOSE

Summary of Rotamer Calculations

Mode	GT	Δ	GG	Δ	TG	Δ	Experimental
36	949	0.3	919	30.3	945	4.4	949
37	880	26.2	901	5.3	909	2.8	906
38	871	17.2	864	25.1	864	25.4	889
39	793	8.7	827	42.8	759	24.7	784
40	705	1.7	734	31.3	674	28.8	703
41	605	18.2	611	12.5	617	6.0	623
42	560	0.1	555	4.7	579	18.7	560
43	513	22.8	541	4.8	547	11.2	536
44	491	13.5	490	11.9	459	19.5	478
45	424	11.1	426	9.1	439	3.6	435
46	387	12.6	389	10.6	388	11.9	400
47	346	16.9	329	33.7	347	15.8	363
48	321	8.1	324	5.1	325	4.4	329
49	320	9.2	320	9.4	317	6.4	311
50	293	1.0	286	6.5	288	3.6	292
Error, 36→46		12.05		17.13		14.28	
Error, total		9.05 cm^{-1}		11.35		8.15	

TABLE XXVII

ALPHA MANNOSE

Summary of Rotamer Calculations

Mode	GT	Δ	GG	Δ	TG	Δ	Experimental
36	958	0.4	913	0.9	944	13.7	958, 914
37	889	6.2	892	8.6	886	3.3	883
38	825	6.9	835	8.9	851	19.1	832, 844
39	788	26.0	805	25.4	788	25.7	814, 780
40	685	0.4	687	33.4	677	8.3	685, 720
41	603	3.5	660	24.0	587	19.3	606, 684
42	574	2.3	565	9.8	542	34.1	576
43	533	2.8	513	18.4	524	5.8	530
44	468	7.0	495	19.8	497	21.7	475
45	438	12.3	446	3.4	442	7.9	450
46	390	8.0	411	14.4	390	8.4	398
47	372	0.7	390	17.0	388	15.1	373
48	349	9.7	318	40.4	358	1.2	359
49	309	1.0	300	5.6	308	0.4	308
50	292	18.4	277	9.1	294	20.1	274
Error, 36→46		6.89		15.18		13.48	
Error, total		6.05 cm^{-1}		9.38		8.69	

TABLE XXVIII

BETA MANNOSE

Summary of Rotamer Calculations

Mode	GT	Δ	GG	Δ	TG	Δ	Experimental
36	932	1.1	908	25.1	934	1.2	933
37	895	1.4	898	2.4	859	37.1	896
38	826	29.1	843	11.7	839	16.5	855
39	768	1.2	777	7.9	769	0.5	769
40	728	1.8	726	4.2	722	7.9	730
41	617	0.9	677	59.4	664	45.5	618
42	604	4.6	589	9.6	546	53.0	599
43	501	8.5	528	35.8	510	18.0	492
44	469	24.7	477	32.5	469	24.9	444
45	416	6.6	409	13.8	417	6.3	423
46	387	6.7	395	1.4	391	2.6	394
47	366	4.3	352	18.6	371	0.5	370
48	328	1.9	328	1.6	329	2.9	326
49	309	(0)	306	(0)	316	(0)	--
50	292	4.3	277	10.8	291	2.6	288
Error, 36→46		7.87		18.5		19.41	
Error, total		7.39 cm^{-1}		12.62		10.26	

RESULTS AND DISCUSSION

KNOWN STRUCTURES - GLUCOSE

As a starting point we will examine the calculated results for known structures. The crystal structures of alpha and beta glucose are well known (10,11), and, as mentioned, the hydroxymethylene groups lie close to the staggered conformations pictured in Fig. 44. The experimental and calculated spectra are shown in part, graphically, in Fig. 45-46. The conformation sensitivity in the calculated spectra is confined primarily to the region shown, between 1000 and 200 cm^{-1} . The data are also displayed in tabular form, with some error statistics, in Tables XXIII-XXIV.

For alpha glucose, the overall fit favors the crystallographic GT conformation. The preference is even stronger for normal modes 36-46, which tend to be both quite isolated and conformation sensitive. In addition to these average error tests, large individual mismatches, if well beyond the extrema of fit typical of such calculations, can argue against the acceptability of a particular conformation. Alpha glucose normal modes 40 and 44 show such errors for the GG model, while 41 and 44 show them for the TG. When considered together with the steric arguments against the TG, the spectroscopic data show a very definite preference for the correct GT conformation. For beta glucose, a substantial preference is again shown for the correct GG form, with the incorrect models showing large mismatches at modes 37-39.

It is encouraging to note that the most conformation sensitive bands are found in one of the more sparsely occupied spectral regions and are thus easily assigned. The 714 cm^{-1} band in beta glucose provides the most extreme example of this situation. Detailed examination of the potential energy

distributions suggests that the conformation induced shifts are primarily a result of G matrix changes rather than of conformation dependent coupling constants.

UNKNOWN STRUCTURES — GALACTOSE AND MANNOSE

Both alpha galactose and beta mannose show a definite preference for one sterically favorable rotamer. For alpha galactose, the statistics favor the TG model, and the other two conformations both show several large mismatches. A rather similar situation is found for beta mannose, with the GT conformation favored. Beta galactose represents a more ambiguous situation. The sterically unfavorable GG is clearly the poorest choice, but the two other conformations fit the experimental data to a comparable degree. The GT gives a better match in the most sensitive region, but the TG gives a better overall fit. Since neither the TG nor GT shows totally unreasonable mismatches, we will not venture to declare a choice.

Alpha mannose provides a somewhat more interesting situation. The GT conformation is clearly preferred, but there are a number of weaker experimental bands which do not correspond to the calculated spectrum. Many of these bands can be explained by assuming a mixture of two forms, with GT dominant and GG present in lower concentration. The relatively isolated band at 914 cm^{-1} , for example, is unassignable under the GT model. The nearest calculated GT mode is 25 cm^{-1} away and is more reasonably assigned to a band near its calculated frequency. The GG model, however, calculates the 914 cm^{-1} frequency almost exactly. Several other similar situations are found elsewhere in the spectrum.

Such a mixture proposal is not novel, since a similar condition has previously been established for the hydroxymethylene group in alpha sorbose (83). Comparison of the Raman spectra of alpha sorbose (Fig. 51) and alpha mannose

Figure 51. Raman Spectra of Alpha Sorbose

(Fig. 25) with the spectra of the other hexoses presented here reveals that the first two compounds have a significantly greater number of bands, particularly between 1000 and 400 cm^{-1} , despite the constant molecular weight and similar structures. This is fully consistent with the multiple conformation hypothesis. The temperature dependence of the spectra, however, does not suggest a low barrier to interconversion of the conformers, in contrast to Zhbakov, et al. (87) conclusions.

CONCLUSIONS

Our calculations support the GT hydroxymethylene conformation for beta mannose, the TG for alpha galactose, and a mixture of GT and GG for alpha mannose. In the beta galactose case, we eliminate the GG but cannot distinguish between the GT and TG. While these results are interesting, they could be achieved at a higher level of precision by x-ray crystallography, although at a considerably higher cost in effort expended. The greater importance of this study is as a feasibility demonstration for the method. In five of the six compounds studied, the spectroscopic data definitely favored one conformation over the two alternatives, and in the last case, one of the three was at least eliminated. In both cases with known structures, the spectroscopic data favored the crystallographically correct conformation. We thus conclude that the fortuitous occurrence of high conformation sensitivity in an uncrowded spectral region makes interpretation of spectral data by normal coordinate calculations a very promising technique for determination of hydroxymethylene conformation in carbohydrates. While results are not guaranteed, as evidenced by beta galactose, the possibility of a less ambiguous interpretation than is available from x-ray diffraction would seem to justify the effort required to perform these calculations for higher molecular weight systems.

While we await the results for higher saccharides (16), we can still make some comments on the cellulose problem based on the form of our hexose solutions. The spectral differences between cellulose I and II have been attributed to differences in hydrogen bonding patterns (58), differences in hydroxymethylene conformation (87), and differences in backbone conformation (88). While hydrogen bonding differences are unquestionably a contributing factor, the relative importance of the other two factors remains controversial. Comparison of the Raman spectra of cellulose I and II (88) reveals that the most visible differences are in the $400\text{--}300\text{ cm}^{-1}$ region. Although our calculations could rationalize shifts of this magnitude on hydroxymethylene rotation, such rotations are expected to produce larger shifts at higher frequency. In the absence of such higher frequency shifts, and assuming that most of the modes in the $400\text{--}300\text{ cm}^{-1}$ region are pure internal fundamentals, a change in backbone conformation seems the best explanation yet advanced for these shifts (88). The considerable similarity of the cellulose II and cellobiose (89) spectra below 1000 cm^{-1} tempts us to speculate further that the hydroxymethylene conformations are the same in both systems, namely GT (11).

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APPENDIX I
COMPUTER INPUT — HEXOSES^a

The information reported in this appendix is as follows:

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^aFor details of the input or programs, see References 6 or 32.

Figure 52. Atomic Numbering for Calculations - Hexoses

TABLE XXIX

DESCRIPTION OF THE INTERNAL COORDINATES
USED TO DESCRIBE ALDOHEXOSES

Description Code		Description Code		Description Code	
Bond Stretching Coordinates					
1. C1-C2	C1C2	8. C1-O6	C-O6	69. C3-H18	C3-H
2. C2-C3	C2C3	9. C2-O7	C-O7	70. C4-H17	C4-H
3. C3-C4	C3C4	10. C3-O8	C-O8	71. C5-H15	C5-H
4. C4-C5	C4C5	11. C4-O9	C-O9	72. C16-H21	C-HA
5. C5-C16	C5C'	12. C16-O23	C-O*	73. C16-H22	C-HB
6. C5-O10	C5O'	67. C1-H20	C1-H		
7. O10-C1	O'C1	68. C2-H19	C2-H		
Valence Angle Bending Coordinates					
13. C1-C2-C3	C1CC	27. C16-C5-O10	CCO'	41. H21-C16-H22	HCH
14. C2-C3-C4	C2CC	28. C2-C1-O10	O'CC	42. O6-C1-H20	OC1H
15. C3-C4-C5	C3CC	29. C4-C5-O10	CCO'	43. O10-C1-H20	'C1H
16. C4-C5-C16	C4CC	30. C2-C1-H20	CC1H	44. O7-C2-H19	OC2H
17. C5-O10-C1	CO'C	31. C1-C2-H19	CCH2	45. O8-C3-H18	OC3H
18. O10-C1-O6	OCO	32. C3-C2-H19	HC2C	46. O9-C4-H17	OC4H
19. C2-C1-O6	CCO6	33. C2-C3-H18	CC3H	47. O10-C5-H15	'C5H
20. C1-C2-O7	CCO7	34. C4-C3-H18	HC3C	48. O23-C16-H21	OCHA
21. C3-C2-O7	O7CC	35. C3-C4-H17	CC4H	49. O23-C16-H22	OCHB
22. C2-C3-O8	CCO8	36. C5-C4-H17	HC4C	50. C1-O6-H11	C1OH
23. C4-C3-O8	O8CC	37. C4-C5-H15	CC5H	51. C2-O7-H12	C2OH
24. C3-C4-O9	CCO9	38. C16-C5-H15	HC5C	52. C3-O8-H13	C3OH
25. C5-C5-O9	O9CC	39. C5-C16-H21	CCHA	53. C4-O9-H14	C4OH
26. C5-C16-O23	CCO*	40. C5-C16-H22	CCHB	54. C16-O23-H24	C'OH

TABLE XXIX (Continued)
DESCRIPTION OF THE INTERNAL COORDINATES
USED TO DESCRIBE ALDOHEXOSSES

Linear Combination Of:	Description Code	Linear Combination Of:	Description Code
Torsional Coordinates			
55. H11-06-C1-C2	TH-1	61. C2-C3-C4-09	TCC2
H11-06-C1-010		08-C3-C4-C5	
H11-06-C1-H20		H17-C3-C4-C16	
56. H12-07-C2-C3	TH-2	62. C3-C4-C5-C16	TCC3
H12-07-C2-C1		09-C4-C5-010	
H12-07-C2-H19		C16-C4-C5-H15	
57. H13-08-C3-C4	TH-3	63. 010-C1-C2-07	TCC4
H13-08-C3-C2		06-C1-C2-C3	
H13-08-C3-H18		H20-C1-C2-H19	
58. H14-09-C4-C5	TH-4	64. C4-C5-C16-023	TCC5
H14-09-C4-C3		010-C5-C16-H21	
H14-09-C4-H17		H15-C5-C16-H22	
59. H24-023-C16-C5	TH-5	65. C2-C1-010-C5	TC01
H24-023-C16-H21		06-C1-010-C5	
H24-023-C16-H22		H20-C1-010-C5	
60. C1-C2-C3-08	TCC1	66. C1-010-C5-C16	TC02
07-C2-C3-C4		C1-010-C5-C4	
H18-C2-C3-H17		C1-010-C5-H15	

TABLE XXX

CART AND CARTSET INPUT - HEXOSES

CARTSET INPUT- ALPHA GLUCOSE		CART INPUT CALCULATION -- ALPHA GLUCOSE		CELL 10.36 14.84 4.97		-- BRUNN AND LEVY STRUCTURE 90. 90.	
PARAMETERS		24					
C	1	.3329	.6007	-.0762			
C	2	.4184	.6746	.0455			
C	3	.5611	.6514	.0154			
C	4	.5860	.5369	.1200			
C	5	.4956	.4886	-.0123			
O	6	.3470	.6007	-.3541			
O	7	.3880	.7598	-.0657			
O	8	.6334	.7154	.1634			
O	9	.7116	.5348	.0668			
O	10	.3654	.5154	.0329			
H	11	.2753	.5674	-.4299			
H	12	.4485	.7776	-.2031			
H	13	.7247	.7137	.1178			
H	14	.7517	.5082	.2326			
H	15	.5136	.4865	-.2312			
C	16	.5141	.3953	.1026			
H	17	.5677	.5565	.3385			
H	18	.5888	.6543	-.1995			
H	19	.3958	.6776	.2599			
H	20	.2327	.6124	-.0154			
H	21	.6112	.3792	.1032			
H	22	.4804	.3947	.1116			
O	23	.4458	.3311	-.0518			
H	24	.4127	.2861	.0699			

1	1	1	1
2	2	2	2
3	3	3	3
4	4	4	4
5	5	5	5
6	6	6	6
7	7	7	7
8	8	8	8
9	9	9	9
10	10	10	10
11	11	11	11
12	12	12	12
13	13	13	13
14	14	14	14
15	15	15	15
16	16	16	16
17	17	17	17
18	18	18	18
19	19	19	19
20	20	20	20
21	21	21	21
22	22	22	22
23	23	23	23
24	24	24	24

CARTSET INPUT- BETA GLUCOSE		CART INPUT CALCULATION -- BETA GLUCOSE		CELL 9.21 12.64 6.65		-- CHU AND JEFFREY STRUCT. 90.0 90.0	
ATOMS		24					
C	1	.0198	.1614	.4610			
C	2	-.0786	.0717	.3902			
C	3	-.0081	.0059	.2259			
C	4	.0486	.0764	.0600			
C	5	.1479	.1614	.1486			
O	6	-.0611	.2279	.5825			
O	7	-.1119	.0060	.5587			
O	8	-.1147	-.0647	.1445			
O	9	.1297	.0173	-.0825			
O	10	.0636	.2220	.2893			
H	11	.010	.252	.676			
H	12	-.212	.020	.622			
H	13	-.085	-.128	.188			
H	14	.067	-.002	-.196			
H	15	.238	.125	.218			
C	16	.2099	.2385	-.0027			
H	17	-.041	.107	-.008			
H	18	-.081	-.035	.296			
H	19	-.175	.104	.337			
H	20	.116	.137	.540			
H	21	.289	.292	.071			
H	22	.271	.196	-.109			
O	23	.0992	.2936	-.1079			
H	24	.085	.370	-.120			

1	1	1	1
2	2	2	2
3	3	3	3
4	4	4	4
5	5	5	5
6	6	6	6
7	7	7	7
8	8	8	8
9	9	9	9
10	10	10	10
11	11	11	11
12	12	12	12
13	13	13	13
14	14	14	14
15	15	15	15
16	16	16	16
17	17	17	17
18	18	18	18
19	19	19	19
20	20	20	20
21	21	21	21
22	22	22	22
23	23	23	23
24	24	24	24

TABLE XXX (Continued)

CART INPUT- GLUCOSE- C(6) CONFORMATION CALCULATIONS

-09 24 0 -1
-09 ALPHA GLUCOSE---STRUCTURE OF BROWN AND LEVY--NEUTRON DIFFRACTION
EXACT GT CONFORMATION. (+60.0) 12/26/75

1	1	1.533997			12.00000
2	2	1.525286	111.125610		12.00000
3	3	1.517718	109.968340	-51.229874	12.00000
4	4	1.528656	111.221664	-53.256958	12.00000
5	5	1.388865	109.461672	-68.780151	15.99491
6	6	1.420000	110.914780	-125.564804	15.99491
7	7	1.420000	108.135361	-120.774780	15.99491
8	8	1.420000	108.355042	-122.077377	15.99491
9	9	1.424113	109.152575	-56.743073	15.99491
10	10	0.986000	0.0	-74.788040	1.00783
11	11	0.986000	0.0	-79.490433	1.00783
12	12	0.986000	0.0	-73.816467	1.00783
13	13	0.986000	0.0	-76.421066	1.00783
14	14	1.110000	109.867004	-62.454690	1.00783
15	15	1.509924	111.612885	-119.815826	12.00000
16	16	1.110000	108.360217	-118.893417	1.00783
17	17	1.110000	109.754349	-119.569397	1.00783
18	18	1.110000	106.916183	-117.845078	1.00783
19	19	1.110000	109.029770	-65.908249	1.00783
20	20	1.110000	109.019501	-60.000000	1.00783
21	21	1.110000	107.901779	-118.183350	1.00783
22	22	1.420000	110.164309	-121.242249	15.99491
23	23	0.986000	0.0	84.239273	1.00783

CGL3 10
CGL3 20
CGL3 30
CGL3 40
CGL3 50
CGL3 60
CGL3 70
CGL3 80
CGL3 90
CGL3 100
CGL3 110
CGL3 120
CGL3 130
CGL3 140
CGL3 150
CGL3 160
CGL3 170
CGL3 180
CGL3 190
CGL3 200
CGL3 210
CGL3 220
CGL3 230
CGL3 240
CGL3 250
CGL3 260
CGL3 270
CGL3 280
CGL3 290
CGL3 300

-09 24 0 -1
-09 ALPHA GLUCOSE---STRUCTURE OF BROWN AND LEVY--NEUTRON DIFFRACTION
EXACT GT CONFORMATION. (-60.0) 12/26/75

1	1	1.533997			12.00000
2	2	1.525286	111.125610		12.00000
3	3	1.517718	109.968340	-51.229874	12.00000
4	4	1.528656	111.221664	-53.256958	12.00000
5	5	1.388865	109.461672	-68.780151	15.99491
6	6	1.420000	110.914780	-125.564804	15.99491
7	7	1.420000	108.135361	-120.774780	15.99491
8	8	1.420000	108.355042	-122.077377	15.99491
9	9	1.424113	109.152575	-56.743073	15.99491
10	10	0.986000	0.0	-74.788040	1.00783
11	11	0.986000	0.0	-79.490433	1.00783
12	12	0.986000	0.0	-73.816467	1.00783
13	13	0.986000	0.0	-76.421066	1.00783
14	14	1.110000	109.867004	-62.454690	1.00783
15	15	1.509924	111.612885	-119.815826	12.00000
16	16	1.110000	108.360217	-118.893417	1.00783
17	17	1.110000	109.754349	-119.569397	1.00783
18	18	1.110000	106.916183	-117.845078	1.00783
19	19	1.110000	109.029770	-65.908249	1.00783
20	20	1.110000	109.019501	-60.000000	1.00783
21	21	1.110000	107.901779	-118.183350	1.00783
22	22	1.420000	110.164309	-121.242249	15.99491
23	23	0.986000	0.0	84.239273	1.00783

CGL3 310
CGL3 320
CGL3 330
CGL3 340
CGL3 350
CGL3 360
CGL3 370
CGL3 380
CGL3 390
CGL3 400
CGL3 410
CGL3 420
CGL3 430
CGL3 440
CGL3 450
CGL3 460
CGL3 470
CGL3 480
CGL3 490
CGL3 500
CGL3 510
CGL3 520
CGL3 530
CGL3 540
CGL3 550
CGL3 560
CGL3 570
CGL3 580
CGL3 590
CGL3 600

-09 24 0 -1
-09 ALPHA GLUCOSE---STRUCTURE OF BROWN AND LEVY--NEUTRON DIFFRACTION
EXACT GT CONFORMATION. (180.0) 12/26/75

1	1	1.533997			12.00000
2	2	1.525286	111.125610		12.00000
3	3	1.517718	109.968340	-51.229874	12.00000
4	4	1.528656	111.221664	-53.256958	12.00000
5	5	1.388865	109.461672	-68.780151	15.99491
6	6	1.420000	110.914780	-125.564804	15.99491
7	7	1.420000	108.135361	-120.774780	15.99491
8	8	1.420000	108.355042	-122.077377	15.99491
9	9	1.424113	109.152575	-56.743073	15.99491
10	10	0.986000	0.0	-74.788040	1.00783
11	11	0.986000	0.0	-79.490433	1.00783
12	12	0.986000	0.0	-73.816467	1.00783
13	13	0.986000	0.0	-76.421066	1.00783
14	14	1.110000	109.867004	-62.454690	1.00783
15	15	1.509924	111.612885	-119.815826	12.00000
16	16	1.110000	108.360217	-118.893417	1.00783
17	17	1.110000	109.754349	-119.569397	1.00783
18	18	1.110000	106.916183	-117.845078	1.00783
19	19	1.110000	109.029770	-65.908249	1.00783
20	20	1.110000	109.019501	-60.000000	1.00783
21	21	1.110000	107.901779	-118.183350	1.00783
22	22	1.420000	110.164309	-121.242249	15.99491
23	23	0.986000	0.0	84.239273	1.00783

CGL3 610
CGL3 620
CGL3 630
CGL3 640
CGL3 650
CGL3 660
CGL3 670
CGL3 680
CGL3 690
CGL3 700
CGL3 710
CGL3 720
CGL3 730
CGL3 740
CGL3 750
CGL3 760
CGL3 770
CGL3 780
CGL3 790
CGL3 800
CGL3 810
CGL3 820
CGL3 830
CGL3 840

CARD INPUT ... GALACTOSE AND HANNOSE										CTHX	TO
-09 24 0 -1 ALPHA GALACTOSE. STRUCTURE ASSUMED SIMILAR TO ALPHA GLUCOSE. H(04)										CTHX	10
IS CIS TO H(C4). C6 IN IN GT POSITION.										CTHX	30
1	2	3	4	5	6	7	8	9	10	CTHX	40
1	1	1	1	1	1	1	1	1	1	CTHX	50
2	1	2	1	1	1	1	1	1	1	CTHX	60
3	2	3	2	1	1	1	1	1	1	CTHX	70
4	3	4	3	2	1	1	1	1	1	CTHX	80
5	4	5	4	3	2	1	1	1	1	CTHX	90
6	5	6	5	4	3	2	1	1	1	CTHX	100
7	6	7	6	5	4	3	2	1	1	CTHX	110
8	7	8	7	6	5	4	3	2	1	CTHX	120
9	8	9	8	7	6	5	4	3	2	CTHX	130
10	9	10	9	8	7	6	5	4	3	CTHX	140
11	10	11	10	9	8	7	6	5	4	CTHX	150
12	11	12	11	10	9	8	7	6	5	CTHX	160
13	12	13	12	11	10	9	8	7	6	CTHX	170
14	13	14	13	12	11	10	9	8	7	CTHX	180
15	14	15	14	13	12	11	10	9	8	CTHX	190
16	15	16	15	14	13	12	11	10	9	CTHX	200
17	16	17	16	15	14	13	12	11	10	CTHX	210
18	17	18	17	16	15	14	13	12	11	CTHX	220
19	18	19	18	17	16	15	14	13	12	CTHX	230
20	19	20	19	18	17	16	15	14	13	CTHX	240
21	20	21	20	19	18	17	16	15	14	CTHX	250
22	21	22	21	20	19	18	17	16	15	CTHX	260
23	22	23	22	21	20	19	18	17	16	CTHX	270
24	23	24	23	22	21	20	19	18	17	CTHX	280
-09	24	0	-1							CTHX	290
ALPHA GALACTOSE. STRUCTURE ASSUMED SIMILAR TO ALPHA GLUCOSE. H(04)										CTHX	300
IS CIS TO H(C4). C6 IN IN GG POSITION.										CTHX	310
1	2	3	4	5	6	7	8	9	10	CTHX	320
1	1	1	1	1	1	1	1	1	1	CTHX	330
2	1	2	1	1	1	1	1	1	1	CTHX	340
3	2	3	2	1	1	1	1	1	1	CTHX	350
4	3	4	3	2	1	1	1	1	1	CTHX	360
5	4	5	4	3	2	1	1	1	1	CTHX	370
6	5	6	5	4	3	2	1	1	1	CTHX	380
7	6	7	6	5	4	3	2	1	1	CTHX	390
8	7	8	7	6	5	4	3	2	1	CTHX	400
9	8	9	8	7	6	5	4	3	2	CTHX	410
10	9	10	9	8	7	6	5	4	3	CTHX	420
11	10	11	10	9	8	7	6	5	4	CTHX	430
12	11	12	11	10	9	8	7	6	5	CTHX	440
13	12	13	12	11	10	9					

TABLE XXX (Continued)

-09 24 0 -1 ALPHA MANNOSE. STRUCTURE IS ASSUMED SIMILAR TO ALPHA GLUCOSE. H(02) IS CIS TO H(2). C6 IS IN GT CONFORMATION. 11/23/75										CTHX1690
1	2	1	1	1.533997	111.125610	-51.229874	12.00000	CTHX1700		
2	1	2	1	1.525286	109.908340	-53.256958	12.00000	CTHX1710		
3	2	3	1	1.517718	109.908340	-53.256958	12.00000	CTHX1720		
4	3	4	2	1.528656	109.401672	-68.780151	15.99490	CTHX1730		
5	4	5	3	1.388865	110.914780	-119.000000	15.99490	CTHX1740		
6	1	2	1	1.420000	108.135361	-120.774780	15.99490	CTHX1750		
7	2	1	3	1.420000	108.355042	122.077377	15.99490	CTHX1760		
8	3	2	4	1.420000	109.152575	-56.743073	15.99490	CTHX1770		
9	4	3	5	0.986000	0.0	74.788040	1.00783	CTHX1800		
10	5	4	3	0.986000	0.0	-120.000000	1.00783	CTHX1810		
11	6	7	1	0.986000	0.0	73.816467	1.00783	CTHX1820		
12	7	2	1	0.986000	0.0	-76.421066	1.00783	CTHX1830		
13	8	3	4	1.110000	109.867004	62.494690	1.00783	CTHX1840		
14	9	4	5	1.509924	111.612885	-119.815826	12.00000	CTHX1850		
15	5	4	3	1.110000	108.300217	-118.893417	1.00783	CTHX1860		
16	5	4	3	1.110000	109.754349	119.569397	1.00783	CTHX1870		
17	4	3	5	1.110000	106.916183	125.000000	1.00783	CTHX1880		
18	3	2	4	1.110000	108.135361	-120.774780	1.00783	CTHX1890		
19	2	1	3	1.110000	109.019501	-60.000000	1.00783	CTHX1900		
20	1	2	19	1.110000	107.901779	-118.183350	1.00783	CTHX1910		
21	16	21	5	1.420000	110.104309	121.242249	15.99491	CTHX1920		
22	16	21	5	0.986000	0.0	84.239273	1.00783	CTHX1930		
23	16	21	5					CTHX1940		
24	23	16	21					CTHX1950		
-09 24 0 -1 ALPHA MANNOSE. STRUCTURE IS ASSUMED SIMILAR TO ALPHA GLUCOSE. H(02) IS CIS TO H(2). C6 IS IN GG CONFORMATION. 11/23/75										CTHX1960
1	2	1	1	1.533997	111.125610	-51.229874	12.00000	CTHX1970		
2	1	2	1	1.525286	109.908340	-53.256958	12.00000	CTHX1980		
3	2	3	1	1.517718	109.908340	-53.256958	12.00000	CTHX1990		
4	3	4	2	1.528656	109.401672	-68.780151	15.99490	CTHX2000		
5	4	5	3	1.388865	110.914780	-119.000000	15.99490	CTHX2010		
6	1	2	1	1.420000	108.135361	-120.774780	15.99490	CTHX2020		
7	2	1	3	1.420000	108.355042	122.077377	15.99490	CTHX2030		
8	3	2	4	1.420000	109.152575	-56.743073	15.99490	CTHX2040		
9	4	3	5	0.986000	0.0	74.788040	1.00783	CTHX2050		
10	5	4	3	0.986000	0.0	-120.000000	1.00783	CTHX2060		
11	6	7	1	0.986000	0.0	73.816467	1.00783	CTHX2070		
12	7	2	1	0.986000	0.0	-76.421066	1.00783	CTHX2080		
13	8	3	4	1.110000	109.867004	62.494690	1.00783	CTHX2090		
14	9	4	5	1.509924	111.612885	-119.815826	12.00000	CTHX2100		
15	5	4	3	1.110000	108.300217	-118.893417	1.00783	CTHX2110		
16	5	4	3	1.110000	109.754349	119.569397	1.00783	CTHX2120		
17	4	3	5	1.110000	106.916183	125.000000	1.00783	CTHX2130		
18	3	2	4	1.110000	108.135361	-120.774780	1.00783	CTHX2140		
19	2	1	3	1.110000	109.019501	-60.000000	1.00783	CTHX2150		
20	1	2	19	1.110000	107.901779	-118.183350	1.00783	CTHX2160		
21	16	21	5	1.420000	110.104309	121.242249	15.99491	CTHX2170		
22	16	21	5	0.986000	0.0	84.239273	1.00783	CTHX2180		
23	16	21	5					CTHX2190		
24	23	16	21					CTHX2200		
-09 24 0 -1 ALPHA MANNOSE. STRUCTURE IS ASSUMED SIMILAR TO ALPHA GLUCOSE. H(02) IS CIS TO H(2). C6 IS IN TG CONFORMATION. 11/23/75										CTHX2210
1	2	1	1	1.533997	111.125610	-51.229874	12.00000	CTHX2220		
2	1	2	1	1.525286	109.908340	-53.256958	12.00000	CTHX2230		
3	2	3	1	1.517718	109.908340	-53.256958	12.00000	CTHX2240		
4	3	4	2	1.528656	109.401672	-68.780151	15.99490	CTHX2250		
5	4	5	3	1.388865	110.914780	-119.000000	15.99490	CTHX2260		
6	1	2	1	1.420000	108.135361	-120.774780	15.99490	CTHX2270		
7	2	1	3	1.420000	108.355042	122.077377	15.99490	CTHX2280		
8	3	2	4	1.420000	109.152575	-56.743073	15.99490	CTHX2290		
9	4	3	5	0.986000	0.0	74.788040	1.00783	CTHX2300		
10	5	4	3	0.986000	0.0	-120.000000	1.00783	CTHX2310		
11	6	7	1	0.986000	0.0	73.816467	1.00783	CTHX2320		
12	7	2	1	0.986000	0.0	-76.421066	1.00783	CTHX2330		
13	8	3	4	1.110000	109.867004	62.494690	1.00783	CTHX2340		
14	9	4	5	1.509924	111.612885	-119.815826	12.00000	CTHX2350		
15	5	4	3	1.110000	108.300217	-118.893417	1.00783	CTHX2360		
16	5	4	3	1.110000	109.754349	119.569397	1.00783	CTHX2370		
17	4	3	5	1.110000	106.916183	125.000000	1.00783	CTHX2380		
18	3	2	4	1.110000	108.135361	-120.774780	1.00783	CTHX2390		
19	2	1	3	1.110000	109.019501	-60.000000	1.00783	CTHX2400		
20	1	2	19	1.110000	107.901779	-118.183350	1.00783	CTHX2410		
21	16	21	5	1.420000	110.104309	121.242249	15.99491	CTHX2420		
22	16	21	5	0.986000	0.0	84.239273	1.00783	CTHX2430		
23	16	21	5					CTHX2440		
24	23	16	21					CTHX2450		

TABLE XXX (Continued)

-09	24	0	-1	STRUCTURE ASSUMED TO BE SIMILAR TO BETA GLUCOSE.				CTHX2530
-09	24	0	-1	BETA MANNOSE. H(C2) PLACED CIS TO H(C2). C6 IS GT.				CTHX2540
								CTHX2550
								CTHX2560
1	1			1.533997			12.00000	CTHX2570
2	1			1.525286	111.125610		12.00000	CTHX2580
3	2	1		1.517718	109.908340	-51.229874	12.00000	CTHX2590
4	3	2	1	1.528656	111.221664	53.256958	12.00000	CTHX2600
5	4	3	2	1.388865	109.401672	-169.461227	15.99491	CTHX2610
6	1	2	3	1.420000	110.914780	-119.000000	15.99491	CTHX2620
7	2	1	3	1.420000	108.135361	-120.774780	15.99491	CTHX2630
8	3	2	4	1.420000	108.355042	122.077377	15.99491	CTHX2640
9	4	3	5	1.424113	109.152575	-56.743073	15.99491	CTHX2650
10	5	4	3	0.986000	0.0	-84.135406	1.00783	CTHX2660
11	6	1	10	0.986000	0.0	-120.000000	1.00783	CTHX2670
12	7	2	1	0.986000	0.0	129.423325	1.00783	CTHX2680
13	8	3	4	0.986000	0.0	-143.396088	1.00783	CTHX2690
14	9	4	5	1.110000	109.867004	62.494690	1.00783	CTHX2700
15	5	4	3	1.509924	111.612885	-119.815826	12.00000	CTHX2710
16	5	4	10	1.110000	108.300217	-118.893417	1.00783	CTHX2720
17	4	3	5	1.110000	109.754349	119.569397	1.00783	CTHX2730
18	3	2	4	1.110000	106.916183	125.000000	1.00783	CTHX2740
19	2	1	3	1.110000	109.029770	53.600000	1.00783	CTHX2750
20	1	2	19	1.110000	109.019501	-60.000000	1.00783	CTHX2760
21	16	5	15	1.110000	107.901779	-118.183350	1.00783	CTHX2770
22	16	21	5	1.420000	110.104309	121.242249	15.99491	CTHX2780
23	16	21	5	0.986000	0.0	1.025115	1.00783	CTHX2790
24	23	16	21					CTHX2800
-09	24	0	-1	STRUCTURE ASSUMED TO BE SIMILAR TO BETA GLUCOSE.				CTHX2810
-09	24	0	-1	BETA MANNOSE. H(C2) PLACED CIS TO H(C2). C6 IS GG				CTHX2820
								CTHX2830
								CTHX2840
1	1			1.533997			12.00000	CTHX2850
2	1			1.525286	111.125610		12.00000	CTHX2860
3	2	1		1.517718	109.908340	-51.229874	12.00000	CTHX2870
4	3	2	1	1.528656	111.221664	53.256958	12.00000	CTHX2880
5	4	3	2	1.388865	109.401672	-169.461227	15.99491	CTHX2890
6	1	2	3	1.420000	110.914780	-119.000000	15.99491	CTHX2900
7	2	1	3	1.420000	108.135361	-120.774780	15.99491	CTHX2910
8	3	2	4	1.420000	108.355042	122.077377	15.99491	CTHX2920
9	4	3	5	1.424113	109.152575	-56.743073	15.99491	CTHX2930
10	5	4	3	0.986000	0.0	-84.135406	1.00783	CTHX2940
11	6	1	10	0.986000	0.0	-120.000000	1.00783	CTHX2950
12	7	2	1	0.986000	0.0	129.423325	1.00783	CTHX2960
13	8	3	4	0.986000	0.0	-143.396088	1.00783	CTHX2970
14	9	4	5	1.110000	109.867004	62.494690	1.00783	CTHX2980
15	5	4	3	1.509924	111.612885	-119.815826	12.00000	CTHX2990
16	5	4	10	1.110000	108.300217	-118.893417	1.00783	CTHX3000
17	4	3	5	1.110000	109.754349	119.569397	1.00783	CTHX3010
18	3	2	4	1.110000	106.916183	125.000000	1.00783	CTHX3020
19	2	1	3	1.110000	109.029770	53.600000	1.00783	CTHX3030
20	1	2	19	1.110000	109.019501	-60.000000	1.00783	CTHX3040
21	16	5	15	1.110000	107.901779	-118.183350	1.00783	CTHX3050
22	16	21	5	1.420000	110.104309	121.242249	15.99491	CTHX3060
23	16	21	5	0.986000	0.0	1.025115	1.00783	CTHX3070
24	23	16	21					CTHX3080
-09	24	0	-1	STRUCTURE ASSUMED TO BE SIMILAR TO BETA GLUCOSE.				CTHX3090
-09	24	0	-1	BETA MANNOSE. H(C2) PLACED CIS TO H(C2). C6 IS TG				CTHX3100
								CTHX3110
								CTHX3120
								CTHX3130
								CTHX3140
1	1			1.533997			12.00000	CTHX3150
2	1			1.525286	111.125610		12.00000	CTHX3160
3	2	1		1.517718	109.908340	-51.229874	12.00000	CTHX3170
4	3	2	1	1.528656	111.221664	53.256958	12.00000	CTHX3180
5	4	3	2	1.388865	109.401672	-169.461227	15.99491	CTHX3190
6	1	2	3	1.420000	110.914780	-119.000000	15.99491	CTHX3200
7	2	1	3	1.420000	108.135361	-120.774780	15.99491	CTHX3210
8	3	2	4	1.420000	108.355042	122.077377	15.99491	CTHX3220
9	4	3	5	1.424113	109.152575	-56.743073	15.99491	CTHX3230
10	5	4	3	0.986000	0.0	-84.135406	1.00783	CTHX3240
11	6	1	10	0.986000	0.0	-120.000000	1.00783	CTHX3250
12	7	2	1	0.986000	0.0	129.423325	1.00783	CTHX3260
13	8	3	4	0.986000	0.0	-143.396088	1.00783	CTHX3270
14	9	4	5	1.110000	109.867004	62.494690	1.00783	CTHX3280
15	5	4	3	1.509924	111.612885	-119.815826	12.00000	CTHX3290
16	5	4	10	1.110000	108.300217	-118.893417	1.00783	CTHX3300
17	4	3	5	1.110000	109.754349	119.569397	1.00783	CTHX3310
18	3	2	4	1.110000	106.916183	125.000000	1.00783	CTHX3320
19	2	1	3	1.110000	109.029770	53.600000	1.00783	CTHX3330
20	1	2	19	1.110000	109.019501	-60.000000	1.00783	CTHX3340
21	16	5	15	1.110000	107.901779	-118.183350	1.00783	CTHX3350
22	16	21	5	1.420000	110.104309	121.242249	15.99491	CTHX3360
23	16	21	5	0.986000	0.0	1.025115	1.00783	
24	23	16	21					

TABLE XXXI

GMAT INPUT - HEXOSES

GMAT INPUT- ALPHA GLUCOSE

ALPHA GLUCOSE. BROWN AND LEVY STRUCTURE WITH THERMAL CORRECTIONS. (GT)										GGL1	
26 DEC. 1975										10	
-09	400	24	73	1	1	1				GGL1	20
-09										GGL1	30
1	2	1.533997	1	3	2.083728	2	3	1.422775	1	4	1.436452
2	4	2.226911	3	4	1.112595	1	5	-0.088425	2	5	2.158811
3	5	1.029504	1	6	-0.461363	2	6	-0.474150	3	6	-1.221175
1	7	2.040905	2	7	-0.771486	3	7	-1.079003	1	8	3.489556
2	8	1.353429	3	8	-0.187702	1	9	1.888399	2	9	3.569534
3	9	1.015119	1	10	-0.498086	2	10	0.795465	1	10	1.069115
1	11	-1.409983	2	11	-0.229020	3	11	-1.331758	1	12	1.999842
2	12	-0.241742	3	12	-1.905595	1	13	3.894056	2	13	2.225017
3	13	-0.033450	1	14	1.733835	2	14	4.031411	3	14	1.872426
1	15	-0.434720	2	15	2.609021	3	15	0.075832	1	16	-0.741163
2	16	2.886507	3	16	2.180268	1	17	1.752197	2	17	1.793928
3	17	2.084671	1	18	1.859258	2	18	1.911700	3	18	-0.970910
1	19	-1.856975	2	19	-0.496027	3	19	-0.939011	1	20	-0.361925
2	20	-1.028370	3	20	-0.208719	1	21	-0.287562	2	21	3.895217
3	21	-2.274326	1	22	-0.537138	2	22	2.331695	3	22	3.119768
1	23	-2.140265	2	23	2.958626	3	23	1.964992	1	24	-2.599423
2	24	3.096355	3	24	2.832065	1	0	0.0	2	0	0.0
1	1	0.0	2	1	0.0	3	1	0.0	3	1	0.0
4	1	0.0	5	1	0.0	6	1	0.0	6	1	0.0
7	1	0.0	8	1	0.0	9	1	0.0	9	1	0.0
10	1	0.0	11	1	0.0	12	1	0.0	12	1	0.0
13	1	0.0	14	1	0.0	15	1	0.0	15	1	0.0
16	1	0.0	17	1	0.0	18	1	0.0	18	1	0.0
19	1	0.0	20	1	0.0	21	1	0.0	21	1	0.0
22	1	0.0	23	1	0.0	24	1	0.0	24	1	0.0
25	1	0.0	26	1	0.0	27	1	0.0	27	1	0.0
28	1	0.0	29	1	0.0	30	1	0.0	30	1	0.0
31	1	0.0	32	1	0.0	33	1	0.0	33	1	0.0
34	1	0.0	35	1	0.0	36	1	0.0	36	1	0.0
37	1	0.0	38	1	0.0	39	1	0.0	39	1	0.0
40	1	0.0	41	1	0.0	42	1	0.0	42	1	0.0
43	1	0.0	44	1	0.0	45	1	0.0	45	1	0.0
46	1	0.0	47	1	0.0	48	1	0.0	48	1	0.0
49	1	0.0	50	1	0.0	51	1	0.0	51	1	0.0
52	1	0.0	53	1	0.0	54	1	0.0	54	1	0.0
55	1	0.0	56	1	0.0	57	1	0.0	57	1	0.0
56	1	0.0	58	1	0.0	59	1	0.0	59	1	0.0
57	1	0.0	60	1	0.0	61	1	0.0	61	1	0.0
58	1	0.0	62	1	0.0	63	1	0.0	63	1	0.0
59	1	0.0	64	1	0.0	65	1	0.0	65	1	0.0
60	1	0.0	66	1	0.0	67	1	0.0	67	1	0.0
61	1	0.0	68	1	0.0	69	1	0.0	69	1	0.0
62	1	0.0	70	1	0.0	71	1	0.0	71	1	0.0
63	1	0.0	72	1	0.0	73	1	0.0	73	1	0.0
64	1	0.0	74	1	0.0	75	1	0.0	75	1	0.0
65	1	0.0	76	1	0.0	77	1	0.0	77	1	0.0
66	1	0.0	78	1	0.0	79	1	0.0	79	1	0.0
67	1	0.0	80	1	0.0	81	1	0.0	81	1	0.0
68	1	0.0	82	1	0.0	83	1	0.0	83	1	0.0
69	1	0.0	84	1	0.0	85	1	0.0	85	1	0.0
70	1	0.0	86	1	0.0	87	1	0.0	87	1	0.0
71	1	0.0	88	1	0.0	89	1	0.0	89	1	0.0
72	1	0.0	90	1	0.0	91	1	0.0	91	1	0.0
73	1	0.0	92	1	0.0	93	1	0.0	93	1	0.0
74	1	0.0	94	1	0.0	95	1	0.0	95	1	0.0
75	1	0.0	96	1	0.0	97	1	0.0	97	1	0.0
76	1	0.0	98	1	0.0	99	1	0.0	99	1	0.0
77	1	0.0	100	1	0.0	101	1	0.0	101	1	0.0
78	1	0.0	102	1	0.0	103	1	0.0	103	1	0.0
79	1	0.0	104	1	0.0	105	1	0.0	105	1	0.0
80	1	0.0	106	1	0.0	107	1	0.0	107	1	0.0
81	1	0.0	108	1	0.0	109	1	0.0	109	1	0.0
82	1	0.0	110	1	0.0	111	1	0.0	111	1	0.0
83	1	0.0	112	1	0.0	113	1	0.0	113	1	0.0
84	1	0.0	114	1	0.0	115	1	0.0	115	1	0.0
85	1	0.0	116	1	0.0	117	1	0.0	117	1	0.0
86	1	0.0	118	1	0.0	119	1	0.0	119	1	0.0
87	1	0.0	120	1	0.0	121	1	0.0	121	1	0.0
88	1	0.0	122	1	0.0	123	1	0.0	123	1	0.0
89	1	0.0	124	1	0.0	125	1	0.0	125	1	0.0
90	1	0.0	126	1	0.0	127	1	0.0	127	1	0.0
91	1	0.0	128	1	0.0	129	1	0.0	129	1	0.0
92	1	0.0	130	1	0.0	131	1	0.0	131	1	0.0
93	1	0.0	132	1	0.0	133	1	0.0	133	1	0.0
94	1	0.0	134	1	0.0	135	1	0.0	135	1	0.0
95	1	0.0	136	1	0.0	137	1	0.0	137	1	0.0
96	1	0.0	138	1	0.0	139	1	0.0	139	1	0.0
97	1	0.0	140	1	0.0	141	1	0.0	141	1	0.0
98	1	0.0	142	1	0.0	143	1	0.0	143	1	0.0
99	1	0.0	144	1	0.0	145	1	0.0	145	1	0.0
100	1	0.0	146	1	0.0	147	1	0.0	147	1	0.0
101	1	0.0	148	1	0.0	149	1	0.0	149	1	0.0
102	1	0.0	150	1	0.0	151	1	0.0	151	1	0.0
103	1	0.0	152	1	0.0	153	1	0.0	153	1	0.0
104	1	0.0	154	1	0.0	155	1	0.0	155	1	0.0
105	1	0.0	156	1	0.0	157	1	0.0	157	1	0.0
106	1	0.0	158	1	0.0	159	1	0.0	159	1	0.0
107	1	0.0	160	1	0.0	161	1	0.0	161	1	0.0
108	1	0.0	162	1	0.0	163	1	0.0	163	1	0.0
109	1	0.0	164	1	0.0	165	1	0.0	165	1	0.0
110	1	0.0	166	1	0.0	167	1	0.0	167	1	0.0
111	1	0.0	168	1	0.0	169	1	0.0	169	1	0.0
112	1	0.0	170	1	0.0	171	1	0.0	171	1	0.0
113	1	0.0	172	1	0.0	173	1	0.0	173	1	0.0
114	1	0.0	174	1	0.0	175	1	0.0	175	1	0.0
115	1	0.0	176	1	0.0	177	1	0.0	177	1	0.0
116	1	0.0	178	1	0.0	179	1	0.0	179	1	0.0
117	1	0.0	180	1	0.0	181	1	0.0	181	1	0.0
118	1	0.0	182	1	0.0	183	1	0.0	183	1	0.0
119	1	0.0	184	1	0.0	185	1	0.0	185	1	0.0
120	1	0.0	186	1	0.0	187	1	0.0	187	1	0.0
121	1	0.0	188	1	0.0	189	1	0.0	189	1	0.0
122	1	0.0	190	1	0.0	191	1	0.0	191	1	0.0
123	1	0.0	192	1	0.0	193	1	0.0	193	1	0.0
124	1	0.0	194	1	0.0	195	1	0.0	195	1	0.0
125	1	0.0	196	1	0.0	197	1	0.0	197	1	0.0
126	1	0.0	198	1	0.0	199	1	0.0	199	1	0.0
127	1	0.0	200	1	0.0	201	1	0.0	201	1	0.0
128	1	0.0	202	1	0.0	203	1	0.0	203	1	0.0
129	1	0.0	204	1	0.0	205	1	0.0	205	1	0.0
130	1	0.0	206	1	0.0	207	1	0.0	207	1	0.0
131	1	0.0	208	1	0.0	209	1	0.0	209	1	0.0
132	1	0.0	210	1	0.0	211	1	0.0	211	1	0.0
133	1	0.0	212	1	0.0	213	1	0.0	213	1	0.0
134	1	0.0	214	1	0.0	215	1	0.0	215	1	0.0
135	1	0.0	216	1	0.0	217	1	0.0	217	1	0.0
136	1	0.0	218	1	0.0	219	1	0.0	219	1	0.0
137	1	0.0	220	1	0.0	221	1	0.0	221	1	0.0
138	1	0.0	222	1	0.0	223	1	0.0	223	1	0.0
139	1	0.0	224	1	0.0	225	1	0.0	225	1	0.0
140	1	0.0	226	1	0.0	227	1	0.0	227	1	0.0
141	1	0.0	228	1	0.0	229	1	0.0	229	1	0.0
142	1	0.0	230	1	0.0	231	1	0.0	231	1	0.0
143	1	0.0	232	1	0.0	233	1	0.0	233	1	0.0
144	1	0.0	234	1	0.0	235	1	0.0	235	1	0.0

[illegible]

[illegible]

BETA GALACTOSE. STRUCTURE IS ASSUMED SIMILAR TO BETA GLUCOSE. H(04) IS 1/29/76									
CIS	TO H(C4).	C6	IS IN	GG	POSITION.				
-09	1	2	1	3	2.083728	2	3	1.422775	1 4
-09	1	2	1	3	1.112595	2	3	-0.088425	2 5
-09	1	2	1	3	-0.461363	2	3	-1.287897	3 6
-09	1	2	1	3	-0.771486	2	3	-1.079003	1 8
-09	1	2	1	3	-0.187702	2	3	1.841619	2 9
-09	1	2	1	3	-0.498086	2	3	-0.795465	3 10
-09	1	2	1	3	-1.282773	2	3	-0.779264	1 11
-09	1	2	1	3	-0.841859	2	3	3.945788	2 13
-09	1	2	1	3	-2.328889	2	3	2.357819	3 14
-09	1	2	1	3	-2.609021	2	3	0.075832	1 17
-09	1	2	1	3	-2.180268	2	3	1.789299	2 16
-09	1	2	1	3	-1.859238	2	3	1.911700	3 18
-09	1	2	1	3	-0.960227	2	3	-0.939011	1 20
-09	1	2	1	3	-0.997733	2	3	-1.842323	2 22
-09	1	2	1	3	-0.489367	2	3	3.965539	3 22
-09	1	2	1	3	-2.503000	2	3	4.318875	1 24
-09	1	2	1	3	3.931212	-1	0	0.0	-1.076615
-09	1	2	1	3	2.5	16	0	0	0
-09	1	2	1	3	1.1	4	0	0	0
-09	1	2	1	3	1.4	3	0	0	0
-09	1	2	1	3	1.5	10	1	0	0
-09	1	2	1	3	1.2	7	0	0	0
-09	1	2	1	3	1.1	1	0	0	0
-09	1	2	1	3	1.0	2	0	0	0
-09	1	2	1	3	0.9	3	0	0	0
-09	1	2	1	3	0.8	4	0	0	0
-09	1	2	1	3	0.7	5	0	0	0
-09	1	2	1	3	0.6	6	0	0	0
-09	1	2	1	3	0.5	7	0	0	0
-09	1	2	1	3	0.4	8	0	0	0
-09	1	2	1	3	0.3	9	0	0	0
-09	1	2	1	3	0.2	10	0	0	0
-09	1	2	1	3	0.1	11	0	0	0
-09	1	2	1	3	0.0	12	0	0	0
-09	1	2	1	3	0.0	13	0	0	0
-09	1	2	1	3	0.0	14	0	0	0
-09	1	2	1	3	0.0	15	0	0	0
-09	1	2	1	3	0.0	16	0	0	0
-09	1	2	1	3	0.0	17	0	0	0
-09	1	2	1	3	0.0	18	0	0	0
-09	1	2	1	3	0.0	19	0	0	0
-09	1	2	1	3	0.0	20	0	0	0
-09	1	2	1	3	0.0	21	0	0	0
-09	1	2	1	3	0.0	22	0	0	0
-09	1	2	1	3	0.0	23	0	0	0
-09	1	2	1	3	0.0	24	0	0	0
-09	1	2	1	3	0.0	25	0	0	0
-09	1	2	1	3	0.0	26	0	0	0
-09	1	2	1	3	0.0	27	0	0	0
-09	1	2	1	3	0.0	28	0	0	0
-09	1	2	1	3	0.0	29	0	0	0
-09	1	2	1	3	0.0	30	0	0	0
-09	1	2	1	3	0.0	31	0	0	0
-09	1	2	1	3	0.0	32	0	0	0
-09									

TABLE XXXI (Continued)

[illegible]

TABLE XXXI (Continued)

-09		404	24	73	1	1	1	1/29/76	
BETA		MANNOSE		STRUCTURE		ASSUMED TO BE		SIMILAR TO BETA GLUCOSE	
H(2)		PLACED		CIS TO H(C2)		C6 IS GT			
1	1	1	1	1	1	1	1	3	1
4	1	1	1	1	1	1	1	6	1
7	1	1	1	1	1	1	1	9	1
10	1	1	1	1	1	1	1	12	1
13	1	1	1	1	1	1	1	15	1
16	1	1	1	1	1	1	1	18	1
19	1	1	1	1	1	1	1	21	1
22	1	1	1	1	1	1	1	24	1
25	1	1	1	1	1	1	1	27	1
28	1	1	1	1	1	1	1	30	1
31	1	1	1	1	1	1	1	33	1
34	1	1	1	1	1	1	1	36	1
37	1	1	1	1	1	1	1	39	1
40	1	1	1	1	1	1	1	42	1
43	1	1	1	1	1	1	1	45	1
46	1	1	1	1	1	1	1	48	1
49	1	1	1	1	1	1	1	51	1
52	1	1	1	1	1	1	1	54	1
55	1	1	1	1	1	1	1	57	1
58	1	1	1	1	1	1	1	60	1
61	1	1	1	1	1	1	1	63	1
64	1	1	1	1	1	1	1	66	1
67	1	1	1	1	1	1	1	69	1
70	1	1	1	1	1	1	1	72	1
73	1	1	1	1	1	1	1		
-06									
12.000000		12.000000		12.000000		12.000000		12.000000	
15.994910		15.994910		15.994910		15.994910		15.994910	
1.0078250		1.0078250		1.0078250		1.0078250		1.0078250	
1.0078250		1.0078250		1.0078250		1.0078250		1.0078250	
-06									
12.000000		12.000000		12.000000		12.000000		12.000000	
15.994910		15.994910		15.994910		15.994910		15.994910	
1.0078250		1.0078250		1.0078250		1.0078250		1.0078250	
1.0078250		1.0078250		1.0078250		1.0078250		1.0078250	
-09									
BETA		MANNOSE		STRUCTURE		ASSUMED TO BE		SIMILAR TO BETA GLUCOSE	
H(2)		PLACED		CIS TO H(C2)		C6 IS GT			
1	1	1	1	1	1	1	1	1.422775	1
4	1	1	1	1	1	1	1	1.436452	1
7	1	1	1	1	1	1	1	1.450129	1
10	1	1	1	1	1	1	1	1.463806	1
13	1	1	1	1	1	1	1	1.477483	1
16	1	1	1	1	1	1	1	1.491160	1
19	1	1	1	1	1	1	1	1.504837	1
22	1	1	1	1	1	1	1	1.518514	1
25	1	1	1	1	1	1	1	1.532191	1
28	1	1	1	1	1	1	1	1.545868	1
31	1	1	1	1	1	1	1	1.559545	1
34	1	1	1	1	1	1	1	1.573222	1
37	1	1	1	1	1	1	1	1.586899	1
40	1	1	1	1	1	1	1	1.600576	1
43	1	1	1	1	1	1	1	1.614253	1
46	1	1	1	1	1	1	1	1.627930	1
49	1	1	1	1	1	1	1	1.641607	1
52	1	1	1	1	1	1	1	1.655284	1
55	1	1	1	1	1	1	1	1.668961	1
58	1	1	1	1	1	1	1	1.682638	1
61	1	1	1	1	1	1	1	1.696315	1
64	1	1	1	1	1	1	1	1.709992	1
67	1	1	1	1	1	1	1	1.723669	1
70	1	1	1	1	1	1	1	1.737346	1
73	1	1	1	1	1	1	1	1.751023	1
-06									
12.000000		12.000000		12.000000		12.000000		12.000000	
15.994910		15.994910		15.994910		15.994910		15.994910	
1.0078250		1.0078250		1.0078250		1.0078250		1.0078250	
1.0078250		1.0078250		1.0078250		1.0078250		1.0078250	
-06									
12.000000		12.000000		12.000000		12.000000		12.000000	
15.994910		15.994910		15.994910		15.994910		15.994910	
1.0078250		1.0078250		1.0078250		1.0078250		1.0078250	
1.0078250		1.0078250		1.0078250		1.0078250		1.0078250	

PAMOLE AND PAM1 INPUT — HEXOSES

TABLE XXXII (Continued)

		PAHOLE INPUT		GALACTOSE AND MANNOSE			
-9	43	2	1	0.0	0.20	0.21	
-6	NG=1235	ALPHA	GALACTOSE				TG
SCALE	1.200	0	0.0				
C1	0.0	0.0	0.0	0.0	C2	0.03	H20 010 .0
C2	1.534	0.0	0.0	0.0	C3	0.07	H19
C3	2.084	1.423	0.0	0.0	C4	0.08	H18
C4	1.436	2.227	1.113	C5	0.09	H17	
C5	-0.088	2.159	1.029	H15	C16	0.10	
O6	-0.461	0.474	-1.221	H11			
O7	2.041	-0.771	-1.079	H12			
O8	3.490	1.353	0.188	H13			
O9	1.842	1.675	2.357	H14			
O10	-0.498	0.795	1.069				
H11	-1.410	0.229	-1.332				
H12	2.000	-0.242	-1.910				
H13	3.894	2.225	-0.033				
H14	2.329	2.358	2.876				
H15	-0.435	2.609	0.076				
C16	-0.741	2.886	2.180				
H17	1.789	3.276	1.035				
H18	1.859	1.912	-0.971				
H19	1.857	-0.496	0.939				
H20	-0.362	-1.028	0.209				
H21	-0.396	2.437	3.135	C16			
H22	-1.841	2.749	2.116	C16			
O23	-0.412	4.267	2.143	C16			
H24	-1.110	4.784	2.610	O23			
VIEW	20.	0.	20.				
VIEW	-20.	0.	-20.				
-9	42	2	1	0.0	0.20	0.21	TG
-6	NG=1236	BETA	GALACTOSE				
SCALE	1.200	0	0.0				
C1	0.0	0.0	0.0	0.0	C2	0.03	H20 010 .0
C2	1.534	0.0	0.0	0.0	C3	0.07	H19
C3	2.084	1.423	0.0	0.0	C4	0.08	H18
C4	1.436	2.227	1.113	C5	0.09	H17	
C5	-0.088	2.159	1.029	H15	C16	0.10	
O6	-0.461	-1.288	-0.240	H11			
O7	2.041	-0.771	-1.079	H12			
O8	3.490	1.353	0.188	H13			
O9	1.842	1.675	2.357	H14			
O10	-0.498	0.795	1.069				
H11	-1.285	-1.247	-0.780				
H12	2.010	-1.728	-0.842				
H13	3.946	1.614	-0.647				
H14	2.329	2.358	2.876				
H15	-0.435	2.609	0.076				
C16	-0.741	2.886	2.180				
H17	1.789	3.276	1.035				
H18	1.859	1.912	-0.971				
H19	1.857	-0.496	0.939				
H20	-0.362	0.325	-0.998				
H21	-0.396	2.437	3.135	C16			
H22	-1.841	2.749	2.116	C16			
O23	-0.412	4.267	2.143	C16			
H24	0.037	4.521	2.984	O23			
VIEW	20.	0.	20.				
VIEW	-20.	0.	-20.				
-9	45	2	1	0.0	0.20	0.21	GT
-6	NG=1237	ALPHA	MANNOSE				
SCALE	1.200	0	0.0				
C1	0.0	0.0	0.0	0.0	C2	0.03	H20 010 .0
C2	1.534	0.0	0.0	0.0	C3	0.07	H19
C3	2.084	1.423	0.0	0.0	C4	0.08	H18
C4	1.436	2.227	1.113	C5	0.09	H17	
C5	-0.088	2.159	1.029	H15	C16	0.10	
O6	-0.461	0.474	-1.221	H11			
O7	2.041	-0.771	-1.079	H12			
O8	3.490	1.353	0.188	H13			
O9	1.888	3.569	1.015	H14			
O10	-0.498	0.795	1.069				
H11	-1.410	0.229	-1.332				
H12	2.592	-1.416	0.853				
H13	3.894	2.225	-0.033				
H14	1.734	4.031	1.872				
H15	-0.435	2.609	0.076				
C16	-0.741	2.886	2.180				
H17	1.752	1.794	2.085				
H18	1.859	1.912	-0.971				
H19	1.857	-0.609	-0.870				
H20	-0.362	-1.030	0.159				
H21	-0.454	3.958	2.140	C16			
H22	-0.361	2.466	3.135	C16			
O23	-2.153	2.757	2.110	C16			
H24	-2.539	2.868	3.011	O23			
VIEW	20.	0.	20.				
VIEW	-20.	0.	-20.				
-9	40	2	1	0.0	0.20	0.21	GT
-6	NG=1238	BETA	MANNOSE				
SCALE	1.200	0	0.0				
C1	0.0	0.0	0.0	0.0	C2	0.03	H20 010 .0
C2	1.534	0.0	0.0	0.0	C3	0.07	H19
C3	2.084	1.423	0.0	0.0	C4	0.08	H18
C4	1.436	2.227	1.113	C5	0.09	H17	
C5	-0.088	2.159	1.029	H15	C16	0.10	
O6	-0.461	-1.288	-0.240	H11			
O7	2.041	-0.643	1.160	H12			
O8	3.490	1.353	0.188	H13			
O9	1.888	3.569	1.015	H14			
O10	-0.498	0.795	1.069				
H11	-1.285	-1.247	-0.780				
H12	2.592	-1.416	0.853				
H13	3.946	1.614	-0.647				
H14	2.667	1.698	1.606				
H15	-0.435	2.609	0.076				
C16	-0.741	2.886	2.180				
H17	1.752	1.794	2.085				
H18	1.859	1.912	-0.971				
H19	1.857	-0.609	-0.870				
H20	-0.362	0.335	-0.994				
H21	-0.454	3.958	2.140	C16			
H22	-0.361	2.466	3.135	C16			
O23	-2.153	2.757	2.110	C16			
H24	-2.563	3.653	2.058	O23			
VIEW	20.	0.	20.				
VIEW	-20.	0.	-20.				

TABLE XXXIII

Z MATRICES - HEXOSES

Z MATRIX			ALPHA GLUCOSE (GT)		
1	1	4	1.000000	1	17
1	9	18	1.000000	1	19
1	28	22	1.000000	1	31
1	68	47	1.000000	2	3
2	10	18	1.000000	2	14
2	22	22	1.000000	2	33
2	69	47	1.000000	3	4
3	11	18	1.000000	3	14
3	24	22	1.000000	3	15
3	70	47	1.000000	4	5
4	11	18	1.000000	4	16
4	29	22	1.000000	4	37
4	71	47	1.000000	5	6
5	16	21	1.000000	5	27
5	39	26	1.000000	5	71
5	73	47	1.000000	6	7
6	27	25	1.000000	6	29
7	7	25	1.000000	7	43
7	28	24	1.000000	8	19
8	18	24	1.000000	8	42
8	67	47	1.000000	9	9
9	44	27	1.000000	9	51
10	22	25	1.000000	10	23
10	69	47	1.000000	11	11
11	46	27	1.000000	11	53
12	26	25	1.000000	12	48
12	72	47	1.000000	12	73
13	19	41	1.000000	13	20
13	28	41	1.000000	13	30
13	33	32	1.000000	14	14
14	22	42	1.000000	14	23
14	33	43	1.000000	14	34
15	16	40	1.000000	15	23
15	29	41	1.000000	15	34
15	37	32	1.000000	16	16
16	27	42	1.000000	16	29
16	38	43	1.000000	16	39
17	18	41	1.000000	17	27
17	43	37	1.000000	17	47
18	28	42	1.000000	18	42
19	19	12	1.000000	19	20
19	31	33	1.000000	19	42
20	21	42	1.000000	20	28
20	44	43	1.000000	20	51
21	32	43	1.000000	21	33
22	22	12	1.000000	22	33
22	45	43	1.000000	22	52
23	34	43	1.000000	23	35
24	24	12	1.000000	24	25
24	46	43	1.000000	24	53
25	36	43	1.000000	25	37
26	26	12	1.000000	26	27
26	40	43	1.000000	26	48
27	27	12	1.000000	27	29
27	40	34	1.000000	27	47
28	31	34	1.000000	28	43
29	37	43	1.000000	29	47
30	42	45	1.000000	30	43
31	32	45	1.000000	31	44
32	33	29	1.000000	32	44
33	34	45	1.000000	33	45
34	35	29	1.000000	34	45
35	36	45	1.000000	35	46
36	37	29	1.000000	36	46
37	38	45	1.000000	37	47
38	39	30	1.000000	38	40
39	39	9	1.000000	39	40
39	72	47	1.000000	40	40
40	73	47	1.000000	41	41
41	72	47	1.000000	41	73
42	50	39	1.000000	42	67
44	44	7	1.000000	44	51
45	52	39	1.000000	45	69
46	70	47	1.000000	47	47
48	49	44	1.000000	48	54
49	54	39	1.000000	49	73
52	52	6	1.000000	53	53
56	56	14	1.000000	57	57
60	60	15	1.000000	61	61
64	64	15	1.000000	65	65
68	68	2	1.000000	69	69
72	72	2	1.000000	72	73
1	17	18	1.000000	1	19
1	19	22	1.000000	1	31
1	31	26	1.000000	2	3
2	3	17	1.000000	2	14
2	14	21	1.000000	2	33
3	4	17	1.000000	3	4
3	15	21	1.000000	3	14
3	15	26	1.000000	3	15
4	5	17	1.000000	4	5
4	16	21	1.000000	4	16
4	37	26	1.000000	5	6
5	6	18	1.000000	5	27
5	27	22	1.000000	5	71
6	7	20	1.000000	6	7
6	47	27	1.000000	6	29
7	17	23	1.000000	7	43
7	67	47	1.000000	8	19
8	42	27	1.000000	8	42
9	20	25	1.000000	9	9
9	68	47	1.000000	9	51
10	45	27	1.000000	10	23
11	24	25	1.000000	11	11
11	70	47	1.000000	11	53
12	49	27	1.000000	12	48
13	13	10	1.000000	13	20
13	21	42	1.000000	13	30
13	31	43	1.000000	14	14
14	15	41	1.000000	14	23
14	24	40	1.000000	14	34
15	24	42	1.000000	15	23
15	35	43	1.000000	15	34
16	25	41	1.000000	16	16
16	36	32	1.000000	16	29
16	40	32	1.000000	16	39
17	28	41	1.000000	17	27
17	41	11	1.000000	17	47
18	43	43	1.000000	18	42
18	43	43	1.000000	19	20
19	28	42	1.000000	19	42
19	50	35	1.000000	20	28
20	30	34	1.000000	20	51
21	31	12	1.000000	21	33
21	44	43	1.000000	22	33
22	32	34	1.000000	23	35
23	23	12	1.000000	24	25
23	45	43	1.000000	25	37
24	34	34	1.000000	26	27
25	25	12	1.000000	27	29
25	46	43	1.000000	28	43
26	38	34	1.000000	29	47
26	49	43	1.000000	30	43
27	38	43	1.000000	31	44
28	28	12	1.000000	32	44
29	29	12	1.000000	33	45
30	30	9	1.000000	34	45
31	67	47	1.000000	35	46
32	68	47	1.000000	36	46
33	69	47	1.000000	37	47
34	69	47	1.000000	38	40
35	70	47	1.000000	39	40
36	70	47	1.000000	40	40
37	71	47	1.000000	41	41
38	47	45	1.000000	42	67
39	41	46	1.000000	44	51
40	41	46	1.000000	45	69
41	48	46	1.000000	47	47
42	42	7	1.000000	48	54
43	43	7	1.000000	49	73
44	68	47	1.000000	53	53
46	46	7	1.000000	57	57
47	71	47	1.000000	61	61
48	72	47	1.000000	65	65
50	50	6	1.000000	69	69
54	54	6	1.000000	72	73
58	58	14	1.000000	1	17
62	62	15	1.000000	1	19
66	66	16	1.000000	1	31
70	70	2	1.000000	2	3
73	73	2	1.000000	2	14
-2	-2	-2	1.000000	2	33
				3	4
				3	14
				3	15
				4	5
				4	16
				5	6
				5	27
				6	7
				6	29
				7	43
				8	19
				8	42
				9	9
				9	51
				10	23
				11	11
				11	53
				12	48
				13	20
				13	30
				14	14
				14	23
				15	23
				15	34
				16	16
				16	29
				17	27
				17	47
				18	42
				19	20
				19	42
				20	28
				20	51
				21	33
				22	33
				23	35
				24	25
				25	37
				26	27
				26	48
				27	29
				27	47
				28	43
				29	47
				30	43
				31	44
				32	44
				33	45
				34	45
				35	46
				36	46
				37	47
				38	40
				39	40
				40	40
				41	41
				42	67
				44	51
				45	69
				47	47
				48	54
				49	73
				53	53
				57	57
				61	61
				65	65
				69	69
				72	73
				AGLU	84

TABLE XXXIII (Continued)

Z MATRIX				ALPHA GLUCOSE (TG)							
1	1	4	1.000000	1	7	18	1.000000	1	8	18	1.000000
1	9	18	1.000000	1	13	21	1.000000	1	19	22	1.000000
1	28	22	1.000000	1	30	26	1.000000	1	31	26	1.000000
1	68	47	1.000000	2	2	4	1.000000	2	3	17	1.000000
2	10	18	1.000000	2	13	21	1.000000	2	14	21	1.000000
2	22	22	1.000000	2	32	26	1.000000	2	33	26	1.000000
2	69	47	1.000000	3	3	4	1.000000	3	4	17	1.000000
3	11	18	1.000000	3	14	21	1.000000	3	15	21	1.000000
3	24	22	1.000000	3	34	26	1.000000	3	35	26	1.000000
3	70	47	1.000000	4	4	4	1.000000	4	5	17	1.000000
4	11	18	1.000000	4	15	21	1.000000	4	16	21	1.000000
4	29	22	1.000000	4	36	26	1.000000	4	37	26	1.000000
4	71	47	1.000000	5	5	4	1.000000	5	6	18	1.000000
5	16	21	1.000000	5	26	22	1.000000	5	27	22	1.000000
5	39	26	1.000000	5	40	26	1.000000	5	71	47	1.000000
5	73	47	1.000000	6	6	3	1.000000	6	7	20	1.000000
6	27	25	1.000000	6	29	25	1.000000	6	47	27	1.000000
7	7	3	1.000000	7	8	19	1.000000	7	17	23	1.000000
7	28	25	1.000000	7	43	27	1.000000	7	67	47	1.000000
8	18	24	1.000000	8	19	25	1.000000	8	42	27	1.000000
8	67	47	1.000000	9	5	3	1.000000	9	20	25	1.000000
9	44	27	1.000000	9	51	28	1.000000	9	68	47	1.000000
10	22	25	1.000000	10	23	25	1.000000	10	45	27	1.000000
10	69	47	1.000000	11	11	3	1.000000	11	24	25	1.000000
11	46	27	1.000000	11	53	28	1.000000	11	70	47	1.000000
12	26	25	1.000000	12	48	27	1.000000	12	49	27	1.000000
12	72	47	1.000000	12	73	47	1.000000	13	13	10	1.000000
13	19	41	1.000000	13	20	42	1.000000	13	21	42	1.000000
13	28	41	1.000000	13	30	31	1.000000	13	31	43	1.000000
13	33	32	1.000000	14	14	10	1.000000	14	15	41	1.000000
14	22	42	1.000000	14	23	42	1.000000	14	24	40	1.000000
14	33	43	1.000000	14	34	43	1.000000	14	35	32	1.000000
15	16	40	1.000000	15	23	40	1.000000	15	24	42	1.000000
15	29	41	1.000000	15	34	32	1.000000	15	35	43	1.000000
15	37	32	1.000000	16	16	10	1.000000	16	25	41	1.000000
16	27	42	1.000000	16	29	42	1.000000	16	36	32	1.000000
16	38	43	1.000000	16	39	32	1.000000	16	40	31	1.000000
17	18	41	1.000000	17	27	40	1.000000	17	28	41	1.000000
17	43	37	1.000000	17	47	38	1.000000	18	18	11	1.000000
18	28	42	1.000000	18	42	43	1.000000	18	43	43	1.000000
19	19	12	1.000000	19	20	41	1.000000	19	28	42	1.000000
19	31	33	1.000000	19	42	43	1.000000	19	50	35	1.000000
20	21	42	1.000000	20	28	40	1.000000	20	30	34	1.000000
20	44	43	1.000000	20	51	35	1.000000	21	21	12	1.000000
21	32	43	1.000000	21	33	34	1.000000	21	44	43	1.000000
22	22	12	1.000000	22	23	42	1.000000	22	32	34	1.000000
22	45	43	1.000000	22	52	35	1.000000	23	23	12	1.000000
23	34	43	1.000000	23	35	34	1.000000	23	45	43	1.000000
24	24	12	1.000000	24	25	42	1.000000	24	34	34	1.000000
24	46	43	1.000000	24	53	36	1.000000	25	25	12	1.000000
25	36	43	1.000000	25	37	34	1.000000	25	46	43	1.000000
26	26	12	1.000000	26	27	40	1.000000	26	38	34	1.000000
26	40	43	1.000000	26	48	43	1.000000	26	49	43	1.000000
27	27	12	1.000000	27	29	42	1.000000	27	38	43	1.000000
27	40	34	1.000000	27	47	43	1.000000	28	28	12	1.000000
28	31	34	1.000000	28	43	43	1.000000	29	29	12	1.000000
29	37	43	1.000000	29	47	43	1.000000	30	30	9	1.000000
30	42	45	1.000000	30	43	45	1.000000	30	67	47	1.000000
31	32	45	1.000000	31	44	45	1.000000	31	68	47	1.000000
32	33	29	1.000000	32	44	45	1.000000	32	68	47	1.000000
33	34	45	1.000000	33	45	45	1.000000	33	69	47	1.000000
34	35	29	1.000000	34	45	45	1.000000	34	69	47	1.000000
35	36	45	1.000000	35	46	45	1.000000	35	70	47	1.000000
36	37	29	1.000000	36	46	45	1.000000	36	70	47	1.000000
37	38	45	1.000000	37	47	45	1.000000	37	71	47	1.000000
38	39	29	1.000000	38	40	30	1.000000	38	47	45	1.000000
39	39	9	1.000000	39	40	44	1.000000	39	41	46	1.000000
39	72	47	1.000000	40	40	9	1.000000	40	41	46	1.000000
40	73	47	1.000000	41	41	8	1.000000	41	48	46	1.000000
41	72	47	1.000000	41	73	47	1.000000	42	42	7	1.000000
42	50	39	1.000000	42	67	47	1.000000	43	43	7	1.000000
44	44	7	1.000000	44	51	39	1.000000	44	68	47	1.000000
45	52	39	1.000000	45	69	47	1.000000	46	46	7	1.000000
46	70	47	1.000000	47	47	7	1.000000	47	71	47	1.000000
48	49	44	1.000000	48	54	39	1.000000	48	72	47	1.000000
49	54	39	1.000000	49	73	47	1.000000	50	50	6	1.000000
52	52	6	1.000000	53	53	6	1.000000	54	54	6	1.000000
56	56	14	1.000000	57	57	14	1.000000	58	58	14	1.000000
60	60	15	1.000000	61	61	15	1.000000	62	62	15	1.000000
64	64	15	1.000000	65	65	16	1.000000	66	66	16	1.000000
68	68	2	1.000000	69	69	2	1.000000	70	70	2	1.000000
72	72	2	1.000000	72	73	47	1.000000	73	73	2	1.000000

TABLE XXXIII (Continued)

Z MATRIX				BETA GLUCOSE (GT)			
1	1	4	1.000000	1	2	17	1.000000
1	9	18	1.000000	1	13	21	1.000000
1	28	22	1.000000	1	30	26	1.000000
1	68	47	1.000000	2	2	4	1.000000
2	10	18	1.000000	2	13	21	1.000000
2	22	22	1.000000	2	32	26	1.000000
2	69	47	1.000000	3	3	4	1.000000
3	11	18	1.000000	3	14	21	1.000000
3	24	22	1.000000	3	34	26	1.000000
3	70	47	1.000000	4	4	4	1.000000
4	11	18	1.000000	4	15	21	1.000000
4	29	22	1.000000	4	36	26	1.000000
4	71	47	1.000000	5	5	4	1.000000
5	16	21	1.000000	5	26	22	1.000000
5	39	26	1.000000	5	40	26	1.000000
5	73	47	1.000000	6	6	3	1.000000
6	27	25	1.000000	6	29	25	1.000000
7	7	3	1.000000	7	8	19	1.000000
7	28	25	1.000000	7	43	27	1.000000
8	18	24	1.000000	8	19	25	1.000000
8	67	47	1.000000	9	9	3	1.000000
9	44	27	1.000000	9	51	28	1.000000
10	22	25	1.000000	10	23	25	1.000000
10	69	47	1.000000	11	11	3	1.000000
11	46	27	1.000000	11	53	28	1.000000
12	26	25	1.000000	12	48	27	1.000000
12	72	47	1.000000	12	73	47	1.000000
13	19	40	1.000000	13	20	42	1.000000
13	28	41	1.000000	13	30	32	1.000000
13	33	32	1.000000	14	14	10	1.000000
14	22	42	1.000000	14	23	42	1.000000
14	33	43	1.000000	14	34	43	1.000000
15	16	40	1.000000	15	23	40	1.000000
15	29	41	1.000000	15	34	32	1.000000
15	37	32	1.000000	16	16	10	1.000000
16	27	42	1.000000	16	29	42	1.000000
16	38	43	1.000000	16	39	32	1.000000
17	18	40	1.000000	17	27	40	1.000000
17	43	38	1.000000	17	47	38	1.000000
18	28	42	1.000000	18	42	43	1.000000
19	19	12	1.000000	19	20	41	1.000000
19	31	34	1.000000	19	42	43	1.000000
20	21	42	1.000000	20	28	40	1.000000
20	44	43	1.000000	20	51	35	1.000000
21	32	43	1.000000	21	33	34	1.000000
22	22	12	1.000000	22	23	42	1.000000
22	45	43	1.000000	22	52	35	1.000000
23	34	43	1.000000	23	35	34	1.000000
24	24	12	1.000000	24	25	42	1.000000
24	46	43	1.000000	24	53	36	1.000000
25	36	43	1.000000	25	37	34	1.000000
26	26	12	1.000000	26	27	41	1.000000
26	40	43	1.000000	26	48	43	1.000000
27	27	12	1.000000	27	29	42	1.000000
27	40	34	1.000000	27	47	43	1.000000
28	31	34	1.000000	28	43	43	1.000000
29	37	43	1.000000	29	47	43	1.000000
30	42	45	1.000000	30	43	45	1.000000
31	32	45	1.000000	31	44	45	1.000000
32	33	29	1.000000	32	44	45	1.000000
33	34	45	1.000000	33	45	45	1.000000
34	35	29	1.000000	34	45	45	1.000000
35	36	45	1.000000	35	46	45	1.000000
36	37	29	1.000000	36	46	45	1.000000
37	38	45	1.000000	37	47	45	1.000000
38	39	30	1.000000	38	40	29	1.000000
39	39	9	1.000000	39	40	44	1.000000
39	72	47	1.000000	40	40	9	1.000000
40	73	47	1.000000	41	41	8	1.000000
41	72	47	1.000000	41	73	47	1.000000
42	50	39	1.000000	42	67	47	1.000000
44	44	7	1.000000	44	51	39	1.000000
45	52	39	1.000000	45	69	47	1.000000
46	70	47	1.000000	47	47	7	1.000000
48	49	44	1.000000	48	54	39	1.000000
49	54	39	1.000000	49	73	47	1.000000
52	52	6	1.000000	53	53	5	1.000000
56	56	14	1.000000	57	57	14	1.000000
60	60	15	1.000000	61	61	15	1.000000
64	64	15	1.000000	65	65	16	1.000000
68	68	2	1.000000	69	69	2	1.000000
72	72	2	1.000000	72	73	75	1.000000
1	8	18	1.000000	1	19	22	1.000000
1	20	22	1.000000	1	31	26	1.000000
1	67	47	1.000000	2	3	17	1.000000
2	21	22	1.000000	2	14	21	1.000000
2	9	18	1.000000	2	33	26	1.000000
2	21	22	1.000000	3	4	17	1.000000
2	68	47	1.000000	3	15	21	1.000000
3	10	18	1.000000	3	35	26	1.000000
3	23	22	1.000000	4	5	17	1.000000
3	69	47	1.000000	4	16	21	1.000000
4	25	22	1.000000	4	37	26	1.000000
4	70	47	1.000000	5	6	18	1.000000
5	12	18	1.000000	5	27	22	1.000000
5	38	26	1.000000	5	71	47	1.000000
5	72	47	1.000000	6	7	20	1.000000
6	17	23	1.000000	6	47	27	1.000000
6	71	47	1.000000	7	17	23	1.000000
7	18	24	1.000000	7	67	47	1.000000
8	8	3	1.000000	8	42	27	1.000000
8	50	28	1.000000	9	20	25	1.000000
9	21	25	1.000000	9	68	47	1.000000
10	52	28	1.000000	10	45	27	1.000000
10	25	25	1.000000	11	24	25	1.000000
12	12	3	1.000000	11	70	47	1.000000
12	54	28	1.000000	12	49	27	1.000000
13	14	41	1.000000	13	13	10	1.000000
13	22	40	1.000000	13	21	42	1.000000
13	32	43	1.000000	14	15	41	1.000000
14	21	40	1.000000	14	24	40	1.000000
14	32	32	1.000000	14	35	32	1.000000
15	15	10	1.000000	15	24	42	1.000000
15	25	42	1.000000	15	35	43	1.000000
15	36	43	1.000000	16	25	41	1.000000
16	26	42	1.000000	16	36	32	1.000000
16	37	43	1.000000	16	40	32	1.000000
17	17	13	1.000000	17	28	41	1.000000
17	29	41	1.000000	18	18	11	1.000000
18	19	42	1.000000	18	43	43	1.000000
18	50	35	1.000000	19	28	42	1.000000
19	30	43	1.000000	19	50	35	1.000000
20	20	12	1.000000	20	30	34	1.000000
20	31	43	1.000000	21	21	12	1.000000
21	22	41	1.000000	21	44	43	1.000000
21	51	36	1.000000	22	32	34	1.000000
22	33	43	1.000000	22	33	12	1.000000
23	24	41	1.000000	23	45	43	1.000000
23	52	36	1.000000	24	34	34	1.000000
24	35	43	1.000000	25	25	12	1.000000
25	29	40	1.000000	25	46	43	1.000000
25	53	35	1.000000	26	38	34	1.000000
26	39	43	1.000000	26	49	43	1.000000
26	54	35	1.000000	27	38	43	1.000000
27	39	33	1.000000	28	28	12	1.000000
28	30	43	1.000000	29	29	12	1.000000
29	36	34	1.000000	30	30	9	1.000000
30	31	9	1.000000	30	67	47	1.000000
31	32	9	1.000000	31	68	47	1.000000
32	33	9	1.000000	32	68	47	1.000000
33	34	9	1.000000	33	69	47	1.000000
34	35	9	1.000000	34	69	47	1.000000
35	36	9	1.000000	35	36	9	1.000000
36	37	9	1.000000	36	70	47	1.000000
37	38	9	1.000000	37	71	47	1.000000
38	38	9	1.000000	38	47	45	1.000000
38	71	47	1.000000	39	41	46	1.000000
39	48	45	1.000000	40	41	46	1.000000
40	49	45	1.000000	41	48	46	1.000000
41	49	46	1.000000	42	42	7	1.000000
42	43	45	1.000000	43	43	7	1.000000
43	67	47	1.000000	44	68	47	1.000000
45	45	7	1.000000	46	46	7	1.000000
46	48	7	1.000000	47	71	47	1.000000
48	48	7	1.000000	48	72	47	1.000000
49	49	7	1.000000	50	50	6	1.000000
51	51	6	1.000000	54	54	6	1.000000
55	55	14	1.000000	58	58	14	1.000000
59	59	14	1.000000	62	62	15	1.000000
63	63	15	1.000000	66	66	16	1.000000
67	67	2	1.000000	70	70	2	1.000000
71	71	2	1.000000	73	73	2	1.000000
-2							

TABLE XXXIII (Continued)

Z MATRIX			BETA GLUCOSE (GG)		
1	1	4	1	7	18
1	9	18	1	19	22
1	28	22	1	31	26
1	68	47	2	3	17
2	10	18	2	14	21
2	22	22	2	33	26
2	69	47	3	4	17
3	11	18	3	15	21
3	24	22	3	35	26
3	70	47	4	5	17
4	11	18	4	16	21
4	29	22	4	37	26
4	71	47	5	6	18
5	16	21	5	27	22
5	39	26	5	71	47
5	73	47	6	7	20
6	27	25	6	47	27
7	7	3	7	17	23
7	28	25	7	67	47
8	18	24	8	42	27
8	67	47	9	20	25
9	44	27	9	68	47
10	22	25	10	45	27
10	69	47	11	24	25
11	46	27	11	70	47
12	26	25	12	49	27
12	72	47	13	13	10
13	19	40	13	21	42
13	28	41	13	31	43
13	33	32	14	15	41
14	22	42	14	24	40
14	33	43	14	35	32
15	16	40	15	24	42
15	29	41	15	35	43
15	37	32	16	25	41
16	27	42	16	36	32
16	38	43	16	40	32
17	18	40	17	28	41
17	43	38	18	18	11
18	28	42	18	43	43
19	19	12	19	28	42
19	31	34	19	50	35
20	21	42	20	30	34
20	44	43	21	21	12
21	32	43	21	44	43
22	22	12	22	32	34
22	45	43	23	23	12
23	34	43	23	45	43
24	24	12	24	34	34
24	46	43	25	25	12
25	36	43	25	46	43
26	26	12	26	38	33
26	40	43	26	49	43
27	27	12	27	38	43
27	40	33	28	28	12
28	31	34	29	29	12
29	37	43	30	30	9
30	42	45	30	67	47
31	32	45	31	68	47
32	33	29	32	68	47
33	34	45	33	69	47
34	35	29	34	69	47
35	36	45	35	36	9
36	37	29	36	70	47
37	38	45	37	71	47
38	39	30	38	47	45
39	39	9	39	41	46
39	72	47	40	41	46
40	73	47	41	48	46
41	72	47	42	42	7
42	50	39	43	43	7
44	44	7	44	68	47
45	52	39	46	46	7
46	70	47	47	71	47
48	49	44	48	72	47
49	54	39	50	50	6
52	52	6	54	54	6
56	56	14	58	58	14
60	60	15	62	62	15
64	64	15	66	66	16
68	68	2	70	70	2
72	72	2	73	73	2
1	8	18	1	20	22
1	67	47	2	9	18
2	21	22	2	68	47
2	68	47	3	10	18
3	23	22	3	23	22
3	69	47	4	6	18
4	25	22	4	25	22
4	70	47	5	12	18
5	38	26	5	38	26
5	72	47	6	17	23
6	17	23	6	71	47
7	18	24	7	18	24
8	50	28	8	50	28
9	21	25	9	21	25
10	52	28	10	52	28
11	25	25	11	25	25
12	12	3	12	12	3
12	54	28	13	14	41
13	22	40	13	22	40
13	32	43	14	21	40
14	21	40	14	32	32
15	15	10	15	15	10
15	25	42	15	25	42
15	36	43	16	26	41
16	26	41	16	37	43
17	17	13	17	17	13
17	29	41	18	19	42
18	19	42	18	50	35
19	30	43	19	30	43
20	20	12	20	20	12
20	31	43	21	22	41
21	22	41	21	51	36
22	33	43	22	33	43
23	24	41	23	24	41
24	35	43	24	35	43
25	29	40	25	29	40
25	53	35	26	39	43
26	39	43	26	54	35
27	39	34	27	39	34
28	30	43	28	30	43
29	36	34	29	36	34
30	31	29	30	31	29
31	31	9	31	31	9
32	32	9	32	32	9
33	33	9	33	33	9
34	34	9	34	34	9
35	35	9	35	35	9
36	36	9	36	36	9
37	37	9	37	37	9
38	38	9	38	38	9
39	39	9	39	39	9
40	40	9	40	40	9
41	41	9	41	41	9
42	42	9	42	42	9
43	43	9	43	43	9
44	44	9	44	44	9
45	45	9	45	45	9
46	46	9	46	46	9
47	47	9	47	47	9
48	48	9	48	48	9
49	49	9	49	49	9
50	50	9	50	50	9
51	51	9	51	51	9
52	52	9	52	52	9
53	53	9	53	53	9
54	54	9	54	54	9
55	55	9	55	55	9
56	56	9	56	56	9
57	57	9	57	57	9
58	58	9	58	58	9
59	59	9	59	59	9
60	60	9	60	60	9
61	61	9	61	61	9
62	62	9	62	62	9
63	63	9	63	63	9
64	64	9	64	64	9
65	65	9	65	65	9
66	66	9	66	66	9
67	67	9	67	67	9
68	68	9	68	68	9
69	69	9	69	69	9
70	70	9	70	70	9
71	71	9	71	71	9
72	72	9	72	72	9

Z MATRIX				ALPHA GALACTOSE (GT)											
1	1	4	1.000000	1	2	17	1.000000	1	7	18	1.000000	1	8	18	1.000000
1	9	18	1.000000	1	13	21	1.000000	1	19	22	1.000000	1	20	22	1.000000
1	28	22	1.000000	1	30	26	1.000000	1	31	26	1.000000	1	67	22	1.000000
1	68	47	1.000000	2	2	4	1.000000	2	3	17	1.000000	2	9	18	1.000000
2	10	18	1.000000	2	13	21	1.000000	2	14	21	1.000000	2	21	22	1.000000
2	22	22	1.000000	2	32	26	1.000000	2	33	26	1.000000	2	68	47	1.000000
2	69	47	1.000000	3	4	4	1.000000	3	4	17	1.000000	3	10	18	1.000000
3	11	18	1.000000	3	14	21	1.000000	3	15	21	1.000000	3	23	22	1.000000
3	24	22	1.000000	3	34	26	1.000000	3	35	26	1.000000	3	69	47	1.000000
3	70	47	1.000000	4	4	4	1.000000	4	5	17	1.000000	4	6	18	1.000000
4	11	18	1.000000	4	15	21	1.000000	4	16	21	1.000000	4	25	22	1.000000
4	29	22	1.000000	4	36	26	1.000000	4	37	26	1.000000	4	72	47	1.000000
4	71	47	1.000000	5	5	4	1.000000	5	6	18	1.000000	5	12	18	1.000000
5	16	21	1.000000	5	26	22	1.000000	5	27	22	1.000000	5	38	26	1.000000
5	39	26	1.000000	5	46	26	1.000000	5	71	47	1.000000	5	72	47	1.000000
5	73	47	1.000000	6	6	3	1.000000	6	7	20	1.000000	6	17	23	1.000000
6	27	25	1.000000	6	29	25	1.000000	6	47	27	1.000000	6	71	47	1.000000
7	7	3	1.000000	7	8	19	1.000000	7	17	23	1.000000	7	18	24	1.000000
7	28	25	1.000000	7	43	27	1.000000	7	67	47	1.000000	8	8	3	1.000000
7	68	24	1.000000	8	19	25	1.000000	8	42	27	1.000000	8	50	28	1.000000
8	18	47	1.000000	8	9	3	1.000000	8	20	25	1.000000	9	21	25	1.000000
9	44	27	1.000000	9	51	28	1.000000	9	68	47	1.000000	10	10	3	1.000000
10	22	25	1.000000	10	23	25	1.000000	10	45	27	1.000000	10	52	28	1.000000
10	69	47	1.000000	11	11	3	1.000000	11	24	25	1.000000	11	25	25	1.000000
11	46	27	1.000000	11	53	28	1.000000	11	70	47	1.000000	12	12	3	1.000000
12	26	25	1.000000	12	48	27	1.000000	12	49	27	1.000000	12	54	28	1.000000
12	72	47	1.000000	12	73	47	1.000000	13	13	10	1.000000	13	14	41	1.000000
13	19	41	1.000000	13	20	42	1.000000	13	21	42	1.000000	13	22	40	1.000000
13	28	41	1.000000	13	30	31	1.000000	13	31	43	1.000000	13	32	43	1.000000
13	33	32	1.000000	14	14	10	1.000000	14							

TABLE XXXIII (Continued)

Z MATRIX				ALPHA GALACTOSE				TG CONFORMATION			
1	1	18	1.000000	1	2	17	1.000000	1	7	18	1.000000
1	9	18	1.000000	1	13	21	1.000000	1	19	22	1.000000
1	28	22	1.000000	1	30	26	1.000000	1	31	26	1.000000
1	68	47	1.000000	2	2	4	1.000000	2	3	17	1.000000
2	10	18	1.000000	2	13	21	1.000000	2	14	21	1.000000
2	22	22	1.000000	2	32	26	1.000000	2	33	26	1.000000
2	69	47	1.000000	3	3	4	1.000000	3	4	17	1.000000
3	11	18	1.000000	3	14	21	1.000000	3	15	21	1.000000
3	24	22	1.000000	3	34	26	1.000000	3	35	26	1.000000
3	70	47	1.000000	4	4	4	1.000000	4	5	17	1.000000
4	11	18	1.000000	4	15	21	1.000000	4	16	21	1.000000
4	29	22	1.000000	4	36	26	1.000000	4	37	26	1.000000
4	71	47	1.000000	5	5	4	1.000000	5	6	18	1.000000
5	16	21	1.000000	5	26	22	1.000000	5	27	22	1.000000
5	39	26	1.000000	5	40	26	1.000000	5	71	47	1.000000
5	73	47	1.000000	6	6	3	1.000000	6	7	20	1.000000
6	27	25	1.000000	6	29	25	1.000000	6	47	27	1.000000
7	7	3	1.000000	7	8	19	1.000000	7	17	23	1.000000
7	28	25	1.000000	7	43	27	1.000000	7	67	47	1.000000
8	18	24	1.000000	8	19	25	1.000000	8	42	27	1.000000
8	67	47	1.000000	9	9	3	1.000000	9	20	25	1.000000
9	44	27	1.000000	9	51	28	1.000000	9	68	47	1.000000
10	22	25	1.000000	10	23	25	1.000000	10	45	27	1.000000
10	69	47	1.000000	11	11	3	1.000000	11	24	25	1.000000
11	46	27	1.000000	11	53	28	1.000000	11	70	47	1.000000
12	26	25	1.000000	12	48	27	1.000000	12	49	27	1.000000
12	72	47	1.000000	12	73	47	1.000000	13	13	10	1.000000
13	19	41	1.000000	13	20	42	1.000000	13	21	42	1.000000
13	28	41	1.000000	13	30	31	1.000000	13	31	43	1.000000
13	33	32	1.000000	14	14	10	1.000000	14	15	41	1.000000
14	22	42	1.000000	14	23	42	1.000000	14	24	41	1.000000
14	33	43	1.000000	14	34	43	1.000000	14	35	31	1.000000
15	16	40	1.000000	15	23	40	1.000000	15	24	42	1.000000
15	29	41	1.000000	15	34	32	1.000000	15	35	43	1.000000
15	37	32	1.000000	16	16	10	1.000000	16	25	41	1.000000
16	27	42	1.000000	16	29	42	1.000000	16	36	32	1.000000
16	38	43	1.000000	16	39	32	1.000000	16	40	31	1.000000
17	18	41	1.000000	17	27	40	1.000000	17	28	41	1.000000
17	43	37	1.000000	17	47	38	1.000000	18	18	11	1.000000
18	28	42	1.000000	18	42	43	1.000000	18	43	43	1.000000
19	19	12	1.000000	19	20	41	1.000000	19	28	42	1.000000
19	31	33	1.000000	19	42	43	1.000000	19	50	35	1.000000
20	21	42	1.000000	20	28	40	1.000000	20	30	34	1.000000
20	44	43	1.000000	20	51	35	1.000000	21	21	12	1.000000
21	32	43	1.000000	21	33	34	1.000000	21	44	43	1.000000
22	22	12	1.000000	22	23	42	1.000000	22	32	34	1.000000
22	45	43	1.000000	22	52	35	1.000000	23	23	12	1.000000
23	34	43	1.000000	23	35	34	1.000000	23	45	43	1.000000
24	24	12	1.000000	24	25	42	1.000000	24	34	33	1.000000
24	46	43	1.000000	24	53	36	1.000000	25	25	12	1.000000
25	36	43	1.000000	25	37	33	1.000000	25	46	43	1.000000
26	26	12	1.000000	26	27	40	1.000000	26	38	34	1.000000
26	40	43	1.000000	26	48	43	1.000000	26	49	43	1.000000
27	27	12	1.000000	27	29	42	1.000000	27	38	43	1.000000
27	40	34	1.000000	27	47	43	1.000000	28	28	12	1.000000
28	31	34	1.000000	28	43	43	1.000000	29	29	12	1.000000
29	37	43	1.000000	29	47	43	1.000000	30	30	9	1.000000
30	42	45	1.000000	30	43	45	1.000000	30	67	47	1.000000
31	32	45	1.000000	31	44	45	1.000000	31	68	47	1.000000
32	33	29	1.000000	32	44	45	1.000000	32	68	47	1.000000
33	34	45	1.000000	33	45	45	1.000000	33	69	47	1.000000
34	35	30	1.000000	34	45	45	1.000000	34	69	47	1.000000
35	36	45	1.000000	35	46	45	1.000000	35	70	47	1.000000
36	37	30	1.000000	36	46	45	1.000000	36	70	47	1.000000
37	38	45	1.000000	37	47	45	1.000000	37	71	47	1.000000
38	39	29	1.000000	38	40	30	1.000000	38	47	45	1.000000
39	39	9	1.000000	39	40	44	1.000000	39	41	46	1.000000
39	72	47	1.000000	40	40	9	1.000000	40	41	46	1.000000
40	73	47	1.000000	41	41	8	1.000000	41	48	46	1.000000
41	72	47	1.000000	41	73	47	1.000000	42	42	7	1.000000
42	50	39	1.000000	42	67	47	1.000000	43	43	7	1.000000
42	44	7	1.000000	44	51	39	1.000000	44	68	47	1.000000
45	52	39	1.000000	45	69	47	1.000000	46	46	7	1.000000
46	70	47	1.000000	47	47	7	1.000000	47	71	47	1.000000
48	49	44	1.000000	48	54	39	1.000000	48	72	47	1.000000
49	54	39	1.000000	49	73	47	1.000000	50	50	6	1.000000
52	52	6	1.000000	53	53	6	1.000000	54	54	6	1.000000
56	56	14	1.000000	57	57	14	1.000000	58	58	14	1.000000
60	60	15	1.000000	61	61	15	1.000000	62	62	15	1.000000
64	64	15	1.000000	65	65	16	1.000000	66	66	16	1.000000
68	68	2	1.000000	69	69	2	1.000000	70	70	2	1.000000
72	72	2	1.000000	72	73	75	1.000000	73	73	2	1.000000

TABLE XXXIII (Continued)

Z MATRIX			BETA GALACTOSE			(GT)		
1	1	4	1	17	1	1	8	18
1	9	18	1	13	1	1	20	22
1	28	22	1	30	1	1	67	47
1	68	47	1	2	2	2	9	18
2	10	18	2	13	2	2	21	22
2	22	22	2	32	2	2	68	47
2	69	47	3	3	3	3	10	18
3	11	18	3	14	3	3	23	22
3	24	22	3	34	3	3	69	47
3	70	47	4	4	4	4	6	18
4	11	18	4	15	4	4	25	22
4	29	22	4	36	4	4	70	47
4	71	47	5	5	5	5	12	18
5	16	21	5	26	5	5	38	26
5	39	26	5	40	5	5	72	47
5	73	47	6	6	6	6	17	23
6	27	25	6	29	6	6	71	47
7	7	3	7	8	7	7	18	24
7	28	25	7	43	7	7	8	3
8	18	24	8	19	8	8	50	28
8	67	47	9	9	9	9	21	25
9	44	27	9	51	9	9	10	10
10	22	25	10	23	10	10	52	28
10	69	47	11	11	11	11	25	25
11	46	27	11	53	11	11	12	12
12	26	25	12	48	12	12	54	28
12	72	47	12	73	12	12	14	41
13	19	40	13	20	13	13	22	40
13	28	41	13	30	13	13	32	43
13	33	32	14	14	14	14	21	40
14	22	42	14	23	14	14	32	32
14	33	43	14	34	14	14	15	10
15	16	40	15	23	15	15	25	42
15	29	41	15	34	15	15	36	43
15	37	32	16	16	16	16	26	40
16	27	42	16	29	16	16	37	43
16	38	43	16	39	16	16	17	13
17	18	40	17	27	17	17	29	41
17	43	38	17	47	17	17	18	11
18	28	42	18	42	18	18	43	43
19	19	12	19	20	19	19	28	42
19	31	34	19	42	19	19	50	35
20	21	42	20	28	20	20	30	34
20	44	43	20	51	20	20	21	12
21	32	43	21	33	21	21	44	43
22	22	12	22	23	22	22	32	34
22	45	43	22	52	22	22	23	12
23	34	43	23	35	23	23	45	43
24	24	12	24	25	24	24	34	33
24	46	43	24	53	24	24	25	12
25	36	43	25	37	25	25	46	43
26	26	12	26	27	26	26	38	34
26	40	43	26	48	26	26	49	43
27	27	12	27	29	27	27	38	43
27	40	34	27	47	27	27	28	12
28	31	34	28	43	28	28	29	12
29	37	43	29	47	29	29	30	9
30	42	45	30	43	30	30	67	47
31	32	45	31	44	31	31	68	47
32	33	29	32	44	32	32	68	47
33	34	45	33	45	33	33	69	47
34	35	30	34	45	34	34	69	47
35	36	45	35	46	35	35	70	47
36	37	30	36	46	36	36	70	47
37	38	45	37	47	37	37	71	47
38	39	30	38	40	38	38	47	45
39	39	9	39	44	39	39	41	46
39	72	47	40	40	40	40	41	46
40	73	47	41	41	41	41	48	46
41	72	47	41	73	42	42	42	7
42	50	39	42	67	43	43	43	7
44	44	7	44	51	44	44	68	47
45	52	39	45	69	46	46	46	7
46	70	47	47	47	47	47	71	47
48	49	44	48	54	48	48	72	47
49	54	39	49	73	50	50	50	6
52	52	6	53	53	54	54	54	6
56	56	14	57	57	58	58	14	14
60	60	15	61	61	62	62	15	15
64	64	15	65	65	66	66	16	16
68	68	2	69	69	70	70	2	2
72	72	2	72	73	73	73	2	2

TABLE XXXIII (Continued)

Z MATRIX				BETA GALACTOSE (GG)			
1	1	4	1.000000	1	17	18	1.000000
1	9	18	1.000000	1	19	22	1.000000
1	28	22	1.000000	1	31	26	1.000000
1	68	47	1.000000	2	3	17	1.000000
2	10	18	1.000000	2	14	21	1.000000
2	22	22	1.000000	2	33	26	1.000000
2	69	47	1.000000	3	4	17	1.000000
3	11	18	1.000000	3	15	21	1.000000
3	24	22	1.000000	3	35	26	1.000000
3	70	47	1.000000	4	5	17	1.000000
4	11	18	1.000000	4	16	21	1.000000
4	29	22	1.000000	4	37	26	1.000000
4	71	47	1.000000	5	6	18	1.000000
5	16	21	1.000000	5	27	22	1.000000
5	39	26	1.000000	5	71	47	1.000000
5	73	47	1.000000	6	7	20	1.000000
6	27	25	1.000000	6	47	27	1.000000
6	7	3	1.000000	7	17	23	1.000000
7	28	25	1.000000	7	67	47	1.000000
8	18	24	1.000000	8	42	27	1.000000
8	67	47	1.000000	9	20	25	1.000000
9	44	27	1.000000	9	68	47	1.000000
10	22	25	1.000000	10	45	27	1.000000
10	69	47	1.000000	11	24	25	1.000000
11	46	27	1.000000	11	70	47	1.000000
12	26	25	1.000000	12	49	27	1.000000
12	72	47	1.000000	13	13	10	1.000000
13	19	40	1.000000	13	21	42	1.000000
13	28	41	1.000000	13	31	43	1.000000
13	33	32	1.000000	14	15	41	1.000000
14	22	42	1.000000	14	24	41	1.000000
14	33	43	1.000000	14	35	31	1.000000
15	16	40	1.000000	15	24	42	1.000000
15	29	41	1.000000	15	35	43	1.000000
15	37	32	1.000000	16	25	41	1.000000
16	27	42	1.000000	16	36	32	1.000000
16	38	43	1.000000	16	40	32	1.000000
17	18	40	1.000000	17	28	41	1.000000
17	43	38	1.000000	18	18	11	1.000000
18	28	42	1.000000	18	43	43	1.000000
19	19	12	1.000000	19	28	42	1.000000
19	31	34	1.000000	19	50	35	1.000000
20	21	42	1.000000	20	30	34	1.000000
20	44	43	1.000000	21	21	12	1.000000
21	32	43	1.000000	21	44	43	1.000000
22	22	12	1.000000	22	32	34	1.000000
22	45	43	1.000000	23	23	12	1.000000
23	34	43	1.000000	23	45	43	1.000000
24	24	12	1.000000	24	34	33	1.000000
24	46	43	1.000000	25	25	12	1.000000
25	36	43	1.000000	25	46	43	1.000000
26	26	12	1.000000	26	38	33	1.000000
26	40	43	1.000000	26	49	43	1.000000
27	27	12	1.000000	27	38	43	1.000000
27	40	33	1.000000	28	28	12	1.000000
28	31	34	1.000000	29	29	12	1.000000
29	37	43	1.000000	30	30	9	1.000000
30	42	45	1.000000	30	67	47	1.000000
31	32	45	1.000000	31	68	47	1.000000
32	33	29	1.000000	32	68	47	1.000000
33	34	45	1.000000	33	69	47	1.000000
34	35	30	1.000000	34	69	47	1.000000
35	36	45	1.000000	35	70	47	1.000000
36	37	30	1.000000	36	70	47	1.000000
37	38	45	1.000000	37	71	47	1.000000
38	39	30	1.000000	38	47	45	1.000000
39	39	9	1.000000	39	41	46	1.000000
39	72	47	1.000000	40	41	46	1.000000
40	73	47	1.000000	41	48	46	1.000000
41	72	47	1.000000	42	42	7	1.000000
42	50	39	1.000000	43	43	7	1.000000
44	44	7	1.000000	44	68	47	1.000000
45	51	39	1.000000	46	46	7	1.000000
46	70	47	1.000000	47	71	47	1.000000
48	49	44	1.000000	48	72	47	1.000000
49	54	39	1.000000	50	50	6	1.000000
52	52	6	1.000000	54	54	6	1.000000
56	56	14	1.000000	58	58	14	1.000000
60	60	15	1.000000	62	62	15	1.000000
64	64	15	1.000000	66	66	16	1.000000
68	68	2	1.000000	70	70	2	1.000000
72	72	2	1.000000	73	73	2	1.000000

TABLE XXXIII (Continued)

Z MATRIX				BETA GALACTOSE				(TG)				
1	1	4	1.000000	1	17	1.000000	1	17	1.000000	1	18	1.000000
1	1	18	1.000000	1	21	1.000000	1	19	1.000000	1	20	1.000000
1	1	22	1.000000	1	26	1.000000	1	22	1.000000	1	22	1.000000
1	28	47	1.000000	1	30	1.000000	1	31	1.000000	1	67	1.000000
1	68	47	1.000000	2	2	1.000000	2	3	1.000000	2	9	1.000000
2	10	18	1.000000	2	21	1.000000	2	14	1.000000	2	21	1.000000
2	22	22	1.000000	2	26	1.000000	2	33	1.000000	2	68	1.000000
2	69	47	1.000000	2	3	1.000000	2	4	1.000000	2	10	1.000000
3	11	18	1.000000	3	14	1.000000	3	15	1.000000	3	23	1.000000
3	24	22	1.000000	3	34	1.000000	3	35	1.000000	3	69	1.000000
3	70	47	1.000000	4	4	1.000000	4	5	1.000000	4	6	1.000000
4	11	18	1.000000	4	15	1.000000	4	16	1.000000	4	25	1.000000
4	29	22	1.000000	4	36	1.000000	4	37	1.000000	4	70	1.000000
4	71	47	1.000000	5	5	1.000000	5	6	1.000000	5	12	1.000000
5	16	21	1.000000	5	26	1.000000	5	27	1.000000	5	38	1.000000
5	39	26	1.000000	5	40	1.000000	5	71	1.000000	5	72	1.000000
5	73	47	1.000000	6	6	1.000000	6	7	1.000000	6	17	1.000000
6	27	25	1.000000	6	29	1.000000	6	47	1.000000	6	71	1.000000
7	7	3	1.000000	7	2	1.000000	7	17	1.000000	7	18	1.000000
7	28	25	1.000000	7	43	1.000000	7	67	1.000000	8	8	1.000000
8	18	24	1.000000	8	19	1.000000	8	42	1.000000	8	50	1.000000
8	67	47	1.000000	8	9	1.000000	9	20	1.000000	9	21	1.000000
9	44	27	1.000000	9	51	1.000000	9	68	1.000000	10	10	1.000000
10	22	25	1.000000	10	23	1.000000	10	45	1.000000	10	52	1.000000
10	69	47	1.000000	11	11	1.000000	11	24	1.000000	11	25	1.000000
11	46	27	1.000000	11	53	1.000000	11	70	1.000000	12	12	1.000000
12	26	25	1.000000	12	48	1.000000	12	49	1.000000	12	54	1.000000
12	72	47	1.000000	12	73	1.000000	13	13	1.000000	13	14	1.000000
13	19	40	1.000000	13	20	1.000000	13	21	1.000000	13	22	1.000000
13	28	41	1.000000	13	30	1.000000	13	31	1.000000	13	32	1.000000
13	33	32	1.000000	14	14	1.000000	14	15	1.000000	14	21	1.000000
14	22	42	1.000000	14	23	1.000000	14	24	1.000000	14	32	1.000000
14	33	43	1.000000	14	34	1.000000	14	35	1.000000	15	15	1.000000
15	16	40	1.000000	15	23	1.000000	15	24	1.000000	15	25	1.000000
15	29	41	1.000000	15	34	1.000000	15					

TABLE XXXIII (Continued)

Z MATRIX				ALPHA MANNOSE (GT)			
1	1	4	1.000000	1	17	18	1.000000
1	9	18	1.000000	1	19	22	1.000000
2	28	22	1.000000	1	31	26	1.000000
1	68	47	1.000000	2	3	17	1.000000
2	10	18	1.000000	2	14	21	1.000000
2	22	22	1.000000	2	33	26	1.000000
2	69	47	1.000000	3	4	17	1.000000
3	11	18	1.000000	3	15	21	1.000000
3	24	22	1.000000	3	35	26	1.000000
3	70	47	1.000000	4	5	17	1.000000
4	11	18	1.000000	4	16	21	1.000000
4	29	22	1.000000	4	37	26	1.000000
4	71	47	1.000000	5	6	18	1.000000
5	16	21	1.000000	5	27	22	1.000000
5	73	47	1.000000	6	7	20	1.000000
6	27	25	1.000000	6	47	27	1.000000
7	7	3	1.000000	7	17	23	1.000000
7	28	25	1.000000	7	67	47	1.000000
8	18	24	1.000000	8	42	27	1.000000
8	67	47	1.000000	9	20	25	1.000000
9	44	27	1.000000	9	68	47	1.000000
10	22	25	1.000000	10	45	27	1.000000
10	69	47	1.000000	11	24	25	1.000000
11	46	27	1.000000	11	70	47	1.000000
12	26	25	1.000000	12	49	27	1.000000
12	72	47	1.000000	13	13	10	1.000000
13	19	41	1.000000	13	21	42	1.000000
13	28	41	1.000000	13	31	43	1.000000
13	33	32	1.000000	14	15	41	1.000000
14	22	42	1.000000	14	24	40	1.000000
14	33	43	1.000000	14	35	32	1.000000
15	16	40	1.000000	15	24	42	1.000000
15	29	41	1.000000	15	35	43	1.000000
15	37	32	1.000000	16	25	41	1.000000
16	27	42	1.000000	16	36	32	1.000000
16	38	43	1.000000	16	40	32	1.000000
17	18	41	1.000000	17	28	41	1.000000
17	43	37	1.000000	18	18	11	1.000000
18	28	42	1.000000	18	43	43	1.000000
24	46	43	1.000000	25	25	12	1.000000
19	19	12	1.000000	19	28	42	1.000000
19	31	34	1.000000	19	50	35	1.000000
20	21	42	1.000000	20	30	34	1.000000
20	44	43	1.000000	21	21	12	1.000000
21	32	43	1.000000	21	44	43	1.000000
22	22	12	1.000000	22	32	34	1.000000
22	45	43	1.000000	23	23	12	1.000000
23	34	43	1.000000	23	45	43	1.000000
24	24	12	1.000000	24	34	34	1.000000
5	39	26	1.000000	5	71	47	1.000000
25	36	43	1.000000	25	46	43	1.000000
26	26	12	1.000000	26	38	34	1.000000
26	40	43	1.000000	26	49	43	1.000000
27	27	12	1.000000	27	38	43	1.000000
27	40	34	1.000000	28	28	12	1.000000
28	31	33	1.000000	29	29	12	1.000000
28	37	43	1.000000	30	30	9	1.000000
30	42	45	1.000000	30	67	47	1.000000
31	32	45	1.000000	31	68	47	1.000000
32	33	30	1.000000	32	69	47	1.000000
33	34	45	1.000000	33	69	47	1.000000
34	35	29	1.000000	34	69	47	1.000000
35	36	45	1.000000	35	70	47	1.000000
36	37	29	1.000000	36	70	47	1.000000
37	38	45	1.000000	37	71	47	1.000000
38	39	30	1.000000	38	47	45	1.000000
39	39	9	1.000000	39	41	46	1.000000
39	72	47	1.000000	40	41	46	1.000000
40	73	47	1.000000	41	48	46	1.000000
41	72	47	1.000000	42	42	7	1.000000
42	50	39	1.000000	43	43	7	1.000000
44	44	7	1.000000	44	68	47	1.000000
45	52	39	1.000000	45	46	7	1.000000
46	70	47	1.000000	46	46	7	1.000000
48	49	44	1.000000	47	71	47	1.000000
49	54	39	1.000000	48	72	47	1.000000
52	52	6	1.000000	50	50	6	1.000000
56	56	14	1.000000	54	54	6	1.000000
60	60	15	1.000000	58	58	14	1.000000
64	64	15	1.000000	62	62	15	1.000000
68	68	2	1.000000	66	66	16	1.000000
72	72	2	1.000000	70	70	2	1.000000
				73	73	2	1.000000
							-2

TABLE XXXIII (Continued)

Z MATRIX			ALPHA MANNOSE (GG)								
1	1	4	1.000000	1	7	18	1.000000	1	8	18	1.000000
1	9	16	1.000000	1	13	21	1.000000	1	19	22	1.000000
1	28	22	1.000000	1	30	26	1.000000	1	31	26	1.000000
1	68	47	1.000000	2	2	4	1.000000	2	3	17	1.000000
2	10	18	1.000000	2	13	21	1.000000	2	14	21	1.000000
2	22	22	1.000000	2	32	26	1.000000	2	33	26	1.000000
2	69	47	1.000000	3	3	4	1.000000	3	4	17	1.000000
3	11	18	1.000000	3	14	21	1.000000	3	15	21	1.000000
3	24	22	1.000000	3	34	26	1.000000	3	35	26	1.000000
3	70	47	1.000000	4	4	4	1.000000	4	5	17	1.000000
4	11	18	1.000000	4	15	21	1.000000	4	16	21	1.000000
4	29	22	1.000000	4	36	26	1.000000	4	37	26	1.000000
4	71	47	1.000000	5	5	4	1.000000	5	6	18	1.000000
5	16	21	1.000000	5	26	22	1.000000	5	27	22	1.000000
5	39	26	1.000000	5	40	26	1.000000	5	71	47	1.000000
5	73	47	1.000000	6	6	3	1.000000	6	7	20	1.000000
6	27	25	1.000000	6	29	25	1.000000	6	47	27	1.000000
7	27	3	1.000000	7	8	19	1.000000	7	17	23	1.000000
7	28	25	1.000000	7	43	27	1.000000	7	67	47	1.000000
8	18	24	1.000000	8	15	25	1.000000	8	42	27	1.000000
8	67	47	1.000000	9	9	3	1.000000	9	20	25	1.000000
9	44	27	1.000000	9	51	28	1.000000	9	68	47	1.000000
10	22	25	1.000000	10	23	25	1.000000	10	45	27	1.000000
10	69	47	1.000000	11	11	3	1.000000	11	24	25	1.000000
11	46	27	1.000000	11	53	28	1.000000	11	70	47	1.000000
12	26	25	1.000000	12	48	27	1.000000	12	49	27	1.000000
12	72	47	1.000000	12	73	47	1.000000	13	13	10	1.000000
13	19	41	1.000000	13	20	42	1.000000	13	21	42	1.000000
13	28	41	1.000000	13	30	31	1.000000	13	31	43	1.000000
13	33	32	1.000000	14	14	10	1.000000	14	15	43	1.000000
14	22	42	1.000000	14	23	42	1.000000	14	24	40	1.000000
14	33	43	1.000000	14	34	43	1.000000	14	35	32	1.000000
15	16	40	1.000000	15	23	40	1.000000	15	24	42	1.000000
15	29	41	1.000000	15	34	32	1.000000	15	35	43	1.000000
15	37	32	1.000000	16	16	10	1.000000	16	25	41	1.000000
16	27	42	1.000000	16	29	42	1.000000	16	36	32	1.000000
16	38	43	1.000000	16	39	31	1.000000	16	40	32	1.000000
17	18	41	1.000000	17	27	40	1.000000	17	28	41	1.000000
17	43	37	1.000000	17	47	38	1.000000	18	18	11	1.000000
18	28	42	1.000000	18	42	43	1.000000	18	43	43	1.000000
19	19	12	1.000000	19	20	40	1.000000	19	28	42	1.000000
19	31	34	1.000000	19	42	43	1.000000	19	50	35	1.000000
20	41	42	1.000000	20	28	41	1.000000	20	30	34	1.000000
20	44	43	1.000000	20	51	35	1.000000	21	21	12	1.000000
21	32	43	1.000000	21	33	33	1.000000	21	44	43	1.000000
22	22	12	1.000000	22	23	42	1.000000	22	32	34	1.000000
22	45	43	1.000000	22	52	35	1.000000	23	23	12	1.000000
23	34	43	1.000000	23	35	34	1.000000	23	45	43	1.000000
24	24	12	1.000000	24	25	42	1.000000	24	34	34	1.000000
24	46	43	1.000000	24	53	36	1.000000	25	25	12	1.000000
25	36	43	1.000000	25	37	34	1.000000	25	46	43	1.000000
26	26	12	1.000000	26	27	41	1.000000	26	38	33	1.000000
26	40	43	1.000000	26	48	43	1.000000	26	49	43	1.000000
27	27	12	1.000000	27	29	42	1.000000	27	38	43	1.000000
27	40	33	1.000000	27	47	43	1.000000	28	28	12	1.000000
28	31	33	1.000000	28	43	43	1.000000	29	29	12	1.000000
29	37	43	1.000000	29	47	43	1.000000	30	30	9	1.000000
30	42	45	1.000000	30	43	45	1.000000	30	67	47	1.000000
31	32	45	1.000000	31	44	45	1.000000	31	68	47	1.000000
32	31	30	1.000000	32	44	45	1.000000	32	68	47	1.000000
33	34	45	1.000000	33	45	45	1.000000	33	69	47	1.000000
34	35	29	1.000000	34	45	45	1.000000	34	69	47	1.000000
35	36	45	1.000000	35	46	45	1.000000	35	70	47	1.000000
36	37	29	1.000000	36	46	45	1.000000	36	70	47	1.000000
37	38	45	1.000000	37	47	45	1.000000	37	71	47	1.000000
38	39	30	1.000000	38	40	30	1.000000	38	47	45	1.000000
39	39	9	1.000000	39	40	44	1.000000	39	41	46	1.000000
39	72	47	1.000000	40	40	9	1.000000	40	41	46	1.000000
40	73	47	1.000000	41	41	8	1.000000	41	48	46	1.000000
41	72	47	1.000000	41	73	47	1.000000	42	42	7	1.000000
42	50	39	1.000000	42	57	47	1.000000	43	43	7	1.000000
44	44	7	1.000000	44	51	39	1.000000	44	68	47	1.000000
45	52	39	1.000000	45	59	47	1.000000	46	46	7	1.000000
46	70	47	1.000000	47	47	7	1.000000	47	71	47	1.000000
48	49	44	1.000000	48	54	39	1.000000	48	72	47	1.000000
49	54	39	1.000000	49	73	47	1.000000	50	50	6	1.000000
52	52	6	1.000000	53	53	6	1.000000	54	54	6	1.000000
56	56	14	1.000000	57	57	14	1.000000	58	58	14	1.000000
60	60	15	1.000000	61	61	15	1.000000	62	62	15	1.000000
64	64	15	1.000000	65	65	16	1.000000	66	66	16	1.000000
68	68	2	1.000000	69	69	2	1.000000	70	70	2	1.000000
72	72	2	1.000000	72	73	75	1.000000	73	73	2	1.000000

Z MATRIX				...	ALPHA MANNOSE (TG)											
1	1	4	1.000000	1	2	17	1.000000	1	7	18	1.000000	1	8	18	1.000000	
1	9	18	1.000000	1	13	21	1.000000	1	19	22	1.000000	1	20	22	1.000000	
1	1	28	1.000000	1	1	30	26	1.000000	1	31	26	1.000000	1	67	47	1.000000
1	68	47	1.000000	2	2	4	1.000000	2	3	17	1.000000	2	9	18	1.000000	
2	10	18	1.000000	2	13	21	1.000000	2	14	21	1.000000	2	21	22	1.000000	
2	22	22	1.000000	2	32	26	1.000000	2	33	26	1.000000	2	68	47	1.000000	
2	69	47	1.000000	3	3	4	1.000000	3	4	17	1.000000	3	10	18	1.000000	
3	11	18	1.000000	3	14	21	1.000000	3	15	21	1.000000	3	23	22	1.000000	
3	24	22	1.000000	3	34	26	1.000000	3	35	26	1.000000	3	69	47	1.000000	
3	70	47	1.000000	4	4	4	1.000000	4	5	17	1.000000	4	6	18	1.000000	
4	11	18	1.000000	4	15	21	1.000000	4	16	21	1.000000	4	25	22	1.000000	
4	29	22	1.000000	4	36	26	1.000000	4	37	26	1.000000	4	70	47	1.000000	
4	71	47	1.000000	5	5	4	1.000000	5	6	18	1.000000	5	12	18	1.000000	
5	16	21	1.000000	5	26	22	1.000000	5	27	22	1.000000	5	38	26	1.000000	
5	39	26	1.000000	5	40	26	1.000000	5	71	47	1.000000	5	72	47	1.000000	
5	73	47	1.000000	6	6	3	1.000000	6	7	20	1.000000	6	17	23	1.000000	
6	27	25	1.000000	6	25	25	1.000000	6	47	27	1.000000	6	71	47	1.000000	
6	77	7	1.000000	7	8	19	1.000000	7	17	23	1.000000	7	18	24	1.000000	
7	28	25	1.000000	7	43	27	1.000000	7	67	47	1.000000	8	8	3	1.000000	
8	18	24	1.000000	8	19	25	1.000000	8	42	27	1.000000	8	50	28	1.000000	
8	67	47	1.000000	9	9	3	1.000000	9	20	25	1.000000	9	21	25	1.000000	
9	44	27	1.000000	9	51	28	1.000000	9	68	47	1.000000	10	10	3	1.000000	
10	22	25	1.000000	10	23	25	1.000000	10	45	27	1.000000	10	52	28	1.000000	
10	69	47	1.000000	11	11	3	1.000000	11	24	25	1.000000	11	25	25	1.000000	
11	46	27	1.000000	11	53	28	1.000000	11	70	47	1.000000	12	12	3	1.000000	
12	26	25	1.000000	12	48	27	1.000000	12	49	27	1.000000	12	54	28	1.000000	
12	72	47	1.000000	12	73	47	1.000000	13	13	10	1.000000	13	14	41	1.000000	
13	19	41	1.000000	13	20	42	1.000000	13	21	42	1.000000	13	22	40	1.000000	
13	28	41	1.000000	13	30	31	1.000000	13	31	43	1.000000	13	32	43	1.000000	
13	33	32	1.000000	14	14	10	1.0000									

TABLE XXXIII (Continued)

Z MATRIX				BETA MANNOSE (GG)			
1 1 4	1.000000	1 2 17	1.000000	1 7 18	1.000000	1 8 18	1.000000
1 9 18	1.000000	1 13 21	1.000000	1 19 22	1.000000	1 20 22	1.000000
1 28 22	1.000000	1 30 26	1.000000	1 31 26	1.000000	1 67 47	1.000000
1 68 47	1.000000	2 2 4	1.000000	2 3 17	1.000000	2 9 18	1.000000
2 10 18	1.000000	2 13 21	1.000000	2 14 21	1.000000	2 21 22	1.000000
2 22 22	1.000000	2 32 26	1.000000	2 33 26	1.000000	2 68 47	1.000000
2 69 47	1.000000	3 3 4	1.000000	3 4 17	1.000000	3 10 18	1.000000
3 11 18	1.000000	3 14 21	1.000000	3 15 21	1.000000	3 23 22	1.000000
3 24 22	1.000000	3 34 26	1.000000	3 35 26	1.000000	3 69 47	1.000000
3 70 47	1.000000	4 4 4	1.000000	4 5 17	1.000000	4 6 18	1.000000
4 11 18	1.000000	4 15 21	1.000000	4 16 21	1.000000	4 25 22	1.000000
4 29 22	1.000000	4 36 26	1.000000	4 37 26	1.000000	4 70 47	1.000000
4 71 47	1.000000	5 5 4	1.000000	5 6 18	1.000000	5 12 18	1.000000
5 16 21	1.000000	5 26 22	1.000000	5 27 22	1.000000	5 38 26	1.000000
5 39 26	1.000000	5 40 26	1.000000	5 71 47	1.000000	5 72 47	1.000000
5 73 47	1.000000	6 6 3	1.000000	6 7 20	1.000000	6 17 23	1.000000
6 27 25	1.000000	6 24 25	1.000000	6 47 27	1.000000	6 71 47	1.000000
7 7 3	1.000000	7 8 19	1.000000	7 17 23	1.000000	7 18 24	1.000000
7 28 25	1.000000	7 43 27	1.000000	7 67 47	1.000000	8 8 3	1.000000
8 18 24	1.000000	8 19 25	1.000000	8 42 27	1.000000	8 50 28	1.000000
8 67 47	1.000000	9 9 3	1.000000	9 20 25	1.000000	9 21 25	1.000000
9 44 27	1.000000	9 51 28	1.000000	9 68 47	1.000000	10 10 3	1.000000
10 22 25	1.000000	10 23 25	1.000000	10 45 27	1.000000	10 52 28	1.000000
10 69 47	1.000000	11 11 3	1.000000	11 24 25	1.000000	11 25 25	1.000000
11 46 27	1.000000	11 53 28	1.000000	11 70 47	1.000000	12 12 3	1.000000
12 26 25	1.000000	12 48 27	1.000000	12 49 27	1.000000	12 54 28	1.000000
12 72 47	1.000000	12 73 47	1.000000	13 13 10	1.000000	13 14 41	1.000000
13 19 41	1.000000	13 20 42	1.000000	13 21 42	1.000000	13 22 40	1.000000
13 28 41	1.000000	13 30 31	1.000000	13 31 43	1.000000	13 32 43	1.000000
13 33 32	1.000000	14 14 10	1.000000	14 15 41	1.000000	14 21 41	1.000000
14 22 42	1.000000	14 23 42	1.000000	14 24 40	1.000000	14 32 31	1.000000
14 33 43	1.000000	14 34 43	1.000000	14 35 32	1.000000	15 15 10	1.000000
15 16 40	1.000000	15 23 40	1.000000	15 24 42	1.000000	15 25 42	1.000000
15 29 41	1.000000	15 34 32	1.000000	15 35 43	1.000000	15 36 43	1.000000
15 37 32	1.000000	16 16 10	1.000000	16 25 41	1.000000	16 26 41	1.000000
16 27 42	1.000000	16 29 42	1.000000	16 36 32	1.000000	16 37 43	1.000000
16 38 43	1.000000	16 39 31	1.000000	16 40 32	1.000000	17 17 13	1.000000
17 18 41	1.000000	17 27 40	1.000000	17 28 41	1.000000	17 29 41	1.000000
17 43 37	1.000000	17 47 38	1.000000	18 18 11	1.000000	18 19 42	1.000000
18 28 42	1.000000	18 42 43	1.000000	18 43 43	1.000000	18 50 35	1.000000
19 19 12	1.000000	19 20 41	1.000000	19 28 42	1.000000	19 30 43	1.000000
19 31 34	1.000000	19 42 43	1.000000	19 50 35	1.000000	20 20 12	1.000000
20 21 42	1.000000	20 28 41	1.000000	20 30 33	1.000000	20 31 43	1.000000
20 44 43	1.000000	20 51 35	1.000000	21 21 12	1.000000	21 22 41	1.000000
21 32 43	1.000000	21 33 33	1.000000	21 44 43	1.000000	21 51 36	1.000000
22 22 12	1.000000	22 23 42	1.000000	22 32 34	1.000000	22 33 43	1.000000
22 45 43	1.000000	22 52 35	1.000000	23 23 12	1.000000	23 24 41	1.000000
23 34 43	1.000000	23 35 34	1.000000	23 45 43	1.000000	23 52 36	1.000000
24 24 12	1.000000	24 25 42	1.000000	24 34 34	1.000000	24 35 43	1.000000
24 46 43	1.000000	24 53 36	1.000000	25 25 12	1.000000	25 29 40	1.000000
25 36 43	1.000000	25 37 34	1.000000	25 46 43	1.000000	25 53 35	1.000000
26 26 12	1.000000	26 27 41	1.000000	26 38 33	1.000000	26 39 43	1.000000
26 40 43	1.000000	26 48 43	1.000000	26 49 43	1.000000	26 54 35	1.000000
27 27 12	1.000000	27 29 42	1.000000	27 38 43	1.000000	27 39 34	1.000000
27 40 33	1.000000	27 47 43	1.000000	28 28 12	1.000000	28 30 43	1.000000
28 31 33	1.000000	28 43 43	1.000000	29 29 12	1.000000	29 36 34	1.000000
29 37 43	1.000000	29 47 43	1.000000	30 30 9	1.000000	30 31 30	1.000000
30 42 45	1.000000	30 43 45	1.000000	30 67 47	1.000000	31 31 9	1.000000
31 32 45	1.000000	31 44 45	1.000000	31 68 47	1.000000	32 32 9	1.000000
32 33 30	1.000000	32 44 45	1.000000	32 68 47	1.000000	33 33 9	1.000000
33 34 45	1.000000	33 45 45	1.000000	33 69 47	1.000000	34 34 9	1.000000
34 35 29	1.000000	34 45 45	1.000000	34 69 47	1.000000	35 35 9	1.000000
35 36 45	1.000000	35 46 45	1.000000	35 70 47	1.000000	36 36 9	1.000000
36 37 29	1.000000	36 46 45	1.000000	36 70 47	1.000000	37 37 9	1.000000
37 38 45	1.000000	37 47 45	1.000000	37 71 47	1.000000	38 38 9	1.000000
38 39 30	1.000000	38 40 30	1.000000	38 47 45	1.000000	38 71 47	1.000000
39 39 9	1.000000	39 40 44	1.000000	39 41 46	1.000000	39 48 45	1.000000
39 72 47	1.000000	40 40 9	1.000000	40 41 46	1.000000	40 49 45	1.000000
40 73 47	1.000000	41 41 8	1.000000	41 48 46	1.000000	41 49 46	1.000000
41 72 47	1.000000	41 73 47	1.000000	42 42 7	1.000000	42 43 45	1.000000
42 50 39	1.000000	42 67 47	1.000000	43 43 7	1.000000	43 67 47	1.000000
44 44 7	1.000000	44 51 39	1.000000	44 68 47	1.000000	45 45 7	1.000000
45 52 39	1.000000	45 69 47	1.000000	46 46 7	1.000000	46 53 39	1.000000
46 70 47	1.000000	47 47 7	1.000000	47 71 47	1.000000	48 48 7	1.000000
48 49 44	1.000000	48 54 39	1.000000	48 72 47	1.000000	49 49 7	1.000000
49 54 39	1.000000	49 73 47	1.000000	50 50 6	1.000000	51 51 6	1.000000
52 52 6	1.000000	53 53 6	1.000000	54 54 6	1.000000	55 55 14	1.000000
56 56 14	1.000000	57 57 14	1.000000	58 58 14	1.000000	59 59 14	1.000000
60 60 15	1.000000	61 61 15	1.000000	62 62 15	1.000000	63 63 15	1.000000
64 64 15	1.000000	65 65 16	1.000000	66 66 16	1.000000	67 67 2	1.000000
68 68 2	1.000000	69 69 2	1.000000	70 70 2	1.000000	71 71 2	1.000000
72 72 2	1.000000	72 73 75	1.000000	73 73 2	1.000000	-2	

TABLE XXXIII (Continued)

Z MATRIX				BETA MANNOSE (TG)			
1	1	4	1.0000000	1	7	18	1.0000000
1	9	18	1.0000000	1	19	22	1.0000000
1	28	22	1.0000000	1	31	26	1.0000000
1	68	47	1.0000000	2	3	17	1.0000000
2	10	18	1.0000000	2	14	21	1.0000000
2	22	22	1.0000000	2	33	26	1.0000000
2	69	47	1.0000000	3	4	17	1.0000000
3	11	18	1.0000000	3	15	21	1.0000000
3	24	22	1.0000000	3	35	26	1.0000000
3	70	47	1.0000000	4	5	17	1.0000000
4	11	18	1.0000000	4	16	21	1.0000000
4	29	22	1.0000000	4	37	26	1.0000000
4	71	47	1.0000000	5	6	18	1.0000000
5	16	21	1.0000000	5	27	22	1.0000000
5	39	26	1.0000000	5	71	47	1.0000000
5	73	47	1.0000000	6	7	20	1.0000000
6	27	25	1.0000000	6	47	27	1.0000000
7	7	3	1.0000000	7	17	23	1.0000000
7	28	25	1.0000000	7	67	47	1.0000000
8	18	24	1.0000000	8	42	27	1.0000000
8	67	47	1.0000000	9	20	25	1.0000000
9	44	27	1.0000000	9	68	47	1.0000000
10	22	25	1.0000000	10	45	27	1.0000000
10	69	47	1.0000000	11	24	25	1.0000000
11	46	27	1.0000000	11	70	47	1.0000000
12	26	25	1.0000000	12	49	27	1.0000000
12	72	47	1.0000000	13	13	10	1.0000000
13	19	41	1.0000000	13	21	42	1.0000000
13	28	41	1.0000000	13	31	43	1.0000000
13	33	32	1.0000000	14	15	41	1.0000000
14	22	42	1.0000000	14	24	40	1.0000000
14	33	43	1.0000000	14	35	32	1.0000000
15	26	40	1.0000000	15	24	42	1.0000000
15	39	41	1.0000000	15	35	43	1.0000000
15	37	32	1.0000000	16	25	41	1.0000000
16	27	42	1.0000000	16	36	32	1.0000000
16	38	43	1.0000000	16	40	31	1.0000000
17	18	41	1.0000000	17	28	41	1.0000000
17	43	37	1.0000000	18	18	11	1.0000000
18	28	42	1.0000000	18	43	43	1.0000000
19	19	12	1.0000000	19	28	42	1.0000000
19	31	34	1.0000000	19	50	35	1.0000000
20	21	42	1.0000000	20	30	33	1.0000000
20	44	43	1.0000000	21	21	12	1.0000000
21	32	43	1.0000000	21	44	43	1.0000000
22	22	12	1.0000000	22	32	34	1.0000000
22	45	43	1.0000000	23	23	12	1.0000000
23	34	43	1.0000000	23	45	43	1.0000000
24	24	12	1.0000000	24	34	34	1.0000000
24	46	43	1.0000000	25	25	12	1.0000000
25	36	43	1.0000000	25	46	43	1.0000000
26	26	12	1.0000000	26	38	34	1.0000000
26	40	43	1.0000000	26	49	43	1.0000000
27	27	12	1.0000000	27	38	43	1.0000000
27	40	34	1.0000000	28	28	12	1.0000000
28	31	33	1.0000000	29	29	12	1.0000000
29	37	43	1.0000000	30	30	9	1.0000000
30	42	45	1.0000000	30	67	47	1.0000000
31	32	45	1.0000000	31	68	47	1.0000000
32	33	30	1.0000000	32	68	47	1.0000000
33	34	45	1.0000000	33	69	47	1.0000000
34	35	29	1.0000000	34	69	47	1.0000000
35	36	45	1.0000000	35	70	47	1.0000000
36	37	29	1.0000000	36	70	47	1.0000000
37	38	45	1.0000000	37	71	47	1.0000000
38	39	29	1.0000000	38	47	45	1.0000000
39	39	9	1.0000000	39	41	46	1.0000000
39	72	47	1.0000000	40	41	46	1.0000000
40	73	47	1.0000000	41	48	46	1.0000000
41	72	47	1.0000000	42	42	7	1.0000000
42	50	39	1.0000000	43	43	7	1.0000000
44	44	7	1.0000000	44	68	47	1.0000000
45	52	39	1.0000000	46	46	7	1.0000000
46	70	47	1.0000000	47	71	47	1.0000000
48	49	44	1.0000000	48	72	47	1.0000000
49	54	39	1.0000000	50	50	6	1.0000000
52	52	6	1.0000000	54	54	6	1.0000000
56	56	14	1.0000000	58	58	14	1.0000000
60	60	15	1.0000000	62	62	15	1.0000000
64	64	15	1.0000000	66	66	16	1.0000000
68	68	2	1.0000000	70	70	2	1.0000000
72	72	2	1.0000000	73	73	2	1.0000000
							-2

APPENDIX II

CORRELATION MATRIX AND POTENTIAL ENERGY DISTRIBUTIONS — HEXCOSES

The information reported in this appendix is as follows:

Content	Description of Content	Page
1. Table XXXIV	Potential Energy Distributions — Hexoses	197
2. Table XXXV	Correlation Matrix — Glucose Force Field	280

TABLE XXXIV

POTENTIAL ENERGY DISTRIBUTIONS — HEXCSES

Explanation of the table:

1. The molecule name is found on the second line of the body of each page.
2. The observed frequency is the frequency actually used in the force field refinement.
3. The four letter codes in each row identify the force constants and internal coordinates. The keys to these codes are found in Tables XI and XXIX.
4. The definitions of the potential energy distribution elements are given in Appendix VI, page 428.

POTENTIAL ENERGY DISTRIBUTIONS - HEXOSES

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400										PAGE 1	
MOLECULE 1 -6 NG=1236 ALPHA GLUCOSE											
NORMAL MODE 8		OBSERVED= 1457.0 CM-1		CALCULATED= 1455.2 CM-1		ERROR= 1.8 CM-1		OR		0.1 PERCENT	
INTERNAL COORDINATES-		67.93 C0M1		6.05 C0D		1.68 B834					
FORCE CONSTANTS-		68.37 BCOH 6.58 CCH		-1.77 SB25							
OFF DIAGONAL-		4.45 BB36 3.84 SB28									
NORMAL MODE 9		OBSERVED= 1442.0 CM-1		CALCULATED= 1449.8 CM-1		ERROR= -7.8 CM-1		OR		-0.5 PERCENT	
INTERNAL COORDINATES-		61.19 HCH 20.81 OCHB		19.06 OCHA							
FORCE CONSTANTS-		61.19 HCH 40.25 OCH									
OFF DIAGONAL-		-4.08 SB27									
NORMAL MODE 10		OBSERVED= 1427.0 CM-1		CALCULATED= 1422.7 CM-1		ERROR= 4.3 CM-1		OR		0.3 PERCENT	
INTERNAL COORDINATES-		22.48 C3OH 19.61 C4OH		12.95 OCH4 7.14 HC4C		5.54 CC3H					
FORCE CONSTANTS-		42.42 BCOH 20.97 CCH		20.28 CCH 7.70 CO		8.10 SB25		5.95 CCO			
OFF DIAGONAL-		-5.47 SB27 -4.36 SB26		4.04 BB29 3.57 SB28		-3.12 SB25		3.12 BB34 2.24 BB36		-1.81 BB43 -1.63 BB45	
NORMAL MODE 11		OBSERVED= 1409.0 CM-1		CALCULATED= 1413.8 CM-1		ERROR= -4.8 CM-1		OR		-0.3 PERCENT	
INTERNAL COORDINATES-		44.22 BCOH 9.58 OC3H		15.88 CCH 6.61 OC4C		5.64 CO					
FORCE CONSTANTS-		44.22 BCOH 9.58 OCH		-3.66 SB26 3.35 BB29		2.43 BB36		-1.81 BB39 -1.58 BB45			
OFF DIAGONAL-		-4.44 SB27 4.02 SB28									
NORMAL MODE 12		OBSERVED= 1400.0 CM-1		CALCULATED= 1408.8 CM-1		ERROR= 0.0 CM-1		OR		0.0 PERCENT	
INTERNAL COORDINATES-		57.85 C1OH 20.99 OC1H		8.04 C1H							
FORCE CONSTANTS-		57.11 BCOH 30.28 OCH		8.45 CCH							
OFF DIAGONAL-		4.75 SB28 -4.40 SB27		-3.06 BB39							
NORMAL MODE 13		OBSERVED= 1385.0 CM-1		CALCULATED= 1390.4 CM-1		ERROR= -5.4 CM-1		OR		-0.4 PERCENT	
INTERNAL COORDINATES-		66.35 C1OH 6.52 C1H		5.83 OCHB 5.26 C5C*							
FORCE CONSTANTS-		70.58 BCOH 16.11 OCH		10.25 CCH 6.06 CC							
OFF DIAGONAL-		-4.49 SB26 2.12 SB28		-2.11 BB39 -1.67 SB27							
NORMAL MODE 14		OBSERVED= 1381.0 CM-1		CALCULATED= 1385.8 CM-1		ERROR= -4.8 CM-1		OR		-0.3 PERCENT	
INTERNAL COORDINATES-		34.07 C1H 16.91 C1OH		14.50 OC1H 10.01 C1OH		8.96 C4OH					
FORCE CONSTANTS-		62.17 BCOH 33.62 BCOH		7.22 CCH 2.12 BB37		-1.97 SB26					
OFF DIAGONAL-		-4.27 SB27 -2.18 BB45									
NORMAL MODE 15		OBSERVED= 1375.0 CM-1		CALCULATED= 1374.3 CM-1		ERROR= 0.8 CM-1		OR		0.0 PERCENT	
INTERNAL COORDINATES-		33.70 C4OH 18.61 C5H		5.36 HC5C 5.15 C1H		5.12 CCHB		5.09 CC5H			
FORCE CONSTANTS-		33.70 CCH 31.47 BCOH		31.02 CCH							
OFF DIAGONAL-		5.97 BB29 -4.89 SB27		-2.84 BB26 1.86 BB34							
NORMAL MODE 16		OBSERVED= 1371.0 CM-1		CALCULATED= 1369.9 CM-1		ERROR= 1.1 CM-1		OR		0.1 PERCENT	
INTERNAL COORDINATES-		31.76 C4OH 13.44 C3OH		11.85 OC3H 10.02 OC2H		8.57 HC3C		8.22 HC2C			
FORCE CONSTANTS-		49.51 BCOH 24.59 CCH		24.08 OCH							
OFF DIAGONAL-		4.60 BB29 -3.41 SB27		-3.07 SB28 2.57 BB34		-2.08 BB36		-1.90 BB45 1.61 BB39			
NORMAL MODE 17		OBSERVED= 1363.0 CM-1		CALCULATED= 1346.9 CM-1		ERROR= -3.9 CM-1		OR		-0.3 PERCENT	
INTERNAL COORDINATES-		16.81 HC5C 16.02 UC2H		12.26 CCHB 9.15 HC2C		6.47 CC5H					
FORCE CONSTANTS-		56.76 CCH 26.96 OCH		8.27 BCOH							
OFF DIAGONAL-		12.27 BB29 -4.83 SB26		-3.65 SB27 -3.52 BB45		2.01 BB34		-1.81 SB28			
NORMAL MODE 18		OBSERVED= 1328.0 CM-1		CALCULATED= 1326.1 CM-1		ERROR= 1.9 CM-1		OR		0.1 PERCENT	
INTERNAL COORDINATES-		18.73 HC3C 9.98 CC4H		8.49 OC2H 7.34 OC3H		6.39 HC2C		6.12 CC5H 6.01 HC4C		5.89 HC5C 5.63 CCHB	
FORCE CONSTANTS-		68.07 CCH 23.54 CC		5.99 CCH							
OFF DIAGONAL-		14.44 BB29-10.00 SB26		-3.95 BB45 -3.28 SB27							
NORMAL MODE 19		OBSERVED= 1312.0 CM-1		CALCULATED= 1312.0 CM-1		ERROR= 0.0 CM-1		OR		0.0 PERCENT	
INTERNAL COORDINATES-		77.54 CCH2 12.61 C1H		11.91 OC2H 10.94 C1OH		5.55 C1OH					
FORCE CONSTANTS-		49.93 CCH 22.78 OCH		13.90 CO 12.72 BCOH							
OFF DIAGONAL-		-3.34 SB28 -3.18 BB45		2.58 BB34 -2.18 SB26		-2.15 SB25 1.51 BB29					
NORMAL MODE 20		OBSERVED= 1298.0 CM-1		CALCULATED= 1300.2 CM-1		ERROR= -2.2 CM-1		OR		-0.2 PERCENT	
INTERNAL COORDINATES-		19.45 OCHA 18.71 CCHA		13.50 OC4H 9.57 HC4C		9.36 CC5H					
FORCE CONSTANTS-		50.19 OCH 41.35 CCH		5.64 BCOH							
OFF DIAGONAL-		-3.57 BB45 -3.00 SB27		-1.98 BB29							
NORMAL MODE 21		OBSERVED= 1288.0 CM-1		CALCULATED= 1281.3 CM-1		ERROR= 6.8 CM-1		OR		0.5 PERCENT	
INTERNAL COORDINATES-		12.17 CC1H 10.85 OC1H		10.81 OCHA 9.63 CCHA		9.03 CH22		7.22 C1OH 6.62 OC1C		5.25 CC3H	
FORCE CONSTANTS-		43.55 CCH 23.13 OCH		2.99 BB29		-2.74 SB25 2.48 SB27					
OFF DIAGONAL-		-3.13 BB45 3.11 BB34									
NORMAL MODE 22		OBSERVED= 1270.0 CM-1		CALCULATED= 1267.7 CM-1		ERROR= 2.3 CM-1		OR		0.2 PERCENT	
INTERNAL COORDINATES-		55.72 OCH 35.32 CCH		5.01 CO 8.28 CC1H		7.66 CC5H		7.59 CC5H 7.31 CC4H		6.50 CCHA	
FORCE CONSTANTS-		-3.73 BB29 -3.64 BB45		3.63 SB27 2.32 BB34							
OFF DIAGONAL-											
NORMAL MODE 23		OBSERVED= 1261.0 CM-1		CALCULATED= 1259.3 CM-1		ERROR= 1.7 CM-1		OR		0.1 PERCENT	
INTERNAL COORDINATES-		20.58 OC3H 19.93 C5H		12.41 CC4H 7.11 CC3H		6.40 HC4C					
FORCE CONSTANTS-		50.16 OCH 39.75 CCH		3.57 BB34 -3.57 BB45							
OFF DIAGONAL-		4.99 SB27 -4.86 BB29									
NORMAL MODE 24		OBSERVED= 1224.0 CM-1		CALCULATED= 1227.1 CM-1		ERROR= -3.1 CM-1		OR		-0.3 PERCENT	
INTERNAL COORDINATES-		13.57 HC5C 11.73 OC4H		9.70 OCHB 7.80 CC5H		7.47 OC3H		6.52 CC3H 6.50 CCHB			
FORCE CONSTANTS-		43.03 CCH 36.61 OCH		10.18 CO 5.15 BCOH		5.09 CCH					
OFF DIAGONAL-		-8.17 BB29 9.87 SB27		4.55 BB34 -3.23 SB25		-3.10 BB45					
NORMAL MODE 25		OBSERVED= 1203.0 CM-1		CALCULATED= 1192.4 CM-1		ERROR= 10.6 CM-1		OR		0.9 PERCENT	
INTERNAL COORDINATES-		16.77 OC1C 12.35 C5O*		26.87 OCHB 11.92 HC4C		7.84 CC3H		6.41 CC3H 5.79 CC5H		5.87 C2OH	
FORCE CONSTANTS-		36.33 CO 31.32 CCH		26.86 OCH 9.45 CCH		7.73 BCOH					
OFF DIAGONAL-		-6.05 SB25 -4.34 BB29		-2.27 SB26 -1.91 BB45		1.67 BB34					
NORMAL MODE 26		OBSERVED= 1147.0 CM-1		CALCULATED= 1142.3 CM-1		ERROR= 4.7 CM-1		OR		0.4 PERCENT	
INTERNAL COORDINATES-		26.15 OC1C 9.39 CCH2		6.51 C5O* 5.92 HC2C		1.80 HC4C		5.57 C1OH			
FORCE CONSTANTS-		48.07 CO 35.05 CCH		12.02 OCH 9.55 CCO		7.14 CC					
OFF DIAGONAL-		-4.61 BB29 -2.93 SB25		2.44 BB34 -2.26 SB27		-1.72 SB22		-1.67 BB45			
NORMAL MODE 27		OBSERVED= 1126.0 CM-1		CALCULATED= 1135.5 CM-1		ERROR= -9.5 CM-1		OR		-0.8 PERCENT	
INTERNAL COORDINATES-		16.74 C5O* 9.85 OCHB		7.43 OCHA 6.67 C2OH		5.67 CCOH		5.40 CC3H 5.17 C1OH			
FORCE CONSTANTS-		28.51 CO 25.48 OCH		23.02 CCH 13.26 CCO		9.72 BCOH					
OFF DIAGONAL-		-7.91 SB25 -3.54 BB29		3.57 SB27 2.79 BB34		-2.76 SB28		-2.42 SB23 -1.55 SB22			
NORMAL MODE 28		OBSERVED= 1118.0 CM-1		CALCULATED= 1122.8 CM-1		ERROR= -4.8 CM-1		OR		-0.4 PERCENT	
INTERNAL COORDINATES-		35.88 C1OH 4.98 C1OH		9.64 C4C5 6.83 C2C3		6.00 CCOH		5.84 C2OH			
FORCE CONSTANTS-		-9.68 SB25 -8.71 SB28		-4.15 SB22 -3.10 SB26		2.33 SB27		-1.85 SS18			
OFF DIAGONAL-											
NORMAL MODE 29		OBSERVED= 1109.0 CM-1		CALCULATED= 1107.2 CM-1		ERROR= 1.8 CM-1		OR		0.2 PERCENT	
INTERNAL COORDINATES-		44.19 C4C5 1.48 C5C		15.75 C4C5 7.48 C1OH		6.97 CCH		5.48 C1OH			
FORCE CONSTANTS-		77.39 CCH 25.49 CCH		-4.05 SB27 -3.90 SB25		-2.84 SS17		-2.78 SS18 -1.96 SB26		-1.59 SB28	
OFF DIAGONAL-		-10.93 SB22 -4.85 SB21									
NORMAL MODE 30		OBSERVED= 1078.0 CM-1		CALCULATED= 1082.0 CM-1		ERROR= -4.0 CM-1		OR		-0.4 PERCENT	
INTERNAL COORDINATES-		37.46 C1OH 25.05 C3C4		9.75 C1OH 9.27 C5C*		8.52 OC1C					
FORCE CONSTANTS-		63.00 CO 35.25 CCH		7.86 CCH 5.39 CCO		5.07 OCH					
OFF DIAGONAL-		-7.91 SS18 -5.95 SB27		-5.41 SB28 -2.61 SB22		-2.22 SB21		1.59 SB26			
NORMAL MODE 31		OBSERVED= 1072.0 CM-1		CALCULATED= 1064.5 CM-1		ERROR= 7.5 CM-1		OR		0.7 PERCENT	
INTERNAL COORDINATES-		45.06 C1C2 16.73 C1OH		12.21 C1OH 11.66 C2C3		8.07 C1OH		6.13 C1OH 5.42 C1OH			
FORCE CONSTANTS-		65.32 CCH 47.45 CCH		11.84 CCH 9.03 CCH		8.45 OCH		8.10 CCH			
OFF DIAGONAL-		-10.12 SB22 -9.89 SB26		-8.25 SB27 -7.32 SB28		-7.02 SS18		-3.83 SB24 -2.60 BB34		-2.09 SB21 -1.77 BB43	
NORMAL MODE 32		OBSERVED= 1065.0 CM-1		CALCULATED= 1060.8 CM-1		ERROR= 4.2 CM-1		OR		0.4 PERCENT	
INTERNAL COORDINATES-		39.66 C1OH 18.20 C1C2		10.83 CCOH 11.65 OCH		8.19 CCH		5.75 CCH			
FORCE CONSTANTS-		-10.82 SB22 -6.11 SB25		-5.50 SB26 -3.45 SB28		-1.93 BB34		1.73 SS18			
OFF DIAGONAL-											
NORMAL MODE 33		OBSERVED= 1053.0 CM-1		CALCULATED= 1045.0 CM-1		ERROR= 8.0 CM-1		OR		0.8 PERCENT	
INTERNAL COORDINATES-		48.13 C1OH 11.10 C1OH		9.26 C1OH 8.62 C2C3		7.70 C4OH		6.95 C3C4 5.70 C1OH			
FORCE CONSTANTS-		79.34 CO 17.00 CCH		13.16 CCH 12.54 CCH		10.99 BCOH		9.74 CCO 9.69 OCH			
OFF DIAGONAL-		-10.02 SB28 -9.56 SB27		-9.37 SB25 -8.51 SB21		-5.63 SS18		-3.20 BB34 -1.98 BB29		-1.93 BB36	
NORMAL MODE 34		OBSERVED= 1019.0 CM-1		CALCULATED= 1017.0 CM-1		ERROR= 2.0 CM-1		OR		0.2 PERCENT	
INTERNAL COORDINATES-		30.78 C5C* 19.90 C4C5		10.58 C3C4 8.99 C1OH		7.90 C5O*		7.61 C4C4 7.16 C1OH		5.94 OC1C 5.85 CCO*	
FORCE CONSTANTS-		64.17 CCH 31.36 CCH		13.58 CCH 10.55 CCH		10.00 OCH					
OFF DIAGONAL-		-22.47 SB21 -8.85 SS18		-7.92 SB22 -7.48 SB27		4.41 SB25		1.99 SS17 -1.75 SB28		1.65 BB43 -1.56 SB24	
NORMAL MODE 35		OBSERVED= 997.0 CM-1		CALCULATED= 998.9 CM-1		ERROR= -1.9 CM-1		OR		-0.2 PERCENT	
INTERNAL COORDINATES-		25.07 C1OH 6.23 C1OH		8.49 CCH 7.15 HC2C		8.15 C2C3		5.45 CC3H 5.29 HC3C			
FORCE CONSTANTS-		55.77 CCH 36.22 CCH		-4.83 SB25 -4.22 SB22		-3.78 SB24		-3.57 SB21 1.72 BB34		-1.63 SB26	
OFF DIAGONAL-		-6.91 SB27 -6.22 BB29									

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400									
MOLECULE 1 -6 NG=1236 ALPHA GLUCOSE									
PAGE 2									
NORMAL MODE 36									
INTERNAL COORDINATES-	OBSERVED=	0.0 CM-1	CALCULATED=	964.0 CM-1	ERROR=	0.0 CM-1	DR	0.0 PERCENT	
FORCE CONSTANTS-	28.56	C3C2	10.28	C-08	13.54	C-04	12.82	C5C6	8.67
OFF DIAGONAL-	51.17	CC	38.27	CO	18.37	CC	13.68	CCO	5.74
	-12.22	SB22	-6.61	SB26	5.06	SS18	-3.44	BB29	-3.12
									SB25 -2.82 SB28 -2.56 SB21 -2.48 SB27 -1.54 BB43
NORMAL MODE 37									
INTERNAL COORDINATES-	OBSERVED=	915.0 CM-1	CALCULATED=	904.2 CM-1	ERROR=	10.8 CM-1	DR	1.2 PERCENT	
FORCE CONSTANTS-	25.74	C2C3	21.83	C-06	10.08	CC22	9.51	CC08	7.13
OFF DIAGONAL-	44.45	CO	37.67	CC	23.50	CCH	16.87	CCO	6.80
	-9.67	SB22	-7.22	SB21	3.77	SB26	2.41	BB43	2.16
									SS18 -2.06 SB24 -1.68 SB27 -1.59 BB29
NORMAL MODE 38									
INTERNAL COORDINATES-	OBSERVED=	837.0 CM-1	CALCULATED=	837.3 CM-1	ERROR=	-0.3 CM-1	DR	-0.0 PERCENT	
FORCE CONSTANTS-	31.74	C5O1	17.52	CCHA	15.56	CCHR	7.85	O1C1	5.77
OFF DIAGONAL-	44.49	CO	37.67	CC	8.33	CCO	7.49	OCH	6.80
	-3.72	BB29	-2.87	SB23	-2.64	SB24	-2.24	SB25	2.13
									SB26 1.53 SS18
NORMAL MODE 39									
INTERNAL COORDINATES-	OBSERVED=	775.0 CM-1	CALCULATED=	760.8 CM-1	ERROR=	14.2 CM-1	DR	1.8 PERCENT	
FORCE CONSTANTS-	10.86	CO1C	10.06	C-06	7.79	CC06	7.13	CC11	6.59
OFF DIAGONAL-	20.96	CCO	16.93	CC	13.72	CCH	12.53	CC	10.86
	6.06	BB43	5.39	SB25	-3.33	SB27	-2.83	BB34	2.48
									SB22 -2.26 BB41 2.16 SB24 -1.71 SB26 1.62 BB42
NORMAL MODE 40									
INTERNAL COORDINATES-	OBSERVED=	620.0 CM-1	CALCULATED=	633.8 CM-1	ERROR=	-13.8 CM-1	DR	-2.2 PERCENT	
FORCE CONSTANTS-	9.89	OC01	7.81	CC06	7.21	OBCC	6.02	CO1C	5.28
OFF DIAGONAL-	33.62	CCO	20.27	CCH	10.68	CC	9.89	UCO	8.73
	-5.56	BB34	5.52	BB43	4.21	SB25	-4.16	BB29	2.81
									SB24 2.63 SB22 -2.43 SB27 1.89 SS18 -1.83 SB26
NORMAL MODE 41									
INTERNAL COORDINATES-	OBSERVED=	605.0 CM-1	CALCULATED=	622.1 CM-1	ERROR=	-17.1 CM-1	DR	-2.8 PERCENT	
FORCE CONSTANTS-	17.95	CC04	10.99	OBCC	10.17	CC06	7.69	CC5H	7.55
OFF DIAGONAL-	67.46	CCO	30.27	CCH	6.03	CCC	5.71	HC4C	6.82
	-12.96	BB34	7.35	BB43	-6.68	BB29	2.24	SB25	-2.19
									BB41 -1.84 BB42
NORMAL MODE 42									
INTERNAL COORDINATES-	OBSERVED=	556.0 CM-1	CALCULATED=	555.4 CM-1	ERROR=	0.6 CM-1	DR	0.1 PERCENT	
FORCE CONSTANTS-	18.93	O7CC	12.16	CCU9	7.01	CC3H	6.04	C2C3	5.71
OFF DIAGONAL-	46.88	CCO	25.79	CCH	15.03	CC	8.94	CC	8.86
	-11.21	BB34	7.27	BB43	5.74	BB29	2.53	SS18	-2.07
									SB22 -1.86 BB36 1.79 SB21 1.64 SB24
NORMAL MODE 43									
INTERNAL COORDINATES-	OBSERVED=	539.0 CM-1	CALCULATED=	533.3 CM-1	ERROR=	5.7 CM-1	DR	1.0 PERCENT	
FORCE CONSTANTS-	18.72	4CO1	14.67	OCU	10.96	O7CC	7.60	C-09	5.49
OFF DIAGONAL-	41.59	CCO	14.67	CC	7.59	CC	7.01	OC0	6.86
	6.69	SB25	4.92	SB22	-4.48	BB34	-3.48	SB21	-2.76
									BB42 2.43 SS18 -2.36 SB27
NORMAL MODE 44									
INTERNAL COORDINATES-	OBSERVED=	439.0 CM-1	CALCULATED=	447.4 CM-1	ERROR=	-8.4 CM-1	DR	-1.9 PERCENT	
FORCE CONSTANTS-	11.78	C2CC	9.56	C3CC	8.60	CC0*	6.61	CC06	6.07
OFF DIAGONAL-	30.95	CCO	27.33	CCC	22.37	CC	5.06	CC	5.75
	7.17	BB43	-4.98	BB29	-4.46	BB34	-1.64	BB41	CC09
									CC3H 5.75 CC09
NORMAL MODE 45									
INTERNAL COORDINATES-	OBSERVED=	422.0 CM-1	CALCULATED=	429.4 CM-1	ERROR=	-7.4 CM-1	DR	-1.8 PERCENT	
FORCE CONSTANTS-	15.75	U1CC	14.13	O9CC	13.97	OC0	10.35	CCD*	9.44
OFF DIAGONAL-	52.35	CCO	13.97	CC	13.97	CC	6.47	CCO	6.12
	-5.50	SB22	-4.71	BB34	4.58	SB25	-4.91	SB21	-4.33
									BB42
NORMAL MODE 46									
INTERNAL COORDINATES-	OBSERVED=	404.0 CM-1	CALCULATED=	387.4 CM-1	ERROR=	16.6 CM-1	DR	4.1 PERCENT	
FORCE CONSTANTS-	13.45	C2CC	12.81	OBCC	10.55	CC08	7.01	UCO	6.23
OFF DIAGONAL-	51.64	CCO	12.81	CC	8.24	OC0	6.23	O9CC	5.68
	-6.57	BB34	-4.41	BB42	4.29	SB25	-4.22	SB21	-1.53
									BB41 -1.51 SB26
NORMAL MODE 47									
INTERNAL COORDINATES-	OBSERVED=	361.0 CM-1	CALCULATED=	372.2 CM-1	ERROR=	-11.2 CM-1	DR	-3.1 PERCENT	
FORCE CONSTANTS-	16.94	CCO*	12.45	O7CC	6.24	OC0	5.38	CC08	
OFF DIAGONAL-	49.10	CCO	21.25	CCH	10.55	CC	6.24	OC0	
	-7.09	BB34	3.74	BB43	-3.21	BB29	-3.12	SB26	2.99
									SB21 -2.12 BB33 1.97 SB24
NORMAL MODE 48									
INTERNAL COORDINATES-	OBSERVED=	327.0 CM-1	CALCULATED=	320.0 CM-1	ERROR=	7.0 CM-1	DR	2.1 PERCENT	
FORCE CONSTANTS-	16.87	CC09	12.72	CC08	7.35	O7CC	6.80	C3C4	6.51
OFF DIAGONAL-	62.59	CCO	15.28	CC	9.02	CCH	5.74	T-OH	5.74
	-7.15	BB34	4.44	SB22	2.53	BB43	-2.29	BB42	2.10
									SB21
NORMAL MODE 49									
INTERNAL COORDINATES-	OBSERVED=	316.0 CM-1	CALCULATED=	312.1 CM-1	ERROR=	3.9 CM-1	DR	1.3 PERCENT	
FORCE CONSTANTS-	23.01	CC07	13.87	CC08	7.64	OBCC	7.43	CC01	7.37
OFF DIAGONAL-	72.20	CCO	9.22	CC	8.30	T-OH	5.47	CCH	6.42
	-6.92	BB34	-3.82	BB42	2.56	SB22	2.38	SB21	5.23
									TH-2
NORMAL MODE 50									
INTERNAL COORDINATES-	OBSERVED=	302.0 CM-1	CALCULATED=	302.8 CM-1	ERROR=	-0.8 CM-1	DR	-0.3 PERCENT	
FORCE CONSTANTS-	19.95	OBCC	18.00	O9CC	10.55	4CO1	7.78	CC08	6.95
OFF DIAGONAL-	23.52	CCO	12.93	CCH	9.84	CCO9	7.35	CC2	5.19
	-11.24	BB34	-2.58	BB42	-2.33	SB25	2.12	BB43	-1.80
									BB29
NORMAL MODE 51									
INTERNAL COORDINATES-	OBSERVED=	0.0 CM-1	CALCULATED=	257.5 CM-1	ERROR=	0.0 CM-1	DR	0.0 PERCENT	
FORCE CONSTANTS-	20.52	CC06	9.63	O1CC	12.94	T-UH	8.26	CCC	7.21
OFF DIAGONAL-	57.06	CCO	18.64	CCH	12.94	T-UH	8.26	CCC	
	-8.92	BB34	7.12	BB43	-3.59	SB25	-3.24	BB33	-2.47
									BB29 1.62 SB22
NORMAL MODE 52									
INTERNAL COORDINATES-	OBSERVED=	0.0 CM-1	CALCULATED=	242.2 CM-1	ERROR=	0.0 CM-1	DR	0.0 PERCENT	
FORCE CONSTANTS-	51.62	TH-5	7.81	CCU*	6.13	C4CC	8.05	CCC	
OFF DIAGONAL-	63.15	T-OH	19.54	CCO					
	-1.63	BB34							
NORMAL MODE 53									
INTERNAL COORDINATES-	OBSERVED=	0.0 CM-1	CALCULATED=	229.0 CM-1	ERROR=	0.0 CM-1	DR	0.0 PERCENT	
FORCE CONSTANTS-	54.79	TH-1	25.13	TH-3	8.10	TH-2	6.13	TH-4	
OFF DIAGONAL-	94.17	T-OH							
	NONE								
NORMAL MODE 54									
INTERNAL COORDINATES-	OBSERVED=	0.0 CM-1	CALCULATED=	222.8 CM-1	ERROR=	0.0 CM-1	DR	0.0 PERCENT	
FORCE CONSTANTS-	45.75	TH-4	17.29	TH-1	17.04	TH-5	9.66	TH-3	
OFF DIAGONAL-	89.78	T-UH	5.28	CCO					
	NONE								
NORMAL MODE 55									
INTERNAL COORDINATES-	OBSERVED=	0.0 CM-1	CALCULATED=	215.2 CM-1	ERROR=	0.0 CM-1	DR	0.0 PERCENT	
FORCE CONSTANTS-	35.79	TH-3	30.09	TH-4	9.81	TH-1	7.11	TH-2	
OFF DIAGONAL-	83.12	T-OH	14.35	CCO					
	-1.81	BB34							
NORMAL MODE 56									
INTERNAL COORDINATES-	OBSERVED=	0.0 CM-1	CALCULATED=	213.4 CM-1	ERROR=	0.0 CM-1	DR	0.0 PERCENT	
FORCE CONSTANTS-	69.03	TH-2	12.71	TH-3					
OFF DIAGONAL-	83.65	T-OH	14.46	CCO					
	NONE								
NORMAL MODE 57									
INTERNAL COORDINATES-	OBSERVED=	0.0 CM-1	CALCULATED=	199.3 CM-1	ERROR=	0.0 CM-1	DR	0.0 PERCENT	
FORCE CONSTANTS-	26.03	TH-5	24.39	CCU*	12.94	C4CC	6.33	TCC5	5.72
OFF DIAGONAL-	37.19	CCO	32.11	T-OH	14.41	CCC	8.07	T-CC	6.35
	-4.66	BB34	-2.68	BB42	-2.33	BB33			CCH 5.72 CUC
NORMAL MODE 58									
INTERNAL COORDINATES-	OBSERVED=	0.0 CM-1	CALCULATED=	130.2 CM-1	ERROR=	0.0 CM-1	DR	0.0 PERCENT	
FORCE CONSTANTS-	21.94	CO1C	14.79	C4CC	10.26	TCC4	6.53	C1CC	6.39
OFF DIAGONAL-	23.72	CCO	21.94	CUC	12.50	T-CC	11.63	CCO	9.94
	3.87	BB43	-3.49	SB21	-2.38	BB37	1.95	BB41	-1.67
									BB34
NORMAL MODE 59									
INTERNAL COORDINATES-	OBSERVED=	0.0 CM-1	CALCULATED=	97.7 CM-1	ERROR=	0.0 CM-1	DR	0.0 PERCENT	
FORCE CONSTANTS-	6.67	TCC5	9.93	C3CC	5.05	C4CC	5.04	TCC2	
OFF DIAGONAL-	63.50	T-CC	18.78	CCC	17.18	CCO			
	-3.29	SB25	-2.58	BB34	-2.36	SB21	-2.26	BB42	-1.52
									BB43
NORMAL MODE 60									
INTERNAL COORDINATES-	OBSERVED=	0.0 CM-1	CALCULATED=	81.6 CM-1	ERROR=	0.0 CM-1	DR	0.0 PERCENT	
FORCE CONSTANTS-	21.35	C2CC	14.66	C1CC	8.55	CO1C	7.57	TCC1	6.66
OFF DIAGONAL-	41.39	CCO	27.33	CCC	18.11	CCO	8.55	COC	5.99
	-4.11	SB25	-3.99	BB42	-3.07	SB21	2.40	BB41	
NORMAL MODE 61									
INTERNAL COORDINATES-	OBSERVED=	0.0 CM-1	CALCULATED=	65.9 CM-1	ERROR=	0.0 CM-1	DR	0.0 PERCENT	
FORCE CONSTANTS-	23.18	TCC5	14.12	C3CC	9.86	TCC4	7.39	TCC3	7.17
OFF DIAGONAL-	42.06	T-OH	4.66	CCO	21.95	CC			
	-2.67	BB42	-2.21	BB34	-1.71	SB25			

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400									
MOLECULE 2 -6 NG-1236 ALPHA GLUCOSE-0-05									
PAGE 1									
NORMAL MODE 8	OBSERVED=	1457.0 CM-1	CALCULATED=	1449.8 CM-1	ERROR=	7.2 CM-1	OR	0.5 PERCENT	
INTERNAL COORDINATES-	61.45	HCH 20.68	18.99	OCHA					
FORCE CONSTANTS-	61.45	HCH 40.07							
OFF DIAGONAL-	-4.05	SB27							
NORMAL MODE 9	OBSERVED=	1410.0 CM-1	CALCULATED=	1411.1 CM-1	ERROR=	-1.1 CM-1	OR	-0.1 PERCENT	
INTERNAL COORDINATES-	16.25	OC4H 12.12	11.39	CC5H 8.92	6.94	CC5H 6.89	5.97	OC3H 5.46	HC3C
FORCE CONSTANTS-	46.24	OC4H 38.10	12.94	CC5H 8.92					
OFF DIAGONAL-	-8.96	SB27 7.72	5.48	BB34 -4.56	SB25 -3.67	SB26 -3.22	BB45		
NORMAL MODE 10	OBSERVED=	1395.0 CM-1	CALCULATED=	1391.8 CM-1	ERROR=	3.2 CM-1	OR	0.2 PERCENT	
INTERNAL COORDINATES-	41.05	UCH 39.04	12.31	CC1H 7.82					
FORCE CONSTANTS-	90.67	UCH 10.61	6.55	CC1H 7.17					
OFF DIAGONAL-	-9.78	SB27 -3.77	1.98	BB37 1.54	BB29				
NORMAL MODE 11	OBSERVED=	1380.0 CM-1	CALCULATED=	1378.4 CM-1	ERROR=	1.6 CM-1	OR	0.1 PERCENT	
INTERNAL COORDINATES-	15.56	OC3H 13.16	12.44	HC2C 9.39	CC3H 8.98	CC5H 6.60	CC4H 5.44	CC6H	
FORCE CONSTANTS-	47.27	CC4H 41.29	9.26	CC3H 8.98					
OFF DIAGONAL-	10.28	BB29 -8.41	-4.26	SB26 -3.56	BB45 3.54	BB34 -2.63	SB25		
NORMAL MODE 12	OBSERVED=	1340.0 CM-1	CALCULATED=	1353.1 CM-1	ERROR=	-13.1 CM-1	OR	-1.0 PERCENT	
INTERNAL COORDINATES-	20.28	CC6H 17.71	9.32	OC2H 8.27	7.37	CC3H 5.65	HC2C		
FORCE CONSTANTS-	61.88	CC6H 26.43	9.04	OC2H 8.27					
OFF DIAGONAL-	13.85	BB29 -8.97	-4.67	SB27 -3.68	BB45 1.66	BB34			
NORMAL MODE 13	OBSERVED=	1320.0 CM-1	CALCULATED=	1331.0 CM-1	ERROR=	-11.0 CM-1	OR	-0.8 PERCENT	
INTERNAL COORDINATES-	14.00	HC3C 12.41	8.87	HC2C 8.25	CC4H 6.75	OC1H 6.06	CC4H 5.59	CC3H	
FORCE CONSTANTS-	7.17	CC1H 12.41	8.57	CC2H 7.82					
OFF DIAGONAL-	-11.43	SB26 9.75	-3.96	BB45 -3.10	SB27				
NORMAL MODE 14	OBSERVED=	1310.0 CM-1	CALCULATED=	1325.8 CM-1	ERROR=	-15.8 CM-1	OR	-1.2 PERCENT	
INTERNAL COORDINATES-	26.84	UCH 12.82	12.31	CC1H 8.81	5.28	HC3C			
FORCE CONSTANTS-	54.79	CC4H 31.44	8.24	CC1H 8.81					
OFF DIAGONAL-	4.39	BB29 -3.67	2.64	BB34 -2.52	SB26 -1.83	SB25 -1.79	BB43 -1.60	SB27	
NORMAL MODE 15	OBSERVED=	1300.0 CM-1	CALCULATED=	1308.9 CM-1	ERROR=	8.9 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	20.75	CC4H 16.54	11.35	OC4H 10.34	9.19	CC5H 8.48	OC3H		
FORCE CONSTANTS-	50.89	UCH 47.79							
OFF DIAGONAL-	-4.00	BB45 -3.09	SB27						
NORMAL MODE 16	OBSERVED=	1298.0 CM-1	CALCULATED=	1298.1 CM-1	ERROR=	-0.1 CM-1	OR	-0.0 PERCENT	
INTERNAL COORDINATES-	26.62	OC2H 20.47	8.09	CC2H 7.15	OC3H				
FORCE CONSTANTS-	38.83	UCH 37.76	9.09	BCOH					
OFF DIAGONAL-	3.85	SB27 3.14	-3.05	BB45 1.58	BB36				
NORMAL MODE 17	OBSERVED=	1281.0 CM-1	CALCULATED=	1279.2 CM-1	ERROR=	1.8 CM-1	OR	0.1 PERCENT	
INTERNAL COORDINATES-	10.63	UCH 9.87	24.83	CC2H 9.06	8.46	OC1H 7.82	CC1H 6.66	CC5H 6.13	CC4H 6.06
FORCE CONSTANTS-	26.26	UCH 26.26	27.12	CC2H 9.06					
OFF DIAGONAL-	-9.21	SB25 4.16	4.07	BB34 -2.58	SB26 -2.58	BB45 1.96	BB33 1.59	BB43	
NORMAL MODE 18	OBSERVED=	1270.0 CM-1	CALCULATED=	1274.6 CM-1	ERROR=	-4.6 CM-1	OR	-0.4 PERCENT	
INTERNAL COORDINATES-	24.63	UCH 12.82	8.73	CC5H 8.45	CC4H 7.37	UCH 7.12	CC4H 7.06	OC3H 5.44	CC1H
FORCE CONSTANTS-	54.63	UCH 41.79	2.54	SB27 2.00	BB34				
OFF DIAGONAL-	-4.06	BB29 -3.87	BB45						
NORMAL MODE 19	OBSERVED=	1260.0 CM-1	CALCULATED=	1254.8 CM-1	ERROR=	5.2 CM-1	OR	0.4 PERCENT	
INTERNAL COORDINATES-	18.74	UCH 11.86	10.12	HC3C 7.93	CC4H 5.13	CC1H 5.12	CC6H		
FORCE CONSTANTS-	50.58	UCH 31.36	11.66	CC5H 5.42	CCO				
OFF DIAGONAL-	-4.84	BB29 3.83	3.65	SB27 -3.14	BB45 -3.09	SB25			
NORMAL MODE 20	OBSERVED=	1231.0 CM-1	CALCULATED=	1226.2 CM-1	ERROR=	4.8 CM-1	OR	0.4 PERCENT	
INTERNAL COORDINATES-	15.41	OC3H 11.55	10.95	CC5H 10.86	HC3C 8.74	HC4C 7.57	CC4H		
FORCE CONSTANTS-	42.65	UCH 34.55	9.44	BCOH 7.58	CCO 6.70	CCO			
OFF DIAGONAL-	-7.69	BB29 4.31	3.97	SB27 -2.66	SB25 -2.50	BB45 -1.52	SB22		
NORMAL MODE 21	OBSERVED=	1195.0 CM-1	CALCULATED=	1201.2 CM-1	ERROR=	-6.2 CM-1	OR	-0.5 PERCENT	
INTERNAL COORDINATES-	24.74	CC2C 14.79	7.26	C1C2 7.19	OC6H 5.00	C-09			
FORCE CONSTANTS-	35.24	CC2 24.11	18.17	BCOH 14.79	CCO 9.77	CCO 8.55	CCO		
OFF DIAGONAL-	-7.45	SB22 4.46	-3.29	SB25 2.77	BB36 -1.66	BB29 1.64	SB28		
NORMAL MODE 22	OBSERVED=	1168.0 CM-1	CALCULATED=	1165.8 CM-1	ERROR=	2.2 CM-1	OR	0.2 PERCENT	
INTERNAL COORDINATES-	17.74	UCH 17.74	22.51	CC1H 14.17	5.91	C-01 5.83	OC6H 5.59	C4C5 5.28	C1OH
FORCE CONSTANTS-	48.28	CC 25.08	16.68	CCO 10.99	UCH 8.76	BCOH 5.85	UCH		
OFF DIAGONAL-	-6.86	SB22 -4.28	-3.35	SB26 -2.86	SB24 1.91	SB28 -1.78	SS18		
NORMAL MODE 23	OBSERVED=	1153.0 CM-1	CALCULATED=	1158.2 CM-1	ERROR=	-5.2 CM-1	OR	-0.4 PERCENT	
INTERNAL COORDINATES-	13.75	C5C1 8.42	7.15	C-08 6.84	CCO 5.96	C5C1 5.51	UCH 5.29	C4OH 5.18	OCHA 5.10
FORCE CONSTANTS-	28.31	CC 17.38	16.54	UCH 14.36	BCOH 12.58	CCO 9.08	CCO 6.21	CCC	
OFF DIAGONAL-	-6.78	SB22 -3.96	3.10	SB28 -1.59	SB26 1.55	BB34			
NORMAL MODE 24	OBSERVED=	1145.0 CM-1	CALCULATED=	1149.1 CM-1	ERROR=	-4.1 CM-1	OR	-0.3 PERCENT	
INTERNAL COORDINATES-	29.83	C1C2 18.40	9.45	CC2H 6.97	OC1H 6.21	C-09 5.77	HC2C 5.74	OC1H 5.44	CCO7
FORCE CONSTANTS-	34.94	CC 22.64	21.95	CCO 19.54	CCO 17.68	CCO 14.36	UCH		
OFF DIAGONAL-	-13.00	SB22 -10.01	-2.75	SB25 -1.68	BB29				
NORMAL MODE 25	OBSERVED=	1130.0 CM-1	CALCULATED=	1134.9 CM-1	ERROR=	-4.9 CM-1	OR	-0.4 PERCENT	
INTERNAL COORDINATES-	37.47	C3C4 13.02	13.00	C-08 5.56	OC1H 5.54	C4C5 5.02	CCO9		
FORCE CONSTANTS-	45.27	CC 28.94	19.02	BCOH 13.95	CCO 9.42	UCH			
OFF DIAGONAL-	-7.71	SB22 5.33	-4.91	SS18 -3.75	SB21 -2.87	SB27 -1.57	BB36		
NORMAL MODE 26	OBSERVED=	1108.0 CM-1	CALCULATED=	1110.2 CM-1	ERROR=	-2.2 CM-1	OR	-0.5 PERCENT	
INTERNAL COORDINATES-	42.63	UCH 27.52	13.93	BCOH 11.35	CCO 8.81	UCH 5.97	C1OH 6.27	CCC	
FORCE CONSTANTS-	55.99	SB21 -4.77	-3.79	SB25 -2.78	SS18 2.37	SB26 2.30	SB28		
NORMAL MODE 27	OBSERVED=	1097.0 CM-1	CALCULATED=	1109.5 CM-1	ERROR=	-12.5 CM-1	OR	-1.1 PERCENT	
INTERNAL COORDINATES-	36.72	C-07 15.94	14.83	C-09 11.90	C1C2 8.39	CCO 5.83	C1C2 5.40	C4C5	
FORCE CONSTANTS-	71.64	CC 30.26	9.28	CCC 7.14	UCH 6.54	CCO 5.55	CCO		
OFF DIAGONAL-	-7.39	SS18 -5.81	-5.75	SB21 -4.81	SB25 -4.15	SB28 -1.65	SB24		
NORMAL MODE 28	OBSERVED=	1080.0 CM-1	CALCULATED=	1074.3 CM-1	ERROR=	5.7 CM-1	OR	0.5 PERCENT	
INTERNAL COORDINATES-	22.10	C-08 18.46	7.77	C5C1 6.34	C5O1 5.44	C3C4			
FORCE CONSTANTS-	47.71	CC 15.89	15.07	CC 11.48	CCO 10.03	UCH 8.34	CCC 7.98	BCOH	
OFF DIAGONAL-	-6.77	SB25 -3.37	-2.86	SB28 -2.31	SB24 -1.96	SS18 -1.62	BB29		
NORMAL MODE 29	OBSERVED=	1062.0 CM-1	CALCULATED=	1057.7 CM-1	ERROR=	4.3 CM-1	OR	0.4 PERCENT	
INTERNAL COORDINATES-	34.11	C4C5 21.05	19.80	C-09 5.81	C-08				
FORCE CONSTANTS-	26.11	CC 19.93	17.15	BCOH					
OFF DIAGONAL-	-7.64	SB27 -6.79	-6.16	SS18 4.40	SB28 -2.52	SB22			
NORMAL MODE 30	OBSERVED=	1035.0 CM-1	CALCULATED=	1042.3 CM-1	ERROR=	-7.3 CM-1	OR	-0.7 PERCENT	
INTERNAL COORDINATES-	22.10	C-08 18.46	16.46	C-09 9.69	C3OH 9.34	C1OH			
FORCE CONSTANTS-	68.64	CC 23.73	14.36	CC 10.12	CCO 8.08	UCH 5.76	UCH		
OFF DIAGONAL-	-10.60	SB28 -6.59	-4.14	SB27 -2.68	SB21 -1.79	BB35 -1.69	SB22 -1.56	BB29	
NORMAL MODE 31	OBSERVED=	1019.0 CM-1	CALCULATED=	1027.6 CM-1	ERROR=	-8.6 CM-1	OR	-0.8 PERCENT	
INTERNAL COORDINATES-	43.98	C-07 19.72	13.64	C2OH 7.34	C-07 6.94	C-09 5.88	CC5H		
FORCE CONSTANTS-	58.32	CC 40.50	18.94	UCH					
OFF DIAGONAL-	-15.05	SB28 -5.03	-4.68	SB27 -3.87	BB29 1.52	SS18			
NORMAL MODE 32	OBSERVED=	1007.0 CM-1	CALCULATED=	1000.8 CM-1	ERROR=	6.2 CM-1	OR	0.6 PERCENT	
INTERNAL COORDINATES-	30.54	C2OH 16.21	15.13	C-06 8.46	C-09 8.34	C-07 6.55	CC3H 5.57	C3OH	
FORCE CONSTANTS-	55.69	BCOH 33.79	16.40	CC 6.28	CC 5.21	CCO			
OFF DIAGONAL-	-9.34	SB28 -2.80	-2.53	SB24 -2.24	SB22 -2.22	SB25 -2.04	BB36		
NORMAL MODE 33	OBSERVED=	967.0 CM-1	CALCULATED=	970.3 CM-1	ERROR=	-3.3 CM-1	OR	-0.3 PERCENT	
INTERNAL COORDINATES-	32.68	C-06 23.58	10.51	HC2C 9.63	C4OH 9.31	CC1H 6.13	C-07 5.93	CC2H 5.85	C1C2 5.19
FORCE CONSTANTS-	31.16	CC 40.35	37.90	CC 9.14	CC				
OFF DIAGONAL-	-14.95	SB28 -5.93	-5.96	SB27 -4.77	BB29 -4.32	SB24 -3.25	SB25 -2.36	BB35 -2.25	BB34 -2.09
NORMAL MODE 34	OBSERVED=	955.0 CM-1	CALCULATED=	956.0 CM-1	ERROR=	-1.0 CM-1	OR	-0.1 PERCENT	
INTERNAL COORDINATES-	61.84	BCOH 26.83	12.67	C5C1 8.68	C3OH				
FORCE CONSTANTS-	61.84	BCOH 26.83	8.99	CC 8.99	UCH 5.01	CCO			
OFF DIAGONAL-	-4.40	SB28 -4.01	-3.68	SB22 -1.82	SB27 -1.51	SS18			
NORMAL MODE 35	OBSERVED=	947.0 CM-1	CALCULATED=	935.3 CM-1	ERROR=	11.7 CM-1	OR	0.2 PERCENT	
INTERNAL COORDINATES-	15.53	C1OH 19.38	14.66	C3OH 12.45	C1C2 8.94	C5C1 7.23	C4OH 6.09	C2C3	
FORCE CONSTANTS-	53.01	BCOH 31.32	8.23	CC 7.14	UCH 6.89	UCH			
OFF DIAGONAL-	-5.41	SB21 -4.82	-2.09	SB27 -1.61	SS18				

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR		PROBLEM 400		PAGE 2	
MOLECULE 2		-6 NG=1236 ALPHA		GLUCOSE-O-D5	
NORMAL MODE 36	OBSERVED= 893.0 CM-1	CALCULATED= 911.3 CM-1	ERROR= -18.3 CM-1	OR	-2.0 PERCENT
INTERNAL COORDINATES-	28.75 C3C4 28.75 C4OH	10.62 C-OB	5.99 C3OH		
FORCE CONSTANTS-	42.3 CBOH 36.4 C	19.98 CO	19.62 CCH	8.72 CCO	
OFF DIAGONAL-	-6.69 SB22 -4.83 SB28	-4.33 SB26	-3.89 SB21	-2.36 SB27	-1.92 BB29
NORMAL MODE 37	OBSERVED= 868.0 CM-1	CALCULATED= 853.8 CM-1	ERROR= 14.2 CM-1	OR	1.6 PERCENT
INTERNAL COORDINATES-	25.88 C2C3 14.69 C3OH	11.89 C2OH	5.08 CCOH	5.42 C1C2	5.14 CCO9
FORCE CONSTANTS-	35.06 CC 28.39 CBOH	14.48 CCO	12.00 CCH	11.08 CO	
OFF DIAGONAL-	-9.12 SB21 -8.01 SB22	2.06 SB26	1.62 SS18		
NORMAL MODE 38	OBSERVED= 835.0 CM-1	CALCULATED= 834.7 CM-1	ERROR= 0.3 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	29.03 CCO 15.67 CCHA	14.80 CCHB	7.49 CCH1	5.62 CCO6	5.29 C5C*
FORCE CONSTANTS-	42.78 CC 36.04 CCH	9.27 CCO	7.61 CC	6.95 CCH	
OFF DIAGONAL-	-3.79 BB29 -2.85 SB24	-2.57 SB23	2.12 SB26	-1.96 SB25	1.59 SS18
NORMAL MODE 39	OBSERVED= 754.0 CM-1	CALCULATED= 753.4 CM-1	ERROR= 0.6 CM-1	OR	0.1 PERCENT
INTERNAL COORDINATES-	12.00 COTC 9.51 C-U6	6.87 CCH	6.41 C2C3	6.34 CCO6	5.96 CCH
FORCE CONSTANTS-	18.53 CCO 15.72 CC	13.49 CC	12.00 CCO	11.92 CCH	6.42 CCO
OFF DIAGONAL-	5.66 BB43 5.00 SB25	-3.30 SB27	7.73 SB24	-2.43 BB34	2.30 SB22
NORMAL MODE 40	OBSERVED= 630.0 CM-1	CALCULATED= 622.1 CM-1	ERROR= 7.9 CM-1	OR	1.3 PERCENT
INTERNAL COORDINATES-	17.76 OBCC 13.91 CCO*	10.69 CCH	8.15 HC4C	6.16 U9CC	5.97 C4CC
FORCE CONSTANTS-	50.16 CCO 29.31 CCH	9.23 CCO	5.98 CO		
OFF DIAGONAL-	-11.48 BB34 9.10 BB43	-6.59 BB29	4.05 SB25	-1.92 BB36	-1.74 SB27
NORMAL MODE 41	OBSERVED= 600.0 CM-1	CALCULATED= 611.9 CM-1	ERROR= -11.9 CM-1	OR	-2.0 PERCENT
INTERNAL COORDINATES-	18.46 CCO6 11.67 CCO7	9.67 CCO1	9.62 CCO	7.00 CCHB	5.44 CCO*
FORCE CONSTANTS-	49.71 CCO 19.12 CCH	13.41 CCO	12.00 CCO	11.92 CCH	5.29 C1C2
OFF DIAGONAL-	-6.24 BB34 -3.71 BB29	3.49 BB43	-2.07 BB41	2.05 SB25	-1.83 BB42
NORMAL MODE 42	OBSERVED= 565.0 CM-1	CALCULATED= 547.7 CM-1	ERROR= 17.3 CM-1	OR	3.1 PERCENT
INTERNAL COORDINATES-	13.79 COTC 10.88 CCO9	7.89 C2C3	5.08 C1C2	5.14 CCH4	
FORCE CONSTANTS-	40.32 CCO 22.49 CCH	19.51 CC	12.35 CO		
OFF DIAGONAL-	-9.14 BB34 5.92 BB43	-4.87 BB29	3.65 SS18	3.41 SB25	-1.99 BB36
NORMAL MODE 43	OBSERVED= 518.0 CM-1	CALCULATED= 523.3 CM-1	ERROR= -5.3 CM-1	OR	-1.0 PERCENT
INTERNAL COORDINATES-	15.68 CCO 15.32 CCO	13.69 CCH	6.21 COTC	5.09 C-09	
FORCE CONSTANTS-	48.12 CCO 15.32 CCO	10.65 CCH	10.03 CO	8.90 CCO	5.56 CC
OFF DIAGONAL-	-6.25 BB34 4.29 SB25	-3.75 SB21	-3.31 BB42	2.92 SB22	2.25 BB43
NORMAL MODE 44	OBSERVED= 465.0 CM-1	CALCULATED= 442.9 CM-1	ERROR= 22.1 CM-1	OR	4.8 PERCENT
INTERNAL COORDINATES-	11.49 C2CC 8.69 C3CC	8.01 CCO*	7.10 CCO6	6.54 CCO9	5.64 CCH3
FORCE CONSTANTS-	30.91 CCO 26.00 CCO	21.12 CCH	5.30 CC		
OFF DIAGONAL-	6.58 BB43 -4.67 BB29	-3.92 BB34	1.90 SB22	-1.62 BB41	
NORMAL MODE 45	OBSERVED= 420.0 CM-1	CALCULATED= 423.2 CM-1	ERROR= -3.2 CM-1	OR	-0.8 PERCENT
INTERNAL COORDINATES-	17.11 COTC 13.99 CCO	13.41 CCO	11.88 CCO*	9.42 CCO7	6.44 C1CC
FORCE CONSTANTS-	54.23 CCO 13.53 CCO	13.41 CCO	11.88 CCO*	9.42 CCO7	5.75 C4C5
OFF DIAGONAL-	-5.3 BB34 4.82 SB22	-4.58 SB21	4.43 SB25	-4.26 BB42	
NORMAL MODE 46	OBSERVED= 395.0 CM-1	CALCULATED= 383.6 CM-1	ERROR= 11.4 CM-1	OR	2.9 PERCENT
INTERNAL COORDINATES-	14.97 CCO8 12.23 C2CC	10.41 OBCC	7.56 CCO	6.18 C3CC	5.10 CCO9
FORCE CONSTANTS-	54.71 CCO 22.95 CCO	8.92 CCH	8.87 CC		
OFF DIAGONAL-	-7.23 BB34 4.66 SB21	4.56 SB25	-4.01 BB42	-2.14 SB26	-1.61 BB36
NORMAL MODE 47	OBSERVED= 372.0 CM-1	CALCULATED= 366.8 CM-1	ERROR= 5.2 CM-1	OR	1.4 PERCENT
INTERNAL COORDINATES-	19.81 CCO* 13.26 COTC	8.57 CCO			
FORCE CONSTANTS-	45.07 CCO 20.89 CCH	8.57 CCO	8.24 CC	5.43 CCO	5.16 CO
OFF DIAGONAL-	-6.78 BB34 4.10 BB43	-3.41 BB29	2.58 SB24	2.39 SB21	-2.35 SB26
NORMAL MODE 48	OBSERVED= 325.0 CM-1	CALCULATED= 313.8 CM-1	ERROR= 11.2 CM-1	OR	3.4 PERCENT
INTERNAL COORDINATES-	13.56 CCO9 9.98 CCOH	8.34 COTC	6.71 C3C4	6.06 CCO6	5.25 CCO7
FORCE CONSTANTS-	62.07 CCO 15.18 CC	9.46 CCH	6.33 CO		
OFF DIAGONAL-	-7.26 BB34 4.10 SB22	2.90 SB21	2.89 BB43	-2.30 BB42	
NORMAL MODE 49	OBSERVED= 300.0 CM-1	CALCULATED= 308.5 CM-1	ERROR= -8.5 CM-1	OR	-2.8 PERCENT
INTERNAL COORDINATES-	23.87 CCO7 11.12 CCO8	9.30 CCO*	8.72 CCO*	6.11 COTC	5.94 OBCC
FORCE CONSTANTS-	73.62 CCO 9.65 CC	5.62 CCH			
OFF DIAGONAL-	-7.09 BB34 -3.91 BB42	2.93 SB21	2.81 SB22		
NORMAL MODE 50	OBSERVED= 278.0 CM-1	CALCULATED= 296.1 CM-1	ERROR= -18.1 CM-1	OR	-6.5 PERCENT
INTERNAL COORDINATES-	17.46 OBCC 18.50 COTC	12.52 CCO8	8.74 CCO*	8.38 COTC	
FORCE CONSTANTS-	87.25 CCO 11.80 CCH	6.27 T-OH	6.14 CCO		
OFF DIAGONAL-	-11.55 BB34 -3.63 BB42	-2.13 BB36	-2.00 SB25		
NORMAL MODE 51	OBSERVED= 245.0 CM-1	CALCULATED= 249.0 CM-1	ERROR= -4.0 CM-1	OR	-1.6 PERCENT
INTERNAL COORDINATES-	24.97 CCO6 9.57 COTC	9.13 COTC	8.92 CCH2	7.91 CCO9	6.10 CCO7
FORCE CONSTANTS-	64.29 CCO 21.57 CCH	7.79 CCO			
OFF DIAGONAL-	-9.77 BB34 8.20 BB43	-4.23 SB25	-3.93 BB33	-2.82 BB29	2.15 SB22
NORMAL MODE 52	OBSERVED= 225.0 CM-1	CALCULATED= 219.6 CM-1	ERROR= 5.3 CM-1	OR	2.4 PERCENT
INTERNAL COORDINATES-	24.73 CCO* 16.15 C4CC	12.85 TH-5	10.45 COTC	5.30 CCO*	
FORCE CONSTANTS-	44.63 CCO 18.95 CCO	16.56 T-OH	10.45 CCO	5.46 CCH	
OFF DIAGONAL-	-4.07 BB34 -2.88 BB42	-1.85 BB33			
NORMAL MODE 53	OBSERVED= 0.0 CM-1	CALCULATED= 174.4 CM-1	ERROR= 0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	TH-1 14.83 TH-3				
FORCE CONSTANTS-	79.20 T-OH 9.41 CCO				
OFF DIAGONAL-	NONE				
NORMAL MODE 54	OBSERVED= 0.0 CM-1	CALCULATED= 164.2 CM-1	ERROR= 0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	TH-2 23.27 TH-3	13.96 TH-5	10.57 TH-1		
FORCE CONSTANTS-	92.76 T-OH				
OFF DIAGONAL-	NONE				
NORMAL MODE 55	OBSERVED= 0.0 CM-1	CALCULATED= 159.0 CM-1	ERROR= 0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	TH-5 13.10 TH-4	7.85 TCC5	5.24 CCO*		
FORCE CONSTANTS-	78.47 T-OH 8.75 CCO	8.58 T-CC			
OFF DIAGONAL-	NONE				
NORMAL MODE 56	OBSERVED= 0.0 CM-1	CALCULATED= 156.4 CM-1	ERROR= 0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	TH-3 31.94 TH-4	8.07 TH-1			
FORCE CONSTANTS-	97.70 T-OH 6.57 CCO				
OFF DIAGONAL-	NONE				
NORMAL MODE 57	OBSERVED= 0.0 CM-1	CALCULATED= 154.3 CM-1	ERROR= 0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	TH-4 7.39 TH-3				
FORCE CONSTANTS-	90.42 T-OH 6.90 CCO				
OFF DIAGONAL-	NONE				
NORMAL MODE 58	OBSERVED= 0.0 CM-1	CALCULATED= 120.9 CM-1	ERROR= 0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	TH-1 17.34 COTC	11.98 C4CC	8.16 TCC1	5.33 C1CC	5.29 CCO
FORCE CONSTANTS-	20.00 T-OH 18.14 CCO	17.34 CCO	10.55 T-CC	9.61 CCO	8.19 T-CC
OFF DIAGONAL-	3.18 BB43 -2.84 SB21	-1.73 BB37	1.61 BB41		
NORMAL MODE 59	OBSERVED= 0.0 CM-1	CALCULATED= 94.8 CM-1	ERROR= 0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	TH-5 9.03 C3CC	6.73 C9CC			
FORCE CONSTANTS-	60.23 T-CC 17.77 CCO	17.18 CCO	5.06 T-OH		
OFF DIAGONAL-	-3.11 SB25 -2.63 BB44	-2.18 BB42	-2.17 SB21		
NORMAL MODE 60	OBSERVED= 0.0 CM-1	CALCULATED= 78.9 CM-1	ERROR= 0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	TH-3 15.08 C1CC	8.39 COTC	7.71 TCC1	6.91 TCC4	6.66 TCC2
FORCE CONSTANTS-	41.62 CCO 25.63 T-CC	18.51 CCO	8.39 CCO	5.87 T-CC	
OFF DIAGONAL-	-4.21 SB25 -4.03 BB42	-3.04 SB21	2.43 BB41		
NORMAL MODE 61	OBSERVED= 0.0 CM-1	CALCULATED= 63.9 CM-1	ERROR= 0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	TH-4 14.20 C3CC	9.53 TCC4			
FORCE CONSTANTS-	48.10 T-CC 23.13 CCO	21.10 CCO			
OFF DIAGONAL-	-2.65 BB42 -2.24 BB34	-1.71 SB25			

44. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 7.12

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400									
MOLECULE 3 -6 NG=1236 ALPHA GLUCOSE-1,2-D2									
PAGE 1									
NORMAL MODE 8	OBSERVED=	1457.0 CM-1	CALCULATED=	1449.8 CM-1	ERROR=	7.2 CM-1	OR	0.5 PERCENT	
INTERNAL COORDINATES-	61.25	HCH 20.83	OC4H	19.06	OC4H				
FORCE CONSTANTS-	61.25	HCH 40.26	UCH						
OFF DIAGONAL-	-4.08	SB27							
NORMAL MODE 9	OBSERVED=	1447.0 CM-1	CALCULATED=	1433.9 CM-1	ERROR=	13.1 CM-1	OR	0.9 PERCENT	
INTERNAL COORDINATES-	69.06	C2OH							
FORCE CONSTANTS-	70.33	BCOH	6.41	CCH	5.05	CCO			
OFF DIAGONAL-	4.18	BB36	6.52	SB28	1.69	BB34			
NORMAL MODE 10	OBSERVED=	1421.0 CM-1	CALCULATED=	1421.9 CM-1	ERROR=	-0.9 CM-1	OR	-0.1 PERCENT	
INTERNAL COORDINATES-	27.13	C3OH 20.21	C4OH	12.25	OC4H	6.58	HC4C	5.04	CC5H
FORCE CONSTANTS-	47.91	BCOH 19.13	CCH	16.85	UCH	6.78	CC	6.52	CCO
OFF DIAGONAL-	-4.95	SB27	-4.35	SB26	3.83	SB28	3.81	BB29	-2.76
NORMAL MODE 11	OBSERVED=	1409.2 CM-1	CALCULATED=	1409.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	46.74	C3OH 8.40	OC4H	8.12	OC3H				
FORCE CONSTANTS-	51.39	BCOH 20.59	UCH	15.69	CCH	5.08	CO		
OFF DIAGONAL-	-4.75	SB27	3.98	SB28	3.26	BB29	-2.24	SB26	2.14
NORMAL MODE 12	OBSERVED=	1394.7 CM-1	CALCULATED=	1394.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	88.20	C1OH	5.66	C1C2					
FORCE CONSTANTS-	89.02	BCOH	5.79	CC					
OFF DIAGONAL-	3.19	SB28	-2.12	SB22					
NORMAL MODE 13	OBSERVED=	1389.7 CM-1	CALCULATED=	1389.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	77.36	C1OH	7.72	OC4H	6.87	CC4H	5.35	C5C1	
FORCE CONSTANTS-	77.89	BCOH	11.74	CCH	8.37	UCH	5.61	CC	
OFF DIAGONAL-	-4.73	SB26	-2.74	BB39	2.62	SB28			
NORMAL MODE 14	OBSERVED=	1374.8 CM-1	CALCULATED=	1374.8 CM-1	ERROR=	-4.8 CM-1	OR	-0.3 PERCENT	
INTERNAL COORDINATES-	57.34	BCOH 22.68	CC5H	5.51	HC4C				
FORCE CONSTANTS-	57.34	BCOH 22.68	UCH	15.59	UCH				
OFF DIAGONAL-	3.98	BB29	-2.83	SB27	-2.28	BB36	-2.21	SB26	
NORMAL MODE 15	OBSERVED=	1360.8 CM-1	CALCULATED=	1360.8 CM-1	ERROR=	-19.8 CM-1	OR	-1.5 PERCENT	
INTERNAL COORDINATES-	17.00	HC3H 13.99	OC3H	13.22	C4OH	11.48	HC5C	8.32	CC5H
FORCE CONSTANTS-	46.54	CCH 26.92	UCH	18.02	BCOH				
OFF DIAGONAL-	9.91	BB29	-4.82	SB27	-3.02	BB45	-2.59	SB28	2.55
NORMAL MODE 16	OBSERVED=	1333.0 CM-1	CALCULATED=	1333.0 CM-1	ERROR=	-4.0 CM-1	OR	-0.3 PERCENT	
INTERNAL COORDINATES-	14.63	HC5C 12.38	CC4H	12.14	CC5H	10.95	OC3H	9.50	HC3C
FORCE CONSTANTS-	68.18	CCH 16.70	UCH	6.13	BCOH				
OFF DIAGONAL-	15.56	BB29	-8.66	SB26	-3.66	BB45	-3.57	SB27	
NORMAL MODE 17	OBSERVED=	1298.8 CM-1	CALCULATED=	1298.8 CM-1	ERROR=	-4.8 CM-1	OR	-0.4 PERCENT	
INTERNAL COORDINATES-	25.32	OC4H 24.49	CC4H	14.46	OC4H	10.69	HC4C	5.74	CC5H
FORCE CONSTANTS-	50.86	UCH 43.01	CCH	6.03	BCOH				
OFF DIAGONAL-	-3.67	BB45	-3.56	SB27					
NORMAL MODE 18	OBSERVED=	1278.9 CM-1	CALCULATED=	1278.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	35.50	CC5H 12.06	OC4H	10.49	CC4H	7.70	CC5H	6.42	UCHB
FORCE CONSTANTS-	42.53	UCH	3.43	BB45					
OFF DIAGONAL-	5.40	SB27	-3.43	BB45					
NORMAL MODE 19	OBSERVED=	1270.5 CM-1	CALCULATED=	1270.5 CM-1	ERROR=	-2.5 CM-1	OR	-0.2 PERCENT	
INTERNAL COORDINATES-	27.62	OC3H 22.07	CC3H	17.11	CC4C	7.40	OC4H	5.37	C2OH
FORCE CONSTANTS-	46.37	CCH 38.24	UCH	7.09	BCOH				
OFF DIAGONAL-	-4.18	SB26	-3.54	BB45	2.73	BB29	2.26	SB27	1.71
NORMAL MODE 20	OBSERVED=	1245.6 CM-1	CALCULATED=	1245.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	19.18	UC4H 17.36	CC3H	10.92	HC3C	8.40	HC5C	5.28	CC5H
FORCE CONSTANTS-	51.68	CCH 28.32	UCH	8.03	BCOH	7.89	CO		
OFF DIAGONAL-	4.57	SB27	4.44	BB34	-4.08	SB26	-3.70	BB29	-3.29
NORMAL MODE 21	OBSERVED=	1227.8 CM-1	CALCULATED=	1227.8 CM-1	ERROR=	-7.8 CM-1	OR	-0.6 PERCENT	
INTERNAL COORDINATES-	46.79	UC1C 26.76	C-U6	6.32	C5O1	5.87	OC1C	5.57	CC1H
FORCE CONSTANTS-	84.00	UCH 17.29	CC	15.96	UCH	9.22	CCH	2.86	BB3H
OFF DIAGONAL-	-12.92	SB29	-12.92	SB27	-4.18	SB28	2.71	BB34	-2.02
NORMAL MODE 22	OBSERVED=	1200.2 CM-1	CALCULATED=	1200.2 CM-1	ERROR=	-5.8 CM-1	OR	0.5 PERCENT	
INTERNAL COORDINATES-	10.44	UCHB 10.39	HC5C	9.71	CC5H	8.65	HC4C	8.36	CC3H
FORCE CONSTANTS-	59.83	CCH 17.08	UCH	16.13	CO	6.83	BCOH	6.22	CCO
OFF DIAGONAL-	-7.12	BB29	6.34	BB34	-3.83	SB25	-3.00	BB45	-2.99
NORMAL MODE 23	OBSERVED=	1170.7 CM-1	CALCULATED=	1170.7 CM-1	ERROR=	-7.7 CM-1	OR	-0.7 PERCENT	
INTERNAL COORDINATES-	27.93	C5O1 18.11	OC4H	12.60	OC4H	10.11	CCO	5.26	C-U8
FORCE CONSTANTS-	42.24	UCH 38.89	CO	10.17	CCH	10.11	CCO		
OFF DIAGONAL-	-9.24	SB25	1.69	SB27	-1.61	SB23	-1.57	SB28	
NORMAL MODE 24	OBSERVED=	1136.4 CM-1	CALCULATED=	1136.4 CM-1	ERROR=	6.6 CM-1	OR	0.6 PERCENT	
INTERNAL COORDINATES-	26.37	C-U6 16.02	C-U9	11.34	C2C3				
FORCE CONSTANTS-	52.67	CO 18.38	CC	17.30	UCH	15.68	CCO	12.20	CC5H
OFF DIAGONAL-	-6.39	SB27	-6.34	SB25	-4.03	SB28	-3.32	SB22	-2.05
NORMAL MODE 25	OBSERVED=	1112.7 CM-1	CALCULATED=	1112.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	45.66	C4C5 17.51	C3C4	10.37	C5C1	9.68	C2C3		
FORCE CONSTANTS-	83.28	CC 17.33	CCO	14.66	CO	5.38	CCH		
OFF DIAGONAL-	-13.33	SB22	-3.73	SB21	-3.28	SB25	-3.22	SS17	-2.24
NORMAL MODE 26	OBSERVED=	1106.3 CM-1	CALCULATED=	1106.3 CM-1	ERROR=	-0.3 CM-1	OR	-0.0 PERCENT	
INTERNAL COORDINATES-	32.28	C-U8 16.69	C5C1	11.15	C-U7	8.15	C5O1	6.91	C3C4
FORCE CONSTANTS-	59.83	CCH 17.08	UCH	14.48	C3C4	11.11	CCO	9.00	CCO
OFF DIAGONAL-	-7.37	SB25	-5.90	SB27	-5.51	SB28	-5.13	SS18	-3.33
NORMAL MODE 27	OBSERVED=	1088.4 CM-1	CALCULATED=	1088.4 CM-1	ERROR=	-1.6 CM-1	OR	0.1 PERCENT	
INTERNAL COORDINATES-	60.06	CC 25.05	CO	18.60	CCO	14.14	CCH	10.64	BCOH
FORCE CONSTANTS-	12.27	SB22	-5.17	SB21	-5.17	SB28	-3.44	SB27	-3.36
OFF DIAGONAL-									
NORMAL MODE 28	OBSERVED=	1069.3 CM-1	CALCULATED=	1069.3 CM-1	ERROR=	-4.3 CM-1	OR	-0.4 PERCENT	
INTERNAL COORDINATES-	46.42	C-U8 20.43	C3C4	12.91	C-U7				
FORCE CONSTANTS-	67.40	CO 27.05	CC	7.60	CCO	6.98	CCH	6.50	UCH
OFF DIAGONAL-	-5.64	SB27	-4.58	SB22	-4.41	SB25	-4.35	SB28	-2.54
NORMAL MODE 29	OBSERVED=	1050.6 CM-1	CALCULATED=	1050.6 CM-1	ERROR=	-2.3 CM-1	OR	0.2 PERCENT	
INTERNAL COORDINATES-	23.14	C-U6 19.31	OC1C	10.65	C4C5	8.49	C1C2	6.39	CC1H
FORCE CONSTANTS-	68.80	CC 21.87	CC	18.30	CCH	13.09	UCH	6.69	CCO
OFF DIAGONAL-	-8.80	SB24	-6.32	SB27	-6.14	SB21	-5.74	SS18	-4.74
NORMAL MODE 30	OBSERVED=	1050.0 CM-1	CALCULATED=	1050.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	19.84	C-U8 23.19	C-U9	15.60	C1C2	12.57	C-U8	11.81	C-U7
FORCE CONSTANTS-	76.91	CC 17.79	CC	13.26	UCH	9.69	CCO	8.00	CCO
OFF DIAGONAL-	-8.42	SB28	-7.84	SB27	-7.38	SB25	-3.46	SB22	-3.19
NORMAL MODE 31	OBSERVED=	1020.4 CM-1	CALCULATED=	1020.4 CM-1	ERROR=	11.6 CM-1	OR	1.1 PERCENT	
INTERNAL COORDINATES-	17.26	C5C1 15.20	C3C4	10.90	C-U8	9.45	OC1C	8.44	C-U8
FORCE CONSTANTS-	48.01	CC 40.98	CC	17.82	UCH	11.66	CCO	6.95	CC1H
OFF DIAGONAL-	-17.17	SB21	-11.33	SB27	-8.65	SS18	-5.73	SB22	-4.96
NORMAL MODE 32	OBSERVED=	993.7 CM-1	CALCULATED=	993.7 CM-1	ERROR=	9.3 CM-1	OR	0.9 PERCENT	
INTERNAL COORDINATES-	29.07	C1H 16.40	C5C1	10.45	OC1H	6.68	C-U8	6.26	C4C5
FORCE CONSTANTS-	43.48	UCH 23.22	CC	13.74	CO	11.58	CCH	6.06	CCO
OFF DIAGONAL-	-4.78	SB21	2.31	SB27	-2.21	SB22	1.76	BB34	1.59
NORMAL MODE 33	OBSERVED=	974.1 CM-1	CALCULATED=	974.1 CM-1	ERROR=	12.8 CM-1	OR	1.3 PERCENT	
INTERNAL COORDINATES-	16.56	C3C4 12.55	OC1H	10.93	C-U8	10.04	C5C1	6.01	CC4H
FORCE CONSTANTS-	29.69	CC 25.62	CCH	24.49	CO	21.80	UCH	9.39	CCO
OFF DIAGONAL-	-7.49	SB22	-4.85	BB29	-3.50	SB21	2.39	SB27	-2.22
NORMAL MODE 34	OBSERVED=	951.5 CM-1	CALCULATED=	951.5 CM-1	ERROR=	7.5 CM-1	OR	0.8 PERCENT	
INTERNAL COORDINATES-	28.56	OC1H 18.02	CC1H	6.27	C2C3				
FORCE CONSTANTS-	40.92	UCH 28.07	CCH	11.38	CC				
OFF DIAGONAL-	-4.15	SB22	3.97	SB27	2.67	BB34	-1.95	BB45	-1.92
NORMAL MODE 35	OBSERVED=	951.2 CM-1	CALCULATED=	951.2 CM-1	ERROR=	-2.8 CM-1	OR	0.3 PERCENT	
INTERNAL COORDINATES-	15.69	C2C3 13.22	C-U8	13.26	HC4C	10.24	C3C4	8.81	C1C2
FORCE CONSTANTS-	37.83	CC 27.09	CO	18.80	UCH	15.95	UCH	9.49	UCH
OFF DIAGONAL-	-9.12	SB22	-4.34	SB27	3.66	SS18	-3.53	SB28	3.28

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400											PAGE 2	
MOLECULE 3 -6 NG-1236 ALPHA GLUCOSE-1,2-D2												
NORMAL MODE 36		OBSERVED=	924.0 CM-1	CALCULATED=		935.1 CM-1	ERROR=		-11.1 CM-1	OR	-1.2 PERCENT	
INTERNAL COORDINATES-		60.11 UC2H	8.37 C-07	6.35 CCH2		5.76 C2OH	5.18 C1C2		11.60 CO	6.16 BCOH		
FORCE CONSTANTS-		62.21 UCH	12.93 CCH	11.60 CO		9.39 CC	6.45 CCO		6.48 CCH	6.16 BCOH		
OFF DIAGONAL-		10.20 SB27	-4.51 SB26	3.03 SB25		-2.92 SB21	-2.92 SB28		-2.90 SB22	-2.45 BB45 -2.03 BB34 1.67 SS18		
NORMAL MODE 37		OBSERVED=	812.0 CM-1	CALCULATED=		807.6 CM-1	ERROR=		4.4 CM-1	OR	0.5 PERCENT	
INTERNAL COORDINATES-		29.08 C507	14.18 CCHA	12.61 CCHB		11.66 C1H	7.18 O1C1		5.63 C5C7			
FORCE CONSTANTS-		39.01 CO	32.12 CCH	15.66 OCH		8.63 CCO	7.29 CC					
OFF DIAGONAL-		-4.83 SB25	-3.11 BB29	2.36 SB27		-1.83 SB24	1.78 SB26					
NORMAL MODE 38		OBSERVED=	761.0 CM-1	CALCULATED=		772.6 CM-1	ERROR=		-11.6 CM-1	OR	-1.5 PERCENT	
INTERNAL COORDINATES-		31.91 CH2	20.14 HC2C	16.76 C-06		12.21 CC1H	6.08 C2C3					
FORCE CONSTANTS-		66.89 CCH	21.14 CO	8.59 CC		6.48 OCH						
OFF DIAGONAL-		-4.38 SB27	-3.14 BB45	-2.86 BB29		2.46 SB26	-2.26 SB22		-2.10 SB21			
NORMAL MODE 39		OBSERVED=	724.0 CM-1	CALCULATED=		733.8 CM-1	ERROR=		-9.8 CM-1	OR	-1.3 PERCENT	
INTERNAL COORDINATES-		13.54 CC1H	12.27 CO1C	9.69 C-06		5.64 C1CC	5.39 CCO6					
FORCE CONSTANTS-		23.89 CCH	17.00 CCO	15.98 CO		12.27 CCO	11.02 CC		6.43 CCC			
OFF DIAGONAL-		5.89 BB43	4.74 SB25	-4.37 BB34		3.03 SB24	2.82 SB22		-2.46 SB27	-2.14 SB26 -2.09 BB41 -1.59 BB29		
NORMAL MODE 40		OBSERVED=	640.0 CM-1	CALCULATED=		631.7 CM-1	ERROR=		8.3 CM-1	OR	1.3 PERCENT	
INTERNAL COORDINATES-		10.30 UBCC	7.82 OCU	6.14 HC3C		5.88 CCO9	5.20 CC5H					
FORCE CONSTANTS-		36.97 CCO	22.08 CCH	9.55 CO		7.82 CCH	6.57 CC					
OFF DIAGONAL-		-7.25 BB34	6.97 BB43	-4.75 BB29		4.52 SB25	-2.69 SB27		2.63 SB22 2.20 SB24 2.01 SB21			
NORMAL MODE 41		OBSERVED=	624.0 CM-1	CALCULATED=		612.1 CM-1	ERROR=		11.9 CM-1	OR	1.9 PERCENT	
INTERNAL COORDINATES-		16.49 CCO7	14.53 CCU6	8.45 CCO7		6.86 CCO7	6.60 OBCC		6.21 HC4C 6.01 CCHB 5.56 CC5H			
FORCE CONSTANTS-		61.96 CCO	31.88 CCO6									
OFF DIAGONAL-		-11.62 BB34	6.93 BB43	-6.25 BB29		-2.05 BB41	1.71 SB25					
NORMAL MODE 42		OBSERVED=	552.0 CM-1	CALCULATED=		542.9 CM-1	ERROR=		9.1 CM-1	OR	1.6 PERCENT	
INTERNAL COORDINATES-		14.53 OTCC	8.96 CCU9	7.50 C2C3		5.60 CC4H						
FORCE CONSTANTS-		40.97 CCO	24.30 CCH	17.44 CC		11.46 CO						
OFF DIAGONAL-		-9.38 BB34	6.19 BB43	-5.23 BB29		3.24 SS18	2.78 SB25		2.55 SB21 -2.15 SB27			
NORMAL MODE 43		OBSERVED=	533.0 CM-1	CALCULATED=		525.1 CM-1	ERROR=		7.9 CM-1	OR	1.5 PERCENT	
INTERNAL COORDINATES-		18.05 OCO	15.82 4CU7	10.99 O1CC		6.29 C-09	5.90 OTCC		5.84 C3CC			
FORCE CONSTANTS-		42.28 CCO	18.05 CCO	12.57 CCH		11.52 CO	10.20 CCC		6.04 CC			
OFF DIAGONAL-		-6.12 BB34	4.75 SB25	-3.89 SB21		3.37 SB22	-3.33 BB42		2.67 BB43 -2.03 BB29 -1.82 SB27 1.59 SS18			
NORMAL MODE 44		OBSERVED=	451.0 CM-1	CALCULATED=		436.8 CM-1	ERROR=		14.2 CM-1	OR	3.1 PERCENT	
INTERNAL COORDINATES-		10.44 CCO7	9.32 C2CC	9.23 C3CC		7.45 CCO9	7.23 CC3H		6.38 O1CC 6.01 HC2C 5.86 CC06 5.11 HC5C			
FORCE CONSTANTS-		38.02 CCO	26.52 CCH	23.36 CCO		5.85 CC						
OFF DIAGONAL-		7.10 BB43	-6.86 BB34	-5.92 BB29								
NORMAL MODE 45		OBSERVED=	427.0 CM-1	CALCULATED=		422.3 CM-1	ERROR=		4.7 CM-1	OR	1.1 PERCENT	
INTERNAL COORDINATES-		14.86 UBCC	14.75 OCU	12.39 O1CC		10.02 CCO7	8.04 C1CC		7.42 CC08 5.16 CO1C			
FORCE CONSTANTS-		48.76 CCO	14.75 UCO	13.30 CCO		6.51 CO	6.47 CC					
OFF DIAGONAL-		6.20 SB22	-4.60 BB34	-4.27 BB42		4.25 SB25	-3.98 SB21		-1.91 SB27			
NORMAL MODE 46		OBSERVED=	403.0 CM-1	CALCULATED=		387.1 CM-1	ERROR=		15.9 CM-1	OR	3.9 PERCENT	
INTERNAL COORDINATES-		13.41 C2CC	13.01 OBCC	10.32 CCO8		7.10 OCO	5.99 O9CC		5.58 C3CC 5.36 C1CC			
FORCE CONSTANTS-		51.06 CCO	24.35 CCH	7.80 CCH		7.51 CC	7.10 CCO					
OFF DIAGONAL-		-6.69 BB34	-4.40 BB42	4.23 SB25		4.18 SB21	-1.60 SB26		-1.52 BB41			
NORMAL MODE 47		OBSERVED=	370.4 CM-1	CALCULATED=		370.4 CM-1	ERROR=		0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-		16.10 CCO7	12.27 OTCC	6.44 OCO		5.42 CCO8						
FORCE CONSTANTS-		48.42 CCO	21.21 CCH	11.17 CC		6.44 OCO						
OFF DIAGONAL-		-6.94 BB34	3.45 BB43	-3.26 SB26		3.15 SB21	-2.92 BB29		-2.20 BB33 1.89 SB24 1.65 SB22			
NORMAL MODE 48		OBSERVED=	317.9 CM-1	CALCULATED=		317.9 CM-1	ERROR=		0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-		17.85 CCO9	11.30 CCO8	8.46 OTCC		6.34 C3C4	5.96 CCO7		5.77 CC08 5.09 TH-2			
FORCE CONSTANTS-		63.97 CCO	13.55 CCO	9.15 CCH		7.07 T-OH						
OFF DIAGONAL-		-7.30 BB34	5.02 SB22	2.71 BB43		-2.52 BB42						
NORMAL MODE 49		OBSERVED=	311.6 CM-1	CALCULATED=		311.6 CM-1	ERROR=		0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-		21.02 CCO7	17.65 CCO8	8.88 OBCC		7.99 4CO7	7.89 CCO7		5.32 C4C5 5.23 OTCC			
FORCE CONSTANTS-		72.61 CCO	10.09 CC	7.25 T-OH		6.74 CCH						
OFF DIAGONAL-		-7.60 BB34	-3.78 BB42	3.18 SB21		1.88 SB22						
NORMAL MODE 50		OBSERVED=	302.5 CM-1	CALCULATED=		302.5 CM-1	ERROR=		0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-		19.20 UBCC	17.48 O9CC	11.04 4CO7		7.53 OTCC	6.71 CCO8		5.41 CCO7 5.06 TH-4			
FORCE CONSTANTS-		74.86 CCO	13.32 CCH	12.89 T-OH		6.86 CCO						
OFF DIAGONAL-		-11.35 BB34	2.42 BB43	-2.40 BB42		-2.36 SB25	-1.96 BB29					
NORMAL MODE 51		OBSERVED=	254.9 CM-1	CALCULATED=		254.9 CM-1	ERROR=		0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-		18.82 CCO6	9.30 O1CC	8.98 CCO9		7.40 CCH2	6.84 OTCC		5.48 HC2C 5.12 C1CC			
FORCE CONSTANTS-		54.60 CCO	19.42 CCH	14.58 T-OH		8.89 CCC						
OFF DIAGONAL-		-9.03 BB34	7.20 BB43	-3.68 SB25		-3.12 BB33	-2.58 BB29					
NORMAL MODE 52		OBSERVED=	241.7 CM-1	CALCULATED=		241.7 CM-1	ERROR=		0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-		52.75 TH-5	7.37 CCO7	5.73 C4CC								
FORCE CONSTANTS-		63.12 T-OH	20.02 CCO	7.85 CCC								
OFF DIAGONAL-		-1.73 BB34										
NORMAL MODE 53		OBSERVED=	228.8 CM-1	CALCULATED=		228.8 CM-1	ERROR=		0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-		55.10 TH-1	25.06 TH-3	7.59 TH-2		6.20 TH-4						
FORCE CONSTANTS-		93.98 T-UH										
OFF DIAGONAL-		NONE										
NORMAL MODE 54		OBSERVED=	222.7 CM-1	CALCULATED=		222.7 CM-1	ERROR=		0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-		46.83 TH-4	17.17 TH-1	16.05 TH-5		9.32 TH-3						
FORCE CONSTANTS-		89.46 T-OH	5.50 CCO									
OFF DIAGONAL-		NONE										
NORMAL MODE 55		OBSERVED=	215.1 CM-1	CALCULATED=		215.1 CM-1	ERROR=		0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-		37.42 TH-3	29.30 TH-4	9.84 TH-1		5.86 TH-2	5.09 OBCC					
FORCE CONSTANTS-		82.72 T-OH	14.59 CCO									
OFF DIAGONAL-		-1.89 BB34										
NORMAL MODE 56		OBSERVED=	213.2 CM-1	CALCULATED=		213.2 CM-1	ERROR=		0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-		70.17 TH-2	11.17 TH-3									
FORCE CONSTANTS-		83.32 T-UH	14.64 CCO									
OFF DIAGONAL-		NONE										
NORMAL MODE 57		OBSERVED=	199.0 CM-1	CALCULATED=		199.0 CM-1	ERROR=		0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-		25.71 TH-5	24.63 CCO7	13.12 C4CC		6.48 TCC5	5.74 CO1C		5.74 COC			
FORCE CONSTANTS-		37.57 CCO	31.35 T-UH	14.60 CCC		8.24 T-CC	6.38 CCH					
OFF DIAGONAL-		-4.69 BB34	-2.71 BB42	-2.36 BB33								
NORMAL MODE 58		OBSERVED=	129.7 CM-1	CALCULATED=		129.7 CM-1	ERROR=		0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-		22.25 CO1C	14.84 C4CC	10.11 TCC4		6.40 TCO1	6.37 C1CC		5.21 OCO			
FORCE CONSTANTS-		22.33 CC	22.25 CCO	12.30 T-CC		11.59 CCO	10.08 T-CO		5.48 CCH 5.21 OCO			
OFF DIAGONAL-		3.88 BB43	-3.56 SB21	-2.46 BB37		1.97 BB41	-1.69 BB34					
NORMAL MODE 59		OBSERVED=	97.5 CM-1	CALCULATED=		97.5 CM-1	ERROR=		0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-		25.80 TCC5	9.86 C3CC	6.65 O9CC		5.06 C4CC						
FORCE CONSTANTS-		25.88 T-CC	18.22 CCC	17.15 CCO								
OFF DIAGONAL-		-3.25 SB25	-2.59 BB34	-2.31 SB21		-2.24 BB42	-1.51 BB43					
NORMAL MODE 60		OBSERVED=	80.9 CM-1	CALCULATED=		80.9 CM-1	ERROR=		0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-		21.73 C2CC	14.18 C1CC	8.33 CO1C		7.50 TCC1	7.04 TCC2		6.89 TCC5 6.39 TCC4			
FORCE CONSTANTS-		41.50 CCC	27.81 T-CC	18.06 CCO		8.33 CCO	5.81 T-CO					
OFF DIAGONAL-		-4.15 SB25	-3.99 BB42	-3.14 SB21		2.41 BB41						
NORMAL MODE 61		OBSERVED=	65.4 CM-1	CALCULATED=		65.4 CM-1	ERROR=		0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-		22.56 TCC5	13.70 C3CC	10.41 TCC4		7.38 TCC3	6.82 TCC2		6.04 4CO7 5.71 C1CC			
FORCE CONSTANTS-		48.10 T-CC	23.36 CCO	21.85 CCC								
OFF DIAGONAL-		-2.68 BB42	-2.29 BB34	-1.71 SB25								

32. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 7.70

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400				PAGE 1	
MOLECULE 4 -6 NG=1236 ALPHA GLUCOSE-1-D					
NORMAL MODE 8	OBSERVED=	1457.0 CM-1	CALCULATED= 1454.6 CM-1	ERROR= 2.4 CM-1	0.2 PERCENT
INTERNAL COORDINATES-	68.83	BCOH	6.25 CCH	6.00 CCO	
FORCE CONSTANTS-	4.42	BB36	3.92 SB28	1.77 BB34	-1.77 SB25
OFF DIAGONAL-					
NORMAL MODE 9	OBSERVED=	1445.9 CM-1	CALCULATED= 1449.8 CM-1	ERROR= -4.8 CM-1	OR -0.3 PERCENT
INTERNAL COORDINATES-	61.19	HCH	20.82 OCHB	19.04 OCHA	
FORCE CONSTANTS-	61.19	HCH	40.24 OCH		
OFF DIAGONAL-	-4.08	SB27			
NORMAL MODE 10	OBSERVED=	1425.0 CM-1	CALCULATED= 1422.0 CM-1	ERROR= 3.0 CM-1	OR 0.2 PERCENT
INTERNAL COORDINATES-	26.07	C3OH	20.45 C4OH	12.69 OC4H	6.70 HC4C
FORCE CONSTANTS-	46.70	BCOH	19.77 CCH	17.45 OCH	6.70 CO
OFF DIAGONAL-	-5.10	SB27	-4.30 SB26	3.87 BB29	3.73 SB28
NORMAL MODE 11	OBSERVED=	1410.0 CM-1	CALCULATED= 1411.9 CM-1	ERROR= -1.9 CM-1	OR -0.1 PERCENT
INTERNAL COORDINATES-	42.47	C3OH	10.52 OC3H	7.62 OC4H	
FORCE CONSTANTS-	46.28	BCOH	23.83 UCH	18.13 CCH	5.36 CO
OFF DIAGONAL-	-5.33	SB27	4.27 SB28	4.03 BB29	-3.67 SB26
NORMAL MODE 12	OBSERVED=	0.0 CM-1	CALCULATED= 1399.8 CM-1	ERROR= 0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	78.49	C1OH			
FORCE CONSTANTS-	79.65	BCOH	5.32 UCH		
OFF DIAGONAL-	4.76	SB28	-1.96 SB22		
NORMAL MODE 13	OBSERVED=	1385.0 CM-1	CALCULATED= 1389.7 CM-1	ERROR= -4.7 CM-1	OR -0.3 PERCENT
INTERNAL COORDINATES-	77.44	C4OH	7.78 OCHB	6.96 CCHB	5.38 C5C*
FORCE CONSTANTS-	77.70	BCOH	11.86 CCH	8.43 OCH	5.63 CC
OFF DIAGONAL-	-4.75	SB26	-2.74 BB39	2.62 SB28	
NORMAL MODE 14	OBSERVED=	1373.0 CM-1	CALCULATED= 1375.4 CM-1	ERROR= -2.4 CM-1	OR -0.2 PERCENT
INTERNAL COORDINATES-	37.20	C4OH	15.64 C5H	6.80 HC4C	6.13 CCHB
FORCE CONSTANTS-	40.77	BCOH	31.35 CCH	21.88 OCH	5.33 CC5H
OFF DIAGONAL-	-5.93	BB29	-4.30 SB27	-3.24 SB26	-2.12 BB45
NORMAL MODE 15	OBSERVED=	1365.0 CM-1	CALCULATED= 1369.8 CM-1	ERROR= -4.8 CM-1	OR -0.3 PERCENT
INTERNAL COORDINATES-	26.46	C4OH	12.74 C3OH	12.59 OC3H	11.48 OC2H
FORCE CONSTANTS-	40.46	BCOH	27.14 CCH	26.35 OCH	8.76 HC3C
OFF DIAGONAL-	-5.20	BB29	-4.01 SB27	-3.09 SB28	2.67 BB34
NORMAL MODE 16	OBSERVED=	1348.0 CM-1	CALCULATED= 1346.8 CM-1	ERROR= 1.2 CM-1	OR 0.1 PERCENT
INTERNAL COORDINATES-	15.75	OC2H	16.50 HC5C	8.13 HC2C	6.59 CC5H
FORCE CONSTANTS-	55.04	CCH	17.97 UCH	9.24 BCOH	
OFF DIAGONAL-	11.88	BB29	-4.40 SB26	-4.11 SB27	-3.48 BB45
NORMAL MODE 17	OBSERVED=	1329.0 CM-1	CALCULATED= 1325.9 CM-1	ERROR= 3.1 CM-1	OR 0.2 PERCENT
INTERNAL COORDINATES-	17.04	HC3C	14.85 OC2H	10.63 CC4H	7.06 OC3H
FORCE CONSTANTS-	64.87	CCH	25.60 UCH	10.63 CC4H	6.73 HC3C
OFF DIAGONAL-	13.73	BB29	-9.40 SB26	-4.02 SB27	-3.91 BB45
NORMAL MODE 18	OBSERVED=	0.0 CM-1	CALCULATED= 1308.1 CM-1	ERROR= 0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	25.51	CC2H	11.06 O1C1	10.86 C-06	10.46 HC2C
FORCE CONSTANTS-	51.77	CCH	24.53 CO	20.02 OCH	9.29 BCOH
OFF DIAGONAL-	-7.08	SB27	-3.63 SB28	-3.62 SB25	3.23 BB34
NORMAL MODE 19	OBSERVED=	1292.0 CM-1	CALCULATED= 1295.4 CM-1	ERROR= -3.4 CM-1	OR -0.3 PERCENT
INTERNAL COORDINATES-	20.79	OCHA	20.09 CCHA	10.85 OC4H	8.56 HC4C
FORCE CONSTANTS-	52.08	CCH	38.71 UCH	5.63 CCH	5.58 BCOH
OFF DIAGONAL-	-3.72	BB45	-2.88 SB26	-2.47 SB27	
NORMAL MODE 20	OBSERVED=	1277.0 CM-1	CALCULATED= 1278.4 CM-1	ERROR= -1.4 CM-1	OR -0.1 PERCENT
INTERNAL COORDINATES-	34.22	CCH	11.65 UCHA	9.94 CCHA	8.80 OC4H
FORCE CONSTANTS-	62.88	UCH	6.11 CCH	9.11 CO	8.59 CC5H
OFF DIAGONAL-	6.36	SB27	-3.47 BB45	-3.25 BB29	
NORMAL MODE 21	OBSERVED=	1268.0 CM-1	CALCULATED= 1263.2 CM-1	ERROR= 4.7 CM-1	OR 0.4 PERCENT
INTERNAL COORDINATES-	28.99	OC3H	18.70 CC4H	11.81 OC4H	5.66 C5H
FORCE CONSTANTS-	48.78	UCH	36.44 CCH	5.17 CO	
OFF DIAGONAL-	7.45	SB27	-4.39 BB29	-3.37 BB45	3.02 BB34
NORMAL MODE 22	OBSERVED=	1231.0 CM-1	CALCULATED= 1230.9 CM-1	ERROR= 0.1 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	15.04	OC4H	10.77 HC5C	10.17 CC5H	10.11 OC3H
FORCE CONSTANTS-	46.06	CCH	33.33 OCH	8.94 CO	5.37 CCO
OFF DIAGONAL-	-8.78	BB29	7.13 SB27	5.26 BB34	-3.16 SB25
NORMAL MODE 23	OBSERVED=	1207.0 CM-1	CALCULATED= 1193.5 CM-1	ERROR= 13.5 CM-1	OR 1.1 PERCENT
INTERNAL COORDINATES-	19.37	O1C1	13.32 C5O*	10.21 OC2H	7.61 OC2H
FORCE CONSTANTS-	40.11	UCH	28.55 CCH	23.80 OCH	10.17 CCO
OFF DIAGONAL-	-6.62	SB25	-3.76 BB29	-2.78 SB26	2.59 SB27
NORMAL MODE 24	OBSERVED=	1167.0 CM-1	CALCULATED= 1164.2 CM-1	ERROR= 2.8 CM-1	OR 0.2 PERCENT
INTERNAL COORDINATES-	15.07	UCH	13.15 O1C1	11.23 CCO	12.08 C5O*
FORCE CONSTANTS-	45.07	CCH	33.16 CCH	10.23 CCO	8.26 BCOH
OFF DIAGONAL-	-7.77	SB25	-5.02 SB27	-3.59 SB23	2.20 BB37
NORMAL MODE 25	OBSERVED=	1132.0 CM-1	CALCULATED= 1143.8 CM-1	ERROR= -11.8 CM-1	OR -1.0 PERCENT
INTERNAL COORDINATES-	20.25	C5O*	10.53 O1C1	9.50 CC4H	8.34 C-09
FORCE CONSTANTS-	48.22	CCH	40.45 CO	10.14 CCO	9.15 OCH
OFF DIAGONAL-	-8.91	BB29	5.06 BB34	-3.32 SB25	-2.60 BB43
NORMAL MODE 26	OBSERVED=	1119.0 CM-1	CALCULATED= 1130.8 CM-1	ERROR= -11.8 CM-1	OR -1.0 PERCENT
INTERNAL COORDINATES-	49.74	C-07	14.91 C2C3	7.72 C-09	5.30 C2OH
FORCE CONSTANTS-	65.78	CO	22.89 CCH	15.00 CCO	7.92 BCOH
OFF DIAGONAL-	-8.64	SB25	-7.51 SB28	-4.16 SB27	-3.52 SS18
NORMAL MODE 27	OBSERVED=	1106.0 CM-1	CALCULATED= 1110.4 CM-1	ERROR= -4.4 CM-1	OR -0.4 PERCENT
INTERNAL COORDINATES-	49.60	C4C5	16.15 C3C4	11.92 C5C*	5.92 C2C3
FORCE CONSTANTS-	83.65	CC	19.07 CCO	12.14 CO	7.47 OCH
OFF DIAGONAL-	-14.16	SB22	-3.28 SB21	-3.18 SS17	-3.11 SB25
NORMAL MODE 28	OBSERVED=	1095.0 CM-1	CALCULATED= 1089.5 CM-1	ERROR= 5.5 CM-1	OR 0.5 PERCENT
INTERNAL COORDINATES-	16.81	C-09	13.43 C-08	12.92 C5C*	10.34 C1C2
FORCE CONSTANTS-	43.93	CO	43.26 CC	13.00 CCH	7.74 CCO
OFF DIAGONAL-	-6.82	SB22	-4.90 SB28	-3.66 SS18	-2.64 SB27
NORMAL MODE 29	OBSERVED=	1075.0 CM-1	CALCULATED= 1078.8 CM-1	ERROR= -3.8 CM-1	OR -0.3 PERCENT
INTERNAL COORDINATES-	28.77	C-08	16.71 C2C3	14.43 C3C4	13.99 C1C2
FORCE CONSTANTS-	49.79	CO	46.57 CC	16.63 CCO	10.34 CCC
OFF DIAGONAL-	-8.31	SB21	-8.08 SB22	-7.78 SB27	-6.89 SS18
NORMAL MODE 30	OBSERVED=	1070.0 CM-1	CALCULATED= 1062.6 CM-1	ERROR= 7.3 CM-1	OR 0.7 PERCENT
INTERNAL COORDINATES-	38.41	C-08	16.41 C1C2	7.66 C-08	7.55 C-06
FORCE CONSTANTS-	69.70	CO	27.60 CC	10.61 CCH	7.03 UCH
OFF DIAGONAL-	-6.75	SB27	-6.34 SB28	-5.04 SB25	-4.20 SB26
NORMAL MODE 31	OBSERVED=	1042.0 CM-1	CALCULATED= 1050.2 CM-1	ERROR= -8.2 CM-1	OR -0.8 PERCENT
INTERNAL COORDINATES-	29.52	C-09	21.79 C1C2	19.47 C-08	10.28 C-07
FORCE CONSTANTS-	75.40	CO	24.80 CC	12.39 CCH	9.74 CCO
OFF DIAGONAL-	-9.16	SB27	-8.94 SB28	-6.89 SB25	-4.29 SB21
NORMAL MODE 32	OBSERVED=	1020.0 CM-1	CALCULATED= 1026.2 CM-1	ERROR= -6.2 CM-1	OR -0.6 PERCENT
INTERNAL COORDINATES-	15.52	C3C4	11.31 C5C*	13.90 C4C5	12.88 C1C2
FORCE CONSTANTS-	50.52	CCH	31.94 UCH	17.71 CO	13.09 CCH
OFF DIAGONAL-	-18.14	SB21	-9.31 SB27	-8.53 SB22	-6.53 SS18
NORMAL MODE 33	OBSERVED=	1001.0 CM-1	CALCULATED= 1003.1 CM-1	ERROR= -2.1 CM-1	OR -0.2 PERCENT
INTERNAL COORDINATES-	10.95	C-08	10.31 C1H	9.83 C5C*	7.05 C-08
FORCE CONSTANTS-	37.69	CO	23.39 UCH	19.42 CC	19.19 CCH
OFF DIAGONAL-	-6.26	SB21	-4.78 SB28	-3.43 SB24	-3.18 BB29
NORMAL MODE 34	OBSERVED=	994.0 CM-1	CALCULATED= 987.8 CM-1	ERROR= 6.2 CM-1	OR 0.6 PERCENT
INTERNAL COORDINATES-	12.90	C1H	12.56 C5C*	10.98 C-06	9.73 C-09
FORCE CONSTANTS-	30.75	CO	28.41 CC	19.52 OCH	17.40 CCH
OFF DIAGONAL-	-6.68	SB22	-6.16 SB21	3.63 SB27	-3.32 SB28
NORMAL MODE 35	OBSERVED=	963.0 CM-1	CALCULATED= 968.3 CM-1	ERROR= -5.3 CM-1	OR -0.5 PERCENT
INTERNAL COORDINATES-	21.30	C3C4	19.43 OC1H	16.39 C-08	9.63 C-08
FORCE CONSTANTS-	33.08	CC	31.80 CC	23.08 OCH	14.37 CCH
OFF DIAGONAL-	-6.45	SB22	-3.55 SB25	2.83 SS18	-7.72 SB28

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400
MOLECULE 4 -6 NG=1236 ALPHA GLUCOSE-1-D

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NORMAL MODE 36	OBSERVED=	955.0 CM-1	CALCULATED=	952.1 CM-1	ERROR=	1.9 CM-1	OR	0.2 PERCENT
INTERNAL COORDINATES-	17.17	CC14	14.95	CC12	10.86	CC1H	6.06	C3C4
FORCE CONSTANTS-	34.30	OCH	24.70	CC	19.36	CCH	17.92	CO
OFF DIAGONAL-	-8.95	S822	-7.10	S826	4.74	S827	3.81	SS18
NORMAL MODE 37	OBSERVED=	875.0 CM-1	CALCULATED=	870.5 CM-1	ERROR=	4.4 CM-1	OR	0.5 PERCENT
INTERNAL COORDINATES-	27.57	CC06	14.24	CC1H	11.88	C2C3	10.69	CCH2
FORCE CONSTANTS-	33.54	CCH	31.36	CC	16.33	CCO	15.44	CC
OFF DIAGONAL-	-8.83	S827	-4.58	S821	-4.39	S822	4.18	S826
NORMAL MODE 38	OBSERVED=	810.0 CM-1	CALCULATED=	806.4 CM-1	ERROR=	3.6 CM-1	OR	0.4 PERCENT
INTERNAL COORDINATES-	29.66	CC04	14.03	CCHA	13.28	*C1H	12.41	CCH8
FORCE CONSTANTS-	37.06	CC	33.07	CCH	17.38	OCH	8.61	CCO
OFF DIAGONAL-	-4.81	S825	-2.88	BB29	2.80	S827	1.66	S826
NORMAL MODE 39	OBSERVED=	761.0 CM-1	CALCULATED=	739.5 CM-1	ERROR=	21.5 CM-1	OR	2.8 PERCENT
INTERNAL COORDINATES-	17.28	CC1H	13.00	CC04	6.90	C2C3	5.92	C-06
FORCE CONSTANTS-	27.19	CCH	18.02	CCO	13.63	CC	13.00	COC
OFF DIAGONAL-	5.70	BB43	4.28	S825	-3.77	BB34	-3.18	S826
NORMAL MODE 40	OBSERVED=	637.0 CM-1	CALCULATED=	633.0 CM-1	ERROR=	3.9 CM-1	OR	0.6 PERCENT
INTERNAL COORDINATES-	19.86	OBCC	8.24	CCO	6.04	HC3C	6.02	CCO9
FORCE CONSTANTS-	36.04	CCO	21.63	CCH	9.97	CO	8.24	CCO
OFF DIAGONAL-	-6.97	BB34	6.61	BB43	-4.61	BB29	4.52	S825
NORMAL MODE 41	OBSERVED=	621.0 CM-1	CALCULATED=	614.5 CM-1	ERROR=	6.5 CM-1	OR	1.0 PERCENT
INTERNAL COORDINATES-	17.65	CC04	13.53	CCO6	7.56	CCO7	6.02	CCO9
FORCE CONSTANTS-	62.05	CCO	32.37	CCH	5.21	CCH	7.21	HC4C
OFF DIAGONAL-	-12.12	BB34	7.57	BB43	-6.66	BB29	2.18	S825
NORMAL MODE 42	OBSERVED=	552.0 CM-1	CALCULATED=	547.6 CM-1	ERROR=	4.4 CM-1	OR	0.8 PERCENT
INTERNAL COORDINATES-	18.30	OBCC	10.54	CCO9	7.81	C2C3	5.96	C1C2
FORCE CONSTANTS-	45.12	CCO	22.98	CCH	17.33	CC	9.30	CO
OFF DIAGONAL-	-10.15	BB34	6.64	BB43	-4.69	BB29	2.76	SS18
NORMAL MODE 43	OBSERVED=	532.0 CM-1	CALCULATED=	530.6 CM-1	ERROR=	1.3 CM-1	OR	0.3 PERCENT
INTERNAL COORDINATES-	17.62	CCO4	16.91	CCO	11.70	O1CC	7.15	C-09
FORCE CONSTANTS-	41.33	CCO	16.91	CCO	14.29	CO	8.51	CCH
OFF DIAGONAL-	6.52	S825	-4.71	BB34	4.32	S822	-3.30	S821
NORMAL MODE 44	OBSERVED=	420.0 CM-1	CALCULATED=	445.9 CM-1	ERROR=	4.1 CM-1	OR	0.9 PERCENT
INTERNAL COORDINATES-	10.79	C2CC	10.05	CCO*	9.84	C3CC	6.18	CC3H
FORCE CONSTANTS-	33.19	CCO	26.04	CCC	22.93	CCO	5.98	CCO6
OFF DIAGONAL-	7.24	BB43	5.08	BB34	-5.04	BB29	-1.53	BB41
NORMAL MODE 45	OBSERVED=	433.0 CM-1	CALCULATED=	425.8 CM-1	ERROR=	7.2 CM-1	OR	1.7 PERCENT
INTERNAL COORDINATES-	15.15	O9CC	13.91	O1CC	13.43	CCO	9.95	CCO7
FORCE CONSTANTS-	59.84	CCO	13.94	CCC	13.93	CCO	6.83	CCO
OFF DIAGONAL-	6.03	S827	-4.63	BB34	4.52	S825	-4.51	S821
NORMAL MODE 46	OBSERVED=	404.0 CM-1	CALCULATED=	387.2 CM-1	ERROR=	16.8 CM-1	OR	4.1 PERCENT
INTERNAL COORDINATES-	13.64	C2CC	12.84	OBCC	10.36	CCO8	7.00	CCO
FORCE CONSTANTS-	50.87	CCO	24.78	CCC	7.52	CCH	7.44	CC
OFF DIAGONAL-	-6.59	BB34	-4.44	BB42	4.25	S825	4.24	S821
NORMAL MODE 47	OBSERVED=	375.0 CM-1	CALCULATED=	371.9 CM-1	ERROR=	3.1 CM-1	OR	0.8 PERCENT
INTERNAL COORDINATES-	16.92	CCO4	12.49	O7CC	6.42	CCO	5.39	CCO8
FORCE CONSTANTS-	49.37	CCO	21.53	CCH	10.50	CC	6.42	CCO
OFF DIAGONAL-	-7.20	BB34	3.75	BB43	-3.20	BB29	-3.18	S826
NORMAL MODE 48	OBSERVED=	0.0 CM-1	CALCULATED=	319.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	16.66	CCO9	13.14	CCO8	7.26	O7CC	6.71	C3C4
FORCE CONSTANTS-	62.95	CCO	13.09	CC	7.96	CCH	7.96	T-0H
OFF DIAGONAL-	-7.19	BB34	4.41	S822	2.47	BB43	-2.36	BB42
NORMAL MODE 49	OBSERVED=	0.0 CM-1	CALCULATED=	312.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	23.47	CCO7	13.67	CCO8	7.52	OBCC	7.37	CCO*
FORCE CONSTANTS-	72.23	CCO	9.12	CC	8.37	T-0H	5.49	CCH
OFF DIAGONAL-	-6.94	BB34	-3.83	BB42	2.58	S822	2.32	S821
NORMAL MODE 50	OBSERVED=	0.0 CM-1	CALCULATED=	302.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	19.75	OBCC	17.75	O9CC	10.71	4C04	7.86	CCO8
FORCE CONSTANTS-	75.85	CCO	13.08	CCH	12.65	T-0H	6.63	CCC
OFF DIAGONAL-	-11.30	BB34	-2.53	BB42	-2.33	S825	2.21	BB43
NORMAL MODE 51	OBSERVED=	0.0 CM-1	CALCULATED=	257.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	20.85	CCO6	9.72	O1CC	8.91	CCO9	7.43	CH2
FORCE CONSTANTS-	57.35	CCO	18.76	CCH	12.65	T-0H	8.34	CCC
OFF DIAGONAL-	-8.91	BB34	7.20	BB43	-3.59	S825	-3.28	BB33
NORMAL MODE 52	OBSERVED=	0.0 CM-1	CALCULATED=	242.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	63.72	T-0H	19.05	CCO*	6.99	C4CC	6.99	CCC
FORCE CONSTANTS-	63.72	T-0H	19.05	CCO	7.99	CCC		
OFF DIAGONAL-	-1.59	BB34						
NORMAL MODE 53	OBSERVED=	0.0 CM-1	CALCULATED=	228.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	54.49	TH-1	25.34	TH-3	8.09	TH-2	6.30	TH-4
FORCE CONSTANTS-	94.22	T-0H						
OFF DIAGONAL-	NONE							
NORMAL MODE 54	OBSERVED=	0.0 CM-1	CALCULATED=	222.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	45.79	TH-4	17.93	TH-1	16.59	TH-5	9.48	TH-3
FORCE CONSTANTS-	89.85	T-0H	5.23	CCO				
OFF DIAGONAL-	NONE							
NORMAL MODE 55	OBSERVED=	0.0 CM-1	CALCULATED=	215.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	36.15	TH-3	30.04	TH-4	9.90	TH-1	6.73	TH-2
FORCE CONSTANTS-	83.14	T-0H	14.33	CCO				
OFF DIAGONAL-	-1.82	BB34						
NORMAL MODE 56	OBSERVED=	0.0 CM-1	CALCULATED=	213.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	69.40	TH-2	12.22	TH-3				
FORCE CONSTANTS-	85.63	T-0H	14.50	CCO				
OFF DIAGONAL-	NONE							
NORMAL MODE 57	OBSERVED=	0.0 CM-1	CALCULATED=	199.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	23.81	TH-2	24.62	CCO*	13.13	C4CC	6.44	CC5
FORCE CONSTANTS-	37.40	CCO	31.58	T-0H	14.56	CCC	8.19	T-CC
OFF DIAGONAL-	-4.07	BB34	-2.70	BB42	-2.35	BB33	6.36	CCH
NORMAL MODE 58	OBSERVED=	0.0 CM-1	CALCULATED=	129.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	22.21	CCO*	14.82	C4CC	10.16	TCC4	6.42	C1CC
FORCE CONSTANTS-	22.37	CCC	22.21	CCC	12.34	T-CC	11.60	CCO
OFF DIAGONAL-	3.88	BB43	-3.56	S821	-2.46	BB37	1.97	BB41
NORMAL MODE 59	OBSERVED=	0.0 CM-1	CALCULATED=	97.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	54.50	TCC5	9.88	C3CC	6.66	O9CC	5.03	TCC2
FORCE CONSTANTS-	63.52	T-CC	18.67	CCC	17.19	CCO		
OFF DIAGONAL-	-3.28	S825	-2.59	BB34	-2.33	S821	-2.25	BB42
NORMAL MODE 60	OBSERVED=	0.0 CM-1	CALCULATED=	81.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	21.35	C2CC	14.61	C1CC	8.42	CCO*	7.34	TCC5
FORCE CONSTANTS-	27.62	CCC	17.62	CCC	11.09	CCO	8.42	CCO
OFF DIAGONAL-	-4.11	S825	-3.98	BB42	-3.10	S821	2.40	BB41
NORMAL MODE 61	OBSERVED=	0.0 CM-1	CALCULATED=	74.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	22.87	TCC5	14.03	C3CC	7.40	TCC3	7.08	TCC2
FORCE CONSTANTS-	48.27	T-CC	23.15	CCO	21.99	CCC	5.94	4C0*
OFF DIAGONAL-	-2.67	BB42	-7.23	BB34	-1.71	S825	5.44	C1CC

3b. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 5.40

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400									
MOLECULE 5 -6 NG=1236 ALPHA GLUCOSE-C1-D,-O-D5									
PAGE 1									
NORMAL MODE 8	OBSERVED=	1457.0	CM-1	CALCULATED=	1449.7	CM-1	ERROR=	7.3	CM-1 OR 0.5 PERCENT
INTERNAL COORDINATES-	61.46	HCH	20.69	OCBH	18.98	OCBA			
FORCE CONSTANTS-	61.46	HCH	40.06	OCBH					
OFF DIAGONAL-	-4.05	SB27							
NORMAL MODE 9	OBSERVED=	1410.0	CM-1	CALCULATED=	1408.1	CM-1	ERROR=	1.9	CM-1 OR 0.1 PERCENT
INTERNAL COORDINATES-	19.98	OC4H	13.67	HCAC	13.44	CC5H	10.24	CC5H	7.27
FORCE CONSTANTS-	43.73	CC4H	40.75	OCBH	11.17	CO	9.94	CC5H	7.05
OFF DIAGONAL-	-9.97	SB27	9.24	BB29	6.08	BB34	-4.23	SB25	-3.78
NORMAL MODE 10	OBSERVED=	1378.3	CM-1	CALCULATED=	1378.3	CM-1	ERROR=	0.0	CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	15.31	OC3H	14.24	OC2H	11.84	HC2C	0.41	CC5H	9.36
FORCE CONSTANTS-	46.46	CC4H	42.24	OCBH	9.32	CO	9.32	CC5H	6.35
OFF DIAGONAL-	10.06	BB29	-8.73	SB27	-3.95	SB26	-3.55	BB45	3.53
NORMAL MODE 11	OBSERVED=	1353.6	CM-1	CALCULATED=	1353.6	CM-1	ERROR=	0.0	CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	19.82	CCBH	16.52	HC5C	10.16	OC2H	0.13	OCBH	7.02
FORCE CONSTANTS-	60.47	CCH	27.40	UCH	6.25	CO			
OFF DIAGONAL-	13.18	BB29	-8.07	SB26	-5.57	SB27	-3.65	BB45	2.01
NORMAL MODE 12	OBSERVED=	1330.9	CM-1	CALCULATED=	1330.9	CM-1	ERROR=	0.0	CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	16.30	HC3C	11.10	OC2H	10.11	CC4H	7.89	CCBH	7.66
FORCE CONSTANTS-	65.88	CCH	26.78	OCBH	6.09	CO	3.61	CC	
OFF DIAGONAL-	11.88	BB29	-10.53	SB26	-5.72	SB27	-3.96	BB45	-1.70
NORMAL MODE 13	OBSERVED=	1317.8	CM-1	CALCULATED=	1317.8	CM-1	ERROR=	0.0	CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	23.31	CC2H	9.86	C-06	8.77	CC4H	8.24	CC3H	7.27
FORCE CONSTANTS-	94.68	CC4H	28.94	OCBH	19.53	CO	19.53	CO	19.53
OFF DIAGONAL-	-7.30	SB27	-3.55	BB45	3.08	BB34	2.90	BB29	-2.84
NORMAL MODE 14	OBSERVED=	1303.9	CM-1	CALCULATED=	1303.9	CM-1	ERROR=	0.0	CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	17.57	CC4H	14.16	OCBA	12.08	HC3C	9.77	HC4C	7.61
FORCE CONSTANTS-	62.20	CC4H	31.16	UCH					
OFF DIAGONAL-	-4.46	SB26	-3.99	BB45	3.32	BB29			
NORMAL MODE 15	OBSERVED=	1292.8	CM-1	CALCULATED=	1292.8	CM-1	ERROR=	0.0	CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	21.06	OC2H	14.33	OC3H	13.44	HC2C	8.49	CC3H	7.50
FORCE CONSTANTS-	38.87	UCH	27.11	CC4H	13.32	CO	9.04	BCOH	8.82
OFF DIAGONAL-	-5.15	BB29	-4.32	SB25	4.19	SB27	3.84	BB34	-2.50
NORMAL MODE 16	OBSERVED=	1281.0	CM-1	CALCULATED=	1281.0	CM-1	ERROR=	0.0	CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	28.56	*C5H	13.02	OC4H	12.39	CC5H	12.11	OCBA	11.64
FORCE CONSTANTS-	61.09	UCH	31.10	CC4H					
OFF DIAGONAL-	5.16	SB27	-3.62	BB45	-2.62	BB29			
NORMAL MODE 17	OBSERVED=	1262.4	CM-1	CALCULATED=	1262.4	CM-1	ERROR=	0.0	CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	17.42	OC4H	12.34	CC4H	11.71	HC5C	9.87	*C5H	7.33
FORCE CONSTANTS-	49.81	CC4H	36.33	CC4H	13.22	CO	9.87	OCBH	7.06
OFF DIAGONAL-	7.34	SB27	-6.30	BB29	3.87	BB34	-3.12	BB45	-2.57
NORMAL MODE 18	OBSERVED=	1226.2	CM-1	CALCULATED=	1226.2	CM-1	ERROR=	0.0	CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	19.72	OC3H	11.35	CC5H	10.42	OCBH	10.34	HC5C	9.15
FORCE CONSTANTS-	42.75	CC4H	34.11	UCH	8.84	BCOH	7.90	CCO	7.57
OFF DIAGONAL-	-7.79	BB29	4.54	BB34	3.74	SB27	-2.89	SB25	-2.54
NORMAL MODE 19	OBSERVED=	1201.9	CM-1	CALCULATED=	1201.9	CM-1	ERROR=	0.0	CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	27.95	C2C3	15.67	C3OH	7.45	OCBH			
FORCE CONSTANTS-	35.12	CC	23.59	BCOH	17.60	UCH	14.52	CCO	9.12
OFF DIAGONAL-	-7.11	SB22	-5.04	SB21	-3.53	SB25	2.94	BB36	1.62
NORMAL MODE 20	OBSERVED=	1182.9	CM-1	CALCULATED=	1182.9	CM-1	ERROR=	0.0	CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	11.33	C2C3	9.52	OCBH	8.45	C4C1	8.10	OCBA	6.84
FORCE CONSTANTS-	28.45	UCH	24.95	CC	19.59	CO	12.62	CCO	11.42
OFF DIAGONAL-	-5.53	SB22	-4.07	SB25	-2.88	SB23	-2.27	SB27	1.99
NORMAL MODE 21	OBSERVED=	1170.4	CM-1	CALCULATED=	1170.4	CM-1	ERROR=	0.0	CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	26.44	*C1C	22.51	C5O*	9.28	C5C*	10.01	C1OH	7.78
FORCE CONSTANTS-	50.70	CC	21.04	CC	10.97	CC4H	12.43	UCH	11.38
OFF DIAGONAL-	-4.95	SB22	-4.02	SB24	-3.17	SB26	-2.91	SB25	-2.63
NORMAL MODE 22	OBSERVED=	1144.3	CM-1	CALCULATED=	1144.3	CM-1	ERROR=	0.0	CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	17.86	C-07	15.36	C3C4	17.86	C-07	15.36	C-07	6.58
FORCE CONSTANTS-	37.06	CC	34.76	CC	20.84	CC2	13.12	CC4H	6.32
OFF DIAGONAL-	-8.49	SB22	-4.76	SB25	-3.16	SB26	-2.38	SS18	1.97
NORMAL MODE 23	OBSERVED=	1141.4	CM-1	CALCULATED=	1141.4	CM-1	ERROR=	0.0	CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	31.16	C1C2	21.15	C1OH	11.33	C3C4	8.20	C4OH	
FORCE CONSTANTS-	48.58	CC	34.87	BCOH	15.03	CC2	15.03	CC4H	9.50
OFF DIAGONAL-	-12.80	SB22	-9.74	SB26	-3.62	SB27	-2.57	SS18	-2.54
NORMAL MODE 24	OBSERVED=	1127.5	CM-1	CALCULATED=	1127.5	CM-1	ERROR=	0.0	CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	26.97	C-07	19.79	C3C4	9.39	C4OH	7.69	C1C2	6.30
FORCE CONSTANTS-	45.32	CC	34.99	CC	15.71	OC4H	11.97	BCOH	11.56
OFF DIAGONAL-	-10.10	SB27	-6.75	SB21	-6.31	SB25	-4.16	SS18	-3.06
NORMAL MODE 25	OBSERVED=	1112.8	CM-1	CALCULATED=	1112.8	CM-1	ERROR=	0.0	CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	21.22	C5C*	18.56	C4C5	14.66	C-09	8.92	C-09	8.42
FORCE CONSTANTS-	50.70	CC	21.04	CC	10.97	CC4H	12.43	UCH	11.38
OFF DIAGONAL-	-5.55	SB27	-4.64	SS18	-3.22	SB22	1.95	SB28	-1.63
NORMAL MODE 26	OBSERVED=	1095.9	CM-1	CALCULATED=	1095.9	CM-1	ERROR=	0.0	CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	18.98	C-09	15.36	C4C5	18.98	C-09	15.36	C-09	6.18
FORCE CONSTANTS-	39.11	CC	20.50	CC	16.32	UCH	13.25	CC4H	13.15
OFF DIAGONAL-	-8.21	SB21	-6.80	SB25	-5.96	SB27	-2.64	SS18	-1.78
NORMAL MODE 27	OBSERVED=	1057.8	CM-1	CALCULATED=	1057.8	CM-1	ERROR=	0.0	CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	30.62	C4C5	21.93	C-08	19.99	C-08	8.59	C-09	6.53
FORCE CONSTANTS-	55.13	CC	33.02	CC	7.31	UCH	6.61	BCOH	6.53
OFF DIAGONAL-	-6.32	SB27	-5.14	SS18	-4.68	SB22	-4.42	SB21	
NORMAL MODE 28	OBSERVED=	1050.8	CM-1	CALCULATED=	1050.8	CM-1	ERROR=	0.0	CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	28.93	C-09	23.41	C-07	14.59	C-08	12.37	C3OH	
FORCE CONSTANTS-	74.39	CC	14.02	BCOH	12.89	CC4H	8.52	CCO	6.00
OFF DIAGONAL-	-7.15	SB25	-6.01	SB28	-4.08	SB27	-2.71	BB29	
NORMAL MODE 29	OBSERVED=	1029.8	CM-1	CALCULATED=	1029.8	CM-1	ERROR=	0.0	CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	41.94	C-08	19.58	C4OH	10.84	C2OH	5.89	C-07	
FORCE CONSTANTS-	51.42	CC	18.95	BCOH	13.99	CC4H	13.99	CC4H	6.00
OFF DIAGONAL-	-14.74	SB28	-6.25	SB25	-9.11	SB27	-3.12	BB29	-2.90
NORMAL MODE 30	OBSERVED=	1008.3	CM-1	CALCULATED=	1008.3	CM-1	ERROR=	0.0	CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	18.98	C2OH	10.67	C1OH	15.27	CC4H	6.87	C1C2	6.33
FORCE CONSTANTS-	39.99	BCOH	22.11	CC	2.04	BB34	1.98	SB26	-1.67
OFF DIAGONAL-	-7.66	SB28	3.57	SB27					
NORMAL MODE 31	OBSERVED=	997.7	CM-1	CALCULATED=	997.7	CM-1	ERROR=	0.0	CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	20.76	C2OH	18.42	C-06	14.55	C4OH	9.27	C-09	7.12
FORCE CONSTANTS-	47.41	BCOH	38.01	CC	15.33	CC4H	6.63	CC	6.25
OFF DIAGONAL-	-8.93	SB28	-3.24	SB24	-2.67	SB29	-2.25	SB25	-1.65
NORMAL MODE 32	OBSERVED=	995.5	CM-1	CALCULATED=	995.5	CM-1	ERROR=	0.0	CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	28.85	OC1H	24.76	*C1H	8.01	C1C2	6.75	C1OH	6.62
FORCE CONSTANTS-	56.69	UCH	14.26	BCOH	14.09	CC	9.36	CC	9.17
OFF DIAGONAL-	-4.17	SB28	3.57	SB27	-1.97	BB45	-1.59	SS18	-1.58
NORMAL MODE 33	OBSERVED=	952.4	CM-1	CALCULATED=	952.4	CM-1	ERROR=	0.0	CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	32.28	C*UH	13.53	C5C*	11.28	C4OH	7.28	C3OH	6.27
FORCE CONSTANTS-	54.61	CC	20.95	CC	14.86	CC	8.95	CC4H	5.32
OFF DIAGONAL-	-6.18	SB28	4.78	SB21	-2.57	SB22	-2.17	SB24	-1.82
NORMAL MODE 34	OBSERVED=	936.2	CM-1	CALCULATED=	936.2	CM-1	ERROR=	0.0	CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	37.30	C*UH	21.85	C3OH	21.14	CC4H	20.41	CC	5.49
FORCE CONSTANTS-	47.96	BCOH	21.85	CC	21.14	CC4H	20.41	CC	5.29
OFF DIAGONAL-	-4.96	SB21	-3.48	SB22	-2.85	BB29	-1.73	SB28	1.65
NORMAL MODE 35	OBSERVED=	916.7	CM-1	CALCULATED=	916.7	CM-1	ERROR=	0.0	CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	34.25	C4OH	27.38	C3C4	8.00	C-08	7.92	C3OH	6.78
FORCE CONSTANTS-	48.88	BCOH	31.13	CC	15.17	CO	10.61	UCH	10.21
OFF DIAGONAL-	-6.93	SB28	-4.84	SB22	-3.63	SB21	-3.01	SB26	-2.62

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400										PAGE 2	
MOLECULE 5 -6 NG=1236 ALPHA GLUCOSE-C1-D,-O-D5											
NORMAL MODE 36	OBSERVED=	0.0 CM-1	CALCULATED=	897.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	28.32 C1OH	23.50 OC1H	16.33 C1C2	15.05 CC1H							
FORCE CONSTANTS-	33.66 BC0H	26.16 OCH	22.22 CCH	20.57 CC	10.44 CO	5.96 CCO					
OFF DIAGONAL-	-8.09 SB26	-5.19 SB22	-2.63 SB27	-2.39 SB28	2.35 BB39						
NORMAL MODE 37	OBSERVED=	0.0 CM-1	CALCULATED=	841.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	18.04 C2C3	15.38 C-U6	9.93 C3OH	9.59 C2OH	8.88 CC08	6.83 CCH2					
FORCE CONSTANTS-	23.19 CC	19.84 BC0H	19.69 CO	19.59 CCH	16.28 CCO	7.89 OCH					
OFF DIAGONAL-	-6.66 SB21	-5.25 SB22	-4.54 SB27	2.86 SB28	2.74 SB25	2.38 BB43	-2.09 SB24	-1.54 BB29	-1.54 SB28		
NORMAL MODE 38	OBSERVED=	0.0 CM-1	CALCULATED=	802.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	28.47 C5OH	13.98 C1H	12.34 CCHA	11.43 CCHB	6.33 C5C	5.99 OC1					
FORCE CONSTANTS-	34.55 CO	32.14 CCH	17.91 OCH	9.16 CC	9.03 CCO						
OFF DIAGONAL-	-4.79 SB25	-5.72 SB27	-2.71 BB29	-2.02 SB22	-1.89 BB34	-1.58 SB23					
NORMAL MODE 39	OBSERVED=	0.0 CM-1	CALCULATED=	733.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	16.50 CC1H	13.94 C-U6	13.94 C3C3	13.48 CC	12.77 CO	5.57 CCC					
FORCE CONSTANTS-	26.23 CCH	16.38 CCO	-3.20 SB26	-2.98 BB34	2.82 SB24	2.48 SB22	-2.14 BB41	-1.79 SB23			
OFF DIAGONAL-	5.18 BB43	4.05 SB25									
NORMAL MODE 40	OBSERVED=	0.0 CM-1	CALCULATED=	621.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	16.70 OCH	11.88 CCU*	9.94 CC5H	7.38 HC4C	5.62 C4CC	5.43 OC9C	5.12 HC3C				
FORCE CONSTANTS-	45.24 CCO	27.73 CCH	7.65 CCC	7.03 CO							
OFF DIAGONAL-	-10.10 BB34	8.59 BB43	-6.12 BB29	4.17 SB25	1.92 SB22	-1.90 SB27	-1.86 BB36	1.65 SB21			
NORMAL MODE 41	OBSERVED=	0.0 CM-1	CALCULATED=	604.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	19.44 CCO6	10.41 CCU7	8.41 CCO*	8.30 CCO*	7.17 OCO	6.42 CCHB					
FORCE CONSTANTS-	52.02 CCO	23.63 CCH	8.11 CC	7.17 OCO							
OFF DIAGONAL-	-8.27 BB34	5.31 BB43	-4.54 BB29	2.14 SB25	-2.04 BB41						
NORMAL MODE 42	OBSERVED=	0.0 CM-1	CALCULATED=	541.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	12.41 O7CC	9.50 C2C3	8.92 CCO9	5.94 C1C2	5.00 CC4H						
FORCE CONSTANTS-	38.55 CCH	21.63 CCO	20.23 CCO	13.11 CCO							
OFF DIAGONAL-	-3.06 BB34	4.93 BB43	3.76 SS18	-3.96 BB29	3.57 SB25	-2.27 SB27	2.18 SB21	-1.64 BB36			
NORMAL MODE 43	OBSERVED=	0.0 CM-1	CALCULATED=	520.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	17.61 CCO	14.29 O*CC	13.89 CCO*	7.57 O7CC							
FORCE CONSTANTS-	44.82 CCH	17.61 CCO	10.25 CCH	9.44 CCO	9.15 CCC						
OFF DIAGONAL-	-6.64 BB34	3.90 SB25	-3.51 BB42	-3.43 SB21	2.75 BB43	2.00 SB22	-1.95 BB29	-1.55 SB27			
NORMAL MODE 44	OBSERVED=	0.0 CM-1	CALCULATED=	441.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	10.61 C2CC	9.42 CCO*	8.96 C3C3	6.58 CCO6	6.58 CCO9	5.79 CC3H					
FORCE CONSTANTS-	32.88 CCO	24.78 CCC	21.81 CCH	6.25 CC							
OFF DIAGONAL-	6.64 BB34	-4.76 BB29	-4.49 BB34	1.89 SB22	-1.51 BB41						
NORMAL MODE 45	OBSERVED=	0.0 CM-1	CALCULATED=	419.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	15.49 O*CC	15.20 O9CC	13.09 OCO	10.18 CCO*	9.98 CCO7	6.89 C1CC	5.51 C4C5				
FORCE CONSTANTS-	53.18 CCO	13.60 CUC	13.09 OCO	6.49 CO	5.96 CC						
OFF DIAGONAL-	5.35 SB22	-5.16 BB34	-4.60 SB21	4.39 SB25	-4.29 BB42	-1.56 SB27					
NORMAL MODE 46	OBSERVED=	0.0 CM-1	CALCULATED=	383.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	14.75 CCH	12.47 C2CC	10.50 O8CC	7.19 O9CC	6.15 C3CC	5.75 CCO9	5.01 CCO6				
FORCE CONSTANTS-	44.82 CCH	23.30 CCO	9.05 CCH	8.69 CC							
OFF DIAGONAL-	-7.30 BB34	4.68 SB21	4.53 SB25	-4.05 BB42	-2.21 SB26	-1.64 BB36	-1.53 BB41	-1.52 BB29			
NORMAL MODE 47	OBSERVED=	0.0 CM-1	CALCULATED=	366.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	19.80 CCO	13.34 C7CC	8.72 OCO	8.27 CC	5.21 CCC	5.07 CO					
FORCE CONSTANTS-	45.30 CCO	21.11 CCH	8.72 OCO	2.57 SB24	-2.40 SB26	2.40 SB21	-2.00 BB33				
OFF DIAGONAL-	-6.85 BB34	4.10 BB43	-3.41 BB29								
NORMAL MODE 48	OBSERVED=	0.0 CM-1	CALCULATED=	312.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	13.23 CCO9	10.46 CCO8	8.19 O7CC	6.63 C3C4	5.95 CCO6	5.22 CCO*	5.00 CCO7				
FORCE CONSTANTS-	62.24 CCO	15.06 CC	9.48 CCH	6.48 CCC							
OFF DIAGONAL-	-7.36 BB34	4.01 SB22	3.03 SB21	2.88 BB43	-2.34 BB42						
NORMAL MODE 49	OBSERVED=	0.0 CM-1	CALCULATED=	308.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	23.24 CCO7	10.82 CCO8	9.14 CCO*	8.58 CCO*	6.32 O7CC	5.80 O8CC					
FORCE CONSTANTS-	73.78 CCO	9.50 CC	5.60 CCH								
OFF DIAGONAL-	-7.10 BB34	-3.93 BB42	2.89 SB22	2.79 SB21							
NORMAL MODE 50	OBSERVED=	0.0 CM-1	CALCULATED=	296.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	27.31 O8CC	18.33 O9CC	12.16 CCO8	8.57 O7CC	8.54 CCO*						
FORCE CONSTANTS-	87.66 CCO	13.89 C4H	9.15 O7CC	8.54 CCO*							
OFF DIAGONAL-	-11.59 BB34	3.60 BB42	-2.13 BB36	-2.00 SB25							
NORMAL MODE 51	OBSERVED=	0.0 CM-1	CALCULATED=	248.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	25.66 CCO	9.59 O*CC	9.15 O7CC	8.96 CCH2	7.81 CCO9	6.01 CCO7	5.96 HC2C	5.34 C1CC			
FORCE CONSTANTS-	64.39 CCO	21.60 CCH	7.83 CCC	-4.23 SB25	-3.96 BB33	-2.81 BB29	2.14 SB22	-1.59 BB36			
OFF DIAGONAL-	-9.75 BB34	8.26 BB43									
NORMAL MODE 52	OBSERVED=	0.0 CM-1	CALCULATED=	219.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	24.79 CCO	16.35 C4CC	13.07 TH-5	10.40 COC*	5.31 CCO*						
FORCE CONSTANTS-	44.41 CCO	19.02 CCC	16.73 T-OH	10.40 CCO	5.41 CCH						
OFF DIAGONAL-	-4.05 BB34	-2.88 BB42	-1.83 BB33								
NORMAL MODE 53	OBSERVED=	0.0 CM-1	CALCULATED=	174.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	58.17 TH-1	15.22 TH-3									
FORCE CONSTANTS-	79.67 T-OH	5.26 CCC									
OFF DIAGONAL-	NONE										
NORMAL MODE 54	OBSERVED=	0.0 CM-1	CALCULATED=	164.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	43.64 TH-4	23.04 TH-3									
FORCE CONSTANTS-	92.70 T-OH										
OFF DIAGONAL-	NONE										
NORMAL MODE 55	OBSERVED=	0.0 CM-1	CALCULATED=	158.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	60.40 TH-4	12.89 TH-4									
FORCE CONSTANTS-	78.32 T-OH	8.80 CCO									
OFF DIAGONAL-	NONE										
NORMAL MODE 56	OBSERVED=	0.0 CM-1	CALCULATED=	156.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	43.82 TH-3	31.82 TH-4									
FORCE CONSTANTS-	91.66 T-OH	6.58 CCO									
OFF DIAGONAL-	NONE										
NORMAL MODE 57	OBSERVED=	0.0 CM-1	CALCULATED=	154.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	75.30 TH-2	7.30 TH-3									
FORCE CONSTANTS-	90.46 T-OH	6.91 CCO									
OFF DIAGONAL-	NONE										
NORMAL MODE 58	OBSERVED=	0.0 CM-1	CALCULATED=	120.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	17.61 CO	16.94 TH-1									
FORCE CONSTANTS-	18.56 T-OH	2.91 SB21									
OFF DIAGONAL-	3.20 BB43	-2.91 SB21									
NORMAL MODE 59	OBSERVED=	0.0 CM-1	CALCULATED=	94.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	54.97 TCC	8.99 C3CC									
FORCE CONSTANTS-	60.26 T-CC	17.67 CCC									
OFF DIAGONAL-	-3.10 SB25	-2.64 BB34									
NORMAL MODE 60	OBSERVED=	0.0 CM-1	CALCULATED=	78.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	21.34 C2CC	15.03 C1CC									
FORCE CONSTANTS-	41.62 CCC	25.86 T-CC									
OFF DIAGONAL-	-4.22 SB25	-4.03 BB42									
NORMAL MODE 61	OBSERVED=	0.0 CM-1	CALCULATED=	63.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	22.80 TCC5	14.09 C3CC									
FORCE CONSTANTS-	48.01 T-CC	23.21 CCO									
OFF DIAGONAL-	-2.66 BB42	-2.26 BB34									

2. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 4.58

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400									
MOLECULE 6 -6 NG-1236 ALPHA GLUCOSE-6-6-D2									
PAGE 1									
NORMAL MODE 8	OBSERVED=	1443.0	CM-1	CALCULATED=	1455.2	CM-1	ERROR=	-12.2	CM-1 OR -0.8 PERCENT
INTERNAL COORDINATES-	68.02	C2CH							
FORCE CONSTANTS-	68.45	CCCH	6.58 CCH	6.05 CCO					
OFF DIAGONAL-		BB36	3.84 SB28	-1.77 SB25	1.68 BB34				
NORMAL MODE 9	OBSERVED=	1416.0	CM-1	CALCULATED=	1420.6	CM-1	ERROR=	-5.6	CM-1 OR -0.4 PERCENT
INTERNAL COORDINATES-	85.60	C3CH	24.05 C4OH	10.72 CCH					
FORCE CONSTANTS-	55.97	BCCH	15.29 CCH	13.72 CCH	7.76 CC	5.32 CO	5.24 CCO		
OFF DIAGONAL-	-4.45	SB26	-3.91 SB27	3.90 SB28	3.01 BB36	2.99 BB29	-2.21 SB25	1.92 BB34	-1.76 BB43 -1.58 SB21
NORMAL MODE 10	OBSERVED=	0.0	CM-1	CALCULATED=	1412.6	CM-1	ERROR=	0.0	CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	30.63	C3OH	9.89 OC3H	8.98 OC4H					
FORCE CONSTANTS-	37.79	BCCH	31.12 UCH	19.11 CCH	6.74 CO				
OFF DIAGONAL-	-6.17	SB27	4.26 BB29	4.17 SB28	-3.79 SB26	-1.96 BB45	-1.95 BB39	1.82 BB34	-1.69 SB25 1.66 BB36
NORMAL MODE 11	OBSERVED=	0.0	CM-1	CALCULATED=	1408.8	CM-1	ERROR=	0.0	CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	53.38	C1OH	20.18 OC1H						
FORCE CONSTANTS-	56.47	BCCH	29.73 UCH	-9.42 CCH					
OFF DIAGONAL-	-4.77	SB28	-4.48 SB27	-3.07 BB39	-1.51 BB45				
NORMAL MODE 12	OBSERVED=	1382.0	CM-1	CALCULATED=	1386.2	CM-1	ERROR=	-4.2	CM-1 OR -0.3 PERCENT
INTERNAL COORDINATES-	42.41	C1H	21.72 C1OH	17.36 OC1H	5.54 C1OH				
FORCE CONSTANTS-	61.44	CCCH	32.01 BCCH						
OFF DIAGONAL-	-4.22	SB27	2.79 BB37	-2.31 BB45	-1.65 SB26				
NORMAL MODE 13	OBSERVED=	1379.0	CM-1	CALCULATED=	1377.4	CM-1	ERROR=	1.6	CM-1 OR 0.1 PERCENT
INTERNAL COORDINATES-	88.31	BCCH	7.11 UCH						
FORCE CONSTANTS-	1.85	SB28	-1.54 BB39						
OFF DIAGONAL-									
NORMAL MODE 14	OBSERVED=	1372.0	CM-1	CALCULATED=	1370.6	CM-1	ERROR=	1.4	CM-1 OR 0.1 PERCENT
INTERNAL COORDINATES-	58.65	C4OH	8.58 C3OH	6.12 HC3C	6.16 OC3H				
FORCE CONSTANTS-	65.85	BCCH	15.97 CCH	15.02 CCH					
OFF DIAGONAL-	-3.04	BB36	-2.73 SB28	2.53 BB29	-1.61 SB27	1.59 BB34			
NORMAL MODE 15	OBSERVED=	1360.0	CM-1	CALCULATED=	1363.8	CM-1	ERROR=	-3.8	CM-1 OR -0.3 PERCENT
INTERNAL COORDINATES-	19.24	OC2H	13.13 HC2C	11.82 C5H	10.71 HC4C	9.29 CC5H	5.97 C3OH	5.93 OC3H	5.14 CC4H
FORCE CONSTANTS-	45.23	CCH	38.23 UCH	10.83 BCCH	6.61 CO				
OFF DIAGONAL-	9.45	BB29	-6.65 SB27	-3.77 SB26	-3.45 BB45	2.94 BB34	-1.91 SB28	-1.84 SB25	
NORMAL MODE 16	OBSERVED=	1326.0	CM-1	CALCULATED=	1330.9	CM-1	ERROR=	-4.9	CM-1 OR -0.4 PERCENT
INTERNAL COORDINATES-	21.72	HC3C	18.83 OC2H	11.34 CC4H	9.17 HC2C	8.99 C5H	6.50 OC3H	6.37 CC3H	
FORCE CONSTANTS-	58.75	CCH	16.37 UCH						
OFF DIAGONAL-	12.56	BB29	7.91 SB26	-4.55 SB27	-4.11 BB45				
NORMAL MODE 17	OBSERVED=	0.0	CM-1	CALCULATED=	1312.9	CM-1	ERROR=	0.0	CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	45.57	CCCH	25.98 C1H	11.65 BCCH	9.57 CCO	6.93 OC1H	6.53 OC2H	5.12 HC2C	
FORCE CONSTANTS-	49.94	CCH	39.83 CCH	-2.55 SB28	2.24 BB34				
OFF DIAGONAL-	-3.31	BB45	-3.20 SB26						
NORMAL MODE 18	OBSERVED=	1298.0	CM-1	CALCULATED=	1301.3	CM-1	ERROR=	-3.3	CM-1 OR -0.3 PERCENT
INTERNAL COORDINATES-	28.27	C5H	21.52 HC5C	10.25 CCH2	8.98 OC4H	7.85 HC4C			
FORCE CONSTANTS-	45.51	CCH	44.32 UCH	11.53 CO					
OFF DIAGONAL-	-5.49	SB26	-3.74 BB45	3.68 BB29	-3.52 SB27	-1.56 SB25			
NORMAL MODE 19	OBSERVED=	1283.0	CM-1	CALCULATED=	1276.2	CM-1	ERROR=	-6.8	CM-1 OR 0.5 PERCENT
INTERNAL COORDINATES-	26.02	CC1H	9.05 OC1H	7.69 OC1C	7.14 C1H	6.77 HC3C	6.62 C-06	5.94 CC3H	
FORCE CONSTANTS-	51.67	CCH	20.30 CCH	16.67 CO	5.52 CCO				
OFF DIAGONAL-	-4.81	BB34	3.67 BB29	-3.16 BB45	-3.03 SB25				
NORMAL MODE 20	OBSERVED=	0.0	CM-1	CALCULATED=	1268.8	CM-1	ERROR=	0.0	CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	30.21	OC4H	17.65 OC3H	13.85 CC4H	9.52 HC5C	8.79 CC5H			
FORCE CONSTANTS-	49.94	OC4H	39.83 CCH	5.09 CO					
OFF DIAGONAL-	5.98	SB27	-3.68 BB45	-3.60 BB29	2.89 BB34	-2.64 SB26			
NORMAL MODE 21	OBSERVED=	1240.0	CM-1	CALCULATED=	1246.1	CM-1	ERROR=	-6.1	CM-1 OR -0.5 PERCENT
INTERNAL COORDINATES-	18.82	C5H	15.91 C5H	10.77 HC5C	9.89 HC5C	8.02 CC3H	6.35 OC4H	5.53 CC4H	
FORCE CONSTANTS-	59.17	CCH	32.81 UCH	9.97 CO					
OFF DIAGONAL-	-6.36	BB29	5.10 BB34	4.06 SB27	-3.57 BB45	-2.16 SB25	-2.06 SB26		
NORMAL MODE 22	OBSERVED=	1210.0	CM-1	CALCULATED=	1202.1	CM-1	ERROR=	-7.9	CM-1 OR 0.6 PERCENT
INTERNAL COORDINATES-	18.32	C5H	16.53 C5C1	10.75 CC5H	8.85 OC2H	6.53 C2OH	5.46 C5H		
FORCE CONSTANTS-	41.30	CO	27.47 CCH	22.80 CCH	10.99 CCO	8.85 BCCH			
OFF DIAGONAL-	-8.21	SB25	3.11 SB27	-3.00 SB26	-1.91 BB29	-1.78 SB28	-1.76 BB45		
NORMAL MODE 23	OBSERVED=	1156.0	CM-1	CALCULATED=	1149.9	CM-1	ERROR=	-6.9	CM-1 OR 0.6 PERCENT
INTERNAL COORDINATES-	23.35	O1C1	13.62 C5H	10.22 CCH2	7.08 HC2C	6.12 C-09	5.76 HC4C	5.47 CC4H	5.43 C5H
FORCE CONSTANTS-	51.38	CO	37.34 CCH	13.73 CCH	8.32 CCO	5.13 CC			
OFF DIAGONAL-	-5.66	SB27	-4.45 BB29	-3.74 SB25	2.50 BB34	-1.97 BB45	-1.82 SB24		
NORMAL MODE 24	OBSERVED=	1147.0	CM-1	CALCULATED=	1136.6	CM-1	ERROR=	-10.4	CM-1 OR 0.9 PERCENT
INTERNAL COORDINATES-	12.71	C5H	9.48 C-U8	8.04 C-06	7.25 OC2H	6.59 CCO	6.17 CCH	6.12 C2OH	
FORCE CONSTANTS-	59.17	CO	20.05 CCH	14.43 CCO	11.69 CCH	8.11 BCCH	7.33 CC	6.17 CCH	
OFF DIAGONAL-	-9.04	SB25	5.53 SB27	-3.95 SB23	3.06 BB34	-2.58 SB22	2.96 BB43	2.13 SB26	-2.11 SB28
NORMAL MODE 25	OBSERVED=	1117.0	CM-1	CALCULATED=	1125.6	CM-1	ERROR=	-8.6	CM-1 OR -0.8 PERCENT
INTERNAL COORDINATES-	25.08	C-07	11.87 C5C	10.78 C5C	11.08 CCH	8.96 CCH	5.43 C-09	5.31 CCH	
FORCE CONSTANTS-	52.08	CO	38.02 CC	10.78 CCO	11.08 CCH	8.96 CCH	5.43 C-09	5.31 CCH	
OFF DIAGONAL-	-8.69	SB28	-7.85 SB25	-5.13 SB22	-4.87 SB26	-2.19 SS18			
NORMAL MODE 26	OBSERVED=	1112.0	CM-1	CALCULATED=	1107.9	CM-1	ERROR=	-4.1	CM-1 OR 0.4 PERCENT
INTERNAL COORDINATES-	39.59	C4C5	4.66 C-U9	12.40 C5C	10.91 C-07	9.01 CCH			
FORCE CONSTANTS-	65.34	CC	32.78 CCH	12.10 CCO	8.89 CCH	7.25 CCH	7.14 CCH		
OFF DIAGONAL-	-7.63	SB22	-4.36 SB21	-4.36 SB27	-4.10 SB25	-3.52 SS18	-2.55 SB28	-2.32 SS17	-1.98 SU26 -1.53 BB29
NORMAL MODE 27	OBSERVED=	1092.0	CM-1	CALCULATED=	1091.0	CM-1	ERROR=	-1.0	CM-1 OR 0.1 PERCENT
INTERNAL COORDINATES-	28.68	C3C4	25.83 C-0*	15.26 C-08	10.21 OC4H	8.75 UCHB	6.58 HCH		
FORCE CONSTANTS-	49.03	CO	36.56 CC	20.94 CCH	10.97 CCH	6.58 HCH	6.28 BCCH	5.82 CCO	
OFF DIAGONAL-	-17.43	SB27	-5.64 SB28	-5.41 SS18	-4.39 SB22	-1.89 SB26	-1.59 BB29		
NORMAL MODE 28	OBSERVED=	1074.0	CM-1	CALCULATED=	1070.2	CM-1	ERROR=	-3.8	CM-1 OR 0.4 PERCENT
INTERNAL COORDINATES-	35.32	C-08	11.77 HCH	10.83 C-0*	10.01 O-C1	7.91 C1C2	6.17 OC4H	5.03 C2C3	
FORCE CONSTANTS-	59.17	CCH	21.15 CC	14.94 CCH	11.77 HCH	8.57 CCO	8.46 CCH	7.90 CCC	6.61 BCCH
OFF DIAGONAL-	-13.02	SB27	-6.07 SB28	-5.31 SB25	-1.69 SS18	-2.75 SB22	-2.03 SB24	-1.93 BB34	
NORMAL MODE 29	OBSERVED=	1062.0	CM-1	CALCULATED=	1062.0	CM-1	ERROR=	-0.0	CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	78.43	C1C4	12.63 C2C3	11.82 C-08	7.45 C1OH	5.82 CCH			
FORCE CONSTANTS-	17.47	SB22	-14.29 SB26	-6.94 SB27	-4.65 SS18	-4.08 SB28	8.98 BCCH		
OFF DIAGONAL-									
NORMAL MODE 30	OBSERVED=	1050.0	CM-1	CALCULATED=	1043.6	CM-1	ERROR=	-6.4	CM-1 OR 0.6 PERCENT
INTERNAL COORDINATES-	49.05	C-09	11.91 C-U7	10.78 C2C3	7.40 C4OH	6.48 C-08	6.34 C3CC		
FORCE CONSTANTS-	74.24	CO	18.35 CC	14.48 CCH	10.84 CCH	10.12 BCCH	10.10 CCO	9.85 CCH	
OFF DIAGONAL-	-9.23	SB28	-8.63 SB25	-8.62 SB27	-8.25 SB21	-5.68 SS18	-2.46 BB34	-2.44 BB29	-1.85 BB36 1.65 SB26
NORMAL MODE 31	OBSERVED=	1040.0	CM-1	CALCULATED=	1026.4	CM-1	ERROR=	-13.6	CM-1 OR 1.3 PERCENT
INTERNAL COORDINATES-	33.89	HCH	9.32 C-U*	8.35 C3C4	6.44 CCHA	5.42 OCCHB	5.34 O-C1	5.30 C5H	
FORCE CONSTANTS-	33.89	HCH	21.43 CO	11.07 CCH	10.71 CCH	9.58 CC	6.46 CCC	6.34 CCO	
OFF DIAGONAL-	6.30	SB27	-4.01 SB21	-3.12 SB25	-1.97 SB22				
NORMAL MODE 32	OBSERVED=	1013.0	CM-1	CALCULATED=	1013.2	CM-1	ERROR=	-0.2	CM-1 OR -0.0 PERCENT
INTERNAL COORDINATES-	29.25	C5C	18.64 C4C5	11.69 HCH	9.82 C-0*	7.36 C3C4	7.08 C5H	6.60 C4CC	6.46 C-08
FORCE CONSTANTS-	57.67	CO	29.50 CC	11.69 HCH	11.58 CCH	9.45 CCO	6.83 CCH		
OFF DIAGONAL-	-19.61	SB21	-8.24 SS18	-7.08 SB22	-4.45 SB27	-4.35 SB25	-2.45 SB26	-2.05 SB28	1.81 SS17
NORMAL MODE 33	OBSERVED=	1000.0	CM-1	CALCULATED=	995.9	CM-1	ERROR=	-4.1	CM-1 OR 0.4 PERCENT
INTERNAL COORDINATES-	52.73	C-0	15.99 C-07	9.81 C2C3	6.95 C-09	6.68 C3C4	5.38 HCH		
FORCE CONSTANTS-	52.73	CO	10.46 CC	14.46 CCH	13.98 CCH	9.07 BCCH	5.20 CC3H		
OFF DIAGONAL-	-7.03	SB28	-5.46 BB29	-4.47 SB22	-4.35 SB25	-4.32 SB24	-3.84 SB21	2.76 BB34	
NORMAL MODE 34	OBSERVED=	977.0	CM-1	CALCULATED=	962.4	CM-1	ERROR=	-14.6	CM-1 OR 1.5 PERCENT
INTERNAL COORDINATES-	31.43	C-0*	2.49 OC4H	10.82 CCHA	9.73 C5C	7.49 C3C4	5.38 HCH	5.04 CCHB	
FORCE CONSTANTS-	35.53	CO	20.70 CCH	18.36 CC	16.25 CCH	8.38 CCH	5.38 HCH		
OFF DIAGONAL-	14.48	SB27	-9.04 SB26	-5.46 SB25	-5.36 SB22	3.46 SS18	-1.78 SB21		
NORMAL MODE 35	OBSERVED=	964.0	CM-1	CALCULATED=	954.0	CM-1	ERROR=	-10.0	CM-1 OR 1.0 PERCENT
INTERNAL COORDINATES-	18.72	C3C4	13.94 CCHB	13.35 C-08	7.62 C1C2	6.60 C5C	5.48 OC4H		
FORCE CONSTANTS-	33.79	CC	30.04 CCH	20.60 CO	11.43 CCO	11.24 CCH			
OFF DIAGONAL-	-7.75	SB22	-3.88 BB29	2.90 BB34	-2.86 SB27	2.48 SS18	-1.93 SB28	-1.56 BB45	1.53 SB26

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400									
MOLECULE 6 -6 NG=1236 ALPHA GLUCOSE-6,6-D2									
PAGE 2									
NORMAL MODE 36	OBSERVED=	917.0 CM-1	CALCULATED=	910.7 CM-1	ERROR=	6.3 CM-1	OR	0.7 PERCENT	
INTERNAL COORDINATES-	49.42	OCBH 37.76	OCHA	5.40	CCBH				
FORCE CONSTANTS-	31.11	CC 28.43	CO	21.11	CCH 16.02	CCO	7.16	OCH	
OFF DIAGONAL-	-2.01	BB45							
NORMAL MODE 37	OBSERVED=	911.0 CM-1	CALCULATED=	901.7 CM-1	ERROR=	9.3 CM-1	OR	1.0 PERCENT	
INTERNAL COORDINATES-	24.51	C-06 22.71	C2C3	9.58	CCH2	9.13	CCO8	7.13	C1C2
FORCE CONSTANTS-	17.02	C-06 10.60	CO	3.74	SB26	-2.94	SB24	2.86	BB43
OFF DIAGONAL-	-8.76	SB22	-5.96	SB21					2.08
NORMAL MODE 38	OBSERVED=	764.0 CM-1	CALCULATED=	758.9 CM-1	ERROR=	5.1 CM-1	OR	0.7 PERCENT	
INTERNAL COORDINATES-	22.26	CCO 18.37	CO	17.52	CCH 10.60	CCO	10.07	CC	6.22
FORCE CONSTANTS-	6.64	SB25	5.91	BB43	-3.78	SB27	-3.18	BB34	2.11
OFF DIAGONAL-									5.89
NORMAL MODE 39	OBSERVED=	745.0 CM-1	CALCULATED=	737.1 CM-1	ERROR=	7.9 CM-1	OR	1.1 PERCENT	
INTERNAL COORDINATES-	29.51	CCHA 22.85	C5O*	8.66	CCBH	7.39	C5C*		
FORCE CONSTANTS-	39.16	CCH 25.92	CO	8.90	CCO	8.34	CC		
OFF DIAGONAL-	3.63	SB26	2.10	BB34	1.81	BB33	-1.61	SB27	1.55
NORMAL MODE 40	OBSERVED=	630.0 CM-1	CALCULATED=	628.9 CM-1	ERROR=	1.0 CM-1	OR	0.2 PERCENT	
INTERNAL COORDINATES-	14.85	OBCC 9.78	CCO*	7.67	CC5H	6.08	HC3C	5.86	CCO9
FORCE CONSTANTS-	44.15	CCO 25.15	CCH	9.37	CO	6.81	CCC		
OFF DIAGONAL-	-9.38	BB34	8.01	BB43	-5.42	BB29	4.49	SB25	-2.49
NORMAL MODE 41	OBSERVED=	599.0 CM-1	CALCULATED=	606.6 CM-1	ERROR=	-7.6 CM-1	OR	-1.3 PERCENT	
INTERNAL COORDINATES-	16.96	CCO6 11.02	CCBH	10.09	CCO7	6.72	OCO	6.64	CCO*
FORCE CONSTANTS-	49.78	CCO 8.95	CCH	7.55	CC	7.12	CO	6.72	OCO
OFF DIAGONAL-	-7.89	BB34	-3.35	BB29	3.86	BB43	2.34	SB24	-2.19
NORMAL MODE 42	OBSERVED=	554.0 CM-1	CALCULATED=	551.9 CM-1	ERROR=	2.1 CM-1	OR	0.4 PERCENT	
INTERNAL COORDINATES-	20.52	OCF 13.64	CCO9	9.85	CC3H	8.45	CO		
FORCE CONSTANTS-	12.11	CCO 10.30	CCH	6.45	CC				
OFF DIAGONAL-	-12.38	BB34	8.00	BB43	-6.85	BB29	-2.67	SB22	-2.10
NORMAL MODE 43	OBSERVED=	537.0 CM-1	CALCULATED=	528.3 CM-1	ERROR=	8.7 CM-1	OR	1.6 PERCENT	
INTERNAL COORDINATES-	17.63	OCO 17.62	4CC*	9.89	O*CC	7.88	C-09	6.64	O9CC
FORCE CONSTANTS-	37.61	CCO 17.63	OCO	13.65	CO	9.80	CC	9.74	CCH
OFF DIAGONAL-	5.94	SB25	5.35	SB22	-3.44	BB34	-3.25	SB21	-2.98
NORMAL MODE 44	OBSERVED=	438.0 CM-1	CALCULATED=	440.2 CM-1	ERROR=	-2.2 CM-1	OR	-0.5 PERCENT	
INTERNAL COORDINATES-	13.88	C2CC 9.36	C3CC	7.84	CCO*	6.31	CCO6	5.15	CC3H
FORCE CONSTANTS-	29.39	CCC 28.64	CCO	23.23	CCH				
OFF DIAGONAL-	6.74	BB43	-5.19	BB29	-3.42	BB34	1.94	SB22	-1.59
NORMAL MODE 45	OBSERVED=	424.0 CM-1	CALCULATED=	426.6 CM-1	ERROR=	-2.6 CM-1	OR	-0.6 PERCENT	
INTERNAL COORDINATES-	16.34	O*CC 13.93	O9CC	13.63	OCO	12.20	CCO*	9.27	CCO7
FORCE CONSTANTS-	54.15	CCO 13.63	OCO	13.48	CC	6.33	CC	6.02	C1CC
OFF DIAGONAL-	5.41	SB22	-5.04	BB34	-4.97	SB21	4.38	SB25	-4.25
NORMAL MODE 46	OBSERVED=	398.0 CM-1	CALCULATED=	386.3 CM-1	ERROR=	11.7 CM-1	OR	2.9 PERCENT	
INTERNAL COORDINATES-	19.49	CCO8 12.48	OBCC	11.39	C2CC	8.33	O9CC		
FORCE CONSTANTS-	55.33	CCO 21.13	CCC	10.14	CC	9.44	CC		
OFF DIAGONAL-	-7.80	BB34	4.50	SB25	4.29	SB21	-3.73	BB42	-2.16
NORMAL MODE 47	OBSERVED=	357.0 CM-1	CALCULATED=	355.6 CM-1	ERROR=	1.4 CM-1	OR	0.4 PERCENT	
INTERNAL COORDINATES-	18.13	O7CC 14.46	CCU*	7.87	OCO	6.75	CCBH	5.20	C3C4
FORCE CONSTANTS-	45.75	CCO 21.89	CCH	10.33	CC	7.87	OCO	6.01	CCC
OFF DIAGONAL-	-7.79	BB34	3.72	SB21	-3.19	BB29	3.02	BB43	-2.45
NORMAL MODE 48	OBSERVED=	0.0 CM-1	CALCULATED=	318.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	21.51	CCO9 14.39	CCO8	6.22	CCO6	5.90	O9CC	5.47	OBCC
FORCE CONSTANTS-	69.43	CCO 13.05	CC	8.27	CCH	6.89	T-OH		
OFF DIAGONAL-	-6.72	BB34	4.64	SB22	-2.39	BB42			
NORMAL MODE 49	OBSERVED=	0.0 CM-1	CALCULATED=	310.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	21.87	CCO7 14.66	CCU8	8.24	4CO*	7.88	CCO*	7.18	OBCC
FORCE CONSTANTS-	59.90	CCO 9.97	CC	7.77	T-OH	5.31	CCH		
OFF DIAGONAL-	-6.67	BB34	-3.62	BB42	3.29	SB21	2.36	SB22	
NORMAL MODE 50	OBSERVED=	0.0 CM-1	CALCULATED=	298.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	16.04	OBCC 14.51	O9CC	13.48	4CO*	6.53	O7CC	6.32	CCO*
FORCE CONSTANTS-	69.11	CCO 18.46	CCH	12.49	T-OH	6.22	CCC		
OFF DIAGONAL-	-12.98	BB34	4.52	BB43	-3.39	BB29	-2.96	SB25	
NORMAL MODE 51	OBSERVED=	0.0 CM-1	CALCULATED=	257.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	20.72	CCO6 9.91	O*CC	8.80	CCO9	7.40	CH2	7.11	O7CC
FORCE CONSTANTS-	56.89	CCO 18.37	CCH	13.02	T-OH	8.38	CCC		
OFF DIAGONAL-	-8.81	BB34	7.03	BB43	-3.45	SB25	-3.26	BB33	-2.40
NORMAL MODE 52	OBSERVED=	0.0 CM-1	CALCULATED=	238.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	63.07	TH-5 6.94	TH-4	5.70	CCO*				
FORCE CONSTANTS-	76.53	T-OH 12.29	CCO	5.56	CCC				
OFF DIAGONAL-	NONE								
NORMAL MODE 53	OBSERVED=	0.0 CM-1	CALCULATED=	228.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	53.97	TH-1 25.86	TH-3	8.05	TH-2	6.08	TH-4		
FORCE CONSTANTS-	94.09	T-OH							
OFF DIAGONAL-	NONE								
NORMAL MODE 54	OBSERVED=	0.0 CM-1	CALCULATED=	223.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	89.11	TH-4 18.18	TH-1	16.28	TH-5	8.12	TH-3		
FORCE CONSTANTS-	89.11	T-OH							
OFF DIAGONAL-	NONE								
NORMAL MODE 55	OBSERVED=	0.0 CM-1	CALCULATED=	215.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	15.92	TH-3 27.78	TH-4	11.16	TH-1	7.92	TH-2		
FORCE CONSTANTS-	82.69	T-OH 14.37	CCO						
OFF DIAGONAL-	-1.85	BB34							
NORMAL MODE 56	OBSERVED=	0.0 CM-1	CALCULATED=	213.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	68.28	TH-2 13.52	TH-3						
FORCE CONSTANTS-	83.63	T-OH 14.47	CCO						
OFF DIAGONAL-	NONE								
NORMAL MODE 57	OBSERVED=	0.0 CM-1	CALCULATED=	186.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	34.13	CCO*	4CC	15.70	TH-5	6.78	CO*CC	5.28	CCHA
FORCE CONSTANTS-	46.93	CCO 13.36	T-OH	9.65	CCO	8.15	CCO	6.78	CCC
OFF DIAGONAL-	-5.40	BB34	-3.59	BB33	-3.58	BB42			6.40
NORMAL MODE 58	OBSERVED=	0.0 CM-1	CALCULATED=	129.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	22.91	CCO*	4CC	12.48	T-CC	11.71	CCO	9.86	T-CC
FORCE CONSTANTS-	3.88	BB43	-3.43	SB21	-2.33	BB37	1.93	BB41	-1.68
OFF DIAGONAL-									BB34
NORMAL MODE 59	OBSERVED=	0.0 CM-1	CALCULATED=	93.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	47.77	TCC5 11.92	C3CC	7.68	TCC2	7.66	C2CC	6.72	O9CC
FORCE CONSTANTS-	59.87	T-CC 22.97	CCC	17.64	CCO				
OFF DIAGONAL-	-3.93	SB25	-3.00	SB21	-2.62	BB42	-2.32	BB34	1.64
NORMAL MODE 60	OBSERVED=	0.0 CM-1	CALCULATED=	79.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	17.40	C2CC 14.44	C1CC	14.17	TCC5	8.48	CO*CC	7.40	TCC4
FORCE CONSTANTS-	36.32	CCC 33.05	T-CC	16.59	CCO	8.48	CCO	6.19	T-CC
OFF DIAGONAL-	-3.52	BB42	-3.40	SB25	-2.19	SB21	2.06	BB41	
NORMAL MODE 61	OBSERVED=	0.0 CM-1	CALCULATED=	65.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	26.22	TCC5 33.78	C3CC	9.30	TCC4	7.12	TCC2	7.07	TCC3
FORCE CONSTANTS-	50.40	T-CC 22.00	CCO	21.12	CCO				
OFF DIAGONAL-	-2.55	BB42	-2.11	BB34	-1.61	SB25			

36. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 5.76

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400										PAGE 1
MOLECULE 7 -6 NG=1236 ALPHA GLUCOSE-C6,6-D2,-O-D5										
NORMAL MODE 8	OBSERVED=	1410.0 CM-1	CALCULATED=	1406.6 CM-1	ERROR=	3.4 CM-1	OR	0.2 PERCENT		
INTERNAL COORDINATES-	17.95	OC4H 11.25 CC5H	10.81	HC2C	8.63	OC3H	6.94	HC3C	5.66	OC1H
FORCE CONSTANTS-	49.16	OC4H 31.26 CCH	11.74	CO	5.22	CCO				
OFF DIAGONAL-	-10.06	SB27 8.07 BB29	4.84	BB34	-4.04	SB25	-4.03	SB26	-3.32	BB45
NORMAL MODE 9	OBSERVED=	1400.3 CM-1	CALCULATED=	1391.7 CM-1	ERROR=	8.3 CM-1	OR	0.6 PERCENT		
INTERNAL COORDINATES-	39.91	C1H 38.25 OC1H								
FORCE CONSTANTS-	89.37	OC4H 11.59 CCH	6.67	CO						
OFF DIAGONAL-	-9.78	SB27 -3.76 BB45	1.93	BB37	1.78	BB29				
NORMAL MODE 10	OBSERVED=	0.0 CM-1	CALCULATED=	1371.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	16.75	UC2H 15.49 HC2C	13.49	CC3H	13.00	OC3H	8.63	HC4C	7.37	CC5H
FORCE CONSTANTS-	49.42	CCH 39.55 UCH	9.44	CO						
OFF DIAGONAL-	10.88	BB29 -8.10 SB27	-5.43	SB26	3.81	BB34	-3.65	BB45	-3.07	SB25
NORMAL MODE 11	OBSERVED=	0.0 CM-1	CALCULATED=	1332.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	22.98	HC3C 13.08 CC5H	13.02	CC4H	12.40	OC2H	8.44	CC3H		
FORCE CONSTANTS-	61.86	CCH 32.34 CCH								
OFF DIAGONAL-	13.31	BB29 -9.16 SB26	-4.46	SB27	-4.07	BB45				
NORMAL MODE 12	OBSERVED=	0.0 CM-1	CALCULATED=	1327.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	39.51	CC1H 20.88 CCH2	10.15	C1H	8.43	OC1H	6.21	HC2C		
FORCE CONSTANTS-	58.07	CCH 24.56 UCH	10.66	CO	5.19	CC				
OFF DIAGONAL-	-3.65	SB26 -3.63 BB45	2.77	BB34	1.67	BB30	1.53	BB29		
NORMAL MODE 13	OBSERVED=	0.0 CM-1	CALCULATED=	1304.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	24.34	CC5H 16.44 HC5C	11.33	OC3H	10.77	OC4H	9.29	OC2H	6.09	CC2H
FORCE CONSTANTS-	60.31	UCH 34.84 CCH	6.10	CO						
OFF DIAGONAL-	-3.81	BB45 -2.82 SB27	-2.06	SB26						
NORMAL MODE 14	OBSERVED=	0.0 CM-1	CALCULATED=	1296.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	20.54	UC2H 16.55 CC3H	7.90	C2OH	7.64	CC5H	7.19	HC5C		
FORCE CONSTANTS-	41.13	CCH 35.04 UCH	8.65	BCOH	5.78	CCO				
OFF DIAGONAL-	3.25	BB34 -3.04 BB45	2.90	SB27	-2.28	SB26	1.59	BB36		
NORMAL MODE 15	OBSERVED=	0.0 CM-1	CALCULATED=	1276.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	14.24	CC1H 11.64 UC4H	8.48	O*CI	7.69	OC3H	7.39	UC1H	7.23	HC2C
FORCE CONSTANTS-	40.55	CCH 30.80 UCH	19.61	CO	5.00	CCO				
OFF DIAGONAL-	4.50	BB34 -3.92 SB25	3.73	SB27	-3.00	BB45	-1.82	BB29	-1.73	SB28
NORMAL MODE 16	OBSERVED=	0.0 CM-1	CALCULATED=	1269.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	20.98	HC5C 20.39 OC4H	13.43	CC5C	6.47	CC5H	5.23	O*CI		
FORCE CONSTANTS-	51.22	CCH 29.32 CCH	12.73	CO	5.89	CCO				
OFF DIAGONAL-	4.12	BB34 -4.11 SB26	-3.36	BB45	-3.19	SB25				
NORMAL MODE 17	OBSERVED=	0.0 CM-1	CALCULATED=	1233.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	14.02	OC3H 14.07 CC5H	11.55	CC4H	11.13	HC4C	7.73	CC5H	6.73	HC5C
FORCE CONSTANTS-	47.81	CCH 28.96 UCH	12.55	CO	8.00	CCO				
OFF DIAGONAL-	-6.12	BB29 4.68 BB34	-3.77	SB25	3.70	SB27	-2.83	BB45		
NORMAL MODE 18	OBSERVED=	0.0 CM-1	CALCULATED=	1202.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	27.88	C2C3 16.17 C3UH	7.53	C1C2	5.25	C-O9	5.20	C2OH		
FORCE CONSTANTS-	37.92	CCH 24.86 BCOH	16.42	CCO	11.34	CO	11.16	UCH	9.54	CCH
OFF DIAGONAL-	-8.06	SB22 -5.05 SB21	-4.46	SB25	3.01	BB36	-2.33	SB26	1.86	SB28
NORMAL MODE 19	OBSERVED=	0.0 CM-1	CALCULATED=	1169.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	18.84	C5C* 13.80 O*CI	13.33	C2O*	6.47	C4C5	5.92	CCO*	5.69	C1C2
FORCE CONSTANTS-	36.27	CO 33.33 CCH	15.39	CCO	11.92	BCOH	10.78	UCH	10.66	CCH
OFF DIAGONAL-	-7.87	SB22 -4.72 SB26	-2.76	SB25	-2.71	SS18	2.70	SB28	-2.26	SB24
NORMAL MODE 20	OBSERVED=	0.0 CM-1	CALCULATED=	1165.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	18.28	C5U* 22.98 C5C*	11.89	O*CI	10.11	CCOH	7.94	C-O8	7.90	C1OH
FORCE CONSTANTS-	49.16	CO 22.09 CCH	18.05	CC	16.45	UCH	10.43	BCOH	8.53	CCO
OFF DIAGONAL-	-10.63	SB27 -4.70 SB25	-4.25	SB26	3.49	SB28	-2.83	SB22	-1.55	SB24
NORMAL MODE 21	OBSERVED=	0.0 CM-1	CALCULATED=	1145.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	37.13	C1C 18.82 C1OH	9.32	C-O9	7.63	C5C*	5.85	C1OH	5.45	O*CC
FORCE CONSTANTS-	59.13	CO 26.23 BCOH	16.24	CO	16.05	CCO	13.76	CCH	13.10	UCH
OFF DIAGONAL-	-11.47	SB22 -7.89 SB26	3.82	SB28	-2.68	SB27	-2.10	SS18		
NORMAL MODE 22	OBSERVED=	0.0 CM-1	CALCULATED=	1144.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	33.40	C3C4 22.64 C4UH	12.58	CCH	11.24	CO	10.88	CCO	9.86	UCH
FORCE CONSTANTS-	41.83	CCH 24.42 BCOH	-3.04	SB26	-2.60	BB36	-1.95	SB27	1.62	SB28
OFF DIAGONAL-	-9.84	SB22 -3.63 SB21								
NORMAL MODE 23	OBSERVED=	0.0 CM-1	CALCULATED=	1129.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	25.74	C-O8 12.45 C3C4	9.86	C4C5	9.73	O*CI				
FORCE CONSTANTS-	43.02	CO 23.53 CC	14.45	CCO	9.43	CCO	8.78	CCC	8.52	BCOH
OFF DIAGONAL-	-6.31	SB25 -3.92 SB22	-3.78	SB21	3.73	SB28	-2.93	SB27	-2.81	SS18
NORMAL MODE 24	OBSERVED=	0.0 CM-1	CALCULATED=	1109.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	33.44	C-O 23.10 C1C2	10.04	CCO	10.06	UCH	9.03	CCC	6.49	CCO
FORCE CONSTANTS-	60.04	CO 23.10 CC	10.09	CCO	18.06	UCH	9.94	CC2	6.49	CCO
OFF DIAGONAL-	-7.17	SS18 -6.17 SB21	-4.35	SB25	-4.06	SB27	-3.70	SB28	-2.07	SB24
NORMAL MODE 25	OBSERVED=	0.0 CM-1	CALCULATED=	1076.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	11.25	C-O9	8.03	OC8H	6.06	C1OH				
FORCE CONSTANTS-	45.49	CC 20.27 CO	15.77	UCH	13.71	BCOH	8.33	CCH	7.92	CCO
OFF DIAGONAL-	-9.62	SB21 -6.88 SB27	-4.80	SS18	4.34	SB28	-3.58	SB22		
NORMAL MODE 26	OBSERVED=	0.0 CM-1	CALCULATED=	1066.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	24.68	C-O8 16.95 O*CI	8.31	HCH	6.87	C5O*	6.76	C3C4		
FORCE CONSTANTS-	53.41	CO 13.97 CCH	12.28	CC	11.88	CCO	8.38	UCH	8.31	HCH
OFF DIAGONAL-	-6.77	SB25 -3.78 SB28	-3.49	SB27	-1.98	SB24	-1.57	SB21		
NORMAL MODE 27	OBSERVED=	0.0 CM-1	CALCULATED=	1045.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	17.99	C-O8 17.47 C1OH	17.25	HCH	13.85	C-O7	9.92	C-O*	8.06	C-O9
FORCE CONSTANTS-	52.19	CO 26.66 BCOH	17.25	HCH	9.21	CCO	8.48	CCH	7.12	CC
OFF DIAGONAL-	-9.98	SB28 -6.63 SB27	-5.83	SB25	-1.91	SB21	-1.90	BB35	-1.80	SB22
NORMAL MODE 28	OBSERVED=	0.0 CM-1	CALCULATED=	1036.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	25.87	C-O9 22.75 HCH	17.61	C-O7	8.28	C2OH				
FORCE CONSTANTS-	49.52	CO 17.13 BCOH	21.99	BCOH	8.58	UCH				
OFF DIAGONAL-	-8.38	SB28 -4.50 SB25	-3.95	SB27	-1.60	SB21	7.44	CCH	5.57	CC
NORMAL MODE 29	OBSERVED=	0.0 CM-1	CALCULATED=	1015.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	11.21	C-O 13.39 C2OH	13.84	HCH	10.08	C1OH	5.11	ERROR=		
FORCE CONSTANTS-	39.42	CO 30.74 BCOH	16.87	UCH	13.84	HCH				
OFF DIAGONAL-	-9.13	SB28 6.82 SB27	-3.06	BB29	-1.82	SB25				
NORMAL MODE 30	OBSERVED=	0.0 CM-1	CALCULATED=	998.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	22.53	C2OH 18.20 C-U*	16.06	C4OH	10.11	C-O6	8.21	C-O9	5.73	C4C5
FORCE CONSTANTS-	48.39	BCOH 38.98 CO	14.09	CCH	7.56	CC				
OFF DIAGONAL-	-9.77	SB28 -2.62 BB29	-2.05	SB22	-2.03	SB24	-1.86	BB36	-1.57	SB25
NORMAL MODE 31	OBSERVED=	0.0 CM-1	CALCULATED=	988.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	19.25	C5C* 17.00 C1OH	12.08	C-O6	8.24	CCBH	7.33	C1OH		
FORCE CONSTANTS-	27.37	BCOH 23.68 CC	22.60	CO	18.68	UCH				
OFF DIAGONAL-	-7.66	SB28 5.76 SB26	-4.84	SB21	-3.69	SB22	-3.29	SS18	-1.77	SB27
NORMAL MODE 32	OBSERVED=	0.0 CM-1	CALCULATED=	964.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	26.57	C-O6 14.72 C4OH	24.51	C1OH	9.35	C-O8	8.33	HC2C	7.70	CC1H
FORCE CONSTANTS-	54.81	CO 17.13 BCOH	23.94	CO	10.36	CC				
OFF DIAGONAL-	-13.68	SB28 -6.01 SB24	-4.59	SB27	-3.75	BB29	-3.53	SB25	-3.29	SB26
NORMAL MODE 33	OBSERVED=	0.0 CM-1	CALCULATED=	940.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	44.17	BCOH 24.14 C3OH	11.94	CC1H	11.54	UCH	6.92	UCH		
FORCE CONSTANTS-	44.05	SB22								
OFF DIAGONAL-										
NORMAL MODE 34	OBSERVED=	0.0 CM-1	CALCULATED=	933.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	41.12	OCHA 11.52 CCHA	9.36	C5C*	6.86	C1OH	6.19	UCH		
FORCE CONSTANTS-	49.22	UCH 14.20 BCOH	14.11	CCH	13.80	CC	5.86	CO		
OFF DIAGONAL-	-5.07	SB26 -3.18 SB21	2.96	SB26	2.25	SB28	-2.23	SB22	-1.73	BB45
NORMAL MODE 35	OBSERVED=	0.0 CM-1	CALCULATED=	911.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	31.79	C4OH 29.45 C3C4	9.12	C-O8	5.48	C3OH				
FORCE CONSTANTS-	42.84	BCOH 34.26 CCH	16.10	CO	14.42	UCH	9.21	CCO	7.80	UCH
OFF DIAGONAL-	-6.75	SB22 -6.30 SB28	-4.85	SB21	-3.36	SB27	-3.08	SB26	-2.40	BB29

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400									
MOLECULE 7 -6 NG=1236 ALPHA GLUCOSE-C6,6-D2,-O-D5									
PAGE 2									
NORMAL MODE 36	OBSERVED=	0.0 CM-1	CALCULATED=	884.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	49.95	OCCH 24.57 C*OH	9.61 CCHB	8.90 OCMA	5.08	C3C			
FORCE CONSTANTS-	34.54	CC 28.67 BCOH	12.11 CCH	7.82 CC					
OFF DIAGONAL-	-3.06	SB26 -2.32 SB22	1.84 SB28	-1.80 BB34	1.61	SB27			
NORMAL MODE 37	OBSERVED=	0.0 CM-1	CALCULATED=	852.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	25.88	C2C3 15.03 C3OH	11.75 C2OH	8.04 CC08	7.66	C-06	6.16 C1C2	5.25 CCH2	5.15 CC09
FORCE CONSTANTS-	34.54	CC 28.67 BCOH	12.11 CCH	7.82 CC					
OFF DIAGONAL-	-8.61	SB21 -7.79 SB22	2.27 SB26	2.09 BB43	10.42	CO			
NORMAL MODE 38	OBSERVED=	0.0 CM-1	CALCULATED=	751.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	11.96	CU*C 10.49 C-06	7.82 CC06	6.90 CCHH	6.57	C2C3	5.36 C*CC	5.22 C1CC	
FORCE CONSTANTS-	19.40	CCO 17.48 CO	15.25 CCH	11.96 C0C	10.77	CC	5.72 CCC	5.39 OCH	
OFF DIAGONAL-	6.11	SB25 5.55 BB43	-3.79 SB27	-2.73 BB34	2.31	SB24	-2.17 SB23	-2.09 BB41	1.95 SB22 -1.67 SB26
NORMAL MODE 39	OBSERVED=	0.0 CM-1	CALCULATED=	736.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	29.88	CCMA 23.26 C5O*	9.39 CCHB	5.97 C5C					
FORCE CONSTANTS-	40.43	CCO 26.46 CO	12.66 CCO	7.81 CC					
OFF DIAGONAL-	3.52	SB26 2.11 BB34	1.79 BB33	-1.64 SB27	1.55	SB25			
NORMAL MODE 40	OBSERVED=	0.0 CM-1	CALCULATED=	621.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	17.88	OBCC 14.28 CCU*	10.67 CC9H	8.20 HC4C	6.24	U9CC	5.98 C4CC	5.07 HC3C	
FORCE CONSTANTS-	51.00	CCO 29.24 CCH	8.25 CCC	5.67 CO					
OFF DIAGONAL-	-11.58	BB34 9.22 BB43	-6.58 BB29	3.90 SB25	-1.92	BB36	-1.87 SB27		
NORMAL MODE 41	OBSERVED=	0.0 CM-1	CALCULATED=	594.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	18.18	CC06 10.81 CCU*	9.66 CCHB	8.92 CCO	6.66	CO*E	6.53 C1C2		
FORCE CONSTANTS-	42.10	CCO 21.23 CCH	10.57 CC	9.12 CO	8.92	CCO	6.66 C0C		
OFF DIAGONAL-	-4.81	BB34 -3.41 BB29	2.92 SB24	2.32 BB43	-2.13	SB23	-2.04 BB41	2.00 SS18 -1.99 BB42	
NORMAL MODE 42	OBSERVED=	0.0 CM-1	CALCULATED=	542.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	15.67	O*CC 13.55 CCU9	7.12 C2C3	6.46 CC3H	5.08	CC4H			
FORCE CONSTANTS-	43.03	CCO 28.78 CCH	16.90 CC	8.52 CO					
OFF DIAGONAL-	-10.53	BB34 6.96 BB43	-6.48 BB29	3.13 SB25	2.71	SS18	-2.49 BB36	1.64 SB21 -1.58 SB27	
NORMAL MODE 43	OBSERVED=	0.0 CM-1	CALCULATED=	519.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	18.37	OCO 15.72 4CU*	13.54 O*CC	5.61 C-09	5.24	O9CC			
FORCE CONSTANTS-	44.73	CCO 18.37 CCO	10.19 CCO	10.11 C-09	8.40	CC			
OFF DIAGONAL-	-5.17	BB34 3.88 SB25	-3.67 SB21	-3.62 BB42	3.48	SB22	-6.43 CC		
NORMAL MODE 44	OBSERVED=	0.0 CM-1	CALCULATED=	435.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	13.24	C2CC 9.46 C3CC	7.35 CCO	6.54 CCO6	5.11	CC09			
FORCE CONSTANTS-	20.42	CCO 22.78 CCH	9.26 CC	8.94 CCO					
OFF DIAGONAL-	6.33	BB43 -4.98 BB29	-3.13 BB34	2.30 SB22	-1.54	BB41			
NORMAL MODE 45	OBSERVED=	0.0 CM-1	CALCULATED=	420.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	14.49	O*CC 13.72 CCO*	13.61 O9CC	13.09 CCO	9.18	CC07	6.10 C4C5	5.42 C1CC	5.32 C3CC
FORCE CONSTANTS-	55.73	CCO 13.31 CCH	13.09 CCO	6.33 CC	5.70	CCH	5.54 CO		
OFF DIAGONAL-	-5.48	BB34 -5.04 SB21	4.74 SB22	4.18 SB25	-4.16	BB42			
NORMAL MODE 46	OBSERVED=	0.0 CM-1	CALCULATED=	383.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	15.82	CC08 11.40 C2CC	10.23 OBCC	8.14 O9CC	5.82	CC09	5.66 C3CC	5.32 CC06	
FORCE CONSTANTS-	56.30	CCO 21.50 CCH	10.06 CCH	9.40 CC					
OFF DIAGONAL-	-7.70	BB34 4.59 SB21	4.51 SB25	-3.72 BB42	-2.35	SB26	-1.73 BB29	-1.58 BB36	
NORMAL MODE 47	OBSERVED=	0.0 CM-1	CALCULATED=	349.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	18.24	O7CC 15.69 CCO*	8.94 CCO	7.46 CCHB					
FORCE CONSTANTS-	44.24	CCO 22.78 CCH	9.26 CC	8.94 CCO	6.25	CCC			
OFF DIAGONAL-	-8.09	BB34 -3.59 BB29	3.45 BB43	3.39 SB21	-2.12	SB26	2.04 SB24	-1.93 BB36	-1.71 BB33
NORMAL MODE 48	OBSERVED=	0.0 CM-1	CALCULATED=	311.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	17.72	CC09 10.29 CC08	7.99 CCO6	7.09 CCO7	5.78	O9CC	5.54 O7CC	5.05 C3C4	
FORCE CONSTANTS-	69.47	CCO 12.39 CCH	8.74 CCH						
OFF DIAGONAL-	-6.66	BB34 4.89 SB22	-3.03 BB42	1.85 BB43					
NORMAL MODE 49	OBSERVED=	0.0 CM-1	CALCULATED=	306.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	19.85	CC07 13.94 CC08	10.96 4CO*	9.88 CCO*	6.76	OBCC	5.78 C4C5		
FORCE CONSTANTS-	70.95	CCO 11.21 CC	5.91 CCH						
OFF DIAGONAL-	-7.15	BB34 4.52 SB21	-3.62 BB42	2.01 SB22					
NORMAL MODE 50	OBSERVED=	0.0 CM-1	CALCULATED=	292.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	22.87	OBCC 15.61 C9CC	11.61 4CO*	8.88 CCO8	7.95	O7CC	5.74 CCO*		
FORCE CONSTANTS-	79.97	CCO 16.77 CCH	6.34 CCC	6.00 T-OH					
OFF DIAGONAL-	-13.14	BB34 3.32 BB43	-2.68 SB25	-2.58 BB29	-2.12	BB42	-1.81 BB36		
NORMAL MODE 51	OBSERVED=	0.0 CM-1	CALCULATED=	248.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	24.53	CC06 9.43 O*CC	9.08 O7CC	8.81 CCH2	8.27	CC09	5.83 CCO7	5.82 HC2C	5.22 C1CC
FORCE CONSTANTS-	63.46	CCO 21.43 CCH	7.93 CCO	6.00 T-OH					
OFF DIAGONAL-	-9.72	BB34 8.16 BB43	-4.15 SB25	-3.87 BB33	-2.82	BB29	2.17 SB22	-1.59 BB36	
NORMAL MODE 52	OBSERVED=	0.0 CM-1	CALCULATED=	207.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	21.70	CCO 25.95 T-OH	15.74 CCO	8.93 C0C	5.60	CCH			
FORCE CONSTANTS-	41.90	CCO 25.95 T-OH	18.04 CCH						
OFF DIAGONAL-	-3.85	BB34 -3.04 BB42	-2.41 BB33						
NORMAL MODE 53	OBSERVED=	0.0 CM-1	CALCULATED=	174.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	38.57	TH-1 19.06 TH-3							
FORCE CONSTANTS-	79.43	T-OH 5.27 CCC							
OFF DIAGONAL-	NONE								
NORMAL MODE 54	OBSERVED=	0.0 CM-1	CALCULATED=	164.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	41.70	TH-4 22.32 TH-3	16.50 TH-5	10.76 TH-1					
FORCE CONSTANTS-	92.79	T-UH							
OFF DIAGONAL-	NONE								
NORMAL MODE 55	OBSERVED=	0.0 CM-1	CALCULATED=	156.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	41.69	TH-4 20.51 TH-2	19.06 TH-3						
FORCE CONSTANTS-	90.14	T-OH 7.40 CCO							
OFF DIAGONAL-	NONE								
NORMAL MODE 56	OBSERVED=	0.0 CM-1	CALCULATED=	155.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	83.27	TH-2 9.09 CCO	22.22 TH-2						
FORCE CONSTANTS-	83.27	T-OH							
OFF DIAGONAL-	NONE								
NORMAL MODE 57	OBSERVED=	0.0 CM-1	CALCULATED=	153.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	44.57	TH-2 28.94 TH-5	6.73 CCO*						
FORCE CONSTANTS-	79.03	T-OH 12.07 CCO							
OFF DIAGONAL-	-1.57	BB34							
NORMAL MODE 58	OBSERVED=	0.0 CM-1	CALCULATED=	120.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	17.03	CO*E 17.00 TH-1	12.59 C4CC	8.17 TCC4	5.34	C1CC	5.24 TC01	5.21 CCO	
FORCE CONSTANTS-	19.69	T-OH 18.75 CCH	17.03 C0C	10.48 T-CC	9.70	CCO	8.16 T-CCO	5.21 CCO	
OFF DIAGONAL-	3.18	BB43 -2.82 SB21	-1.71 BB37	1.60 BB41					
NORMAL MODE 59	OBSERVED=	0.0 CM-1	CALCULATED=	90.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	48.48	TCC2 10.90 C3CC	6.84 O9CC	6.58 TCC2	5.92	C2CC			
FORCE CONSTANTS-	59.17	T-CC 23.78 CCH	17.12 CCO						
OFF DIAGONAL-	-3.65	SB25 -2.66 SB21	-2.42 BB42	-2.36 BB34	-1.52	BB43			
NORMAL MODE 60	OBSERVED=	0.0 CM-1	CALCULATED=	77.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	18.11	C2CC 15.11 C1CC	17.35 TCC5	8.45 CCO*	7.69	TCC4	7.38 TCC1	5.33 TC02	
FORCE CONSTANTS-	37.67	CCC 30.01 T-CC	17.33 CCO	8.45 C0C	6.15	T-CCO			
OFF DIAGONAL-	-3.67	BB42 -3.61 SB25	-2.30 SB21	2.16 BB41					
NORMAL MODE 61	OBSERVED=	0.0 CM-1	CALCULATED=	63.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	25.95	TCC2 13.86 C3CC	8.99 TCC4	7.42 TCC2	7.04	TCC3	5.40 4CO*		
FORCE CONSTANTS-	50.00	T-CC 22.16 CCO	20.91 CCC						
OFF DIAGONAL-	-2.54	BB42 -2.14 BB34	-1.62 SB25						

2. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 5.84

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400				PAGE 1			
MOLECULE 8 -6 NG-1236 ALPHA GLUCOSE-C-D7							
NORMAL MODE 8	OBSERVED=	0.0 CM-1	CALCULATED=	1426.2 CM-1	ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	24.44 C2OH						
FORCE CONSTANTS-	77.83 BC0H						
OFF DIAGONAL-	4.22 BB36 3.13 SB28						
NORMAL MODE 9	OBSERVED=	0.0 CM-1	CALCULATED=	1412.7 CM-1	ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	67.35 C3OH 13.03 C4OH						
FORCE CONSTANTS-	81.18 BC0H 8.74 CC						
OFF DIAGONAL-	4.21 BB36 4.14 SB28 -2.19 SB26						
NORMAL MODE 10	OBSERVED=	0.0 CM-1	CALCULATED=	1394.5 CM-1	ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	88.03 C1OH 5.68 C1C2						
FORCE CONSTANTS-	89.20 BC0H 5.80 CC						
OFF DIAGONAL-	3.15 SB28 -2.12 SB22						
NORMAL MODE 11	OBSERVED=	0.0 CM-1	CALCULATED=	1384.1 CM-1	ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	87.56 C4OH 14.84 C3OH						
FORCE CONSTANTS-	87.24 BC0H						
OFF DIAGONAL-	4.70 SB28 -1.70 BB36						
NORMAL MODE 12	OBSERVED=	0.0 CM-1	CALCULATED=	1377.2 CM-1	ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	87.93 C*OH						
FORCE CONSTANTS-	92.50 BC0H 5.26 CC						
OFF DIAGONAL-	2.55 SB28 -1.86 SB26 -1.85 BB39						
NORMAL MODE 13	OBSERVED=	0.0 CM-1	CALCULATED=	1236.9 CM-1	ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	39.69 U*CI 29.56 C5O*						
FORCE CONSTANTS-	89.98 CO 15.77 CCO						
OFF DIAGONAL-	-14.36 SB25 -12.99 SB27 3.51 BB34 -3.27 SB28 -2.45 SS18 -2.43 SB26 -2.12 SS20 1.96 SB22 -1.59 SB21						
NORMAL MODE 14	OBSERVED=	0.0 CM-1	CALCULATED=	1224.5 CM-1	ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	14.45 C5U* 12.05 C-O9						
FORCE CONSTANTS-	52.73 CO 21.10 CCH						
OFF DIAGONAL-	-13.65 SB25 -12.24 SB27 -7.38 SB26 -5.76 SB28 5.35 BB34 -3.84 SB23 3.45 BB29 -3.11 SS18 2.41 SB22						
NORMAL MODE 15	OBSERVED=	0.0 CM-1	CALCULATED=	1171.9 CM-1	ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	25.80 C-U8 11.98 C5O*						
FORCE CONSTANTS-	47.93 CO 21.04 CCH						
OFF DIAGONAL-	-12.85 SB27 -9.15 SB26 -7.65 SB25 -6.25 SB28 4.97 BB29 -4.85 SS18 3.05 BB34 -1.82 SB23						
NORMAL MODE 16	OBSERVED=	0.0 CM-1	CALCULATED=	1156.8 CM-1	ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	48.23 C-07 7.13 C2C3						
FORCE CONSTANTS-	48.23 CO 35.66 CO						
OFF DIAGONAL-	-21.11 SB26 -15.36 SB27 -5.93 SB28 -5.73 SB22 5.14 BB29 -4.93 SB25 -4.37 SS18 -1.68 BB43 -1.68 BB45						
NORMAL MODE 17	OBSERVED=	0.0 CM-1	CALCULATED=	1146.2 CM-1	ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	31.45 C-07 7.13 C2C3						
FORCE CONSTANTS-	53.71 CO 41.99 CO						
OFF DIAGONAL-	-17.81 SB26 -8.22 SB27 -7.07 SB25 -5.18 SB22 -4.80 BB22 4.56 BB29 -3.70 SS18 -3.32 SB28 -2.11 BB43						
NORMAL MODE 18	OBSERVED=	0.0 CM-1	CALCULATED=	1122.8 CM-1	ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	33.17 C-09 18.03 C-O8						
FORCE CONSTANTS-	63.69 CO 15.69 CCH						
OFF DIAGONAL-	-10.86 SB25 -9.03 SB28 -6.50 SB26 -5.99 SB27 -3.77 BB22 4.56 BB29 -3.70 SS18 -3.32 SB28 -2.11 BB43						
NORMAL MODE 19	OBSERVED=	0.0 CM-1	CALCULATED=	1093.9 CM-1	ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	18.94 C-07 14.81 C-U*						
FORCE CONSTANTS-	42.07 CO 39.52 CO						
OFF DIAGONAL-	-12.04 SB27 -8.40 SB22 -7.98 SB26 -4.39 SB28 -3.91 BB25 -2.01 BB43						
NORMAL MODE 20	OBSERVED=	0.0 CM-1	CALCULATED=	1073.0 CM-1	ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	28.23 C1C2 8.84 C-U*						
FORCE CONSTANTS-	28.23 CO 29.73 CO						
OFF DIAGONAL-	-13.44 SB22 -9.24 SB27 -4.12 SB28 -2.14 SB25						
NORMAL MODE 21	OBSERVED=	0.0 CM-1	CALCULATED=	1045.7 CM-1	ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	30.88 C-O6 9.98 O*CI						
FORCE CONSTANTS-	52.84 CO 21.95 CC						
OFF DIAGONAL-	-10.69 SB24 -7.13 SB27 -6.55 SS18 -6.15 SB28 -3.56 BB21 -2.65 SB22 2.62 BB34 2.43 SB25 -1.69 SB26						
NORMAL MODE 22	OBSERVED=	0.0 CM-1	CALCULATED=	1030.5 CM-1	ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	35.23 HCH 17.56 C3C4						
FORCE CONSTANTS-	35.23 HCH 19.47 CC						
OFF DIAGONAL-	-4.05 SB21 -4.02 SB22 3.49 SB27						
NORMAL MODE 23	OBSERVED=	0.0 CM-1	CALCULATED=	1018.7 CM-1	ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	22.43 C*CH 9.95 C1H						
FORCE CONSTANTS-	36.39 CO 19.33 CCH						
OFF DIAGONAL-	2.46 SB26 -2.23 SB22 -1.69 SB21 -1.59 BB45 6.93 HCH 5.71 CC5H 5.70 C3C4						
NORMAL MODE 24	OBSERVED=	0.0 CM-1	CALCULATED=	1005.8 CM-1	ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	18.80 C-C6 26.32 CCH						
FORCE CONSTANTS-	18.80 CO 10.49 CCH						
OFF DIAGONAL-	-12.91 SB21 -6.97 SB22 -3.79 SB27 3.23 SB25 -3.18 SS18 2.09 SB26 1.67 BB43						
NORMAL MODE 25	OBSERVED=	0.0 CM-1	CALCULATED=	994.8 CM-1	ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	24.96 C5C* 0.25 C1H						
FORCE CONSTANTS-	34.51 CO 24.61 CCH						
OFF DIAGONAL-	-8.17 SB21 -7.88 SB22 4.36 SB26 3.31 BB34 -3.24 SS18 5.36 CCC 2.52 SB25 -1.84 SB24 1.81 BB43 -1.79 SB27						
NORMAL MODE 26	OBSERVED=	0.0 CM-1	CALCULATED=	975.0 CM-1	ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	16.34 C-O* 11.65 C5C*						
FORCE CONSTANTS-	26.04 CCH 26.01 CO						
OFF DIAGONAL-	9.50 SB27 -6.75 SB26 -2.67 SB22 -2.62 SB25 2.46 BB34 -2.07 BB45 1.88 SS18 -1.70 SB21						
NORMAL MODE 27	OBSERVED=	0.0 CM-1	CALCULATED=	968.6 CM-1	ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	24.21 OC1H 8.81 OC4H						
FORCE CONSTANTS-	43.96 OC1H 29.96 CC						
OFF DIAGONAL-	3.94 BB34 3.41 SB27 -3.31 BB29 -2.96 BB45 -1.51 SB26						
NORMAL MODE 28	OBSERVED=	0.0 CM-1	CALCULATED=	956.0 CM-1	ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	39.87 OC1H 10.60 C-O9						
FORCE CONSTANTS-	39.87 OC1H 21.63 CCH						
OFF DIAGONAL-	6.61 SB27 -3.64 SB22 -2.17 BB45 -1.74 SB25						
NORMAL MODE 29	OBSERVED=	0.0 CM-1	CALCULATED=	950.7 CM-1	ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	1.91 HC2C 1.24 C5H						
FORCE CONSTANTS-	32.42 CCH 18.24 CCH						
OFF DIAGONAL-	8.22 SB26 -5.76 SB21 4.17 SB27 3.53 BB29 3.53 BB34 -2.70 SB22 -1.99 BB45 -1.82 SB28 1.54 BB43						
NORMAL MODE 30	OBSERVED=	0.0 CM-1	CALCULATED=	944.3 CM-1	ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	42.69 OC4H 11.26 C-O9						
FORCE CONSTANTS-	46.79 OC1H 22.19 CCH						
OFF DIAGONAL-	11.80 SB27 3.67 BB29 -2.58 BB45						
NORMAL MODE 31	OBSERVED=	0.0 CM-1	CALCULATED=	939.8 CM-1	ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	52.56 OC3H 15.71 CC3H						
FORCE CONSTANTS-	68.99 OC1H 24.07 CCH						
OFF DIAGONAL-	-5.19 SB27 -4.62 BB29 -3.45 BB45 -2.31 BB43 -1.80 SB22						
NORMAL MODE 32	OBSERVED=	0.0 CM-1	CALCULATED=	935.3 CM-1	ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	45.72 OC2H 8.93 C-O7						
FORCE CONSTANTS-	53.72 OC1H 16.37 CCH						
OFF DIAGONAL-	9.34 SB27 -4.32 SB26 -4.23 SB21 -3.63 SB22 -3.04						
NORMAL MODE 33	OBSERVED=	0.0 CM-1	CALCULATED=	910.0 CM-1	ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	46.47 OC1H 13.04 OC4H						
FORCE CONSTANTS-	47.61 CCH 13.28 CC						
OFF DIAGONAL-	10.48 SB26 9.01 BB29 10.41 OC1H 3.15 BB34 -2.54 SB22 -2.54 BB45						
NORMAL MODE 34	OBSERVED=	0.0 CM-1	CALCULATED=	914.2 CM-1	ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	11.28 CC5H 10.04 HC3C						
FORCE CONSTANTS-	82.20 OC1H 15.02 CCH						
OFF DIAGONAL-	-2.12 BB29 -2.00 BB45						
NORMAL MODE 35	OBSERVED=	0.0 CM-1	CALCULATED=	902.2 CM-1	ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	23.27 C*CH 7.87 CC4H						
FORCE CONSTANTS-	40.01 OC1H 22.75 CCH						
OFF DIAGONAL-	4.66 SB27 2.41 SB26 -2.30 BB43 -1.90 SB25						

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400
MOLECULE 8 -6 NG-1236 ALPHA GLUCOSE-C-D7

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NORMAL MODE 36	OBSERVED=	0.0 CM-1	CALCULATED=	891.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	18.45	CC4H 10.94 HC4C	7.97 C-DH	7.81 C-H	5.90 C3C4	5.83 CCO9		5.13 CCO9
FORCE CONSTANTS-	41.60	CCH 18.97 CCH	18.83 CCH	17.28 CO	11.28 CC			
OFF DIAGONAL-	5.94	BB34 -4.70 BB29	-3.70 SB26	-3.55 BB43	-2.68 SB22	-2.20 BB45		
NORMAL MODE 37	OBSERVED=	0.0 CM-1	CALCULATED=	769.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	34.03	CCH2 21.49 C-06	16.64 HC2C	7.30 CCH				
FORCE CONSTANTS-	61.10	CCH 24.27 CO	7.76 CC	6.10 CCH				
OFF DIAGONAL-	-5.56	SB27 4.19 SB26	-3.21 BB29	-2.76 BB45	-2.43 SB21	2.30 SB25	-2.03 SB22	1.73 BB43
NORMAL MODE 38	OBSERVED=	0.0 CM-1	CALCULATED=	721.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	15.16	CCHA 15.04 C5U*	9.93 C5C*					
FORCE CONSTANTS-	23.49	CCH 20.02 CO	13.42 CC	10.81 CCO				
OFF DIAGONAL-	3.82	SB26 3.24 BB43	2.31 SB23					
NORMAL MODE 39	OBSERVED=	0.0 CM-1	CALCULATED=	702.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	15.45	CC1H 12.17 CCHA	9.47 C5U*	9.52 C5C*	7.74 CCH	5.98 C2C3		
FORCE CONSTANTS-	45.43	CCH 20.35 CO	12.36 CCO	9.52 CCH	7.96 CCH	6.59 CC		
OFF DIAGONAL-	-4.60	SB23 -3.86 BB29	3.83 SB25	2.88 BB43	-2.06 SB27	-1.86 BB37		
NORMAL MODE 40	OBSERVED=	0.0 CM-1	CALCULATED=	594.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	17.33	CCO6 17.76 CCO	11.11 CCO	6.39 C2C	5.60 CCH			
FORCE CONSTANTS-	33.44	CCO 18.93 CCH	12.61 CC	11.92 CO	10.76 CCO	5.60 CCH		
OFF DIAGONAL-	3.84	SB24 -3.15 BB29	-3.13 SB27	-3.04 BB34	2.69 SS18	2.59 BB43	-2.21 SB23	2.11 SB25
NORMAL MODE 41	OBSERVED=	0.0 CM-1	CALCULATED=	543.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	18.56	CC5H 17.22 HC4C	14.94 CCO*	14.66 O8CC	9.42 CC4H	6.61 HC3C	6.21 HC5C	
FORCE CONSTANTS-	64.99	CCH 50.80 CCO	6.30 CCO					
OFF DIAGONAL-	-19.01	BB34 -14.71 BB29	9.60 BB43	-1.98 BB45	1.53 SB25			
NORMAL MODE 42	OBSERVED=	0.0 CM-1	CALCULATED=	518.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	17.52	4CO* 15.51 CCO	7.69 C-09	7.14 O9CC	6.26 O1CC	5.54 C4C5		
FORCE CONSTANTS-	32.87	CCO 15.51 CCO	13.59 CC	12.79 CC	12.13 CCH	5.08 CCH		
OFF DIAGONAL-	6.63	SB25 6.28 SB22	-3.82 BB34	-3.06 SB27	3.01 SS18	-2.88 SB21	-2.33 BB42	-1.51 BB29
NORMAL MODE 43	OBSERVED=	0.0 CM-1	CALCULATED=	498.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	18.13	O7CC 15.24 CC3H	11.31 CCO9	10.43 HC2C	9.11 HC3C	7.01 O1CC	6.46 CCO8	5.21 CCO
FORCE CONSTANTS-	51.67	CCH 47.17 CCO	8.81 CCO	8.31 CCO	7.21 SB22	-1.82 BB36		5.03 CC4H
OFF DIAGONAL-	-17.26	BB34 -11.66 BB29	8.86 BB43	2.11 SB22				
NORMAL MODE 44	OBSERVED=	0.0 CM-1	CALCULATED=	414.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	22.33	C2CC 8.74 C1CC	8.54 CCO5	7.15 O9CC	6.32 CCH	6.00 CCO		
FORCE CONSTANTS-	28.53	CCO 24.32 CCH	16.39 CCH	6.33 CC	6.32 CCH	6.00 CCO		
OFF DIAGONAL-	4.64	SB22 -3.08 BB29	2.90 BB43	-1.78 BB41	-1.69 BB42	1.83 SB25		
NORMAL MODE 45	OBSERVED=	0.0 CM-1	CALCULATED=	412.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	18.68	O1CC 7.19 CCO*	11.56 C3CC	9.27 OCO	8.52 O9CC	5.74 CCO7	5.42 HC5C	
FORCE CONSTANTS-	52.43	CCO 18.87 CCH	15.87 CCH	9.27 CCO				
OFF DIAGONAL-	-8.16	BB34 -4.62 SB21	3.43 BB43	3.25 SB22	-3.01 BB42	-2.93 BB29	2.07 SB25	
NORMAL MODE 46	OBSERVED=	0.0 CM-1	CALCULATED=	382.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	13.75	O8CC 13.40 CCO8	8.60 C2CC	8.12 O9CC	7.71 CCO*	5.78 CCO6	5.29 C4C5	
FORCE CONSTANTS-	19.12	CCO 16.43 CCH	15.64 CCH	9.88 CC				
OFF DIAGONAL-	-10.33	BB34 3.85 SB25	3.15 SB21	-3.07 BB29	-2.95 BB42	-2.47 SB26	2.12 BB43	
NORMAL MODE 47	OBSERVED=	0.0 CM-1	CALCULATED=	349.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	20.51	O7CC 13.31 CCO*	6.37 CCO	5.76 C3C4	5.34 CCH			
FORCE CONSTANTS-	46.31	CCO 21.28 CCH	12.27 CC	6.39 CCH	6.37 CCO			
OFF DIAGONAL-	-7.46	BB34 4.28 SB21	-2.82 BB29	-2.67 SB26	2.41 BB43	-1.65 BB33	-1.63 SB27	1.55 SB24
NORMAL MODE 48	OBSERVED=	0.0 CM-1	CALCULATED=	314.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	22.83	CCO9 11.77 CCO8	9.60 CCO	8.84 CCO6	7.09 CCO7	5.75 O8CC		
FORCE CONSTANTS-	71.88	CCO 10.10 CC	9.26 T-OH	6.84 CCH				
OFF DIAGONAL-	-6.15	BB34 5.40 SB22	-3.71 BB42					
NORMAL MODE 49	OBSERVED=	0.0 CM-1	CALCULATED=	309.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	22.40	CCO8 19.09 CCO7	12.41 O8CC	6.71 CCO*	6.68 4CO*	5.75 C4C5		
FORCE CONSTANTS-	73.40	CCO 10.88 CC	7.26 T-OH	6.84 CCH				
OFF DIAGONAL-	-7.83	BB34 -3.81 BB42	3.37 SB21					
NORMAL MODE 50	OBSERVED=	0.0 CM-1	CALCULATED=	291.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	15.77	4CO* 13.31 O9CC	9.70 O8CC	8.83 CCO*	5.91 HC4C	5.12 CC5H		
FORCE CONSTANTS-	61.19	CCO 23.77 CCH	12.57 CCH	8.09 CCH				
OFF DIAGONAL-	-14.29	BB34 6.11 BB43	-4.94 BB29	-3.60 SB25				
NORMAL MODE 51	OBSERVED=	0.0 CM-1	CALCULATED=	251.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	17.99	CCO6 9.09 O1CC	8.65 CCO	7.84 O7CC	7.34 CCH2	5.71 HC2C	5.45 TH-3	5.40 C1CC
FORCE CONSTANTS-	59.22	CCH 20.93 CCH	14.82 T-OH	8.93 CCH				5.29 TH-1
OFF DIAGONAL-	-9.45	BB34 7.60 BB43	-3.71 SB25	-3.03 BB29	-3.03 BB33			
NORMAL MODE 52	OBSERVED=	0.0 CM-1	CALCULATED=	237.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	18.83	TH-5 5.70 TH-4	5.08 CCC					
FORCE CONSTANTS-	77.53	T-OH 11.37 CCO						
OFF DIAGONAL-	NONE							
NORMAL MODE 53	OBSERVED=	0.0 CM-1	CALCULATED=	228.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	51.96	TH-1 27.45 TH-3	7.33 TH-2	6.57 TH-4				
FORCE CONSTANTS-	93.33	T-OH						
OFF DIAGONAL-	NONE							
NORMAL MODE 54	OBSERVED=	0.0 CM-1	CALCULATED=	222.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	47.82	TH-4 17.99 TH-1	15.58 TH-5	6.90 TH-3				
FORCE CONSTANTS-	88.42	T-OH 5.89 CCO						
OFF DIAGONAL-	NONE							
NORMAL MODE 55	OBSERVED=	0.0 CM-1	CALCULATED=	214.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	31.11	TH-3 25.38 TH-4	12.23 TH-2	11.93 TH-1				
FORCE CONSTANTS-	80.87	T-OH 15.35 CCO						
OFF DIAGONAL-	-2.05	BB34						
NORMAL MODE 56	OBSERVED=	0.0 CM-1	CALCULATED=	213.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	18.63	TH-2 16.80 TH-3						
FORCE CONSTANTS-	83.26	T-OH 14.77 CCO						
OFF DIAGONAL-	-1.65	BB34						
NORMAL MODE 57	OBSERVED=	0.0 CM-1	CALCULATED=	185.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	33.81	CCO* 17.26 C4CC	14.25 TH-5	7.00 COTC	5.16 CCHA			
FORCE CONSTANTS-	47.20	CCO 19.16 CCH	17.50 T-OH	9.56 CCH	7.00 CCH	6.32 T-CC		
OFF DIAGONAL-	-5.42	BB34 -3.60 BB42	-3.55 BB33					
NORMAL MODE 58	OBSERVED=	0.0 CM-1	CALCULATED=	128.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	22.03	COTC 15.14 C4CC	10.20 TCC4	6.47 C1CC	6.42 TCO1	5.01 CCO		
FORCE CONSTANTS-	22.70	CCC 22.03 CCO	12.28 T-CC	11.57 CCO	10.05 T-CC	5.63 CCH	5.01 CCO	
OFF DIAGONAL-	3.90	BB43 -3.48 SB21	-2.44 BB37	1.94 BB41	-1.66 BB34			
NORMAL MODE 59	OBSERVED=	0.0 CM-1	CALCULATED=	92.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	50.58	TC5 11.38 C3CC	7.09 TCC2	6.72 C2CC	6.52 U9CC			
FORCE CONSTANTS-	61.89	T-CC 21.49 CCH	16.97 CCO					
OFF DIAGONAL-	-3.71	SB25 -2.74 SB21	-2.47 BB42	-2.28 BB34	-1.56 BB43	1.54 BB41		
NORMAL MODE 60	OBSERVED=	0.0 CM-1	CALCULATED=	78.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	18.43	C2CC 14.53 C1CC	12.62 TCC3	8.47 COTC	7.26 TCC4	7.21 TCC1	5.19 TCO2	
FORCE CONSTANTS-	37.48	CCC 31.99 T-CC	16.80 CCO	8.47 CCH	6.09 T-CC			
OFF DIAGONAL-	-3.62	BB42 -3.56 SB25	-2.32 SB21	2.14 BB41				
NORMAL MODE 61	OBSERVED=	0.0 CM-1	CALCULATED=	64.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	25.03	TC5 13.84 C3CC	9.60 TCC4	7.21 TCC3	7.14 TCC2	5.70 4CO*		
FORCE CONSTANTS-	49.73	T-CC 22.47 CCO	21.36 CCH					
OFF DIAGONAL-	-2.59	BB42 -2.15 BB34	-1.63 SB25					

2. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 0.0

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400										PAGE 1	
MOLECULE 9 -6 NG=1236 ALPHA GLUCOSE-D12											
NORMAL MODE 8	OBSERVED=	0.0 CM-1	CALCULATED=	1256.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	34.62	O*CH 21.54 C-U6	10.85 CCH 10.52 C5O1	7.32	O*CC 6.88 CCO6	6.47	CCH2	5.20	CCO7		
FORCE CONSTANTS-	72.93	CC 23.79 CCO	18.28 CCH 10.31 CCH								
OFF DIAGONAL-	-15.84	SB25-13.15 SB27	3.88 BB34 -2.24 SB26	1.72	BB33 -1.55 BB43	1.52	SB28				
NORMAL MODE 9	OBSERVED=	0.0 CM-1	CALCULATED=	1241.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	24.75	C5O1 19.80 C-U9	9.91 CC5H 6.43 C4C5	5.77	O9CC 5.61 HC4C						
FORCE CONSTANTS-	50.67	CO 22.30 CCH	17.28 CCH 11.26 CC	10.39	OCH						
OFF DIAGONAL-	-15.17	SB25 -8.98 SB27	-7.47 SB26	6.08	BB34 4.17	BB29 -4.01	SS18	3.97	SB22 -2.72	SB21 -1.79	SB23
NORMAL MODE 10	OBSERVED=	0.0 CM-1	CALCULATED=	1205.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	44.95	C2C3 14.97 C3OH	12.33 C-O8 8.47 CC3H	6.96	OBCC 5.86 HC2C	5.12	C1C2				
FORCE CONSTANTS-	53.60	CC 23.67 CCO	17.62 BCOH 17.61 CCH	12.72	CCO 6.44 OCH						
OFF DIAGONAL-	-15.09	SB26 -7.00 SB22	-5.49 SB27 -4.51	SB21 4.25	SB28 -4.02	SS18	3.63	BB36 -3.29	SB25 3.26	BB29	
NORMAL MODE 11	OBSERVED=	0.0 CM-1	CALCULATED=	1185.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	27.74	C3C4 16.04 C4C5	13.55 C5O1 10.86 C-O8	8.67	CC4H 7.90 C-O9	5.73	HC3C	5.09	C4OH		
FORCE CONSTANTS-	49.14	CC 33.71 CCH	21.84 CCH 14.83 CCO	10.09	OCH 8.23 BCOH						
OFF DIAGONAL-	-17.41	SB26 -7.32 SB22	-6.56 SB27 -3.89	SS18 -3.89	SB28 3.89	BB29 -1.83	BB43 -1.73	SB23			
NORMAL MODE 12	OBSERVED=	0.0 CM-1	CALCULATED=	1182.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	34.92	C5O1 19.79 C-O*	9.75 CC5H 7.59 HC5C	7.55	CC8H 6.42 CCH4	5.48	C4C5	5.35	C5O1		
FORCE CONSTANTS-	47.86	CC 13.58 CCO	21.44 CCH 18.90 OCH	9.60	CCO 9.14 BCOH						
OFF DIAGONAL-	-19.30	SB26-14.71 SB27	-5.62 SS18 -4.71	SB22 4.55	SB28 3.84	BB29 -2.01	SB25 -1.62	BB45			
NORMAL MODE 13	OBSERVED=	0.0 CM-1	CALCULATED=	1166.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	19.02	C-O6 17.03 C1C2	11.88 C2OH 9.66 OC1H	6.85	C-O7 6.57 C1OH	6.37	O7CC	6.03	O*Cl		
FORCE CONSTANTS-	35.65	CC 20.23 CCH	18.59 BCOH 14.45 OCH	11.30	CCO 6.12 CCH						
OFF DIAGONAL-	-8.99	SB27 7.70 SB28	-5.80 SB22	2.52	BB36 -2.49	SB25 -2.21	SS18	2.08	BB34		
NORMAL MODE 14	OBSERVED=	0.0 CM-1	CALCULATED=	1146.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	27.41	C1CH 20.68 C1C2	12.17 O*Cl 6.24 *C1H								
FORCE CONSTANTS-	32.26	BCOH 25.76 CC	24.96 CCO 13.89 OCH	10.29	CCH 9.21 CCO						
OFF DIAGONAL-	-8.45	SB27 -6.76 SB22	-5.92 SB26	2.57	SB28 -2.34	SB24 -2.19	SS18	-2.13	SB23		
NORMAL MODE 15	OBSERVED=	0.0 CM-1	CALCULATED=	1131.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	15.41	C-O9 12.52 C-U7	12.23 C4C5 11.39 C2OH	9.24	C-O8 7.71 C2C3	6.49	C1CC	5.30	HC4C	5.01	C3C4
FORCE CONSTANTS-	47.97	CC 26.88 CCH	15.23 CCH 14.16 BCOH	11.49	OCH 11.34 CCO	10.28	CCO				
OFF DIAGONAL-	-8.16	SB27 -7.32 SB26	-6.91 SB25 -5.23	SB28 -4.77	SB21 -2.07	SB22 -1.97	SS18	-1.54	SB24		
NORMAL MODE 16	OBSERVED=	0.0 CM-1	CALCULATED=	1115.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	18.74	C4OH 10.34 C-U8	10.20 C-O7 1.38 CCH	6.63	C4C5 5.43 CC09	5.40	C3C4				
FORCE CONSTANTS-	46.93	CC 19.46 CCO	14.64 CCH 13.64 CCH	13.33	CCO 9.14 BCOH						
OFF DIAGONAL-	-7.87	SB27 -5.57 SB22	-5.52 SB25 -5.32	SB28 -3.39	BB36 1.57	BB34					
NORMAL MODE 17	OBSERVED=	0.0 CM-1	CALCULATED=	1079.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	51.03	C*CH 12.42 C-O*	10.90 CCOH 9.21 HC5C	6.17	HCH 5.39 C5C1	5.08	C4C5				
FORCE CONSTANTS-	51.03	BCOH 14.93 CCO	12.44 CCH 11.95 CCO	10.61	CC 6.17 HCH						
OFF DIAGONAL-	-9.59	SB28 -4.19 SB25	-4.07 SB22	4.02	BB34 -3.86	SB21 -3.85	BB35	1.72	SB27		
NORMAL MODE 18	OBSERVED=	0.0 CM-1	CALCULATED=	1074.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	32.51	C3CH 22.36 C-O7	11.12 C-O9 9.93 OC2H	7.99	C2OH 7.21 HC2C						
FORCE CONSTANTS-	41.55	BCOH 41.23 CCO	16.35 OCH 12.98 CCH	5.60	CCO						
OFF DIAGONAL-	-8.31	SB28 -7.96 SB27	3.20	BB34 -2.80	SB25 -1.83	BB35					
NORMAL MODE 19	OBSERVED=	0.0 CM-1	CALCULATED=	1053.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	17.24	HCH 9.60 CCH2	8.83 O*Cl 6.23 C1C2	5.73	CC1H 8.87 CCO	8.10	BCOH				
FORCE CONSTANTS-	21.91	CCH 21.06 CCH2	17.24 CCH 17.10 OCH	15.34	CC						
OFF DIAGONAL-	-7.98	SB27 -3.90 SB22	2.58	BB34 -2.40	SB24 -1.87	SB26					
NORMAL MODE 20	OBSERVED=	0.0 CM-1	CALCULATED=	1052.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	48.94	C4OH 13.31 HCH	9.89 CCH 7.42 CCH	7.39	C1C2 5.42 CCH2	8.18	CCO				
FORCE CONSTANTS-	46.93	CC 18.10 CCH	17.95 OCH 14.84 CCH	13.33	HCH 8.34						
OFF DIAGONAL-	-4.34	SB22 -3.80 SB28	-3.62 SB27 -3.08	SB21 2.05	BB34 -1.80	BB36					
NORMAL MODE 21	OBSERVED=	0.0 CM-1	CALCULATED=	1021.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	29.09	HCH 16.05 C-U*	10.90 CCOH 9.21 HC5C	6.17	HCH 5.39 C5C1	5.08	C4C5				
FORCE CONSTANTS-	29.09	HCH 20.13 CCO	17.23 CCH 16.40 OCH	5.55	BCOH						
OFF DIAGONAL-	-4.08	SB27 -1.87 SB28									
NORMAL MODE 22	OBSERVED=	0.0 CM-1	CALCULATED=	1012.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	26.56	*C*H 16.74 *C1H	10.02 C4C5 8.83 C-O8								
FORCE CONSTANTS-	50.53	OCH 17.72 CCO	13.42 CC 13.38 CCH								
OFF DIAGONAL-	-4.04	SB21 -2.89 SB28	-2.55 SB26 -2.26	BB45 -1.94	SB22 1.73	SB27					
NORMAL MODE 23	OBSERVED=	0.0 CM-1	CALCULATED=	1005.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	28.81	C-O6 27.20 C1OH	9.74 O*Cl 7.36 C1C2	5.95	C-O9 5.46 C4C5	5.09	OC3H				
FORCE CONSTANTS-	51.42	CC 29.94 BCOH	10.04 CC 7.11 CCH	6.83	OCH 5.23						
OFF DIAGONAL-	-12.32	SB28 6.78 SB27	-5.90	SB24 -3.63	SS18 -2.80	SB25 -2.38	BB35				
NORMAL MODE 24	OBSERVED=	0.0 CM-1	CALCULATED=	988.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	39.50	C-O9 7.83 OC1H	7.80 C*CH 7.42 CCH	7.39	CCO 5.46 C4C5	5.09	OC3H				
FORCE CONSTANTS-	39.50	OCH 27.83 CCH	18.05 CC 13.82 CCH	8.22	BCOH 2.86	SB27 1.77	SB25 1.77	BB34 -1.51	SB24		
OFF DIAGONAL-	-7.09	SB21 -3.82 SS18	3.72	SB26 -3.60	SB28 -2.91	SB22					
NORMAL MODE 25	OBSERVED=	0.0 CM-1	CALCULATED=	980.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	33.00	C3C4 0.13 OC1H	9.34 OC2H 6.93 CC4H	6.50	OC3H 5.61 C4OH						
FORCE CONSTANTS-	33.00	UCH 18.58 CC	18.04 CCH 9.87 BCOH	9.63	CC 8.14 CCO						
OFF DIAGONAL-	-4.54	SB22 -3.99 SB21	3.49	SB26 2.59	SB27 2.24	BB34 -1.78	BB45				
NORMAL MODE 26	OBSERVED=	0.0 CM-1	CALCULATED=	961.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	16.94	C-O8 11.27 C-U9	10.01 C-O*	8.94 CC5H	8.48	HC3C 8.20	C4OH				
FORCE CONSTANTS-	41.47	CC 29.97 CCH	11.66 BCOH 11.40 OCH	5.76	CC						
OFF DIAGONAL-	-6.66	SB28 2.46 SB27	-1.81	SB26 1.78	BB34 -1.73	BB45					
NORMAL MODE 27	OBSERVED=	0.0 CM-1	CALCULATED=	948.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	31.71	OC3H 8.79 OC2H	7.35 CC3H 6.92 HC2C	1.63	CC5H						
FORCE CONSTANTS-	41.18	OCH 27.75 CCH	19.99 CCO								
OFF DIAGONAL-	-8.64	SB27 3.52 BB29	-2.68	BB45 2.37	SB26 -1.62	SB21 1.55	BB34				
NORMAL MODE 28	OBSERVED=	0.0 CM-1	CALCULATED=	941.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	32.93	UCH 24.54 HC4C	9.27 C-O8								
FORCE CONSTANTS-	46.93	CCH 23.13 CCH	10.18 CCO	5.43	CCO						
OFF DIAGONAL-	-7.59	SB27 -2.58 BB45	2.03	SB26 1.97	BB34						
NORMAL MODE 29	OBSERVED=	0.0 CM-1	CALCULATED=	933.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	58.33	OC4H 4.36 CCHA	9.06 OCH 7.17 C5C1	6.92	OCBH						
FORCE CONSTANTS-	58.20	UCH 17.19 CCH	9.28 BCOH 7.97 CC								
OFF DIAGONAL-	-4.75	SB26 2.65 SB27	-2.23	BB45 -1.71	SB21						
NORMAL MODE 30	OBSERVED=	0.0 CM-1	CALCULATED=	924.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	10.27	OC1H 9.69 *C5H	9.04 CC5H 6.93 CC4H	6.67	C5C1 6.61 C1OH						
FORCE CONSTANTS-	29.73	OCH 23.75 CCH	15.17 CC 9.02 BCOH	8.21	CCO						
OFF DIAGONAL-	-6.44	SB26 4.52 SB27	3.50	BB29 -3.06	SB21 -2.08	BB45 -1.56	SB22 -1.55	SS18			
NORMAL MODE 31	OBSERVED=	0.0 CM-1	CALCULATED=	915.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	9.86	HC3C 9.02 OC2H	6.53 CC4H 6.48 OC1H	5.50	C1OH 5.08 CCHB						
FORCE CONSTANTS-	35.54	CC 24.69 OCH	13.26 CCO 8.92 BCOH	6.70	CC						
OFF DIAGONAL-	-6.83	BB29 4.95 SB26	-2.64	SB28 2.54	SB27 -2.47	BB45					
NORMAL MODE 32	OBSERVED=	0.0 CM-1	CALCULATED=	895.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	23.14	OC2H 20.30 C2OH	26.29 CC3H 6.29 CCH2	5.86	CC1H						
FORCE CONSTANTS-	23.14	CCH 31.6 CCH	11.83 BCOH								
OFF DIAGONAL-	-2.83	BB45 -2.76 SB28	-1.87	SB26 1.87	SB27 1.74	BB29					
NORMAL MODE 33	OBSERVED=	0.0 CM-1	CALCULATED=	882.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	43.26	UCHB 8.56 *C*UH	10.98 HC5C 9.69 CCH	7.65	C1OH 5.01 CC1H						
FORCE CONSTANTS-	43.27	UCH 26.30 BCOH	21.42 CCH 6.59 CC								
OFF DIAGONAL-	-3.48	BB29 -2.56 SB22	-2.18	BB45 1.61	BB39						
NORMAL MODE 34	OBSERVED=	0.0 CM-1	CALCULATED=	878.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	16.20	UCHB 9.20 C1OH	8.80 C*CH 5.40 *C5H	5.13	C4OH 5.09 OC1H						
FORCE CONSTANTS-	39.25	UCH 25.14 BCOH	18.28 CCH 9.23 CC								
OFF DIAGONAL-	-3.26	SB22 1.61 BB39									
NORMAL MODE 35	OBSERVED=	0.0 CM-1	CALCULATED=	873.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	20.72	C3OH 13.48 OC3H	12.44 C4OH 10.87 C3C4	9.35	C2C3 7.11 C-O8	5.63	OC4H				
FORCE CONSTANTS-	37.64	UCH 25.30 CC	23.48 OCH 12.84 CCH	12.79	CCO 6.72 CCO						
OFF DIAGONAL-	-5.96	SB28 -5.20 SB27	-4.11	SB21 -3.60	SB22 2.36	BB39 -2.09	BB36 -1.89	BB29			

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400										PAGE 2	
MOLECULE 9 NG=1236 ALPHA GLUCOSE-D12											
NORMAL MODE 36	UBSERVED=	0.0 CM-1	CALCULATED=	852.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	32.12 C3OH 13.66 C4H	9.19 C4H	9.19 C4H	9.19 C4H	6.85 C4H	6.19 C4H	5.75 HC4C	5.51 C3C4			
FORCE CONSTANTS-	32.78 CCH 25.69 BCCH	17.04 CC	14.70 CCO	12.23 CCH	7.99 CO						
OFF DIAGONAL-	-58.80 BB29 5.08 BB34	-4.31 SB22	-3.55 SB26	-2.88 BB43	-2.62 SB21	-1.69 BB45	1.52 BB36				
NORMAL MODE 37	UBSERVED=	0.0 CM-1	CALCULATED=	757.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	31.15 CCH2 19.48 C-O6	16.21 HC2C	5.53 C2C3								
FORCE CONSTANTS-	56.80 CCH 20.68 CO	10.26 CC	5.71 CCH	5.40 CCO							
OFF DIAGONAL-	4.76 SB26	-4.71 SB27	-4.02 HB29	-3.62 SB21	-2.49 BB45	2.09 BB43	2.07 SB25	-2.02 SB22	1.54 BB33		
NORMAL MODE 38	UBSERVED=	0.0 CM-1	CALCULATED=	719.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	16.48 C5O1 16.06 CCHA	10.27 C5C1									
FORCE CONSTANTS-	25.13 CCH 20.33 CO	13.82 CC	10.14 CCO								
OFF DIAGONAL-	3.99 SB26	2.96 BB43	2.25 SB23								
NORMAL MODE 39	UBSERVED=	0.0 CM-1	CALCULATED=	701.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	15.63 CCH 11.16 CCHA	10.36 C5C1	8.32 C5O1	7.37 CCH	6.74 C2C3						
FORCE CONSTANTS-	44.02 CCH 19.39 CO	11.77 CCH	10.36 CCH	7.80 CCH	7.33 CC						
OFF DIAGONAL-	-4.71 SB23	3.85 SB25	-3.76 HB29	2.93 BB43	-2.15 SB27	-1.83 BB37					
NORMAL MODE 40	UBSERVED=	0.0 CM-1	CALCULATED=	581.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	17.69 CCO6 10.28 CCO	10.15 CCO6	7.52 C1C2	5.02 C5C1							
FORCE CONSTANTS-	31.45 CCH 15.73 CCH	11.24 CC	10.71 CCO	10.28 CCO	5.02 CCH						
OFF DIAGONAL-	3.41 SB24	-2.86 SB27	-2.82 HB34	2.63 SS18	2.54 BB43	-2.44 BB29	2.08 SB25	-1.94 SB23	-1.67 BB42		
NORMAL MODE 41	UBSERVED=	0.0 CM-1	CALCULATED=	540.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	19.05 CCH5 18.18 HC4C	15.19 CCH	14.68 HBCC	9.13 CCH	6.08 HC3C	5.68 HC5C					
FORCE CONSTANTS-	64.76 CCH 50.37 CCO	6.33 CCH									
OFF DIAGONAL-	-18.87 BB34	-14.63 BB29	9.56 BB43	-1.92 BB45							
NORMAL MODE 42	UBSERVED=	0.0 CM-1	CALCULATED=	514.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	15.76 CCO1 13.37 CCO	7.98 O9CC	6.96 C-O9	5.40 C4C5							
FORCE CONSTANTS-	32.02 CCO 15.34 CCH	13.96 CC	13.37 CCO	12.87 CCO							
OFF DIAGONAL-	6.70 SB25	6.39 SB22	-4.07 HB34	3.16 SS18	-2.90 SB27	-2.46 SB21	-2.34 BB29	-1.81 BB42			
NORMAL MODE 43	UBSERVED=	0.0 CM-1	CALCULATED=	488.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	16.75 U7CC 13.39 CCH	11.35 CCO9	9.88 HC2C	9.47 O1CC	8.60 HC3C	6.67 CCO	6.44 CCO8				
FORCE CONSTANTS-	48.82 CCO 45.73 CCH	6.67 CCO	6.51 CCH	5.98 CCH							
OFF DIAGONAL-	-16.58 BB34	-10.24 BB29	8.53 BB43	-2.10 SB22	-2.09 BB36						
NORMAL MODE 44	UBSERVED=	0.0 CM-1	CALCULATED=	411.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	13.94 C2CC 8.34 CCO9	8.89 C1CC	5.44 O9CC	5.11 CCH							
FORCE CONSTANTS-	27.78 CCH 10.73 CCH	20.93 CCO	10.71 CCO	10.28 CCO							
OFF DIAGONAL-	-4.24 BB29	3.96 BB43	3.45 SB22	1.95 SB21	-1.91 BB34	-1.66 BB41					
NORMAL MODE 45	UBSERVED=	0.0 CM-1	CALCULATED=	407.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	19.98 O1CC 16.52 CCO*	11.97 O9CC	9.01 C3C4	7.56 CCO7							
FORCE CONSTANTS-	54.88 CCO 15.29 CCH	11.92 CCH	11.65 CCO	5.57 CC							
OFF DIAGONAL-	-7.94 BB34	-5.32 SB21	4.05 SB22	-3.60 BB42	2.69 SB25	2.23 BB43	-1.82 BB29				
NORMAL MODE 46	UBSERVED=	0.0 CM-1	CALCULATED=	379.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	15.74 CCO8 11.68 CCH	8.89 C2CC	8.04 O9CC	6.69 CCO*	6.33 CCO6						
FORCE CONSTANTS-	60.01 CCO 16.20 CCH	15.55 CCH	9.60 CC	9.44 CCH							
OFF DIAGONAL-	-9.98 BB34	3.94 SB25	3.54 SB21	-3.05 BB42	-2.78 BB29	-2.62 SB26	1.80 BB43	-1.54 BB36			
NORMAL MODE 47	UBSERVED=	0.0 CM-1	CALCULATED=	342.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	20.77 U7CC 14.51 CCO*	7.07 CCO	6.20 CCH8	5.55 C3C4							
FORCE CONSTANTS-	43.19 CCO 22.18 CCH	10.30 CCH	10.07 CCO	6.59 CCH							
OFF DIAGONAL-	-7.73 BB34	4.01 SB21	-3.27 BB29	2.87 BB43	-2.37 SB26	-2.16 BB36	1.72 SB24	-1.61 SB27	-1.56 BB33		
NORMAL MODE 48	UBSERVED=	0.0 CM-1	CALCULATED=	307.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	21.07 CCO9 18.96 CCO7	10.33 O9CC	9.52 CCO6	6.36 O7CC							
FORCE CONSTANTS-	73.36 CCH 7.48 CCH	5.64 T-OH	5.39 CCH								
OFF DIAGONAL-	6.72 SB22	-5.47 BB34	-3.97 BB42	-2.41 SB21	-1.56 SB24						
NORMAL MODE 49	UBSERVED=	0.0 CM-1	CALCULATED=	305.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	29.36 CCO9 17.35 HBCC	8.36 CCO7	8.14 CCO*	7.72 CCO*	7.32 C4C5						
FORCE CONSTANTS-	75.77 CCO 14.29 CC	9.44 CCH									
OFF DIAGONAL-	-9.00 BB34	5.33 SB21	-3.75 BB42	-2.02 SB26							
NORMAL MODE 50	UBSERVED=	0.0 CM-1	CALCULATED=	286.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	15.02 HBCC 15.01 CCO*	14.87 O9CC	8.47 CCO*	6.11 O7CC	5.18 CCH5						
FORCE CONSTANTS-	71.06 CCO 22.75 CCH	8.63 CCH	5.55 T-OH								
OFF DIAGONAL-	-14.83 BB34	5.55 BB43	-4.37 BB29	-3.50 SB25							
NORMAL MODE 51	UBSERVED=	0.0 CM-1	CALCULATED=	243.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	22.39 CCO6 9.78 O7CC	9.00 CCH2	8.94 O1CC	8.05 CCO9	6.87 HC2C	5.58 C1CC	5.28 CCO7				
FORCE CONSTANTS-	61.85 CCH 24.60 CCH	2.68 CCH									
OFF DIAGONAL-	-16.60 BB34	8.87 BB43	3.55 SB25	-3.74 BB33	-3.55 BB29	1.92 SB22	-1.65 BB36	1.60 BB42			
NORMAL MODE 52	UBSERVED=	0.0 CM-1	CALCULATED=	205.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	19.97 CCO9 21.98 T-H5	15.67 C4C5	8.89 CCO	5.76 CCH							
FORCE CONSTANTS-	39.94 CCO 27.10 T-OH	18.60 CCH	8.89 CCO								
OFF DIAGONAL-	-3.81 BB34	-2.83 BB42	-2.24 BB33								
NORMAL MODE 53	UBSERVED=	0.0 CM-1	CALCULATED=	173.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	58.89 TH-3 15.38 TH-3										
FORCE CONSTANTS-	80.21 T-OH 5.03 CCH										
OFF DIAGONAL-	NONE										
NORMAL MODE 54	UBSERVED=	0.0 CM-1	CALCULATED=	163.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	41.50 TH-4 21.75 TH-3	17.02 TH-5	11.20 TH-1								
FORCE CONSTANTS-	92.94 T-OH										
OFF DIAGONAL-	NONE										
NORMAL MODE 55	UBSERVED=	0.0 CM-1	CALCULATED=	156.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	41.53 TH-4 21.19 TH-2	19.00 TH-3									
FORCE CONSTANTS-	90.21 T-OH 7.40 CCH										
OFF DIAGONAL-	NONE										
NORMAL MODE 56	UBSERVED=	0.0 CM-1	CALCULATED=	155.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	18.97 TH-3 25.58 TH-2	20.72 TH-5									
FORCE CONSTANTS-	89.65 T-OH 9.05 CCO										
OFF DIAGONAL-	NONE										
NORMAL MODE 57	UBSERVED=	0.0 CM-1	CALCULATED=	152.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	40.03 TH-3 31.54 TH-5	7.58 CCO*									
FORCE CONSTANTS-	76.97 T-OH 12.92 CCO										
OFF DIAGONAL-	-1.70 BB34										
NORMAL MODE 58	UBSERVED=	0.0 CM-1	CALCULATED=	119.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	17.62 CCO1 16.25 TH-1	12.62 C4CC	8.21 TCC4	5.34 C1CC	5.34 TCO1	5.17 CCO					
FORCE CONSTANTS-	18.84 CCH 18.77 T-OH	17.62 C4CC	10.38 T-CC	9.69 CCH	8.38 T-CC	5.17 CCO					
OFF DIAGONAL-	3.22 BB43	-2.89 SB21	-1.81 BB37	1.63 BB41							
NORMAL MODE 59	UBSERVED=	0.0 CM-1	CALCULATED=	89.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	50.72 TCC5 10.46 C3CC	6.64 O9CC	6.11 TCC2	5.22 C2CC							
FORCE CONSTANTS-	69.89 T-CC 19.81 CCO	12.61 CCH									
OFF DIAGONAL-	3.47 SB25	-2.65 SB21	12.33 BB34	-2.31 BB42	-1.51 BB43						
NORMAL MODE 60	UBSERVED=	0.0 CM-1	CALCULATED=	76.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	18.97 C2CC 15.11 C1CC	9.16 TCC5	8.42 CCO1	7.53 TCC4	7.46 TCC1	5.16 TCO2	5.05 TCC2				
FORCE CONSTANTS-	38.58 CCH 29.30 T-CC	17.47 CCO	8.42 CCO	6.03 T-CC							
OFF DIAGONAL-	-3.75 SB25	-3.75 BB42	-2.41 SB21	2.22 BB41							
NORMAL MODE 61	UBSERVED=	0.0 CM-1	CALCULATED=	76.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	24.89 TCC1 13.89 C3CC	9.89 TCC4	7.43 TCC2	7.16 TCC3	5.58 CCO*						
FORCE CONSTANTS-	49.43 T-CC 22.53 CCO	21.01 CCH									
OFF DIAGONAL-	-2.58 BB42	-2.18 BB34	-1.54 SB25								

2. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 0.0

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400									
MOLECULE 10 -6 NG-1237 BETA GLUCOSE									
PAGE 1									
NORMAL MODE 8	OBSERVED=	1449.0	CM-1	CALCULATED=	1450.1	CM-1	ERROR=	-1.1	CM-1 OR -0.1 PERCENT
INTERNAL COORDINATES-	61.43	HCH	20.22	OCBH	19.51	OCHA			
FORCE CONSTANTS-	61.43	HCH	39.84	OCH					
OFF DIAGONAL-	-4.11	SB27							
NORMAL MODE 9	OBSERVED=	1415.0	CM-1	CALCULATED=	1421.7	CM-1	ERROR=	-6.7	CM-1 OR -0.5 PERCENT
INTERNAL COORDINATES-	57.68	OC1H	37.48	OC1H	15.34	C1OH	8.55	C2OH	8.15
FORCE CONSTANTS-	57.44	OCH	22.44	BCOH	13.79	CCH	7.41	CO	5.55
OFF DIAGONAL-	-9.47	SB27	3.61	SB28	2.94	BB29	-2.60	BB45	-2.50
								SB25	2.37
								BB34	-2.04
								BB43	-1.96
								BB39	
NORMAL MODE 10	OBSERVED=	0.0	CM-1	CALCULATED=	1410.0	CM-1	ERROR=	0.0	CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	17.44	OC4H	10.85	HC4C	9.93	CC5H	8.96	OC3H	7.26
FORCE CONSTANTS-	46.34	OCH	36.12	CCH	10.20	CCO	5.42	BCOH	
OFF DIAGONAL-	-9.77	SB27	7.60	BB29	-5.12	SB26	4.11	BB34	-3.23
								SB25	-3.20
								BB45	1.79
								SB28	
NORMAL MODE 11	OBSERVED=	1402.0	CM-1	CALCULATED=	1407.1	CM-1	ERROR=	-5.1	CM-1 OR -0.4 PERCENT
INTERNAL COORDINATES-	24.89	C1OH	22.88	C1OH	11.57	C2OH	9.38	OC1H	
FORCE CONSTANTS-	42.91	UCH	37.33	BCOH	12.83	CCH			
OFF DIAGONAL-	2.30	SB28	-2.00	BB45	-1.89	SB26			
NORMAL MODE 12	OBSERVED=	0.0	CM-1	CALCULATED=	1394.0	CM-1	ERROR=	0.0	CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	52.59	C3OH	12.36	OC3H	12.28	C1OH			
FORCE CONSTANTS-	66.26	BCOH	16.77	OCH	10.34	CCH			
OFF DIAGONAL-	4.74	SB28	-3.56	SB27	-2.89	SB26	-2.71	BB39	
NORMAL MODE 13	OBSERVED=	1387.0	CM-1	CALCULATED=	1391.3	CM-1	ERROR=	-4.3	CM-1 OR -0.3 PERCENT
INTERNAL COORDINATES-	53.65	C1OH	12.68	C3OH	7.52	OCHA	7.27	C1OH	
FORCE CONSTANTS-	78.08	BCOH	9.82	OCH	7.97	CCH			
OFF DIAGONAL-	2.96	SB28	-1.82	BB39					
NORMAL MODE 14	OBSERVED=	1375.0	CM-1	CALCULATED=	1387.6	CM-1	ERROR=	-12.6	CM-1 OR -0.9 PERCENT
INTERNAL COORDINATES-	33.99	C1OH	32.14	C2OH	8.04	C1OH			
FORCE CONSTANTS-	74.53	BCOH	10.90	CCH	9.13	OCH	5.11	CC	
OFF DIAGONAL-	3.10	SB28	-2.95	SB26	-1.82	BB29	1.75	BB29	-1.57
								BB39	
NORMAL MODE 15	OBSERVED=	1369.0	CM-1	CALCULATED=	1365.7	CM-1	ERROR=	3.3	CM-1 OR 0.2 PERCENT
INTERNAL COORDINATES-	20.78	C2OH	16.02	C3OH	7.10	OC2H	6.96	HC2C	6.33
FORCE CONSTANTS-	39.38	BCOH	30.52	CCH	20.50	OCH			
OFF DIAGONAL-	5.93	BB29	-4.03	SB27	3.15	BB34	-3.05	SB28	-2.20
								BB36	1.98
								BB39	-1.97
								BB45	1.87
								SB26	
NORMAL MODE 16	OBSERVED=	1351.0	CM-1	CALCULATED=	1345.5	CM-1	ERROR=	5.5	CM-1 OR 0.4 PERCENT
INTERNAL COORDINATES-	15.25	HCH	14.48	CCHB	11.78	OCBH	10.71	CCH	9.64
FORCE CONSTANTS-	46.34	OCH	36.12	CCH	11.01	BCOH	5.46	CO	5.30
OFF DIAGONAL-	-7.00	SB27	-3.27	BB45	2.31	BB29	1.99	BB30	-1.84
								SB28	
NORMAL MODE 17	OBSERVED=	1343.0	CM-1	CALCULATED=	1331.3	CM-1	ERROR=	11.7	CM-1 OR 0.9 PERCENT
INTERNAL COORDINATES-	14.70	HC3C	15.20	CC4H	9.37	OC2H	6.02	CC4H	5.97
FORCE CONSTANTS-	63.60	CCH	17.56	OCH	9.64	BCOH			
OFF DIAGONAL-	12.47	BB29	-6.85	SB26	-3.54	BB45	-2.61	SB27	1.94
								BB34	
NORMAL MODE 18	OBSERVED=	1338.0	CM-1	CALCULATED=	1304.4	CM-1	ERROR=	7.3	CM-1 OR 0.3 PERCENT
INTERNAL COORDINATES-	14.01	CC2H	9.87	HC2C	8.39	CC4H	8.37	OC4H	8.30
FORCE CONSTANTS-	52.74	CCH	26.75	UCH	7.09	CO	6.81	BCOH	5.98
OFF DIAGONAL-	6.93	BB29	-5.32	SB26	-3.36	BB45	-2.65	SB27	1.80
								BB34	
NORMAL MODE 19	OBSERVED=	0.0	CM-1	CALCULATED=	1295.4	CM-1	ERROR=	0.0	CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	13.76	C4OH	12.50	C5H	10.61	OC4H	8.53	HC3C	8.33
FORCE CONSTANTS-	48.30	CCH	30.98	OCH	13.76	BCOH			
OFF DIAGONAL-	3.70	BB29	-3.45	SB26	-3.34	BB45	1.60	BB34	
									5.07
								OC1H	
NORMAL MODE 20	OBSERVED=	1283.0	CM-1	CALCULATED=	1290.6	CM-1	ERROR=	-7.6	CM-1 OR -0.6 PERCENT
INTERNAL COORDINATES-	19.72	UCHB	17.06	CCBH	11.73	OCHA	7.53	C5H	6.48
FORCE CONSTANTS-	44.49	CCH	30.54	CCH	12.98	CO	5.70	CC	
OFF DIAGONAL-	-3.04	BB45	2.16	SB27	1.66	BB34	1.63	SB26	
NORMAL MODE 21	OBSERVED=	1270.0	CM-1	CALCULATED=	1272.6	CM-1	ERROR=	-2.6	CM-1 OR -0.2 PERCENT
INTERNAL COORDINATES-	43.00	OC3H	4.22	OC2H	10.65	CC3H	12.47	C4OH	5.28
FORCE CONSTANTS-	43.50	OCH	24.90	CCH	13.33	CO	7.57	COH	
OFF DIAGONAL-	7.88	SB27	-2.83	SB25	-2.72	BB45	-2.23	BB29	-1.88
								SB26	1.86
								BB34	1.78
								BB43	
NORMAL MODE 22	OBSERVED=	1263.0	CM-1	CALCULATED=	1261.0	CM-1	ERROR=	2.0	CM-1 OR 0.2 PERCENT
INTERNAL COORDINATES-	20.66	C4OH	13.34	OC2H	6.02	CC3H	5.86	OC4H	5.82
FORCE CONSTANTS-	29.23	OCH	22.88	CC5H	20.66	COH	13.72	CO	6.63
OFF DIAGONAL-	4.06	SB27	-3.08	SB25	-2.76	BB29	2.69	BB34	-2.04
								BB45	1.67
								SB28	-1.60
								SB21	
NORMAL MODE 23	OBSERVED=	1250.0	CM-1	CALCULATED=	1253.1	CM-1	ERROR=	-3.1	CM-1 OR -0.3 PERCENT
INTERNAL COORDINATES-	10.23	HC5C	10.12	CC4H	9.78	OC4H	9.42	C5H	9.19
FORCE CONSTANTS-	36.33	CCH	34.13	UCH	16.30	CO	6.44	COH	
OFF DIAGONAL-	6.58	SB27	-2.86	BB45	-2.45	SB25	2.17	BB34	-2.17
								BB29	
NORMAL MODE 24	OBSERVED=	1222.0	CM-1	CALCULATED=	1216.2	CM-1	ERROR=	5.8	CM-1 OR 0.5 PERCENT
INTERNAL COORDINATES-	16.45	C-06	16.44	O1C1	18.89	HC5C	8.44	HC2C	7.70
FORCE CONSTANTS-	42.91	OCH	37.33	CCH	19.78	OCBH	10.71	CCH	
OFF DIAGONAL-	-6.03	SB25	-3.69	BB29	3.28	BB34	-2.37	BB45	-2.08
								SB26	
NORMAL MODE 25	OBSERVED=	1202.0	CM-1	CALCULATED=	1192.5	CM-1	ERROR=	9.5	CM-1 OR 0.8 PERCENT
INTERNAL COORDINATES-	35.93	O1C1	1.01	C-06	27.79	OCBH	9.38	OC1H	9.00
FORCE CONSTANTS-	35.63	CO	33.25	CCH	26.11	OCH			
OFF DIAGONAL-	-5.04	BB29	-4.59	SB25	-2.22	BB45	1.73	BB34	-1.61
								SB28	
NORMAL MODE 26	OBSERVED=	1152.0	CM-1	CALCULATED=	1157.8	CM-1	ERROR=	-5.8	CM-1 OR -0.5 PERCENT
INTERNAL COORDINATES-	22.15	C5O1	10.89	HC5C	7.93	C5C1	6.48	CCO*	6.42
FORCE CONSTANTS-	35.58	CCH	32.04	CO	19.43	CCO	13.50	UCH	11.77
OFF DIAGONAL-	-10.39	SB25	8.55	SB27	-7.54	SB26	-4.64	BB29	-3.82
								SB22	-2.14
								SB28	1.97
								BB34	1.89
								BB33	
								BB39	-1.67
								BB45	
NORMAL MODE 27	OBSERVED=	1126.0	CM-1	CALCULATED=	1127.6	CM-1	ERROR=	-1.6	CM-1 OR -0.1 PERCENT
INTERNAL COORDINATES-	43.92	C5C1	18.07	C-0*	13.93	C4C5	7.28	OCHA	6.30
FORCE CONSTANTS-	61.43	CO	30.22	CO	14.16	CCO	10.11	CCH	9.24
OFF DIAGONAL-	-12.59	SB22	-11.72	SB26	-9.18	SB28	-4.62	SB27	-4.48
								SS18	-3.21
								BB34	-1.60
								SS17	
NORMAL MODE 28	OBSERVED=	1116.0	CM-1	CALCULATED=	1118.6	CM-1	ERROR=	-2.6	CM-1 OR -0.2 PERCENT
INTERNAL COORDINATES-	17.10	C5O1	11.17	OC1H	9.27	CC1H	8.06	CC2H	7.48
FORCE CONSTANTS-	42.88	CCH	27.46	CO	26.92	OCH	12.23	CCO	5.51
OFF DIAGONAL-	-9.39	BB29	-6.58	SB25	4.19	BB34	-3.35	SB27	-2.35
								SB21	-2.35
								BB43	-2.06
								BB45	-1.75
								SB23	-1.59
								SS18	
NORMAL MODE 29	OBSERVED=	1097.0	CM-1	CALCULATED=	1107.2	CM-1	ERROR=	-10.2	CM-1 OR -0.9 PERCENT
INTERNAL COORDINATES-	20.84	C-06	16.94	C-U9	11.60	C5O1	7.93	C4C5	6.53
FORCE CONSTANTS-	59.59	CO	20.85	CC	13.10	OCH	8.90	CCH	7.09
OFF DIAGONAL-	-4.71	SB25	-4.56	SB28	-4.33	SS18	1.84	SB27	-1.57
								BB29	
NORMAL MODE 30	OBSERVED=	1079.0	CM-1	CALCULATED=	1078.8	CM-1	ERROR=	0.2	CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	31.97	C2C3	29.41	C3C4	17.57	C-07	9.45	C2OH	5.05
FORCE CONSTANTS-	69.11	CO	27.70	CO	12.79	CCO	12.11	BCOH	10.27
OFF DIAGONAL-	-9.32	SB22	-6.48	SB28	-6.15	SB27	-3.90	SB26	-3.36
								SB25	-3.18
								SB21	-2.61
								SS17	-2.43
								BB34	-2.39
								SS18	
NORMAL MODE 31	OBSERVED=	1069.0	CM-1	CALCULATED=	1059.0	CM-1	ERROR=	10.0	CM-1 OR 0.9 PERCENT
INTERNAL COORDINATES-	43.18	C-08	24.51	C1C2	22.01	C2C3	11.52	C3OH	8.56
FORCE CONSTANTS-	53.35	CO	50.28	CO	16.04	CO	14.11	BCOH	12.48
OFF DIAGONAL-	-11.70	SB27	-9.69	SB28	-9.05	SB21	-8.11	SB22	-8.07
								SS18	-6.27
								SB25	-3.44
								BB34	-1.98
								SB26	-1.78
								BB36	
NORMAL MODE 32	OBSERVED=	1050.0	CM-1	CALCULATED=	1049.4	CM-1	ERROR=	0.6	CM-1 OR 0.1 PERCENT
INTERNAL COORDINATES-	25.66	C-08	18.12	C1C2	12.38	C3H	11.85	C3H	5.22
FORCE CONSTANTS-	42.88	CO	35.36	CO	15.28	CO	11.48	OCH	9.26
OFF DIAGONAL-	-8.87	SB21	-6.97	SB22	-6.90	SB27	-4.94	SS18	-4.22
								SB28	-2.52
								BB29	
NORMAL MODE 33	OBSERVED=	1024.0	CM-1	CALCULATED=	1031.9	CM-1	ERROR=	-7.9	

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400
MOLECULE 10 -6 NG=1237 BETA GLUCOSE

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NORMAL MODE 36	OBSERVED=	952.0 CM-1	CALCULATED=	965.2 CM-1	ERROR=	-13.2 CM-1	OR	-1.4 PERCENT
INTERNAL COORDINATES-	23.15	C-06 15.53 C-08 14.93 C1C2	7.53 0.01 5.35 C007					
FORCE CONSTANTS-	52.91	CC 19.58 CC 11.05 CCO	7.34 0CH 6.59 CCH					
OFF DIAGONAL-	-6.64	SB22 -4.79 SB24 4.50 SS18	3.26 SB27 -1.72 SB21 -1.55 SB26					
NORMAL MODE 37	OBSERVED=	913.0 CM-1	CALCULATED=	909.3 CM-1	ERROR=	3.7 CM-1	OR	0.4 PERCENT
INTERNAL COORDINATES-	27.16	C5C1 17.19 C-0* 9.96 CCH8	8.85 C50*					
FORCE CONSTANTS-	32.95	CC 31.05 CO 19.82 CCH	6.86 CCO					
OFF DIAGONAL-	6.88	SB26 6.36 SS18 -5.64 SB22	-5.34 SB21 -3.64 SB25 -3.04 SB27 -2.03 SB23					
NORMAL MODE 38	OBSERVED=	898.0 CM-1	CALCULATED=	884.7 CM-1	ERROR=	13.3 CM-1	OR	1.5 PERCENT
INTERNAL COORDINATES-	14.54	C4C5 13.00 CCHA 12.59 C50*	10.30 CCH8 8.05 C-0*	7.16 CCO				
FORCE CONSTANTS-	29.75	CC 27.37 CO 18.42 CC 12.75 CCH	9.07 CCO 7.16 CCO					
OFF DIAGONAL-	-6.18	SB21 -4.00 SB24 -2.87 SB22	-2.68 SB27 -2.35 SB23 -2.22 SS18	1.91 SB25 1.79 BB43				
NORMAL MODE 39	OBSERVED=	714.0 CM-1	CALCULATED=	726.4 CM-1	ERROR=	-12.4 CM-1	OR	-1.7 PERCENT
INTERNAL COORDINATES-	18.92	CC0* 8.50 CCO* 6.05 CCH	5.59 C4C5 5.51 CC4H					
FORCE CONSTANTS-	40.02	CCO 26.06 CCH 8.87 CC	5.68 CO 5.16 CCH					
OFF DIAGONAL-	7.63	BB43 -7.04 BB34 5.36 SB25	-4.46 BB29 3.84 SB21 -2.23 SB27 -1.64 BB41					
NORMAL MODE 40	OBSERVED=	632.0 CM-1	CALCULATED=	621.8 CM-1	ERROR=	10.2 CM-1	OR	1.6 PERCENT
INTERNAL COORDINATES-	14.89	CC06 8.85 C0* 7.61 CCO9	7.38 CC3H 7.19 HC2C	5.19 CCO8 5.16 C-06				
FORCE CONSTANTS-	46.92	CCO 22.95 CCH 11.33 CC	8.85 CCH					
OFF DIAGONAL-	-8.62	BB34 6.84 BB43 -5.26 SB25	-2.47 SB27 -1.80 BB41					
NORMAL MODE 41	OBSERVED=	593.0 CM-1	CALCULATED=	599.3 CM-1	ERROR=	-6.3 CM-1	OR	-1.1 PERCENT
INTERNAL COORDINATES-	14.98	CCO 11.59 C0CC 9.16 C4CC	8.18 C7CC 7.32 CCO9	6.47 CCO6 5.90 CCO*	5.63 C4C5			
FORCE CONSTANTS-	54.75	CCO 17.30 CCH 14.98 CCO	11.21 CCH 7.78 CC	6.71 CO				
OFF DIAGONAL-	-10.41	BB34 4.95 SB24 -4.89 SB22	-4.88 BB42 4.31 BB43	2.43 SB22 -2.29 SB25 -2.28 BB29 -1.89 BB41				
NORMAL MODE 42	OBSERVED=	574.0 CM-1	CALCULATED=	581.8 CM-1	ERROR=	-7.8 CM-1	OR	-1.4 PERCENT
INTERNAL COORDINATES-	18.30	U*CC 12.94 CCO* 6.02 C-07	5.82 HC4C					
FORCE CONSTANTS-	27.70	CCO 21.60 CCH 12.71 CO	6.83 CCH					
OFF DIAGONAL-	-8.08	BB36 6.47 SB25 6.01 BB43	-6.72 BB29 3.88 SB22 -3.22 SB27 -1.68 SB23					
NORMAL MODE 43	OBSERVED=	519.0 CM-1	CALCULATED=	525.9 CM-1	ERROR=	-6.9 CM-1	OR	-1.3 PERCENT
INTERNAL COORDINATES-	19.85	CC04 7.96 C4C5 6.14 C0CC	5.46 CCH2 5.33 C0C1	5.31 C3C4 5.04 C1C2				
FORCE CONSTANTS-	34.21	CCO 21.79 CC 17.33 CCH	17.39 CO					
OFF DIAGONAL-	-7.10	BB34 5.35 BB43 4.24 SS18	3.89 SB21 -3.34 BB29 -1.72 SB27 1.62 SB25					
NORMAL MODE 44	OBSERVED=	454.0 CM-1	CALCULATED=	458.8 CM-1	ERROR=	-4.8 CM-1	OR	-1.1 PERCENT
INTERNAL COORDINATES-	10.25	C7CC 9.58 CCO6 5.84 CCH	5.40 C9CC 5.33 CCH2	5.13 CCO9				
FORCE CONSTANTS-	42.88	CCO 24.93 CCH 9.76 CC	8.02 CCH 7.14 CO					
OFF DIAGONAL-	-7.94	BB34 5.87 BB43 -5.38 BB29	3.54 SB25 -2.12 SB26 -1.57 SB27 1.56 SS18					
NORMAL MODE 45	OBSERVED=	425.0 CM-1	CALCULATED=	414.4 CM-1	ERROR=	10.6 CM-1	OR	2.5 PERCENT
INTERNAL COORDINATES-	20.21	C2CC 11.67 C0* 10.85 C1CC	9.45 CCO9 5.67 C3CC	5.14 CCO8				
FORCE CONSTANTS-	37.12	CCO 20.72 CCO 11.67 CCH	6.60 CO 5.46 CC	5.35 CCH				
OFF DIAGONAL-	4.14	SB21 2.95 SB25 -2.94 BB42	-2.30 BB41 2.22 BB43 1.72 SB23					
NORMAL MODE 46	OBSERVED=	401.0 CM-1	CALCULATED=	388.8 CM-1	ERROR=	12.2 CM-1	OR	3.0 PERCENT
INTERNAL COORDINATES-	17.05	C*CC 16.11 CCO* 13.42 C3CC	8.69 C8CC 6.13 C1CC					
FORCE CONSTANTS-	54.52	CCO 21.25 CCH 10.92 CCH	10.92 CCH					
OFF DIAGONAL-	5.95	SB21 -4.69 BB34 3.25 SB25	3.10 BB43 -2.92 BB42 -1.83 BB41 -1.66 BB29					
NORMAL MODE 47	OBSERVED=	347.0 CM-1	CALCULATED=	347.1 CM-1	ERROR=	-0.1 CM-1	OR	-0.0 PERCENT
INTERNAL COORDINATES-	25.94	C0CC 14.37 CCO7 9.78 CCO8	5.93 C50*					
FORCE CONSTANTS-	65.98	CCO 10.12 CCH 9.14 CC	7.92 CO					
OFF DIAGONAL-	-8.24	BB34 5.19 SB22 -2.98 SB25	2.79 BB43 -2.66 BB42 -2.19 BB29 -2.08 SB21					
NORMAL MODE 48	OBSERVED=	327.0 CM-1	CALCULATED=	333.2 CM-1	ERROR=	-6.2 CM-1	OR	-1.9 PERCENT
INTERNAL COORDINATES-	19.70	CCO7 16.01 CCO 10.69 C8CC	7.55 CCO6					
FORCE CONSTANTS-	51.09	CCO 16.01 CCO 14.23 CCH	8.09 T-0H 7.99 CC	5.94 CCH				
OFF DIAGONAL-	-7.21	BB34 4.77 SB22 -2.76 BB29	2.43 BB43 -2.38 SB24 -1.89 SB21 -1.74 BB42					
NORMAL MODE 49	OBSERVED=	309.0 CM-1	CALCULATED=	313.5 CM-1	ERROR=	-4.5 CM-1	OR	-1.5 PERCENT
INTERNAL COORDINATES-	21.23	C0CC 11.90 C7CC 11.28 CCO8	10.52 C9CC 10.28 CCO7	6.29 CCO9 5.95 CCO6 5.73 TH-3				
FORCE CONSTANTS-	83.56	CCO 12.68 T-0H 7.60 CCH	6.11 CCH					
OFF DIAGONAL-	-8.92	BB34 -4.48 BB42 -3.39 SB22	1.74 BB41 -1.71 SB26					
NORMAL MODE 50	OBSERVED=	289.0 CM-1	CALCULATED=	297.8 CM-1	ERROR=	-8.8 CM-1	OR	-3.0 PERCENT
INTERNAL COORDINATES-	20.71	C7CC 12.87 CCO8 11.68 CCO9	9.69 CCO6 5.33 CC3H					
FORCE CONSTANTS-	57.92	CCO 19.71 CCH 8.89 CCH	6.12 CC					
OFF DIAGONAL-	-12.64	BB34 8.31 BB43 5.00 SB22	-2.27 BB29 -2.61 SB21 -2.27 SB25					
NORMAL MODE 51	OBSERVED=	274.0 CM-1	CALCULATED=	273.2 CM-1	ERROR=	0.8 CM-1	OR	0.3 PERCENT
INTERNAL COORDINATES-	29.52	CCO* 27.51 TH-5 11.54 C4CC	6.99 C9CC					
FORCE CONSTANTS-	45.73	CCO 31.98 T-0H 12.51 CCH	7.35 CCH					
OFF DIAGONAL-	-4.95	BB34 -2.75 BB42 -2.26 BB33	2.23 SB22					
NORMAL MODE 52	OBSERVED=	250.0 CM-1	CALCULATED=	265.6 CM-1	ERROR=	-15.6 CM-1	OR	-6.3 PERCENT
INTERNAL COORDINATES-	13.74	C4CC 11.27 CCO* 9.53 TH-4	8.96 C0CC 7.71 CCO9					
FORCE CONSTANTS-	31.63	CCO 14.87 CCH 14.39 T-0H	9.59 CCH 8.96 CCH	6.95 CC 6.20 T-CC				
OFF DIAGONAL-	4.57	BB43 -4.03 BB34 3.86 SB21	2.51 SB22 -2.33 SB26					
NORMAL MODE 53	OBSERVED=	227.0 CM-1	CALCULATED=	226.7 CM-1	ERROR=	0.3 CM-1	OR	0.1 PERCENT
INTERNAL COORDINATES-	38.13	TH-1 35.67 TH-2 8.81 TH-5	8.68 TH-3 5.10 TH-4					
FORCE CONSTANTS-	96.38	T-0H						
OFF DIAGONAL-	NONE							
NORMAL MODE 54	OBSERVED=	0.0 CM-1	CALCULATED=	216.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	32.16	TH-1 25.18 TH-3 21.96 TH-4						
FORCE CONSTANTS-	84.95	T-0H 8.18 CCO						
OFF DIAGONAL-	NONE							
NORMAL MODE 55	OBSERVED=	0.0 CM-1	CALCULATED=	214.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	29.89	TH-2 28.87 TH-4 11.79 TH-1	5.01 CCO7					
FORCE CONSTANTS-	84.88	T-0H 11.18 CCO						
OFF DIAGONAL-	NONE							
NORMAL MODE 56	OBSERVED=	0.0 CM-1	CALCULATED=	210.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	49.28	TH-3 24.62 TH-4 6.27 TH-2	5.65 CCO8					
FORCE CONSTANTS-	82.93	T-0H 17.30 CCO						
OFF DIAGONAL-	-2.06	BB34						
NORMAL MODE 57	OBSERVED=	0.0 CM-1	CALCULATED=	209.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	56.09	TH-5 9.92 CCO* 8.46 C4CC						
FORCE CONSTANTS-	63.95	T-0H 17.81 CCO 9.67 CCH	5.01 CCH					
OFF DIAGONAL-	-2.18	BB34 -1.51 BB42						
NORMAL MODE 58	OBSERVED=	0.0 CM-1	CALCULATED=	141.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	18.99	CCO 9.11 C4CC 8.02 TCC4	7.85 CCO*	6.45 CCO*	5.97 TCO1 5.43 CCO			
FORCE CONSTANTS-	25.92	CCO 18.99 CCH 14.21 CCH	9.86 T-CC 9.49 T-CC	8.41 CCH 5.43 CCO				
OFF DIAGONAL-	4.51	BB43 -1.95 SB25	1.69 BB41 -1.55 BB33					
NORMAL MODE 59	OBSERVED=	0.0 CM-1	CALCULATED=	89.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	21.25	TCC9 0.05 C2CC 8.13 C3CC	7.67 C1CC					
FORCE CONSTANTS-	41.31	T-CC 37.84 CCH 20.14 CCO	5.52 CO					
OFF DIAGONAL-	-4.94	SB25 -4.00 SB21 -3.85 BB42	2.27 BB41 -1.66 BB34					
NORMAL MODE 60	OBSERVED=	0.0 CM-1	CALCULATED=	74.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	60.03	TCC5 6.34 C2CC 5.63 CCO*	5.22 C0* 5.22 CCH					
FORCE CONSTANTS-	65.67	T-CC 12.80 CCH 11.97 CCO						
OFF DIAGONAL-	-1.53	BB42						
NORMAL MODE 61	OBSERVED=	0.0 CM-1	CALCULATED=	70.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	15.08	TCC4 14.96 C3CC 10.25 CCO*	9.40 TCC3 8.52 C1CC 6.58 TCC2 5.56 C*CC 5.06 C4CC					
FORCE CONSTANTS-	35.26	T-CC 30.78 CCO 28.57 CCH	5.45 T-CC					
OFF DIAGONAL-	-3.78	BB42 -2.62 SB25 -2.18 BB34	1.89 BB41					

43. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 6.54

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400									
MOLECULE 11 -6 NG=1237 BETA GLUCOSE-O-D5									
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NORMAL MODE 8	OBSERVED=	1449.0 CM-1	CALCULATED=	1450.1 CM-1	ERROR=	-1.1 CM-1	OR	-0.1 PERCENT	
INTERNAL COORDINATES-	61.43 HCH	20.22 OCHB	19.52 OCHA						
FORCE CONSTANTS-	61.43 HCH	39.85 OCH							
OFF DIAGONAL-	-4.11 SB27								
NORMAL MODE 9	OBSERVED=	1420.0 CM-1	CALCULATED=	1416.6 CM-1	ERROR=	3.4 CM-1	OR	0.2 PERCENT	
INTERNAL COORDINATES-	16.16 CCH	28.95 OC1H	10.43 CCH						
FORCE CONSTANTS-	92.07 OCH	13.35 CCH							
OFF DIAGONAL-	-7.77 SB27	-3.90 BB45	2.09 BB29	-1.69 BB43					
NORMAL MODE 10	OBSERVED=	1409.0 CM-1	CALCULATED=	1406.4 CM-1	ERROR=	2.6 CM-1	OR	0.2 PERCENT	
INTERNAL COORDINATES-	20.62 OC4H	13.50 CC5H	12.88 HC4C	9.27 OC3H	7.98 HC3C	5.94 CC5H	5.37 C-D9		
FORCE CONSTANTS-	43.38 CCH	43.04 OCH	11.17 CO	5.21 CCO					
OFF DIAGONAL-	-10.36 SB27	9.37 BB29	5.31 BB34	-4.77 SB26	-3.84 SB25	-3.39 BB45			
NORMAL MODE 11	OBSERVED=	1395.0 CM-1	CALCULATED=	1380.9 CM-1	ERROR=	14.1 CM-1	OR	1.0 PERCENT	
INTERNAL COORDINATES-	20.65 OC2H	12.00 HC2C	9.71 CC3H	9.08 CC5H	8.80 OC3H	5.90 HC4C			
FORCE CONSTANTS-	45.23 CCH	43.26 OCH	10.17 CO						
OFF DIAGONAL-	9.15 BB29	-8.61 SB27	-4.06 SB26	3.68 BB34	-3.54 BB45	-3.17 SB25			
NORMAL MODE 12	OBSERVED=	0.0 CM-1	CALCULATED=	1352.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	16.44 HC5C	15.96 CCHB	14.61 CCHA	8.53 CC5H	7.02 OCHB	6.60 HCH	6.52 OCHA	5.93 OC2H	
FORCE CONSTANTS-	49.89 CCH	3.01 OCH	7.19 HCH	5.91 CO					
OFF DIAGONAL-	-7.76 SB27	-3.74 BB45	2.55 BB29	2.28 BB30	-1.88 SB26				
NORMAL MODE 13	OBSERVED=	0.0 CM-1	CALCULATED=	1339.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	HC3C	12.20 OC3H	12.04 CCH						
FORCE CONSTANTS-	62.48 CCH	26.24 OCH	5.57 CC						
OFF DIAGONAL-	11.63 BB29	-7.78 SB26	-3.82 BB45	-3.52 SB27	1.91 BB34	-1.68 BB43	-1.54 SB25		
NORMAL MODE 14	OBSERVED=	0.0 CM-1	CALCULATED=	1311.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	15.08 CCH2	14.28 HC2C	10.04 CC3H	6.67 OCHA	6.27 CCHA	6.20 OC4H			
FORCE CONSTANTS-	58.23 CCH	20.74 CCH	10.99 CO						
OFF DIAGONAL-	10.49 BB29	-4.01 SB26	-3.45 BB45	2.45 BB34					
NORMAL MODE 15	OBSERVED=	0.0 CM-1	CALCULATED=	1297.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	14.36 UCHA	13.98 OC4H	10.64 OCHB	9.29 HC3C	8.41 CCHA	7.10 HC4C	6.82 OC3H	6.46 CCHB	5.59 HC2C
FORCE CONSTANTS-	49.66 OCH	44.11 CCH							
OFF DIAGONAL-	-3.86 BB45	1.80 BB34	1.70 BB29						
NORMAL MODE 16	OBSERVED=	0.0 CM-1	CALCULATED=	1285.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	32.72 CC5H	18.69 OCHB	13.94 CCHB	10.73 OC4H	8.14 CC5H				
FORCE CONSTANTS-	68.37 OCH	27.88 CCH							
OFF DIAGONAL-	3.81 SB27	-3.68 BB45	-2.19 BB29	-2.02 SB26					
NORMAL MODE 17	OBSERVED=	1272.0 CM-1	CALCULATED=	1272.5 CM-1	ERROR=	-0.5 CM-1	OR	-0.0 PERCENT	
INTERNAL COORDINATES-	12.31 OC3H	18.05 OC2H	17.54 CC3H	9.07 CC4H	5.22 CC5H				
FORCE CONSTANTS-	48.43 CCH	18.95 CCH	3.52 BB29	-2.75 SB26	2.58 BB34	-1.98 SB25			
OFF DIAGONAL-	6.03 SB27	-3.60 BB45							
NORMAL MODE 18	OBSERVED=	0.0 CM-1	CALCULATED=	1240.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	15.09 UCH	13.67 C-D6	9.00 CCH2	8.99 OC4H	8.01 OC2H	8.01 CC4H			
FORCE CONSTANTS-	34.36 CO	30.14 CCH	28.92 OCH	9.72 CCO					
OFF DIAGONAL-	-6.28 SB25	4.50 SB27	-2.40 BB29	-2.38 BB45	2.36 BB34	-2.02 SB26			
NORMAL MODE 19	OBSERVED=	1223.0 CM-1	CALCULATED=	1226.4 CM-1	ERROR=	-3.4 CM-1	OR	-0.3 PERCENT	
INTERNAL COORDINATES-	15.76 C-D6	12.88 C-D1	11.06 HC5C	10.01 OC4H	6.71 HC2C	6.04 CC5H	5.43 CCH2		
FORCE CONSTANTS-	43.11 CCH	32.47 CO	23.18 OCH	11.14 CCO					
OFF DIAGONAL-	-6.00 SB25	-3.28 SB26	-2.71 BB45	-1.77 BB29	-1.57 BB43				
NORMAL MODE 20	OBSERVED=	0.0 CM-1	CALCULATED=	1212.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	16.96 CC1H	14.08 OC1H	8.31 HC5C	7.89 OC2H	7.17 CC5H	5.92 C-D6	5.36 HC4C		
FORCE CONSTANTS-	46.50 CCH	31.88 OCH	16.04 CO	5.99 CCO	5.87 BCOH				
OFF DIAGONAL-	-5.24 BB29	-3.09 SB25	-3.00 SB26	-3.00 BB45	2.90 BB34				
NORMAL MODE 21	OBSERVED=	1186.0 CM-1	CALCULATED=	1183.3 CM-1	ERROR=	2.8 CM-1	OR	0.2 PERCENT	
INTERNAL COORDINATES-	12.21 C4C5	18.02 OCHB	8.04 C-D8	6.38 C-D9	17.09 CC01	6.48 C-DH	5.96 OCHA		
FORCE CONSTANTS-	28.49 CCH	18.02 CCH	10.17 CCH	13.29 CCH	11.57 CCO	9.73 BCOH			
OFF DIAGONAL-	-4.05 SB25	3.81 SB28	-3.32 SB25	2.69 BB34	-2.65 SS18	2.56 SB26	-1.95 BB29	-1.79 SB21	-1.54 SB23
NORMAL MODE 22	OBSERVED=	0.0 CM-1	CALCULATED=	1162.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	17.69 CSC	17.39 C-DH	14.61 OC1H	6.37 CC5H	6.20 CC1H	6.14 HC5C	5.39 C10H	5.12 C4C5	5.10 CCHB
FORCE CONSTANTS-	43.72 CCH	25.90 CC	14.89 OCH	14.81 BCOH	13.90 CCO	8.80 CO			
OFF DIAGONAL-	-9.43 SB26	-8.20 SB22	-7.33 SB25	3.67 BB34	-2.65 SS18	-2.09 BB45	1.96 BB33		
NORMAL MODE 23	OBSERVED=	1157.0 CM-1	CALCULATED=	1156.4 CM-1	ERROR=	0.5 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	34.22 C2C3	12.30 C-D8	11.63 C30H	6.62 C2CC	6.61 C20H	6.40 CC09	5.13 D7CC		
FORCE CONSTANTS-	43.48 CC	23.31 C-D8	20.07 BCOH	17.04 CCO	8.70 CCC				
OFF DIAGONAL-	-8.58 SB21	-7.52 SB22	6.83 SB28	-3.72 SS18	-3.13 SB25	-2.29 SB27			
NORMAL MODE 24	OBSERVED=	0.0 CM-1	CALCULATED=	1150.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	16.07 C-D7	14.48 C3C4	7.98 C2C3	6.96 O-C1	6.67 C501	6.39 C10H	5.40 C-D8	5.06 C30H	
FORCE CONSTANTS-	37.63 CC	28.50 CC	13.92 BCOH	11.33 CCO	10.85 CCH	7.74 OCH	7.64 CCC		
OFF DIAGONAL-	-4.49 SB25	-4.24 SB22	3.83 SB28	-3.23 SB27	-1.97 SS18	-1.80 SB21			
NORMAL MODE 25	OBSERVED=	1150.0 CM-1	CALCULATED=	1143.5 CM-1	ERROR=	-3.5 CM-1	OR	-0.3 PERCENT	
INTERNAL COORDINATES-	19.50 C501	11.54 C5C1	10.14 C2C3	8.65 C4C5	7.98 C20H	5.41 O9CC			
FORCE CONSTANTS-	37.79 CCH	28.97 CCOH	19.84 CCH	17.87 CCOH	10.93 CCO	8.16 CCH			
OFF DIAGONAL-	-9.80 SB22	-9.55 SB26	-5.12 SB25	3.56 BB28	-3.20 SB21	-1.72 SS18			
NORMAL MODE 26	OBSERVED=	0.0 CM-1	CALCULATED=	1120.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	17.04 C-D8	11.27 CCO1	17.59 BCOH	11.27 CCO	8.15 OCH				
FORCE CONSTANTS-	42.65 C-D8	25.84 C1C2	17.04 CCOH	11.27 CCO	8.15 OCH				
OFF DIAGONAL-	-4.73 SB22	-3.77 SB25	-3.68 SS18	-3.59 SB21					
NORMAL MODE 27	OBSERVED=	0.0 CM-1	CALCULATED=	1105.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	30.61 C1C2	16.49 C-D7	8.01 C4C5	7.57 O-C1	6.20 CCH2	5.39 C-DH			
FORCE CONSTANTS-	42.90 CC	42.09 CO	13.13 CCH	9.72 CCO	7.64 OCH				
OFF DIAGONAL-	-6.79 SS18	-4.81 SB22	-2.98 SB21	-2.71 BB29	-2.67 SB28	-2.54 SB25	-2.42 SB24	-1.80 SB26	
NORMAL MODE 28	OBSERVED=	0.0 CM-1	CALCULATED=	1088.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	26.32 C3C4	18.15 C-D8	10.46 C4CC	10.10 C-D9	8.99 C5C1	7.77 C3CC			
FORCE CONSTANTS-	42.45 CC	35.15 CO	18.44 CCC	14.86 CCH	10.29 OCH	7.49 CCO	7.08 BCOH		
OFF DIAGONAL-	-17.11 SB21	-6.99 SB27	-6.41 SS18	-3.08 SB22	-2.52 BB34	-2.02 SB25			
NORMAL MODE 29	OBSERVED=	0.0 CM-1	CALCULATED=	1033.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	27.18 C-D8	15.95 C-DH	12.48 C3C4	12.07 C4C5	5.26 C-D7	5.16 C501			
FORCE CONSTANTS-	17.99 C-D8	13.70 C-D8	19.80 BCOH	9.73 CCO					
OFF DIAGONAL-	-4.61 SB22	-3.76 SB25	-3.15 SB26	-2.77 SB25	1.57 SB21				
NORMAL MODE 30	OBSERVED=	0.0 CM-1	CALCULATED=	1025.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	22.10 C-D8	28.38 CCH	14.20 C-DH	7.97 C4C5	7.79 HC3C	5.81 C20H	5.06 C-D8		
FORCE CONSTANTS-	44.92 CO	28.14 CC	19.11 BCOH	7.89 CCO	6.26 CC				
OFF DIAGONAL-	-10.26 SB28	-7.09 SB25	-6.10 BB29	-4.01 SB27					
NORMAL MODE 31	OBSERVED=	0.0 CM-1	CALCULATED=	997.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	36.90 C-DH	23.72 C-DH	7.14 C-D7	5.36 C30H	5.35 C5C1	5.18 C501			
FORCE CONSTANTS-	48.81 CO	44.03 BCOH	17.33 CCH	15.96 CC					
OFF DIAGONAL-	-15.21 SB28	-6.32 SB27	-4.98 SB26	-3.10 SB22	-2.43 SB25	-1.86 BB29			
NORMAL MODE 32	OBSERVED=	0.0 CM-1	CALCULATED=	980.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	33.41 C-D6	19.11 C10H	13.83 C20H	13.79 O-C1	7.32 CCO	6.94 C-DH	6.80 C-D8	5.97 C-D7	5.06 C-D8
FORCE CONSTANTS-	58.71 CO	40.10 BCOH	7.32 CCO	6.80 CCO	6.19 CCH	5.04 CC			
OFF DIAGONAL-	-12.64 SB28	-10.89 SB24	-3.14 SB28	-2.29 SB27	-2.14 BB35				
NORMAL MODE 33	OBSERVED=	0.0 CM-1	CALCULATED=	962.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	41.24 C30H	30.23 C20H	16.78 C-D8	10.28 C3C4	5.44 OCH				
FORCE CONSTANTS-	71.70 BCOH	28.52 SB27	13.97 CC	7.23 CCH	1.66 BB39	-1.51 BB34			
OFF DIAGONAL-	-14.28 SB28	-5.13 SB27	-2.87 SB25	-1.70 BB35					
NORMAL MODE 34	OBSERVED=	0.0 CM-1	CALCULATED=	926.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	21.18 C5C1	20.74 C-D8	6.62 C40H	5.47 HC5C	5.18 C-D8	5.07 C10H			
FORCE CONSTANTS-	34.92 CO	28.14 CC	14.10 CCO	13.79 CCO	10.70 CCO				
OFF DIAGONAL-	6.40 SB26	-5.40 SB22	-5.21 SB27	3.24 SS18	-3.21 SB28	-2.81 SB25	-2.48 SB21	1.52 BB43	
NORMAL MODE 35	OBSERVED=	0.0 CM-1	CALCULATED=	921.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	17.65 C1C2	11.40 C30H	10.37 CCO	10.16 C20H	8.44 C2C3				
FORCE CONSTANTS-	47.33 BCOH	31.42 CC	10.37 CCO	5.36 CO					
OFF DIAGONAL-	-6.17 SB22	-2.95 SB21	-2.30 SB26	2.24 BB36	2.01 SS18	-1.53 BB35			

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400
MOLECULE 11 -6 NG=1237 BETA GLUCOSE-0-D5

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NORMAL MODE 36	OBSERVED=	890.0 CM-1	CALCULATED=	911.5 CM-1	ERROR=	-21.5 CM-1	OR	-2.4 PERCENT
INTERNAL COORDINATES-	13.12 C4CH	15.64 C1OH	19.37 C1CC	7.14 C2OH	8.89 C-08	6.44 C3OH		
FORCE CONSTANTS-	39.50 CCOH	18.77 CCH	17.47 CC	11.48 CCO	9.48 CO	9.32 CCH	5.93 CCH	
OFF DIAGONAL-	-6.03 SB22	-3.96 SB21	-3.80 SB28	1.74 BB43				
NORMAL MODE 37	OBSERVED=	870.0 CM-1	CALCULATED=	876.6 CM-1	ERROR=	-6.6 CM-1	OR	-0.8 PERCENT
INTERNAL COORDINATES-	15.27 C4CH	12.93 CCH8	11.29 C5OH	10.31 C-0H	9.97 CCHA	5.48 CCO	5.45 C2C3	
FORCE CONSTANTS-	28.24 CCH	19.88 CCOH	15.25 CO	13.27 CCH	10.33 CCH	9.00 CC	5.48 CCO	
OFF DIAGONAL-	-2.57 SB23	-2.49 SB21	-2.24 SB22	-2.21 SB22				
NORMAL MODE 38	OBSERVED=	0.0 CM-1	CALCULATED=	832.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	47.05 C4OH	14.85 C4C5	5.26 C5C6	5.18 C-04	5.00 C-09			
FORCE CONSTANTS-	47.05 CCH	21.80 CC	13.98 CO	7.61 CCH	7.54 CCO	6.03 CCH	5.33 CCC	
OFF DIAGONAL-	-7.54 SB21	-4.91 SB28	-3.17 SB27	-2.94 SB22	-1.99 BB36	1.77 SB25	-1.75 SS18	
NORMAL MODE 39	OBSERVED=	721.0 CM-1	CALCULATED=	722.1 CM-1	ERROR=	-1.1 CM-1	OR	-0.2 PERCENT
INTERNAL COORDINATES-	17.91 CCO8	8.16 CCO4	7.06 C4C5	6.67 C8CC	5.73 C5H8	5.15 CC4H		
FORCE CONSTANTS-	39.56 CCO	25.17 CCH	11.02 CC	4.81 SB25	-4.10 BB29	3.89 SB21	-2.04 SB27	-1.58 BB41
OFF DIAGONAL-	-7.05 BB34	7.05 BB43						
NORMAL MODE 40	OBSERVED=	0.0 CM-1	CALCULATED=	617.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	12.37 CCO8	9.11 CCO4	6.19 C3C8	6.11 HC2C	5.87 C-06	5.83 CCO9		
FORCE CONSTANTS-	40.66 CCO	20.52 CCH	11.70 CO	11.70 CO	9.11 CCH			
OFF DIAGONAL-	-6.78 BB34	6.44 BB43	6.42 SB25	-4.66 BB29	-2.88 SB27	2.16 SB24	-1.66 BB41	
NORMAL MODE 41	OBSERVED=	0.0 CM-1	CALCULATED=	594.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	13.45 CCO	10.66 C9CC	9.14 C7CC	8.66 C4C5	8.54 CCO6	6.97 CCO1	5.49 C4C5	
FORCE CONSTANTS-	39.41 CCO	19.77 CCH	13.45 CCO	10.38 CCH	8.14 CC			
OFF DIAGONAL-	-11.81 BB34	-5.13 SB21	-4.87 BB42	4.78 BB43	3.63 SB24	-2.83 BB29	-1.87 SB25	1.83 SB22 -1.80 BB41
NORMAL MODE 42	OBSERVED=	0.0 CM-1	CALCULATED=	577.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	18.71 U*CC	13.18 C4C5	5.99 C-07	5.16 C0*CC	5.10 HC4C			
FORCE CONSTANTS-	47.44 CCO	19.25 CCH	12.73 CO	6.43 CCH	5.16 CCH	5.08 CC		
OFF DIAGONAL-	-7.24 BB34	6.63 SB25	5.36 BB43	-4.21 BB29	4.07 SB22	-3.08 SB27	-1.84 SB23	-1.53 BB41
NORMAL MODE 43	OBSERVED=	0.0 CM-1	CALCULATED=	522.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	9.87 CCO8	7.29 C4C5	6.10 C8CC	5.63 C1C2	5.54 CCH2	5.32 C0*CC1	5.11 C3C4	
FORCE CONSTANTS-	35.15 CCO	21.60 CCH	17.70 CCH	16.54 CO				
OFF DIAGONAL-	-7.35 BB34	5.26 BB43	4.12 SS18	4.12 SB21	-3.34 BB29	1.53 SB24		
NORMAL MODE 44	OBSERVED=	0.0 CM-1	CALCULATED=	456.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	10.12 U7CC	9.78 CCO6	6.09 CCH1	5.63 CCH2	5.52 C9CC	5.50 CCO9		
FORCE CONSTANTS-	43.43 CCO	24.83 CCH	10.07 CC	7.49 CO	6.29 CCH			
OFF DIAGONAL-	-8.18 BB34	5.73 BB43	-5.36 BB29	3.76 SB25	-2.12 SB26	-1.72 SB27	1.65 SS18	
NORMAL MODE 45	OBSERVED=	0.0 CM-1	CALCULATED=	407.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	20.37 C2CC	11.90 C1CC	10.55 C0*CC	9.61 CCO9	5.33 CCO8	5.26 C3CC		
FORCE CONSTANTS-	37.64 CCO	23.02 CCH	12.04 CC	10.55 CCH	5.18 CC			
OFF DIAGONAL-	-4.25 SB21	-3.41 BB42	3.18 SB25	-2.43 BB41	1.66 BB43	1.57 SB23	1.52 SB22	-1.51 BB36
NORMAL MODE 46	OBSERVED=	0.0 CM-1	CALCULATED=	382.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	13.57 U*CC	13.57 C4C5	10.33 C7CC	10.33 C7CC	5.06 CCO8			
FORCE CONSTANTS-	53.38 CCO	20.43 CCH	10.15 CCH	6.60 CO				
OFF DIAGONAL-	5.94 SB21	-4.51 BB34	-3.00 BB42	2.99 SB25	2.82 BB43	-1.71 BB41	-1.61 BB29	
NORMAL MODE 47	OBSERVED=	0.0 CM-1	CALCULATED=	344.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	24.57 U9CC	14.58 CCO7	10.40 CCO8	5.04 C0*CC				
FORCE CONSTANTS-	66.37 CCO	9.96 CCH	9.71 CC	7.69 CO				
OFF DIAGONAL-	-8.04 BB34	5.49 SB22	-3.04 SB25	2.84 BB43	-2.67 BB42	-2.15 SB21	-2.13 BB29	
NORMAL MODE 48	OBSERVED=	0.0 CM-1	CALCULATED=	329.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	21.96 CCO7	16.35 CCO	9.85 C8CC	6.85 CCO6				
FORCE CONSTANTS-	53.04 CCO	16.42 CCH	16.35 CCO	7.61 CCH	6.38 CCH			
OFF DIAGONAL-	-8.09 BB34	4.46 SB22	3.21 BB29	2.98 BB43	-2.41 SB24	-1.83 SB21		
NORMAL MODE 49	OBSERVED=	0.0 CM-1	CALCULATED=	307.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	17.21 CCO8	8.13 CCO8	12.13 C9CC	11.47 C7CC	10.48 CCO7	8.49 CCO9	6.22 CCO6	5.03 C3CC
FORCE CONSTANTS-	89.22 CCO	8.13 CCH	8.86 CCH	6.44 T-OH				
OFF DIAGONAL-	-9.53 BB34	-4.86 BB42	-3.85 SB22	-1.93 SB26	1.91 BB41			
NORMAL MODE 50	OBSERVED=	0.0 CM-1	CALCULATED=	290.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	20.20 C7CC	11.94 CCO8	11.11 CCO9	9.52 CCO6	5.45 C1CC			
FORCE CONSTANTS-	57.67 CCO	18.41 CCH	10.66 CCH	6.34 CC				
OFF DIAGONAL-	-12.04 BB34	7.99 BB43	5.40 SB22	-3.89 BB29	-3.03 SB21	-2.00 SB25		
NORMAL MODE 51	OBSERVED=	0.0 CM-1	CALCULATED=	262.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	38.95 CCO1	24.18 C4CC	8.93 TH-5	7.07 C9CC	5.40 TCC5			
FORCE CONSTANTS-	52.75 CCO	25.80 CCH	10.92 T-OH	8.58 CCH	5.55 T-CC			
OFF DIAGONAL-	-6.55 BB34	-4.66 BB42	-2.75 BB33					
NORMAL MODE 52	OBSERVED=	0.0 CM-1	CALCULATED=	260.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	14.68 CCO8	8.96 C0*CC	8.31 CCO9	6.58 C4CC	6.51 CCO6			
FORCE CONSTANTS-	42.11 CCO	11.71 CCH	8.96 CCO	6.35 CC	7.87 CCH			
OFF DIAGONAL-	6.63 BB43	5.30 SB22	-4.44 BB34	-2.78 SB26	2.07 SB21	-1.90 BB33	-1.68 BB29	-1.59 SB25
NORMAL MODE 53	OBSERVED=	0.0 CM-1	CALCULATED=	166.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	40.09 TH-1	32.98 TH-2	10.52 TH-3	8.01 TH-4				
FORCE CONSTANTS-	90.29 T-OH							
OFF DIAGONAL-	NONE							
NORMAL MODE 54	OBSERVED=	0.0 CM-1	CALCULATED=	163.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	46.17 TH-5	10.09 TH-1	8.09 C0*CC	7.30 C4CC				
FORCE CONSTANTS-	61.06 T-OH	9.73 CCH	8.09 CCH	8.08 CCO	5.13 T-CC			
OFF DIAGONAL-	-1.54 SB21							
NORMAL MODE 55	OBSERVED=	0.0 CM-1	CALCULATED=	158.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	40.76 TH-4	21.26 TH-3	16.16 TH-5	13.27 TH-1				
FORCE CONSTANTS-	91.55 T-OH							
OFF DIAGONAL-	NONE							
NORMAL MODE 56	OBSERVED=	0.0 CM-1	CALCULATED=	155.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	55.19 TH-2	22.99 TH-1	12.14 TH-4					
FORCE CONSTANTS-	92.71 T-OH	5.84 CCO						
OFF DIAGONAL-	NONE							
NORMAL MODE 57	OBSERVED=	0.0 CM-1	CALCULATED=	151.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	59.16 TH-3	26.17 TH-4	5.37 TH-2					
FORCE CONSTANTS-	90.98 T-OH	9.22 CCO						
OFF DIAGONAL-	NONE							
NORMAL MODE 58	OBSERVED=	0.0 CM-1	CALCULATED=	132.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	17.21 TH-5	12.79 C0*CC	8.99 CCO	7.31 TH-1	6.38 CCO8	5.42 TCC4		
FORCE CONSTANTS-	26.32 T-OH	21.46 CCO	12.79 CCH	8.34 T-CC	8.25 CCH	8.24 CCH	6.00 T-CC	
OFF DIAGONAL-	3.79 BB43	-1.69 BB33						
NORMAL MODE 59	OBSERVED=	0.0 CM-1	CALCULATED=	86.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	20.21 TCC5	20.20 C2CC	10.92 TCC2	8.82 C3CC	7.43 C1CC			
FORCE CONSTANTS-	40.20 T-CC	37.40 CCH	20.22 CCH	5.90 CO				
OFF DIAGONAL-	-4.89 SB25	-3.83 BB42	-3.78 SB21	2.25 BB41	-1.67 BB34			
NORMAL MODE 60	OBSERVED=	0.0 CM-1	CALCULATED=	73.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	58.89 TCC5	6.25 C2CC	5.86 CCO1	5.14 C0*CC				
FORCE CONSTANTS-	64.60 T-CC	12.81 CCH	12.27 CCO	5.14 CCH				
OFF DIAGONAL-	-1.55 BB42	-1.53 BB34						
NORMAL MODE 61	OBSERVED=	0.0 CM-1	CALCULATED=	68.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	15.14 TCC4	14.49 C3CC	10.09 C0*CC	9.20 TCC3	8.48 C1CC	6.41 TCC2	5.54 C0*CC	
FORCE CONSTANTS-	33.71 T-CC	30.36 CCH	27.86 CCH	5.38 T-CC				
OFF DIAGONAL-	-3.71 BB42	-2.54 SB25	-2.03 BB34	1.85 BB41				

12. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 5.09

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CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400									
MOLECULE 12 -6 NG-1237 BETA GLUCOSE-1-D									
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NORMAL MODE 8	OBSERVED=	1450.0 CM-1	CALCULATED=	1450.1 CM-1	ERROR=	-0.1 CM-1	OR	-0.0 PERCENT	
INTERNAL COORDINATES-	61.43 HCH 20.22 OCHB	19.51 OCHA							
FORCE CONSTANTS-	61.43 HCH 39.84 OCH								
OFF DIAGONAL-	-4.11 SB27								
NORMAL MODE 9	OBSERVED=	1413.0 CM-1	CALCULATED=	1410.2 CM-1	ERROR=	-2.8 CM-1	OR	-0.2 PERCENT	
INTERNAL COORDINATES-	18.11 OC4H 11.33 HC4C	10.82 CC5H 8.56 OC3H 6.83 C2OH	6.20 HC3C 5.66 C5H 5.17 OC2H	5.06 C-09					
FORCE CONSTANTS-	38.02 OCH 37.86 CCH	10.11 CO 9.94 BCOH 5.20 CCO							
OFF DIAGONAL-	-9.45 SB27 8.11 BB29	-5.25 SB26 4.38 BB34 -3.43 SB25	-2.97 BB45 2.29 SB28						
NORMAL MODE 10	OBSERVED=	0.0 CM-1	CALCULATED=	1405.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	30.29 C1OH 29.39 C2OH	6.52 OC2H							
FORCE CONSTANTS-	62.65 BCOH 11.68 OCH	9.43 CCH							
OFF DIAGONAL-	-6.61 SB28 -3.62 SB27	-2.33 SB25 7.19 CO -5.63 CCO	-1.86 BB39 1.59 BB29						
NORMAL MODE 11	OBSERVED=	0.0 CM-1	CALCULATED=	1394.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	50.87 CCH 14.24 C1OH	12.44 OC1H							
FORCE CONSTANTS-	64.96 BCOH 17.33 OCH	11.16 CCH							
OFF DIAGONAL-	4.81 SB28 -3.77 SB27	-3.18 SB26 -2.77 BB39 1.53 BB29							
NORMAL MODE 12	OBSERVED=	0.0 CM-1	CALCULATED=	1391.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	56.94 C1OH 14.56 C3OH	7.92 OCHA							
FORCE CONSTANTS-	75.70 BCOH 10.99 OCH	8.80 CCH							
OFF DIAGONAL-	2.97 SB28 -1.81 BB39								
NORMAL MODE 13	OBSERVED=	0.0 CM-1	CALCULATED=	1385.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	47.39 C1OH 29.91 C2OH	6.03 OCH							
FORCE CONSTANTS-	79.81 BCOH 7.90 CCH								
OFF DIAGONAL-	3.68 SB28 -1.85 SB26								
NORMAL MODE 14	OBSERVED=	1363.0 CM-1	CALCULATED=	1363.9 CM-1	ERROR=	-0.9 CM-1	OR	-0.1 PERCENT	
INTERNAL COORDINATES-	16.23 C3CH 14.22 C2OH	8.64 HC2C 7.23 C5H 6.97 CC4H	6.81 OC2H 6.49 OC3H 5.93 CC3H						
FORCE CONSTANTS-	33.69 CCH 28.99 OCH	2.45 OCH							
OFF DIAGONAL-	6.31 BB29 -4.52 SB27	3.21 BB34 -3.06 SB28 -2.24 BB45	1.97 BB39 -1.86 BB36 1.74 SB26						
NORMAL MODE 15	OBSERVED=	1350.0 CM-1	CALCULATED=	1345.6 CM-1	ERROR=	-4.4 CM-1	OR	0.3 PERCENT	
INTERNAL COORDINATES-	15.74 HC2C 13.22 CCHB	12.72 CCH 10.92 OCHB	9.29 C5H 8.57 C1OH 5.34 HCH						
FORCE CONSTANTS-	51.87 CCH 28.99 OCH	11.12 BCOH 5.34 HCH							
OFF DIAGONAL-	-6.31 SB27 -3.23 BB45	2.54 BB29 2.02 BB30 -1.83 SB28							
NORMAL MODE 16	OBSERVED=	1332.0 CM-1	CALCULATED=	1325.8 CM-1	ERROR=	6.1 CM-1	OR	0.5 PERCENT	
INTERNAL COORDINATES-	21.32 HC3C 14.75 CC4H	10.00 OC2H 9.90 CC3H	6.52 CCHA						
FORCE CONSTANTS-	66.95 CCH 18.06 OCH	6.08 BCOH 5.18 CC							
OFF DIAGONAL-	13.48 BB29 -7.97 SB26	-3.75 BB45 -2.52 SB27							
NORMAL MODE 17	OBSERVED=	0.0 CM-1	CALCULATED=	1299.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	22.26 C5H 20.92 C4OH	16.79 OC4H 11.32 CC5H	9.75 CCHA 6.74 HC4C 5.45 OCHA						
FORCE CONSTANTS-	47.01 OCH 31.77 CCH	20.92 COH							
OFF DIAGONAL-	-3.87 BB29 -3.06 BB45	-2.88 SB27 2.41 BB34							
NORMAL MODE 18	OBSERVED=	0.0 CM-1	CALCULATED=	1291.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	20.49 OCHB 17.82 CCHB	12.47 OCHA 7.11 CCHA	7.10 C5H						
FORCE CONSTANTS-	45.38 OCH 31.52 CCH	6.53 CC							
OFF DIAGONAL-	-3.12 BB45 2.37 SB27	1.66 BB34 1.54 SB26							
NORMAL MODE 19	OBSERVED=	0.0 CM-1	CALCULATED=	1275.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	22.14 OC2H 19.10 CCH2	17.29 CC3H 12.30 OC3H	5.14 C4OH						
FORCE CONSTANTS-	42.59 CCH 40.93 OCH	7.53 CCH							
OFF DIAGONAL-	-4.36 SB26 -3.47 BB45	2.66 SB27 1.69 BB29 -1.68 SB25							
NORMAL MODE 20	OBSERVED=	1270.0 CM-1	CALCULATED=	1271.0 CM-1	ERROR=	1.0 CM-1	OR	-0.1 PERCENT	
INTERNAL COORDINATES-	18.73 CCHC 13.63 C4OH	11.84 OCH 8.84 HC2C	5.66 OC3H						
FORCE CONSTANTS-	39.36 CCH 25.53 OCH	11.63 COH 10.31 CO	5.73 CC						
OFF DIAGONAL-	-5.13 SB26 3.24 SB27	2.74 BB34 -2.74 BB45 -2.31 SB25							
NORMAL MODE 21	OBSERVED=	1255.0 CM-1	CALCULATED=	1254.6 CM-1	ERROR=	0.3 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	15.36 C4OH 11.56 C5H	10.56 HC5C 10.41 OC3H	7.88 CC4H						
FORCE CONSTANTS-	39.03 CCH 31.54 OCH	15.36 COH	6.03 CO						
OFF DIAGONAL-	5.48 SB27 -2.88 BB45	1.97 BB34							
NORMAL MODE 22	OBSERVED=	1240.0 CM-1	CALCULATED=	1248.8 CM-1	ERROR=	-8.8 CM-1	OR	-0.7 PERCENT	
INTERNAL COORDINATES-	30.85 OC1 18.10 C-06	7.87 OC4H 6.85 C1OH	5.84 CCH2 5.37 C4OH 5.18 C1H						
FORCE CONSTANTS-	55.86 CO 19.26 OCH	18.87 CCH 12.54 CCO	10.00 BCOH 5.37 COH						
OFF DIAGONAL-	9.42 SB25 -7.85 SB27	-4.28 SB28 2.53 BB34 -1.89 SB26							
NORMAL MODE 23	OBSERVED=	1208.0 CM-1	CALCULATED=	1216.7 CM-1	ERROR=	-8.7 CM-1	OR	-0.7 PERCENT	
INTERNAL COORDINATES-	13.48 C-06 2.85 OC1	10.04 HC2C 8.06 HC2C	8.40 OC4H 6.52 CCH2 5.99 CC5H						
FORCE CONSTANTS-	42.47 CCH 33.57 CCH	21.95 OCH							
OFF DIAGONAL-	-5.38 SB25 -4.13 BB29	3.68 BB34 -2.65 BB45 -2.21 SB26							
NORMAL MODE 24	OBSERVED=	1178.0 CM-1	CALCULATED=	1175.5 CM-1	ERROR=	2.5 CM-1	OR	0.2 PERCENT	
INTERNAL COORDINATES-	9.85 HC4C 8.96 C-07	10.78 HC5C 8.70 CC4H	7.95 CCHB						
FORCE CONSTANTS-	54.71 CCH 23.28 CO	10.07 OCH 8.08 CCO	5.96 CC						
OFF DIAGONAL-	-7.64 BB29 5.54 SB27	4.72 BB34 -4.58 SB25 -4.30 SB26	-2.63 BB45						
NORMAL MODE 25	OBSERVED=	0.0 CM-1	CALCULATED=	1147.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	25.28 C5H 12.85 C-07	7.00 OCHB 6.41 C9C	6.14 CCO1 5.86 OC9C 5.57 C-09 5.55 HC5C						
FORCE CONSTANTS-	50.72 CO 23.13 CCO	14.65 OCH 11.77 CCH	8.61 CC						
OFF DIAGONAL-	-15.41 SB25 8.74 SB27	-5.56 SB26 -3.73 SB28 -1.92 SB22	1.79 BB43						
NORMAL MODE 26	OBSERVED=	1130.0 CM-1	CALCULATED=	1128.0 CM-1	ERROR=	2.0 CM-1	OR	0.2 PERCENT	
INTERNAL COORDINATES-	43.81 C5C 18.32 C-08	13.38 C4C5 7.08 OCMA	6.31 CCO1 6.13 C1OH 5.44 C1C						
FORCE CONSTANTS-	61.13 CO 30.89 CO	13.74 CCO 9.59 CCH	9.52 OCH 7.08 BCOH 5.44 CCO						
OFF DIAGONAL-	-12.32 SB22 -11.52 SB26	-5.21 SB28 -4.71 SB27 -4.69 SS18	-3.22 BB34 -1.58 SS17						
NORMAL MODE 27	OBSERVED=	1115.0 CM-1	CALCULATED=	1110.8 CM-1	ERROR=	4.2 CM-1	OR	0.4 PERCENT	
INTERNAL COORDINATES-	23.56 C5H 11.05 C-09	9.52 OCHA 9.13 C4C5 8.98 CCO2	7.28 C3C4 7.15 OCHB 5.15 C-06						
FORCE CONSTANTS-	44.03 CCH 11.24 CO	11.13 OCH 10.78 CCH	11.86 CCH						
OFF DIAGONAL-	-3.68 SB25 -3.37 SS18	-3.31 SB28 -1.89 SB27 -1.76 BB29	-1.64 SB21						
NORMAL MODE 28	OBSERVED=	1085.0 CM-1	CALCULATED=	1080.0 CM-1	ERROR=	5.0 CM-1	OR	0.5 PERCENT	
INTERNAL COORDINATES-	33.72 C2C3 26.00 C3C4	11.92 C1C2 11.05 C-07 7.69 C2OH							
FORCE CONSTANTS-	76.22 CO 21.78 CO	11.71 CCO 10.67 CCH	10.50 BCOH 5.41 OCH						
OFF DIAGONAL-	-10.83 SB22 -5.18 SB26	-4.93 SB28 -4.27 SB27 -2.94 C-07	2.39 SS18 -1.94 SB24 -1.92 BB34 -1.84 SB25						
NORMAL MODE 29	OBSERVED=	0.0 CM-1	CALCULATED=	1060.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	40.49 C-08 27.53 C1C2	13.64 C2C3 11.37 C3OH	9.20 C3C4 8.83 C2CC 8.74 OC3H 7.94 OC7C	6.02 C-07					
FORCE CONSTANTS-	51.62 CO 50.68 CC	17.08 CCO 14.06 BCOH	13.28 OCH 12.95 CCC 6.42 CCH						
OFF DIAGONAL-	-11.39 SB27 -10.09 SB28	-9.78 SB21 -7.87 SS18 -7.59 SB25	-7.56 SB22 -3.42 BB34 -2.11 BB36 -1.88 BB43						
NORMAL MODE 30	OBSERVED=	1050.0 CM-1	CALCULATED=	1051.8 CM-1	ERROR=	-1.8 CM-1	OR	-0.2 PERCENT	
INTERNAL COORDINATES-	19.06 C-07 13.51 C1C2	11.62 C-08 9.12 C1H	6.59 C3C4 5.30 CC3H 5.06 C-09						
FORCE CONSTANTS-	44.80 CO 26.28 CC	20.08 CCH 18.16 OCH	9.14 CCO 5.42 BCOH						
OFF DIAGONAL-	-6.63 SB21 -5.59 SB27	-5.46 SB22 -4.66 SB28 -4.58 SS18	-3.95 BB29 1.65 BB34						
NORMAL MODE 31	OBSERVED=	1032.0 CM-1	CALCULATED=	1034.5 CM-1	ERROR=	-2.5 CM-1	OR	-0.3 PERCENT	
INTERNAL COORDINATES-	32.47 C-09 17.40 C3C4	14.60 C4OH 8.25 C1H	7.26 C4C2 7.05 C3CC 6.26 OC4H	6.18 C-08	5.25 C4CC				
FORCE CONSTANTS-	44.11 CO 26.33 CC	17.93 OCH 14.60 CCH	13.86 CCO 12.38 CCH	8.17 CO					
OFF DIAGONAL-	-10.16 SB28 -8.56 SB21	-7.25 SB27 -4.56 SB25 -3.92 SS18	-2.60 SB22 -1.77 BB34						
NORMAL MODE 32	OBSERVED=	1020.0 CM-1	CALCULATED=	1023.7 CM-1	ERROR=	-3.7 CM-1	OR	-0.4 PERCENT	
INTERNAL COORDINATES-	44.15 C1H 15.08 C-09	12.97 CC 9.32 COH	9.25 CCH						
FORCE CONSTANTS-	49.15 CO 32.20 CC	12.07 CCH							
OFF DIAGONAL-	-6.86 SB28 -2.83 SS18	-2.67 SB25 -2.53 SB21 -1.97 BB45	1.63 SB26 -1.53 BB36						
NORMAL MODE 33	OBSERVED=	1010.0 CM-1	CALCULATED=	1007.2 CM-1	ERROR=	-2.8 CM-1	OR	0.3 PERCENT	
INTERNAL COORDINATES-	33.72 C-08 11.57 C3C4	7.22 C1H 6.49 C5C	6.26 C2C3 5.60 C4C5 5.55 OC1H	5.14 HC5C					
FORCE CONSTANTS-	44.86 CO 30.91 CC	17.50 CCO 16.93 CCH	9.24 CCO						
OFF DIAGONAL-	-5.60 SB22 -5.53 SB26	-4.01 SB28 -3.89 SB21 -3.38 SB27	-2.27 SB25 -2.10 BB29						
NORMAL MODE 34	OBSERVED=	972.0 CM-1	CALCULATED=	1000.4 CM-1	ERROR=	-28.4 CM-1	OR	-2.9 PERCENT	
INTERNAL COORDINATES-	22.47 C2C3 19.28 C1C2	11.97 C-09 8.59 CCO8	6.66 OC1						
FORCE CONSTANTS-	48.11 CC 29.97 CO	21.28 CCO 8.23 CCH	6.41 OCH						
OFF DIAGONAL-	-14.03 SB22 -7.02 SB21	2.85 BB34 -2.17 SB24 1.87 SB25							
NORMAL MODE 35	OBSERVED=	965.0 CM-1	CALCULATED=	967.2 CM-1	ERROR=	-2.2 CM-1	OR	-0.2 PERCENT	
INTERNAL COORDINATES-	29.96 C-06 16.74 C-08	8.43 OC1 7.81 C1H	6.62 C1C2						
FORCE CONSTANTS-	49.15 CO 14.86 CC	13.35 CCH	9.72 CO						
OFF DIAGONAL-	-7.32 SB24 -4.61 SB27	4.11 SS18 3.34 BB34 -3.22 SB22	-2.64 SB28 -1.53 BB29						

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 1-400
MOLECULE 12 -6 NG=1237 BETA GLUCOSE-1-D

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NORMAL MODE 36	OBSERVED=	900.0 CM-1	CALCULATED=	909.3 CM-1	ERROR=	-9.3 CM-1	OR	-1.0 PERCENT
INTERNAL COORDINATES-	27.19 C5C	17.50 C-O*	9.77 CCHB	8.62 C5O*				
FORCE CONSTANTS-	33.11 CC	31.18 CO	19.59 CCH	6.91 CCO				
OFF DIAGONAL-	6.93 SB26	6.37 SS18	-5.69 SB22	-5.41 SB21	-3.65	SB25	-2.96 SB27	-2.00 SB23
NORMAL MODE 37	OBSERVED=	875.0 CM-1	CALCULATED=	897.8 CM-1	ERROR=	-22.8 CM-1	OR	-2.6 PERCENT
INTERNAL COORDINATES-	16.84 OC1H	14.00 CC1H	9.67 C4C5	9.05 C5O*	8.90	C-O*	8.55 CCHA	6.51 CCHB
FORCE CONSTANTS-	34.11 CCH	24.94 OCH	21.78 CO	14.68 CC	7.13	CCO		
OFF DIAGONAL-	-5.00 SB27	-3.99 SB21	-2.94 SB22	2.43 BB34	2.31	SB25	-1.59 SS18	
NORMAL MODE 38	OBSERVED=	835.0 CM-1	CALCULATED=	850.2 CM-1	ERROR=	-15.2 CM-1	OR	-1.8 PERCENT
INTERNAL COORDINATES-	30.28 OC1H	19.06 CC1H	6.90 OC1	5.92 C1H	5.70	C4C5	5.66 CCHA	
FORCE CONSTANTS-	32.43 OCH	32.13 CCH	19.24 CO	11.23 CC	6.93	CCO		
OFF DIAGONAL-	5.78 SB27	-2.98 SB26	2.65 SB22	-2.26 SB25	-2.12	BB34	-2.07 SB21	-2.03 SB23
NORMAL MODE 39	OBSERVED=	710.0 CM-1	CALCULATED=	720.0 CM-1	ERROR=	-10.0 CM-1	OR	-1.4 PERCENT
INTERNAL COORDINATES-	19.46 CCO*	14.27 CCO*	8.08 OCCH	7.78 CCH	6.51	CCO*	5.90 C4CC	
FORCE CONSTANTS-	39.91 CCO	24.97 CCH	8.93 OCH	7.13 CC	5.93	CCO	5.95 CO	
OFF DIAGONAL-	6.26 BB43	-6.99 BB34	5.09 SB25	-4.55 BB29	3.72	SB21	-1.88 SB27	-1.65 BB41
NORMAL MODE 40	OBSERVED=	0.0 CM-1	CALCULATED=	617.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	11.16 CCO*	9.31 CO*	6.06 CC3H	5.99 CCO*	5.99	C-O*	5.76 HC2C	5.46 4CO
FORCE CONSTANTS-	40.95 CCO	18.81 CCH	13.47 CO	9.31 CCO	6.26	CCC		
OFF DIAGONAL-	6.47 SB25	5.82 BB43	-5.77 BB25	-4.17 BB29	-2.75	SB27	2.10 SB24	-1.96 BB41
NORMAL MODE 41	OBSERVED=	0.0 CM-1	CALCULATED=	599.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	13.94 CCO	10.55 CCO*	10.23 OCCH	9.72 OCCH	7.89	CCO6	7.50 C4CC	6.84 CCO*
FORCE CONSTANTS-	59.84 CCO	22.12 BB43	13.94 CCO	9.05 CCH	8.12	CC		
OFF DIAGONAL-	-12.86 BB34	5.62 BB43	-4.91 SB21	-4.77 BB21	-3.54	BB29	3.35 SB24	1.92 SB22
NORMAL MODE 42	OBSERVED=	0.0 CM-1	CALCULATED=	579.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	17.73 U*CC	12.42 4CO*	5.84 C-O*	5.80 HC4C				
FORCE CONSTANTS-	47.02 CCO	21.39 CCH	12.12 CO	7.67 OCH				
OFF DIAGONAL-	-7.93 BB34	6.31 SB25	6.26 BB43	-4.62 BB29	3.74	SB22	-3.36 SB27	-1.54 SB23
NORMAL MODE 43	OBSERVED=	0.0 CM-1	CALCULATED=	518.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	8.23 CCO*	7.78 C4C5	6.40 OBCC	5.32 C1C2	5.32	C3C4	5.31 C1C1	
FORCE CONSTANTS-	31.43 CCO	22.64 CC	17.95 CCH	17.89 CO				
OFF DIAGONAL-	-6.50 BB34	5.12 BB43	4.47 SS18	4.21 SB21	-3.61	BB29	-2.75 SB27	2.04 SB24
NORMAL MODE 44	OBSERVED=	0.0 CM-1	CALCULATED=	455.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	11.11 CCO*	10.93 CCH	12.56 OCCH	9.10 CO	9.24	CCO	5.04 CCO*	5.04 HC3C
FORCE CONSTANTS-	45.04 CCO	25.95 CCH	10.05 CCH	8.04 CC	6.34	CCO		
OFF DIAGONAL-	-7.85 BB34	5.81 BB43	-5.57 BB29	3.61 SB25	-2.07	SB26		
NORMAL MODE 45	OBSERVED=	0.0 CM-1	CALCULATED=	411.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	19.75 C2CC	11.92 CO*	10.31 CCO*	8.73 C1CC	6.94	C3CC	6.16 CCO8	
FORCE CONSTANTS-	35.90 CCH	22.43 CCO	11.92 CCO	6.79 CO	5.84	CCH	5.74 CC	
OFF DIAGONAL-	4.08 SB21	3.55 SB25	-3.16 BB42	-2.32 BB41	1.89	SB23	1.77 BB43	
NORMAL MODE 46	OBSERVED=	0.0 CM-1	CALCULATED=	385.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	16.57 4CO*	16.49 O*CC	12.07 C3CC	7.48 OBCC	7.00	CCO8	6.97 C1CC	
FORCE CONSTANTS-	52.60 CCO	20.12 CCO	12.38 CCO	5.72 CO				
OFF DIAGONAL-	5.85 SB21	-4.99 BB34	3.58 BB43	2.74 SB25	-2.64	BB42	-2.21 BB29	-1.67 BB41
NORMAL MODE 47	OBSERVED=	0.0 CM-1	CALCULATED=	344.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	25.69 OCCH	12.01 CCO*	6.65 CCO8	6.03 CCO	5.35	C5O*	5.28 C2C3	
FORCE CONSTANTS-	51.11 CCH	22.64 CC	9.11 CCH	7.14 CCH				
OFF DIAGONAL-	-7.73 BB34	5.98 SB22	-2.94 BB42	2.89 BB43	-2.69	SB25	-2.33 SB21	-1.91 BB29
NORMAL MODE 48	OBSERVED=	0.0 CM-1	CALCULATED=	331.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	11.11 CCO*	14.31 OCCH	12.56 OCCH	7.06 CCO*				
FORCE CONSTANTS-	53.95 CCO	15.98 CCH	14.31 CCO	8.29 T-OH	7.16	CC	5.47 CCC	
OFF DIAGONAL-	-8.02 BB34	4.46 SB22	-3.12 BB29	-2.50 SB24	2.31	BB43	-1.87 SB21	-1.64 BB42
NORMAL MODE 49	OBSERVED=	0.0 CM-1	CALCULATED=	313.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	20.16 OCCH	12.64 OCCH	11.75 CCO*	10.63 CCO8	9.76	OCCH	6.54 CCO6	5.75 CCO*
FORCE CONSTANTS-	83.38 CCO	12.61 T-OH	7.82 CCH	6.05 CCC				
OFF DIAGONAL-	-9.02 BB34	-4.47 BB42	-3.43 SB22	1.75 BB41	-1.73	SB26		
NORMAL MODE 50	OBSERVED=	0.0 CM-1	CALCULATED=	296.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	19.99 OCCH	13.28 CCO8	11.30 CCO*	9.34 CCO6	5.38	CC3H		
FORCE CONSTANTS-	57.12 CCO	21.65 CCH	8.66 CCH	5.80 CC	5.36	T-OH		
OFF DIAGONAL-	-13.22 BB34	8.95 BB43	-4.82 BB29	4.73 SB22	-2.61	SB21	-2.50 SB25	
NORMAL MODE 51	OBSERVED=	0.0 CM-1	CALCULATED=	273.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	30.18 CCO*	27.55 TH-5	12.77 C4CC	6.43 OCCH				
FORCE CONSTANTS-	48.04 CCO	32.19 T-OH	7.14 CCH	7.14 CCH				
OFF DIAGONAL-	-5.01 BB34	-2.92 BB42	-2.20 BB33	1.85 SB22				
NORMAL MODE 52	OBSERVED=	0.0 CM-1	CALCULATED=	264.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	11.12 C4CC	11.23 CCO*	13.75 CCH	10.04 CCH	7.44	CCO*	6.92 CC	5.87 T-CC
FORCE CONSTANTS-	31.74 CCO	14.79 T-OH	3.68 SB21	2.80 SB22	-2.42	SB26		
OFF DIAGONAL-	4.86 BB43	-4.02 BB34						
NORMAL MODE 53	OBSERVED=	0.0 CM-1	CALCULATED=	226.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	38.54 TH-3	35.54 TH-2	8.67 TH-3	8.57 TH-5				
FORCE CONSTANTS-	96.29 T-OH							
OFF DIAGONAL-	NONE							
NORMAL MODE 54	OBSERVED=	0.0 CM-1	CALCULATED=	216.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	31.05 TH-1	25.77 TH-3	22.16 TH-4					
FORCE CONSTANTS-	84.39 T-OH	8.17 CCO						
OFF DIAGONAL-	NONE							
NORMAL MODE 55	OBSERVED=	0.0 CM-1	CALCULATED=	214.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	42.95 TH-2	28.76 TH-4	12.25 TH-1	5.13 CCO*				
FORCE CONSTANTS-	86.73 T-OH	11.28 CCO						
OFF DIAGONAL-	NONE							
NORMAL MODE 56	OBSERVED=	0.0 CM-1	CALCULATED=	210.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	49.08 TH-3	25.12 TH-4	6.94 TH-2	5.79 CCO8				
FORCE CONSTANTS-	88.02 T-OH	17.49 CCO						
OFF DIAGONAL-	-2.12 BB34							
NORMAL MODE 57	OBSERVED=	0.0 CM-1	CALCULATED=	209.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	56.41 TH-3	10.16 CCO*	8.06 C4CC	5.38 TH-1				
FORCE CONSTANTS-	63.52 T-OH	18.14 CCO	9.24 CCC	5.10 CCH				
OFF DIAGONAL-	-2.17 BB34	1.61 SB22						
NORMAL MODE 58	OBSERVED=	0.0 CM-1	CALCULATED=	140.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	19.38 CO*	9.20 C4CC	8.08 TCC4	7.67 CCO*	6.24	CCO*	6.07 TCO1	5.46 OCO
FORCE CONSTANTS-	24.76 CCO	19.38 CCO	14.39 CCC	9.93 T-CC	9.66	T-CC	8.30 CCH	5.46 OCO
OFF DIAGONAL-	4.38 BB43	-1.94 SB25	1.70 BB41					
NORMAL MODE 59	OBSERVED=	0.0 CM-1	CALCULATED=	89.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	21.25 ICC*	20.43 C2CC	10.85 TCC2	8.79 C3CC	7.60	C1CC		
FORCE CONSTANTS-	41.77 T-CC	37.82 CCO	20.12 CCO	3.21 CO				
OFF DIAGONAL-	-4.54 SB25	-3.99 SB21	-3.85 BB42	2.27 BB41	-1.65	BB34		
NORMAL MODE 60	OBSERVED=	0.0 CM-1	CALCULATED=	74.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	59.94 TCC*	6.34 C2CC	5.65 CCO*	5.23 CCO*				
FORCE CONSTANTS-	65.60 T-CC	12.79 CCO	12.03 CCO	5.23 CCO				
OFF DIAGONAL-	-1.54 BB42							
NORMAL MODE 61	OBSERVED=	0.0 CM-1	CALCULATED=	70.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	19.19 TCC	14.92 C3CC	10.18 4CO*	9.36 TCC*	8.62	C1CC	6.54 TCC2	5.98 O*CC
FORCE CONSTANTS-	35.37 T-CC	30.60 CCO	28.61 CCC	5.45 T-CC				
OFF DIAGONAL-	-3.78 BB42	-2.62 SB25	-2.07 BB34	1.88 BB41				

23. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 6.33

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400									
MOLECULE 13 -6 NG=1237 BETA GLUCOSE-C1-O, -O-D5									
PAGE 1									
NORMAL MODE 8	OBSERVED=	1450.0 CM-1	CALCULATED=	1450.1 CM-1	ERROR=	-0.1 CM-1	OR	-0.0 PERCENT	
INTERNAL COORDINATES-	61.43 HCH	20.22 OCHB	19.52 OCHA						
FORCE CONSTANTS-	61.43 HCH	39.85 OCH							
OFF DIAGONAL-	-4.11 SB27								
NORMAL MODE 9	OBSERVED=	1410.0 CM-1	CALCULATED=	1406.3 CM-1	ERROR=	3.7 CM-1	OR	0.3 PERCENT	
INTERNAL COORDINATES-	21.43 OC4H	34.59 CC5H	13.22 CC5H	8.11 HC3C	7.58 CC5H	5.54 C-O9			
FORCE CONSTANTS-	4.64 CCH	40.99 OCH	11.22 CO	5.38 CCO					
OFF DIAGONAL-	-10.14 SB27	9.70 BB29	5.50 BB34	-4.86 SB26	-3.95 SB25	-3.39 BB45			
NORMAL MODE 10	OBSERVED=	0.0 CM-1	CALCULATED=	1375.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	16.78 OC2H	19.36 HC2C	13.39 OC3H	10.05 CC5H	9.59 CC3H	6.55 HC4C	5.24 CC4H		
FORCE CONSTANTS-	48.58 CCH	42.66 OCH	9.36 CO						
OFF DIAGONAL-	9.38 BB29	-9.32 SB27	-4.46 SB26	-3.70 BB45	3.03 BB34	-2.74 SB25			
NORMAL MODE 11	OBSERVED=	0.0 CM-1	CALCULATED=	1351.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	17.86 HC5C	17.28 CCHA	14.46 CCHB	8.02 OCHA	7.50 CC5H	6.98 HCH	6.24 OCHB	6.15 OC2H	
FORCE CONSTANTS-	62.43 CCH	30.12 OCH	6.98 HCH	5.32 CO					
OFF DIAGONAL-	-7.39 SB27	-3.79 BB45	2.78 BB29	-2.58 SB26	2.42 BB30				
NORMAL MODE 12	OBSERVED=	0.0 CM-1	CALCULATED=	1332.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	22.98 HC3C	14.08 OC2H	12.72 CC4H	7.60 OC3H	7.06 CCHA	5.74 CC3H			
FORCE CONSTANTS-	65.86 CCH	28.55 OCH	7.02 CO						
OFF DIAGONAL-	13.00 BB29	-10.53 SB26	-4.11 BB45	-4.05 SB27	-2.02 BB43				
NORMAL MODE 13	OBSERVED=	0.0 CM-1	CALCULATED=	1301.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	18.36 OC4H	18.31 OCHA	12.43 CCHA	10.67 OCHB	8.94 OC3H	7.35 HC4C	6.25 CCHB		
FORCE CONSTANTS-	61.17 CCH	31.59 OCH							
OFF DIAGONAL-	-3.86 BB45	-3.02 SB27	1.96 BB34						
NORMAL MODE 14	OBSERVED=	0.0 CM-1	CALCULATED=	1288.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	33.49 CC5H	15.89 OCHB	12.43 CCHB	9.50 OC4H	7.56 CC5H				
FORCE CONSTANTS-	63.95 OCH	27.19 CCH	6.92 CO						
OFF DIAGONAL-	3.66 SB27	-3.51 BB45	-2.26 SB26	-2.20 BB29					
NORMAL MODE 15	OBSERVED=	0.0 CM-1	CALCULATED=	1282.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	31.25 CCH2	15.51 OC2H	13.32 CC3H	5.59 HC2C	5.58 HC3C				
FORCE CONSTANTS-	61.08 CCH	24.12 OCH	8.97 CO						
OFF DIAGONAL-	7.26 BB29	-3.70 BB45	-3.62 SB26	2.74 BB34	-2.34 SB27	-1.69 SB25			
NORMAL MODE 16	OBSERVED=	0.0 CM-1	CALCULATED=	1269.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	23.17 OC3H	10.41 CC4H	9.20 CC3H	7.60 HC2C	7.22 OC1	7.10 CC5H	5.39 C-O6	5.09 HC4C	5.04 OC2H
FORCE CONSTANTS-	38.13 CCH	38.04 OCH	19.03 CO	6.62 CCO					
OFF DIAGONAL-	-4.56 SB25	-4.06 BB29	3.88 BB34	3.43 SB27	-3.02 BB45	-2.02 SB26	1.55 BB43		
NORMAL MODE 17	OBSERVED=	0.0 CM-1	CALCULATED=	1263.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	21.37 OC1	18.48 C-O6	10.64 OC4H	7.07 CC4H	5.54 CCH2	5.10 OC2H			
FORCE CONSTANTS-	46.19 CCH	31.50 OCH	23.32 CO	12.50 CCH					
OFF DIAGONAL-	-8.23 SB25	-6.22 SB27	-2.20 BB45	-2.12 BB29	1.92 BB34				
NORMAL MODE 18	OBSERVED=	0.0 CM-1	CALCULATED=	1225.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	15.93 HC5C	15.93 OC4H	9.17 CC5H	6.00 C-O6	7.68 CCH2	7.16 HC2C	6.54 OC1		
FORCE CONSTANTS-	51.82 CCH	25.00 OCH	19.33 CO	8.74 CCO					
OFF DIAGONAL-	-4.33 SB25	-3.58 BB29	-3.12 BB45	-3.07 SB26	3.03 BB34	2.77 SB27	-1.85 SB28		
NORMAL MODE 19	OBSERVED=	0.0 CM-1	CALCULATED=	1189.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	9.17 HC5C	7.59 CC4H	7.30 CC5H	6.60 CC3H	6.34 C-O6	6.24 CCH2	6.09 HC4C	5.73 CC4C5	5.72 HC2C
FORCE CONSTANTS-	55.90 CCH	17.48 CO	11.31 CCO	8.43 OCH	6.45 CC				
OFF DIAGONAL-	-7.65 BB29	7.29 BB34	-4.09 SB25	4.03 SB27	-2.56 BB45				
NORMAL MODE 20	OBSERVED=	0.0 CM-1	CALCULATED=	1178.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	15.27 C-O6	14.64 CC4C5	10.42 C-OH	9.88 OCHA	7.18 CCO	5.00 OCHB			
FORCE CONSTANTS-	36.64 CC	18.48 OCH	15.42 CCH	14.74 BCOH	12.69 BB34	11.91 CCO			
OFF DIAGONAL-	-7.47 SB22	-3.99 SB26	-2.34 SB25	-1.81 SS18	1.67 BB34				
NORMAL MODE 21	OBSERVED=	0.0 CM-1	CALCULATED=	1156.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	39.35 C-C3	10.23 C-O8	9.89 C3OH	7.98 C2OH	5.79 CCO9	5.15 C2CC			
FORCE CONSTANTS-	46.82 CCH	22.62 CO	19.33 BCOH	16.57 CCO	15.06 CC				
OFF DIAGONAL-	-8.37 SB21	-7.88 SB22	6.79 SB28	-4.09 SS18	-2.44 SB27	-2.37 SB25			
NORMAL MODE 22	OBSERVED=	0.0 CM-1	CALCULATED=	1154.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	19.43 C-O6	18.93 C5C	9.24 C5O5	8.61 C-O6	6.44 CCO9	5.65 C3C4	5.40 CCO	5.39 C2CC	5.18 C3OH
FORCE CONSTANTS-	46.19 CCH	22.62 CO	19.33 BCOH	16.57 CCO	15.06 CC				
OFF DIAGONAL-	-7.35 SB25	-5.71 SB22	6.79 SB28	-4.09 SS18	-2.44 SB27	-2.37 SB25			
NORMAL MODE 23	OBSERVED=	0.0 CM-1	CALCULATED=	1142.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	19.01 C5O	11.18 C4C5	11.04 C5C	10.58 C2C3	8.04 C2OH	5.94 OC6	5.42 C3C4	5.06 C-O6	
FORCE CONSTANTS-	39.29 CC	31.37 CCH	19.71 CCH	8.68 BCOH	8.60 CCH	8.46 OCH			
OFF DIAGONAL-	-9.60 SB22	-5.96 SB26	-5.93 SB25	2.88 SB28	-2.31 SB21				
NORMAL MODE 24	OBSERVED=	0.0 CM-1	CALCULATED=	1128.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	37.64 C1C	19.43 C1OH	9.74 C3C4	8.20 C-O7	6.15 CCH1	6.00 C-O8	5.68 OC1		
FORCE CONSTANTS-	52.90 CC	28.06 CO	21.62 BCOH	10.86 CCH	7.53 OCH	6.42 CCO			
OFF DIAGONAL-	-9.30 SB26	-8.86 SB22	-6.68 SS18	-3.62 SB24	-3.48 SB27	2.09 SB28	-1.71 BB43	-1.69 BB34	
NORMAL MODE 25	OBSERVED=	0.0 CM-1	CALCULATED=	1119.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	20.98 C-O9	13.67 C-O8	12.85 C1C2	12.35 C1OH	7.41 C3C4	7.19 C5O			
FORCE CONSTANTS-	47.51 CCH	24.20 CC	17.01 BCOH	10.26 CCO	9.17 OCH				
OFF DIAGONAL-	-4.26 SB25	-3.89 SB22	-3.74 SS18	-3.26 SB21	1.63 SB27	-1.58 SB28			
NORMAL MODE 26	OBSERVED=	0.0 CM-1	CALCULATED=	1090.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	31.67 C-O6	23.16 C3C4	10.75 C4CC	9.36 C5C5	7.99 C4C	7.84 C3CC	6.91 C-O9	5.36 C4OH	5.33 C5O
FORCE CONSTANTS-	31.67 CCH	23.16 CO	10.75 CCH	9.36 CCO	7.99 CCH	7.84 CCO	6.91 CCO	5.36 CCH	
OFF DIAGONAL-	-18.98 SB21	-6.50 SS18	-6.50 SB27	-2.53 SB22	-2.04 SB25	-2.03 BB34	-1.57 BB36		
NORMAL MODE 27	OBSERVED=	0.0 CM-1	CALCULATED=	1041.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	20.74 C-O6	13.00 C3C4	12.92 C4C5	10.07 C1H	8.85 CCOH	7.29 CCO			
FORCE CONSTANTS-	36.16 CCH	26.95 CC	15.83 OCH	15.26 CCH	11.28 BCOH				
OFF DIAGONAL-	-5.40 SB22	-4.34 SB27	-3.00 SB25	-2.60 SB26	1.94 SB21				
NORMAL MODE 28	OBSERVED=	0.0 CM-1	CALCULATED=	1029.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	18.67 C-O7	17.05 C-O9	10.48 C1OH	9.56 C1H	7.33 CCOH	6.86 OC1H	5.38 CC3H	5.06 C2C3	
FORCE CONSTANTS-	42.04 CO	21.64 CCH	19.84 BCOH	16.97 OCH	9.71 CC				
OFF DIAGONAL-	-5.10 SB28	-4.71 BB29	-3.72 SB25	2.06 SB27	-1.53 BB45				
NORMAL MODE 29	OBSERVED=	0.0 CM-1	CALCULATED=	1020.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	30.68 C1H	20.14 OC1H	13.20 C-O6	9.35 C-O9	9.33 CCOH				
FORCE CONSTANTS-	52.38 CCH	35.76 CO	11.56 CCH	6.93 BCOH					
OFF DIAGONAL-	-5.37 SB28	-3.31 SB25	-2.36 BB45	-2.21 BB29					
NORMAL MODE 30	OBSERVED=	0.0 CM-1	CALCULATED=	997.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	35.24 C-OH	22.10 C-O6	7.93 C-O7	5.99 C3OH	5.10 C5C				
FORCE CONSTANTS-	44.11 CCH	24.47 CO	17.70 CCH	15.29 CCOH	10.43 CCH	8.06 CCO			
OFF DIAGONAL-	-15.61 SB28	-5.58 SB27	-4.85 SB26	-3.21 SB22	-2.54 SB25	-1.94 BB29			
NORMAL MODE 31	OBSERVED=	0.0 CM-1	CALCULATED=	980.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	31.67 C1H	17.09 C-O6	11.76 C1C2	11.76 C1C2	10.69 C2OH	9.71 C1OH			
FORCE CONSTANTS-	55.78 BCOH	32.75 CO	15.55 CC						
OFF DIAGONAL-	-10.23 SB28	-6.18 SB24	-3.38 SS18	3.21 SB27	-2.79 BB35	-2.44 SB23			
NORMAL MODE 32	OBSERVED=	0.0 CM-1	CALCULATED=	968.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	26.63 C-O8	16.96 C-O6	13.07 C3OH	12.45 C1H	8.05 C1C2				
FORCE CONSTANTS-	51.54 CO	16.92 CCH	13.43 BCOH	8.75 CCH	8.74 CC	8.33 OCH			
OFF DIAGONAL-	-8.86 SB27	-6.31 SB28	-5.16 SB24	3.96 BB34	3.18 SB26	-2.30 SB22	-1.90 SB21	-1.74 BB29	1.57 SS18
NORMAL MODE 33	OBSERVED=	0.0 CM-1	CALCULATED=	958.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	30.79 C2OH	27.90 C3OH	12.37 C3C4	7.84 C1C2	5.45 CCO8	5.44 C-O7			
FORCE CONSTANTS-	63.26 BCOH	24.80 CC	12.53 CO	10.18 CCO	7.52 OCH	5.59 CCH			
OFF DIAGONAL-	-9.06 SB28	-3.81 SB21	-3.68 SB22	-3.39 SB27	-1.85 SS18	-1.69 BB36	-1.62 SB25		
NORMAL MODE 34	OBSERVED=	0.0 CM-1	CALCULATED=	925.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	20.14 C-O6	20.02 C5C	7.50 C4OH	6.97 C3OH	5.77 C2C3	5.52 HC5C	5.42 CCHB	5.28 C2OH	5.02 C5O
FORCE CONSTANTS-	34.57 CO	26.37 CC	15.99 CCH	13.36 BCOH	7.90 CCH				
OFF DIAGONAL-	6.54 SB26	-4.26 SB27	-4.02 SB22	3.72 SS18	-3.41 SB25	-3.22 SB28	-2.89 SB21		
NORMAL MODE 35	OBSERVED=	0.0 CM-1	CALCULATED=	916.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	18.42 C3OH	16.25 C2OH	13.77 CCH	9.42 CO	8.53 CCO	5.31 OCH			
FORCE CONSTANTS-	41.89 BCOH	20.89 CC	12.37 CCH	9.42 CO	8.53 CCO				
OFF DIAGONAL-	-4.88 SB22	3.20 BB36	-2.39 SB21	-1.81 SB28					

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400									
MOLECULE 13 -6 NG=1237 BETA GLUCOSE-C1-D,-O-D5									
PAGE 2									
NORMAL MODE 36	OBSERVED=	0.0 CM-1	CALCULATED=	875.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	12.22 C4OH 19.77 CCHB		10.93 C5O 9.30 CCHA		9.82 CCH 5.30 C2C5			5.16 OCO	
FORCE CONSTANTS-	18.22 CCH 16.76 BCOH		15.22 CO 14.22 CCH		10.40 OCH 9.04 CC			5.16 OCO	
OFF DIAGONAL-	-2.68 SB28 -2.51 SB21		-2.30 SB22 -2.22 SB24						
NORMAL MODE 37	OBSERVED=	0.0 CM-1	CALCULATED=	848.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	29.10 C4CH 19.77 OC1H		16.49 CCH 9.40 C1CH		6.07 C1C2 6.01 C4C5				
FORCE CONSTANTS-	29.20 CCH 23.24 OCH		20.01 CCH 14.09 CC		11.26 CO 10.26 BCOH				
OFF DIAGONAL-	-4.85 SB28 -3.03 SB26		-2.91 SB27 -2.54 SB22		-1.86 BB29			1.86 BB39	
NORMAL MODE 38	OBSERVED=	0.0 CM-1	CALCULATED=	817.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	20.86 C4CH 17.16 OC1H		11.31 CCH 9.96 C4C5						
FORCE CONSTANTS-	25.46 OCH 20.86 CCH		18.98 CC 17.50 CCH		9.59 CO 7.59 CCO			7.23 BCOH	
OFF DIAGONAL-	-4.97 SB21 -3.72 SB22		-1.95 SB26 -1.82 SB27		-1.54 BB36				
NORMAL MODE 39	OBSERVED=	0.0 CM-1	CALCULATED=	716.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	18.64 CCO* 7.16 CCO*		6.57 OBCC 6.10 C4C5		5.42 CC5H 5.19 CC4H				
FORCE CONSTANTS-	39.47 CCO 23.68 CCH		8.79 CC 8.38 OCH						
OFF DIAGONAL-	7.77 BB43 -6.90 BB34		4.64 SB25 -4.24 BB29		3.80 SB21 -1.79 SB27			-1.58 BB41	
NORMAL MODE 40	OBSERVED=	0.0 CM-1	CALCULATED=	613.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	9.27 CCH 9.26 CCO6		6.66 O9CC 6.29 CCO6		5.08 CC3H				
FORCE CONSTANTS-	36.32 CCH 17.17 CCH		13.17 CO 9.27 CCH		6.60 CCH				
OFF DIAGONAL-	6.13 SB25 5.57 BB43		-4.55 BB34 -3.73 BB29		-3.05 SB27			2.92 SB24	2.22 SB22 -1.79 BB41 -1.53 SB21
NORMAL MODE 41	OBSERVED=	0.0 CM-1	CALCULATED=	590.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	12.07 CCO9		11.37 O7CC 9.38 CCO6		8.24 O9CC 7.43 CCO*			6.90 C4CC 5.78 C4C5 5.54 CCO8	
FORCE CONSTANTS-	63.25 CCO 23.94 CCH		12.25 OCO 8.88 CCH		8.26 CC				
OFF DIAGONAL-	-13.81 BB34 5.94 BB43		-4.95 SB21 -4.62 BB42		-3.97 BB29			2.24 SB24 -1.70 BB41	
NORMAL MODE 42	OBSERVED=	0.0 CM-1	CALCULATED=	575.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	18.29 O*CC 12.93 CCO*		5.76 C-O7 5.31 HC4C						
FORCE CONSTANTS-	47.57 CCO 18.86 CCH		12.03 CC 7.45 OCH						
OFF DIAGONAL-	-7.16 BB34 6.40 SB25		5.59 BB43 -4.05 BB29		3.87 SB22 -3.19 SB27			-1.70 SB23	
NORMAL MODE 43	OBSERVED=	0.0 CM-1	CALCULATED=	514.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	8.21 CCO* 7.30 C4C5		6.28 OBCC 5.92 C1C2		5.28 O*CC 5.15 C3C4				
FORCE CONSTANTS-	30.99 CCO 22.69 CC		17.77 CCH 17.12 CO						
OFF DIAGONAL-	-6.68 BB34 5.05 BB43		4.39 SS18 4.34 SB21		-3.57 BB29 -2.48 SB27			2.23 SB24	
NORMAL MODE 44	OBSERVED=	0.0 CM-1	CALCULATED=	452.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	11.66 CCO6 10.33 U7CC		7.44 CCH 5.97 O9CC		5.70 CCH2				
FORCE CONSTANTS-	42.24 CCO 28.14 CCH		7.2 CCH 6.29 CCH		6.63 CCH				
OFF DIAGONAL-	8.29 BB34 5.70 BB43		-5.62 BB29 3.90 SB25		-2.06 SB26				
NORMAL MODE 45	OBSERVED=	0.0 CM-1	CALCULATED=	405.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	20.30 C2C 10.90 CCO*		10.35 CCO9 10.00 C1CC		6.47 C3CC 6.22 CCO8				
FORCE CONSTANTS-	36.10 CCO 24.49 CCO		10.90 CCH 6.33 CO		5.40 CC				
OFF DIAGONAL-	4.21 SB21 3.63 SB25		-3.59 BB42 -2.48 BB41		1.75 SB23 -1.64 BB36				
NORMAL MODE 46	OBSERVED=	0.0 CM-1	CALCULATED=	379.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	16.99 U*CC 12.05 CCO*		12.92 C3CC 9.17 OBCC		7.72 CCO8 5.63 C1CC				
FORCE CONSTANTS-	53.52 CCO 19.27 CCH		12.01 CCH 5.26 CO		5.16 CC				
OFF DIAGONAL-	5.87 SB21 -4.77 BB34		3.27 BB43 -2.72 BB42		2.55 SB25 -2.12 BB29			-1.56 BB41	
NORMAL MODE 47	OBSERVED=	0.0 CM-1	CALCULATED=	341.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	24.23 U9CC 12.29 CCO7		7.60 CCO8 6.27 OCO		5.45 C2C3 5.23 O*CC 5.19 C5O*				
FORCE CONSTANTS-	62.91 CCO 10.89 CC		8.89 CCH 7.86 CO		6.27 OCO				
OFF DIAGONAL-	-7.34 BB34 6.27 SB22		-2.97 BB42 2.94 BB43		-2.71 SB25 -2.39 SB21			-1.84 BB29 -1.65 SB23	
NORMAL MODE 48	OBSERVED=	0.0 CM-1	CALCULATED=	327.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	24.51 CCO7 14.72 CCO		11.51 OBCC 6.45 CCO6		5.10 CCH1				
FORCE CONSTANTS-	36.10 CCO 18.37 CCH		14.72 CCO 6.75 CC		5.80 CCH				
OFF DIAGONAL-	-8.99 BB34 4.18 SB22		-3.62 BB29 2.85 BB43		-2.54 SB24 -1.82 SB21				
NORMAL MODE 49	OBSERVED=	0.0 CM-1	CALCULATED=	307.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	20.30 O8CC 12.05 O7CC		11.91 CCO8 11.86 CCO7		11.44 O9CC 8.01 CCO9			6.77 CCO6	
FORCE CONSTANTS-	89.05 CCO 8.31 CCH		6.79 CCH 6.42 T-OH						
OFF DIAGONAL-	-9.63 BB34 -4.86 BB42		-3.91 SB22 -1.96 SB26		1.92 BB41				
NORMAL MODE 50	OBSERVED=	0.0 CM-1	CALCULATED=	289.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	19.57 O7CC 12.34 CCO8		11.18 CCO9 9.19 CCO6		5.62 C1CC				
FORCE CONSTANTS-	56.77 CCO 20.21 CCH		10.74 CCH 6.07 CC						
OFF DIAGONAL-	-12.54 BB34 8.62 BB43		5.15 SB22 -4.40 BB29		-3.01 SB21 -2.21 SB25				
NORMAL MODE 51	OBSERVED=	0.0 CM-1	CALCULATED=	262.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	37.93 CCO* 26.41 C4CC		8.24 T-H5 6.74 O9CC		6.07 FCC5				
FORCE CONSTANTS-	50.46 CCO 28.10 CCH		10.41 T-OH 8.21 CCH		6.27 T-CC				
OFF DIAGONAL-	-6.52 BB34 -4.80 BB42		-2.55 BB33						
NORMAL MODE 52	OBSERVED=	0.0 CM-1	CALCULATED=	259.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	15.45 CCO* 8.33 CCO*		7.42 CCO9 6.92 CCO6						
FORCE CONSTANTS-	44.41 CCO 8.15 CCH		8.15 CC 5.62 CCC		5.36 T-OH				
OFF DIAGONAL-	6.19 BB43 5.85 SB22		-4.54 BB34 -2.85 SB26		-2.14 BB33 -1.82 BB29			-1.66 SB25	
NORMAL MODE 53	OBSERVED=	0.0 CM-1	CALCULATED=	166.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	TH-1 32.86 TH-2		10.82 TH-3 8.35 TH-4		5.06 TH-5				
FORCE CONSTANTS-	96.50 T-OH								
OFF DIAGONAL-	NONE								
NORMAL MODE 54	OBSERVED=	0.0 CM-1	CALCULATED=	163.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	46.85 TH-5 10.90 TH-1		11.87 CCH 7.11 C4CC						
FORCE CONSTANTS-	62.15 T-CH 9.49 CCH		7.89 CCO 7.87 CCH						
OFF DIAGONAL-	-1.57 SB21								
NORMAL MODE 55	OBSERVED=	0.0 CM-1	CALCULATED=	158.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	40.80 TH-4 21.23 TH-3		15.89 TH-5 13.52 TH-1						
FORCE CONSTANTS-	91.58 T-OH								
OFF DIAGONAL-	NONE								
NORMAL MODE 56	OBSERVED=	0.0 CM-1	CALCULATED=	155.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	55.13 TH-2 23.06 TH-1		12.05 TH-4						
FORCE CONSTANTS-	92.66 T-OH 5.86 CCO								
OFF DIAGONAL-	NONE								
NORMAL MODE 57	OBSERVED=	0.0 CM-1	CALCULATED=	151.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	90.97 TH-3 26.28 TH-4		5.48 TH-2						
FORCE CONSTANTS-	90.97 T-CH 9.23 CCO								
OFF DIAGONAL-	NONE								
NORMAL MODE 58	OBSERVED=	0.0 CM-1	CALCULATED=	132.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	16.41 TH-5 13.36 CCO*		8.53 CCO* 6.82 TH-1		6.29 CCO*			5.13 C4C	
FORCE CONSTANTS-	24.89 T-OH 21.44 CCO		13.36 CCH 8.61 CCC		8.49 T-CC 8.24 CCH 6.27 T-CC				
OFF DIAGONAL-	3.77 BB43 -1.67 BB33								
NORMAL MODE 59	OBSERVED=	0.0 CM-1	CALCULATED=	86.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	20.20 TCC5 20.19 C2CC		10.96 TCC2 8.87 C3CC		7.38 C1CC				
FORCE CONSTANTS-	40.17 T-CC 37.40 CCH		20.20 CCO 5.50 CO						
OFF DIAGONAL-	-4.88 SB25 -3.83 BB42		-3.77 SB21 2.25 BB41		-1.67 BB34				
NORMAL MODE 60	OBSERVED=	0.0 CM-1	CALCULATED=	73.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	58.93 TCC5 6.25 C2CC		5.85 CCO 5.13 CCO*						
FORCE CONSTANTS-	64.63 T-CC 12.82 CCH		12.24 CCO 5.13 CCH						
OFF DIAGONAL-	-1.55 BB42 -1.52 BB34								
NORMAL MODE 61	OBSERVED=	0.0 CM-1	CALCULATED=	68.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	12.27 TCC4 16.42 C3CC		10.86 CCH 9.18 T-CC		8.61 C1CC 6.35 TCC2 5.56 O*CC				
FORCE CONSTANTS-	32.48 T-CC 30.31 CCO		21.87 CCH 5.40 T-CC						
OFF DIAGONAL-	-3.71 BB42 -2.54 SB25		-2.01 BB34 1.85 BB41						

2. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 1.95

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400									
MOLECULE 14 -6 NC=1237 BETA GLUCOSE-6,6-N2									
PAGE 1									
NORMAL MODE 8	OBSERVED=	1413.0 CM-1	CALCULATED=	1421.6 CM-1	ERROR=	-8.6 CM-1	OR	-0.6 PERCENT	
INTERNAL COORDINATES-	32.58	C1H 17.42 OC1H	13.42 C1OH	9.00 C2OH	8.16 C1H	5.68 OC2H			
FORCE CONSTANTS-	57.26	UCH 22.57 BCOH	13.79 CCH	7.47 CO	5.27 CCO				
OFF DIAGONAL-	-9.49	SB27 3.62 SB28	2.04 BB29	-2.60 BB45	-2.52 SB25	2.38 BB34	-2.04 BB43	-1.97 BB39	
NORMAL MODE 9	OBSERVED=	1405.0 CM-1	CALCULATED=	1408.6 CM-1	ERROR=	-3.6 CM-1	OR	-0.3 PERCENT	
INTERNAL COORDINATES-	19.10	C1H 11.12 OC1H	10.76 OC4H	8.01 C2OH	7.58 OC3H	6.97 OC2H	5.44 HC4C		
FORCE CONSTANTS-	20.99	UCH 23.68 CCH	13.14 BCOH	6.11 CO					
OFF DIAGONAL-	-6.70	SB27 4.79 BB29	-3.78 SB26	-3.03 BB45	2.18 BB34	1.82 SB28	-1.67 SB25		
NORMAL MODE 10	OBSERVED=	0.0 CM-1	CALCULATED=	1406.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	23.41	C1OH 11.54 C1H	8.97 OC4H	7.33 CCH	6.22 HC4C	6.04 C2OH	5.46 C5H		
FORCE CONSTANTS-	34.54	UCH 31.33 BCOH	20.58 CCH	6.32 CO					
OFF DIAGONAL-	-3.91	BB29 -2.84 SB26	-2.75 SB27	2.43 SB28	2.21 BB34	-2.16 BB45	-1.92 SB25		
NORMAL MODE 11	OBSERVED=	0.0 CM-1	CALCULATED=	1393.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	64.91	C3OH 10.20 CC3H	7.40 CCH						
FORCE CONSTANTS-	70.67	BCOH 14.20 OCH	-2.60 SB26	-2.53 BB39					
OFF DIAGONAL-	-4.35	SB28 -3.07 SB27							
NORMAL MODE 12	OBSERVED=	0.0 CM-1	CALCULATED=	1387.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	37.81	C1OH 34.63 C2OH	8.96 OCH	5.39 CC					
FORCE CONSTANTS-	73.75	BCOH 11.30 CCH	-2.07 SB27	1.88 BB29	-1.62 BB39				
OFF DIAGONAL-	-3.29	SB28 -3.12 SB26							
NORMAL MODE 13	OBSERVED=	1375.0 CM-1	CALCULATED=	1375.8 CM-1	ERROR=	-0.8 CM-1	OR	-0.1 PERCENT	
INTERNAL COORDINATES-	85.67	C4OH							
FORCE CONSTANTS-	88.00	BCOH							
OFF DIAGONAL-	-2.77	SB28							
NORMAL MODE 14	OBSERVED=	1359.0 CM-1	CALCULATED=	1363.6 CM-1	ERROR=	-4.6 CM-1	OR	-0.3 PERCENT	
INTERNAL COORDINATES-	20.93	C2OH 13.65 C3OH	9.32 OC2H	8.62 HC2C	8.37 CC3H	5.44 OC3H			
FORCE CONSTANTS-	37.44	UCH 33.99 CCH	19.72 OCH						
OFF DIAGONAL-	-7.20	BB29 -3.68 SB27	3.47 BB34	-2.85 SB28	-2.28 BB36	-2.07 BB45	1.90 BB39		
NORMAL MODE 15	OBSERVED=	1338.0 CM-1	CALCULATED=	1331.0 CM-1	ERROR=	7.0 CM-1	OR	0.5 PERCENT	
INTERNAL COORDINATES-	19.39	HC3C 19.81 CC4H	8.55 OC2H	6.86 C5H	5.53 CC3H	5.30 CCH2	5.28 HC4C		
FORCE CONSTANTS-	59.19	CCH 25.32 OCH	9.38 BCOH						
OFF DIAGONAL-	-13.11	BB29 -5.61 SB26	-4.03 SB27	-3.67 BB45	1.79 BB34				
NORMAL MODE 16	OBSERVED=	1322.0 CM-1	CALCULATED=	1312.5 CM-1	ERROR=	9.5 CM-1	OR	0.7 PERCENT	
INTERNAL COORDINATES-	36.25	C5H 12.51 HC5C	9.95 C4OH	7.25 OC4H	6.87 CCH2	5.20 HC2C			
FORCE CONSTANTS-	46.09	UCH 36.56 CCH	9.95 COH	6.01 CO					
OFF DIAGONAL-	-4.92	SB27 -3.33 BB45	-3.07 SB26	2.59 BB29					
NORMAL MODE 17	OBSERVED=	1308.0 CM-1	CALCULATED=	1297.8 CM-1	ERROR=	10.2 CM-1	OR	0.8 PERCENT	
INTERNAL COORDINATES-	16.10	CCH2 12.12 HC2C	9.21 HC3C	8.67 OC1H	8.35 CC1H	8.13 CC3H	7.51 C5H		
FORCE CONSTANTS-	61.90	CCH 18.61 UCH	3.67 CCH						
OFF DIAGONAL-	-11.29	BB29 -7.36 SB26	2.50 SB27						
NORMAL MODE 18	OBSERVED=	1272.0 CM-1	CALCULATED=	1277.1 CM-1	ERROR=	-5.1 CM-1	OR	-0.4 PERCENT	
INTERNAL COORDINATES-	33.41	C4OH 15.08 HC5C	9.10 OC3H	8.47 CC5H					
FORCE CONSTANTS-	38.40	CCH 28.63 CCH	16.51 OCH	8.00 CO					
OFF DIAGONAL-	-2.08	SB26 -1.88 BB45	1.72 BB34						
NORMAL MODE 19	OBSERVED=	0.0 CM-1	CALCULATED=	1270.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	17.08	OC3H 2.69 OC4H	11.82 HC5C	11.15 OC2H	8.48 CC3H	8.24 CC4H	7.88 CC5H		
FORCE CONSTANTS-	42.78	UCH 41.13 CCH	8.49 CO						
OFF DIAGONAL-	-4.34	SB27 -3.46 BB45	-2.70 SB26	-2.32 BB29	-1.70 SB25				
NORMAL MODE 20	OBSERVED=	1254.0 CM-1	CALCULATED=	1261.7 CM-1	ERROR=	-7.7 CM-1	OR	-0.6 PERCENT	
INTERNAL COORDINATES-	18.80	OC4H 12.77 OC2H	9.52 OC1C	7.60 C-06	6.91 HC3C				
FORCE CONSTANTS-	34.36	UCH 27.39 CCH	23.64 CO	7.70 CCO					
OFF DIAGONAL-	-5.86	SB27 -4.82 SB25	-4.82 BB29	3.49 BB34	-2.46 BB45				
NORMAL MODE 21	OBSERVED=	1230.0 CM-1	CALCULATED=	1228.9 CM-1	ERROR=	1.1 CM-1	OR	0.1 PERCENT	
INTERNAL COORDINATES-	14.10	OC1C 11.33 C-06	8.04 OC3H	8.02 CC5H	7.90 HC2C	6.29 C4OH	5.85 CCH2	5.55 HC5C	5.07 C5O
FORCE CONSTANTS-	36.41	CCH 36.08 CO	19.82 OCH	8.49 CCO	6.25 COH				
OFF DIAGONAL-	-5.19	SB25 -4.94 BB29	3.07 BB34	-2.18 BB45	1.80 SB27				
NORMAL MODE 22	OBSERVED=	1205.0 CM-1	CALCULATED=	1198.8 CM-1	ERROR=	6.2 CM-1	OR	0.5 PERCENT	
INTERNAL COORDINATES-	17.76	C-06 32.22 CCH	8.09 OC2H	8.49 OCCH	7.67 HC4C	7.58 CC1H	6.91 CC4H		
FORCE CONSTANTS-	41.95	CCH 39.42 CCH	8.76 CCH						
OFF DIAGONAL-	-5.01	SB25 -4.81 BB29	-3.08 SB27	-3.03 SB28	-2.12 BB45	1.80 BB34			
NORMAL MODE 23	OBSERVED=	1187.0 CM-1	CALCULATED=	1176.8 CM-1	ERROR=	10.2 CM-1	OR	1.7 PERCENT	
INTERNAL COORDINATES-	39.21	CO 24.56 CCH	18.95 OCH	17.69 CCO					
FORCE CONSTANTS-	-12.18	SB25 7.51 SB27	-3.74 BB29	-2.66 SB28	2.17 BB43	2.14 BB34	1.55 BB33		
NORMAL MODE 24	OBSERVED=	1151.0 CM-1	CALCULATED=	1144.2 CM-1	ERROR=	6.8 CM-1	OR	0.5 PERCENT	
INTERNAL COORDINATES-	18.33	C5C 24.07 C4C5	11.60 C-06	8.92 CCO	7.48 CCO	6.58 C-06	6.40 C3C4		
FORCE CONSTANTS-	70.08	UCH 19.53 CCO	19.49 CO	10.11 CCH	8.15 OCH	6.56 C-06			
OFF DIAGONAL-	-16.64	SB22 -11.04 SB26	-5.08 SB27	-2.51 SS18	-2.23 SS17	-1.90 SB28	1.59 BB33		
NORMAL MODE 25	OBSERVED=	1118.0 CM-1	CALCULATED=	1120.3 CM-1	ERROR=	-2.3 CM-1	OR	-0.2 PERCENT	
INTERNAL COORDINATES-	29.53	C5O 8.84 CC4H	8.44 C5C	8.15 OC1H	7.73 HC4C	7.60 C-06	7.36 CC1H	5.77 CCH2	
FORCE CONSTANTS-	44.19	CO 43.55 CCH	14.20 OCH	11.17 CCH	9.48 CCO	5.19 C-06			
OFF DIAGONAL-	-8.67	SB27 -8.19 BB29	-5.35 SB25	-3.55 SB21	-3.49 SS18	3.47 BB34	-2.84 BB43	-2.49 SB28	-2.39 BB45
NORMAL MODE 26	OBSERVED=	1110.0 CM-1	CALCULATED=	1110.9 CM-1	ERROR=	-0.9 CM-1	OR	-0.1 PERCENT	
INTERNAL COORDINATES-	21.86	C-07 16.20 C-09	7.82 C1C2	7.41 C5O	6.15 C4C5	5.94 OC1H	5.87 CC1H		
FORCE CONSTANTS-	48.87	UCH 12.42 CCH	17.77 CCH						
OFF DIAGONAL-	-5.15	SB25 -4.54 SS18	-4.27 SB28	-3.47 BB29	0.75 BB34	1.53 SB27			
NORMAL MODE 27	OBSERVED=	1084.0 CM-1	CALCULATED=	1077.8 CM-1	ERROR=	6.2 CM-1	OR	0.6 PERCENT	
INTERNAL COORDINATES-	12.44	C3C4 2.29 C3C4	12.63 CCH	12.59 CCO	12.14 BCOH	6.30 OCH	6.02 CCC		
FORCE CONSTANTS-	64.59	UCH 30.57 CO	-6.48 SB27	-3.71 SB26	-3.44 SB25	-3.11 SB21	-2.39 SS17	-2.31 BB34	-2.30 SS18
OFF DIAGONAL-	-8.67	SB22 -6.90 SB28							
NORMAL MODE 28	OBSERVED=	1065.0 CM-1	CALCULATED=	1059.9 CM-1	ERROR=	5.1 CM-1	OR	0.5 PERCENT	
INTERNAL COORDINATES-	49.68	C-08 18.62 C2C3	13.70 C1C2	12.12 C3OH	8.72 OC3H	8.04 C3C4	7.73 C2C2	6.51 OC7CC	
FORCE CONSTANTS-	54.33	CO 41.00 CC	15.95 OCH	14.06 CCO	13.57 BCOH	10.48 CCC	9.02 CCH		
OFF DIAGONAL-	-13.46	SB27 -10.04 SB28	-8.18 SB21	-7.37 SS18	-6.37 SB25	-5.92 SB22	-3.03 BB34	-1.60 BB29	
NORMAL MODE 29	OBSERVED=	1057.0 CM-1	CALCULATED=	1053.4 CM-1	ERROR=	3.6 CM-1	OR	0.3 PERCENT	
INTERNAL COORDINATES-	31.47	C1C2 17.93 C-07	9.13 HCH	7.13 OC4H	5.87 UCHB	5.47 C-08	5.00 C4C5		
FORCE CONSTANTS-	41.84	UCH 33.32 CO	18.68 OCH	17.47 CCH	9.13 HCH	6.98 CCO			
OFF DIAGONAL-	-10.60	SB27 -7.07 SB22	-5.35 SS18	-5.03 SB21	-2.97 SB28	-2.65 BB29	-2.59 SB24	-2.58 SB26	
NORMAL MODE 30	OBSERVED=	0.0 CM-1	CALCULATED=	1035.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	40.77	HCH 17.47 C-09	6.69 C-07	6.52 C4OH	6.25 OCHA	5.31 OC8H			
FORCE CONSTANTS-	48.87	HCH 17.47 C-09	13.84 C-08	9.60 OC1C	8.19 C1C2	5.78 CCH			
OFF DIAGONAL-	-6.28	SB28 -2.51 SB21	-2.36 SS18	-2.21 SB25	-2.19 SB27	-1.80 SB22			
NORMAL MODE 31	OBSERVED=	1028.0 CM-1	CALCULATED=	1028.7 CM-1	ERROR=	-0.7 CM-1	OR	-0.1 PERCENT	
INTERNAL COORDINATES-	40.83	CO 36.01 C3C4	16.12 C4OH	14.05 CCO	11.11 OCH	8.46 CCO	8.28 CCH	5.70 HCH	
FORCE CONSTANTS-	-13.44	SB21 -10.02 SB28	-6.14 SB27	-6.06 SS18	-3.26 SB25	-3.12 SB22	-1.77 BB34	-1.53 SB24	
OFF DIAGONAL-									
NORMAL MODE 32	OBSERVED=	1018.0 CM-1	CALCULATED=	1015.6 CM-1	ERROR=	2.4 CM-1	OR	0.2 PERCENT	
INTERNAL COORDINATES-	19.39	C5C 12.78 C3C4	10.74 HCH	9.65 C-04	8.33 CCHB	8.05 C-09	7.64 CCHA	6.45 C-07	5.90 HC5C
FORCE CONSTANTS-	38.17	UCH 33.43 CO	31.78 CCH	10.76 HCH	8.25 CCO	7.34 OCH	5.24 COH		
OFF DIAGONAL-	-16.01	SB26 -6.25 SB22	-5.37 SB27	-4.96 SB28	-1.94 SB21	-1.85 BB29			
NORMAL MODE 33	OBSERVED=	1005.0 CM-1	CALCULATED=	987.8 CM-1	ERROR=	17.2 CM-1	OR	1.7 PERCENT	
INTERNAL COORDINATES-	24.82	C2C3 11.23 C1C2	9.30 C-09	8.09 C-07	7.28 C-06	6.58 CCOH	5.45 OC1C		
FORCE CONSTANTS-	39.06	UCH 33.64 CO	22.56 CCO	11.16 CCH	10.58 OCH				
OFF DIAGONAL-	-13.80	SB22 -6.67 SB21	-3.56 SB24	2.41 BB34	-2.39 SB27	-2.27 BB29	-2.15 SB26	2.13 SS18	
NORMAL MODE 34	OBSERVED=	973.0 CM-1	CALCULATED=	974.8 CM-1	ERROR=	-1.8 CM-1	OR	-0.2 PERCENT	
INTERNAL COORDINATES-	22.62	C-08 10.74 OC8H	10.29 CCHA	9.23 C1C2	5.78 CCHB	5.73 C-08			
FORCE CONSTANTS-	32.95	UCH 18.05 CCH	17.42 OCH	16.93 CCH	10.93 CCO				
OFF DIAGONAL-	-13.32	SB27 -4.79 SB26	-4.73 SB22	-4.38 SB25	-2.97 SS18	-1.96 SB28			
NORMAL MODE 35	OBSERVED=	951.0 CM-1	CALCULATED=	959.5 CM-1	ERROR=	-8.5 CM-1	OR	-0.9 PERCENT	
INTERNAL COORDINATES-	11.87	C-08 12.20 CC	9.39 CCO	8.02 OCH	8.19 C1C2	5.72 C-06			
FORCE CONSTANTS-	59.85	UCH 12.20 CC	4.46 SB22	4.22 SS18	-2.23 SB28	-2.19 SB23	-2.02 SB25		
OFF DIAGONAL-	-6.79	SB27 -6.45 SB24							

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400									
MOLECULE 14 -6 NG=1237 BETA GLUCOSE-6,6-D2									
PAGE 2									
NORMAL MODE 36	OBSERVED=	917.0 CM-1	CALCULATED=	907.3 CM-1	ERROR=	9.7 CM-1	OR	1.1 PERCENT	
INTERNAL COORDINATES-	48.14	OCH 38.15	6.25 CCHA						
FORCE CONSTANTS-	86.69	OCH 9.65							
OFF DIAGONAL-	-2.38	BB45							
NORMAL MODE 37	OBSERVED=	866.0 CM-1	CALCULATED=	876.2 CM-1	ERROR=	-10.2 CM-1	OR	-1.2 PERCENT	
INTERNAL COORDINATES-	17.86	C5C1 16.57 C-O*	9.28 C4C5	6.98 HC5C	6.11 CCHB	5.52 C-O6	5.11 OCH8		
FORCE CONSTANTS-	27.86	CC 26.18	CO 19.09	CCH 10.38	OCH 8.02	CCC 7.84	CCO		
OFF DIAGONAL-	11.76	SB26 -8.33 SB21	-7.05 SB27	-3.75 SB22	2.62 SS18	2.27 BB43	-1.54 SB24		
NORMAL MODE 38	OBSERVED=	803.0 CM-1	CALCULATED=	787.6 CM-1	ERROR=	15.3 CM-1	OR	1.9 PERCENT	
INTERNAL COORDINATES-	26.31	CCHB 11.91 C5O1	11.45 OCO	9.67 CCHA					
FORCE CONSTANTS-	36.88	CCH 14.37 CO	11.45 OCO	10.26 CCO	9.31 OCH				
OFF DIAGONAL-	3.60	SB25 2.81 BB33	2.56 BB34	-2.38 SB27	2.10 BB43	-1.99 SB23			
NORMAL MODE 39	OBSERVED=	692.0 CM-1	CALCULATED=	706.7 CM-1	ERROR=	-14.7 CM-1	OR	-2.1 PERCENT	5.00 C4C5
INTERNAL COORDINATES-	15.15	CCO* 11.08 CCHA	9.71 OBCC	7.75 C5H	7.04 C4CC	6.55 CC4H	5.93 HC3C	5.41 OTCC	
FORCE CONSTANTS-	39.22	CCO 38.94 CCH	7.42 CC	8.91					
OFF DIAGONAL-	-10.06	BB34 8.66 BB43	-5.85 BB29	3.79 SB21	3.57 SB25	-1.66 BB41			
NORMAL MODE 40	OBSERVED=	627.0 CM-1	CALCULATED=	617.8 CM-1	ERROR=	9.2 CM-1	OR	1.5 PERCENT	
INTERNAL COORDINATES-	17.46	C2CC 8.13 CC3H	7.99 CC2C	7.78	7.59 CD4C	6.34 CCO8			
FORCE CONSTANTS-	50.51	CCO 26.69 CCH	9.22 CO	7.59 COC					
OFF DIAGONAL-	-10.26	BB34 7.53 BB43	6.26 SB25	-5.98 BB29	-1.97 SB27	-1.66 BB41			
NORMAL MODE 41	OBSERVED=	592.0 CM-1	CALCULATED=	584.1 CM-1	ERROR=	7.9 CM-1	OR	1.3 PERCENT	
INTERNAL COORDINATES-	18.77	O1CC 11.81 4CO1	5.60 OTCC	5.07 HC2C					
FORCE CONSTANTS-	51.20	CCO 21.34 CCH	11.24 CO	7.20 CC					
OFF DIAGONAL-	-9.99	BB34 4.61 BB43	-4.42 BB29	3.91 SB22	3.72 SB25	-2.45 SB21	-1.96 BB41	-1.61 BB42	-1.57 SB27
NORMAL MODE 42	OBSERVED=	575.0 CM-1	CALCULATED=	566.8 CM-1	ERROR=	8.1 CM-1	OR	1.4 PERCENT	
INTERNAL COORDINATES-	10.46	OCO 10.42 CCHB	9.19 O9CC	7.85 O1C1	7.44 CCHA	5.70 CCO7			
FORCE CONSTANTS-	36.46	CCO 22.29 CCH	14.02 CO	10.46 OCO	7.07 CC	5.19 CCC	5.11 OCH		
OFF DIAGONAL-	5.56	SB24 -4.82 BB34	3.65 BB43	-3.36 SB27	2.94 SB22	-2.84 SB21	-2.15 BB42	-1.77 BB33	
NORMAL MODE 43	OBSERVED=	510.0 CM-1	CALCULATED=	514.9 CM-1	ERROR=	-4.9 CM-1	OR	-1.0 PERCENT	
INTERNAL COORDINATES-	10.80	CCO* 9.66 C4C5	6.27 OBCC	5.70 CCH2	5.26 C3C4				
FORCE CONSTANTS-	36.44	CCO 22.31 CC	21.78 CCH	13.24 CO					
OFF DIAGONAL-	-7.75	BB34 5.66 BB43	3.62 SS18	-3.53 BB29	3.37 SB21				
NORMAL MODE 44	OBSERVED=	458.0 CM-1	CALCULATED=	458.4 CM-1	ERROR=	-0.4 CM-1	OR	-0.1 PERCENT	
INTERNAL COORDINATES-	19.13	OTCC 9.73 CC06	5.57 CC1H	5.42 O9CC					
FORCE CONSTANTS-	27.46	CCO 23.54 CCH	10.34 CC	8.95					
OFF DIAGONAL-	-7.49	BB34 5.59 BB43	-5.11 BB29	3.73 SB25	-2.01 SB26	1.64 SS18	-1.63 SB27		
NORMAL MODE 45	OBSERVED=	418.0 CM-1	CALCULATED=	413.0 CM-1	ERROR=	5.0 CM-1	OR	1.2 PERCENT	
INTERNAL COORDINATES-	12.42	C2CC 12.18 CO1C	7.39 CC09	9.18 C1CC	6.90 C3CC				
FORCE CONSTANTS-	36.90	CCO 19.76 CCO	12.18 COC	6.93 CO	5.84 CC				
OFF DIAGONAL-	3.96	SB21 -3.00 BB42	2.95 SB25	-2.29 BB41	2.04 BB43	1.87 SB23			
NORMAL MODE 46	OBSERVED=	397.0 CM-1	CALCULATED=	395.4 CM-1	ERROR=	11.6 CM-1	OR	2.9 PERCENT	
INTERNAL COORDINATES-	17.18	4CCO 16.36 C1CC	12.02 C3CC	9.74 OBCC	6.58 C1CC				
FORCE CONSTANTS-	54.50	CCO 19.79 CCH	11.76 CCH	5.44 CO					
OFF DIAGONAL-	6.19	SB21 -5.18 BB34	3.23 BB43	2.80 SB25	-2.76 BB42	-1.79 BB29	-1.73 BB41		
NORMAL MODE 47	OBSERVED=	0.0 CM-1	CALCULATED=	346.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	26.29	O9CC 13.79 CCU7	9.80 CC08	5.06 C5O1					
FORCE CONSTANTS-	86.53	CCO 20.03 CCH	9.08 CC	7.75 CO					
OFF DIAGONAL-	-8.21	BB34 5.31 SB22	-3.11 SB25	2.73 BB43	-2.72 BB42	-2.16 SB21	-2.15 BB29		
NORMAL MODE 48	OBSERVED=	319.0 CM-1	CALCULATED=	332.9 CM-1	ERROR=	-13.9 CM-1	OR	-4.3 PERCENT	
INTERNAL COORDINATES-	20.81	CCO7 16.00 CCU	9.84 OBCC	7.75 CC06					
FORCE CONSTANTS-	51.59	CCO 16.00 OCO	14.49 CCH	8.15 T-OH	7.72 CC	6.06 CCC			
OFF DIAGONAL-	-7.48	BB34 4.48 SB22	-2.77 BB29	-2.35 SB24	2.32 BB43	-1.78 BB42	-1.71 SB21		
NORMAL MODE 49	OBSERVED=	310.0 CM-1	CALCULATED=	313.0 CM-1	ERROR=	-3.0 CM-1	OR	-1.0 PERCENT	3.30 TH-3
INTERNAL COORDINATES-	21.42	OBCC 12.19 OTCC	10.82 O9CC	10.69 CC08	9.71 CC07	5.92 CC09	5.70 CC06	5.67 TH-3	
FORCE CONSTANTS-	82.98	CCO 12.37 T-OH	7.78 CCH	6.57 CCC					
OFF DIAGONAL-	-9.07	BB34 -4.39 BB42	-3.34 SB22	1.67 BB41	-1.61 SB26				
NORMAL MODE 50	OBSERVED=	0.0 CM-1	CALCULATED=	297.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	20.16	OTCC 12.72 CC08	12.07 CC09	10.13 CC06	5.28 CC3H				
FORCE CONSTANTS-	58.46	CCO 19.67 CCH	8.40 CCC	5.72 T-OH	5.47 CC				
OFF DIAGONAL-	-12.71	BB34 8.40 BB43	4.86 SB22	-4.24 BB29	-2.65 SB21	-2.35 SB25			
NORMAL MODE 51	OBSERVED=	268.0 CM-1	CALCULATED=	267.9 CM-1	ERROR=	0.1 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	15.86	TH-5 12.26 CCU*	6.77 CC01	6.52 CC06	5.01 CO1C				
FORCE CONSTANTS-	41.60	CCO 24.24 T-OH	10.67 CCH	6.45 CC	5.01 COC				
OFF DIAGONAL-	5.63	SB22 4.58 BB43	-4.09 BB34	-2.25 SB26	-2.14 BB33	-1.61 BB29			
NORMAL MODE 52	OBSERVED=	250.0 CM-1	CALCULATED=	247.9 CM-1	ERROR=	2.1 CM-1	OR	0.8 PERCENT	
INTERNAL COORDINATES-	27.11	TH-5 15.57 C4CC	15.05 CC01	13.39 TH-4	5.10 TH-3				
FORCE CONSTANTS-	58.32	T-OH 20.33 CCO	16.05 CC						
OFF DIAGONAL-	-3.24	BB34 2.28 SB21	-2.14 BB42						
NORMAL MODE 53	OBSERVED=	0.0 CM-1	CALCULATED=	226.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	27.11	TH-1 34.60 TH-2	16.77 TH-5	6.08 TH-3					
FORCE CONSTANTS-	95.44	T-OH							
OFF DIAGONAL-	NONE								
NORMAL MODE 54	OBSERVED=	0.0 CM-1	CALCULATED=	216.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	41.98	TH-1 21.60 TH-3	10.77 TH-2	9.69 TH-4					
FORCE CONSTANTS-	84.10	T-OH 9.01 CCO							
OFF DIAGONAL-	NONE								
NORMAL MODE 55	OBSERVED=	0.0 CM-1	CALCULATED=	214.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	36.53	TH-2 34.32 TH-4							
FORCE CONSTANTS-	81.98	T-OH 11.85 CCO							
OFF DIAGONAL-	NONE								
NORMAL MODE 56	OBSERVED=	0.0 CM-1	CALCULATED=	210.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	49.78	TH-3 25.00 TH-4	6.69 TH-2	5.82 CC08					
FORCE CONSTANTS-	83.10	T-OH 17.47 CCO							
OFF DIAGONAL-	-2.10	BB34							
NORMAL MODE 57	OBSERVED=	0.0 CM-1	CALCULATED=	198.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	31.40	TH-5 22.36 CCO*	9.57 TH-4	9.51 TH-3					
FORCE CONSTANTS-	39.12	T-OH 29.78 CCO	22.02 CCC	10.07 CCH					
OFF DIAGONAL-	-4.86	BB34 -3.22 BB42	-2.61 BB33						
NORMAL MODE 58	OBSERVED=	0.0 CM-1	CALCULATED=	141.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	19.09	CO1C 9.00 C4CC	8.15 TCC4	7.75 CCO1	6.36 CCO*	6.02 TCO1	5.45 OCO		
FORCE CONSTANTS-	25.13	CCO 19.09 COC	14.15 CCC	10.01 T-CC	9.51 T-CC	8.45 CCH	5.45 OCO		
OFF DIAGONAL-	4.49	BB43 -1.96 SB25	1.68 BB41	-1.56 BB33					
NORMAL MODE 59	OBSERVED=	0.0 CM-1	CALCULATED=	89.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	21.87	C2CC 16.98 TCC5	11.44 TCC2	9.45 C3CC	8.35 C1CC				
FORCE CONSTANTS-	40.31	CCO 38.30 T-CC	20.86 CCO	9.74 CO					
OFF DIAGONAL-	-5.31	SB25 -4.38 SB21	-4.08 BB42	2.46 BB41	-1.62 BB34	-1.54 SB27	1.52 SB22		
NORMAL MODE 60	OBSERVED=	0.0 CM-1	CALCULATED=	72.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	64.17	TCC5 5.39 CCO1	5.05 CO1C						
FORCE CONSTANTS-	63.39	T-CC 11.59 CCO	9.59 CCC	5.05 COC					
OFF DIAGONAL-	NONE								
NORMAL MODE 61	OBSERVED=	0.0 CM-1	CALCULATED=	70.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	5.20 TCC5
INTERNAL COORDINATES-	15.56	C3CC 14.62 TCC4	9.57 TH-4	9.18 TCC3	7.62 C1CC	7.03 TCC2	5.46 O1CC	5.27 C4CC	
FORCE CONSTANTS-	37.16	T-CC 29.22 CCO	28.54 CCC	5.20 T-CC					
OFF DIAGONAL-	-3.68	BB42 -2.55 SB25	-1.86 BB34	1.85 BB41					

38, EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 6.81

PAGE 1

NORMAL MODE 8	OBSERVED=	1210.0 CM-1	CALCULATED=	1416.5 CM-1	ERROR=	-6.5 CM-1	OR	-0.5 PERCENT
INTERNAL COORDINATES-	50.70	OC1H 28.98	OC1H	10.51 CC1H				
FORCE CONSTANTS-	92.23	UCH 13.27	CCM					
OFF DIAGONAL-	-7.84	SB27 -3.90	BB45	2.09 BB29	-1.69	BB43		
NORMAL MODE 9	OBSERVED=	1400.0 CM-1	CALCULATED=	1404.3 CM-1	ERROR=	-4.3 CM-1	OR	-0.3 PERCENT
INTERNAL COORDINATES-	21.42	OC4H 12.35	CC5H	11.88 HC4C	11.01 OC3H	8.81 HC3C	5.41 C-09	
FORCE CONSTANTS-	44.21	UCH 42.67	CCM	10.43				
OFF DIAGONAL-	-10.27	SB27 9.56	BB29	5.11 BB34	-4.30	SB26	-3.47	SB25 -3.40 BB45
NORMAL MODE 10	OBSERVED=	0.0 CM-1	CALCULATED=	1378.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	22.50	OC2H 12.50	HC2C	10.71 CC3H	7.91 HC4C	7.58		
FORCE CONSTANTS-	46.04	UCH 42.78	CCM	-4.81	SB27	4.01	BB34	-3.58 BB45 -3.11 SB25
OFF DIAGONAL-	-12.11	BB29 -						
NORMAL MODE 11	OBSERVED=	0.0 CM-1	CALCULATED=	1340.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	22.50	OC2H 12.50	HC2C	10.71 CC3H	7.91 HC4C	7.58		
FORCE CONSTANTS-	46.04	UCH 42.78	CCM	-4.81	SB27	4.01	BB34	-3.58 BB45 -3.11 SB25
OFF DIAGONAL-	-12.11	BB29 -						
NORMAL MODE 12	OBSERVED=	0.0 CM-1	CALCULATED=	1313.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	22.50	OC2H 12.50	HC2C	10.71 CC3H	7.91 HC4C	7.58		
FORCE CONSTANTS-	46.04	UCH 42.78	CCM	-4.81	SB27	4.01	BB34	-3.58 BB45 -3.11 SB25
OFF DIAGONAL-	-12.11	BB29 -						
NORMAL MODE 13	OBSERVED=	0.0 CM-1	CALCULATED=	1300.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	22.50	OC2H 12.50	HC2C	10.71 CC3H	7.91 HC4C	7.58		
FORCE CONSTANTS-	46.04	UCH 42.78	CCM	-4.81	SB27	4.01	BB34	-3.58 BB45 -3.11 SB25
OFF DIAGONAL-	-12.11	BB29 -						
NORMAL MODE 14	OBSERVED=	0.0 CM-1	CALCULATED=	1276.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	22.50	OC2H 12.50	HC2C	10.71 CC3H	7.91 HC4C	7.58		
FORCE CONSTANTS-	46.04	UCH 42.78	CCM	-4.81	SB27	4.01	BB34	-3.58 BB45 -3.11 SB25
OFF DIAGONAL-	-12.11	BB29 -						
NORMAL MODE 15	OBSERVED=	0.0 CM-1	CALCULATED=	1266.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	22.50	OC2H 12.50	HC2C	10.71 CC3H	7.91 HC4C	7.58		
FORCE CONSTANTS-	46.04	UCH 42.78	CCM	-4.81	SB27	4.01	BB34	-3.58 BB45 -3.11 SB25
OFF DIAGONAL-	-12.11	BB29 -						
NORMAL MODE 16	OBSERVED=	0.0 CM-1	CALCULATED=	1245.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	22.50	OC2H 12.50	HC2C	10.71 CC3H	7.91 HC4C	7.58		
FORCE CONSTANTS-	46.04	UCH 42.78	CCM	-4.81	SB27	4.01	BB34	-3.58 BB45 -3.11 SB25
OFF DIAGONAL-	-12.11	BB29 -						
NORMAL MODE 17	OBSERVED=	0.0 CM-1	CALCULATED=	1216.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	22.50	OC2H 12.50	HC2C	10.71 CC3H	7.91 HC4C	7.58		
FORCE CONSTANTS-	46.04	UCH 42.78	CCM	-4.81	SB27	4.01	BB34	-3.58 BB45 -3.11 SB25
OFF DIAGONAL-	-12.11	BB29 -						
NORMAL MODE 18	OBSERVED=	0.0 CM-1	CALCULATED=	1191.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	22.50	OC2H 12.50	HC2C	10.71 CC3H	7.91 HC4C	7.58		
FORCE CONSTANTS-	46.04	UCH 42.78	CCM	-4.81	SB27	4.01	BB34	-3.58 BB45 -3.11 SB25
OFF DIAGONAL-	-12.11	BB29 -						
NORMAL MODE 19	OBSERVED=	0.0 CM-1	CALCULATED=	1164.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	22.50	OC2H 12.50	HC2C	10.71 CC3H	7.91 HC4C	7.58		
FORCE CONSTANTS-	46.04	UCH 42.78	CCM	-4.81	SB27	4.01	BB34	-3.58 BB45 -3.11 SB25
OFF DIAGONAL-	-12.11	BB29 -						
NORMAL MODE 20	OBSERVED=	0.0 CM-						

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400									
MOLECULE 15 -6 NG=1237 BETA GLUCOSE-C6,6-D2,-O-D5									
PAGE 2									
NORMAL MODE 36	OBSERVED=	0.0 CM-1	CALCULATED=	876.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	57.22	OCCH 22.76	OCBH 15.70	C*OH 6.57	CCHA 6.36	CCBH 5.27	C5C*		
FORCE CONSTANTS-	51.22	OCCH 16.19	OCBH 13.52	CCH 7.54	CO 7.24	CC			
OFF DIAGONAL-	-2.16	BB45 -1.68	SB22						
NORMAL MODE 37	OBSERVED=	0.0 CM-1	CALCULATED=	835.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	47.72	C4CH 11.89	C4C5 8.89	C5C* 5.41	C-O* 8.49	CCH 7.23	CCC 6.58	OCCH 6.57	CCO
FORCE CONSTANTS-	47.72	COH 24.17	CC 11.03	CO 8.49	CCH 7.23	CCC 6.58	OCCH 6.57	CCO	
OFF DIAGONAL-	-9.17	SB21 -5.53	SB28	3.80	SB26 -3.58	SB27 -2.88	SB22 -2.54	BB36	
NORMAL MODE 38	OBSERVED=	0.0 CM-1	CALCULATED=	775.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	21.77	CCBH 11.22	OCO 10.04	C5O* 5.96	OCCH 5.78	C*OH 5.64	CCO* 5.40	CCHA	
FORCE CONSTANTS-	28.03	CCH 13.15	UCH 13.00	CO 11.41	CCO 11.22	OCO 6.50	BCOH		
OFF DIAGONAL-	4.16	SB25 2.99	BB33	2.43	BB34	2.21	BB43		
NORMAL MODE 39	OBSERVED=	0.0 CM-1	CALCULATED=	700.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	13.71	CCO* 11.34	CCHA 10.54	OBCC 7.08	CCO 6.78	C4CC 6.11	CC4H 5.84	C4C5 5.76	HC3C 5.66
FORCE CONSTANTS-	38.16	CCO 37.16	CCH 8.05	CC 7.21	CCC 3.04	SB25 -1.59	BB41		
OFF DIAGONAL-	-9.60	BB34 7.95	BB43	-5.36	BB29	3.99	SB21		
NORMAL MODE 40	OBSERVED=	0.0 CM-1	CALCULATED=	612.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	16.48	CCO6 7.78	CU*C 7.40	CC3H 7.36	CCO9 7.21	HC2C 5.71	CCO8		
FORCE CONSTANTS-	47.92	CCO 25.39	CCH 8.97	CO 7.78	COC				
OFF DIAGONAL-	-9.38	BB34 7.32	BB43	6.22	SB25 -5.66	BB29 -2.15	SB27 -1.56	BB41	
NORMAL MODE 41	OBSERVED=	0.0 CM-1	CALCULATED=	579.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	18.77	O*CC 11.66	4CO* 5.37	O7CC 5.24	CCO8 5.13	HC2C 5.02	CO*C 5.00	C-O7	
FORCE CONSTANTS-	50.10	CCO 20.08	CCH 10.94	CO 7.67	CC 5.02	COC			
OFF DIAGONAL-	-9.10	BB34 4.48	SB25	4.48	BB43	-4.24	BB29		
NORMAL MODE 42	OBSERVED=	0.0 CM-1	CALCULATED=	562.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	10.69	OCO 10.58	CCBH 8.92	O9CC 8.16	CCHA 7.03	O*CC 5.86	CCO7 5.16	CCO6	
FORCE CONSTANTS-	38.89	CCO 23.06	CCH 12.15	CO 10.69	OCO 7.65	CC 5.40	CCC		
OFF DIAGONAL-	-5.50	BB34 5.17	SB24	3.40	BB43	-3.27	SB21		
NORMAL MODE 43	OBSERVED=	0.0 CM-1	CALCULATED=	511.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	11.69	CCO* 8.98	C4C5 6.24	OBCC 5.70	CCH2 5.11	C3C4 5.00	4CO*		
FORCE CONSTANTS-	37.39	CCO 22.08	CCC 21.46	CCH 5.65	CO 5.11	CCC			
OFF DIAGONAL-	-7.91	BB34 5.57	BB43	3.68	SB21	3.53	SS18		
NORMAL MODE 44	OBSERVED=	0.0 CM-1	CALCULATED=	456.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	10.01	O7CC 9.97	CCO6 8.82	CCCH 5.08	O9CC 5.23	CCCH 5.15	CCO9		
FORCE CONSTANTS-	62.93	CCO 24.43	CCH 10.73	CO 7.89	CCO 6.76	CCC			
OFF DIAGONAL-	-7.73	BB34 5.44	BB43	-5.08	BB29	3.94	SB25		
NORMAL MODE 45	OBSERVED=	0.0 CM-1	CALCULATED=	406.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	20.74	C2CC 11.08	CO*C 10.32	C1CC 9.98	CCO9 6.44	C3CC			
FORCE CONSTANTS-	37.78	CCC 22.52	CCO 11.08	COC 6.31	CO 5.49	CC			
OFF DIAGONAL-	4.06	SB21 -3.46	BB42	3.11	SB25 -2.43	BB41	1.72	SB23	
NORMAL MODE 46	OBSERVED=	0.0 CM-1	CALCULATED=	379.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	17.04	O*CC 14.71	4CO* 12.01	C3CC 11.46	OBCC 5.39	C1CC 5.35	CCO8		
FORCE CONSTANTS-	55.43	CCO 18.92	CCC 11.38	CCH 5.15	CC 5.09	CO			
OFF DIAGONAL-	6.19	SB21 -4.98	BB34	2.94	BB43	-2.85	BB42		
NORMAL MODE 47	OBSERVED=	0.0 CM-1	CALCULATED=	343.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	24.87	O9CC 13.97	CCO7 10.94	CCO8 8.96	OBCC 7.01	CCO6			
FORCE CONSTANTS-	62.93	CCO 9.88	CCH 16.33	OCO 7.37	CC 6.49	CCC			
OFF DIAGONAL-	-8.01	BB34 5.61	SB22	-3.15	SB25	2.79	BB43		
NORMAL MODE 48	OBSERVED=	0.0 CM-1	CALCULATED=	328.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	53.45	CCO 16.46	CCH 16.33	OCO 7.37	CC 6.49	CCC			
FORCE CONSTANTS-	62.93	CCO 9.88	CCH 16.33	OCO 7.37	CC 6.49	CCC			
OFF DIAGONAL-	-8.37	BB34 4.17	SB22	-3.23	BB29	2.86	BB43		
NORMAL MODE 49	OBSERVED=	0.0 CM-1	CALCULATED=	306.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	21.91	O8CC 12.34	O9CC 11.86	O7CC 11.76	CCO8 9.98	CCO7 7.98	CCO9 6.03	CCO6 5.31	C3CC
FORCE CONSTANTS-	88.49	CCO 8.30	CCH 7.33	CCC 6.26	T-OH 1.84	BB41	-1.83	SB26	
OFF DIAGONAL-	-9.66	BB34 -4.77	BB42	-3.80	SB22	1.84	BB41		
NORMAL MODE 50	OBSERVED=	0.0 CM-1	CALCULATED=	290.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	19.63	O7CC 12.18	CCO9 11.73	CCO8 9.98	CCO6 5.70	C1CC			
FORCE CONSTANTS-	58.40	CCO 18.44	CCH 10.44	CCC 5.54	CC				
OFF DIAGONAL-	-12.16	BB34 8.12	BB43	5.20	SB22	-3.86	BB29		
NORMAL MODE 51	OBSERVED=	0.0 CM-1	CALCULATED=	260.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	15.29	CCO* 8.16	CCO6 7.35	CO*C 6.43	CCO9 6.44	T-OH			
FORCE CONSTANTS-	47.74	CCO 12.09	CCC 8.33	CCH 7.35	COC				
OFF DIAGONAL-	6.68	SB22 5.77	BB43	-4.55	BB34	-2.73	SB26		
NORMAL MODE 52	OBSERVED=	0.0 CM-1	CALCULATED=	231.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	35.76	CCO 7.89	C4CC 15.67	T-OH 5.44	CCHA 5.15	TCC			
FORCE CONSTANTS-	43.91	CCO 28.90	CCC 10.66	CCH 10.66	CCH 5.54	T-OH			
OFF DIAGONAL-	-6.84	BB34 -4.55	BB42	-3.01	BB33	1.58	SB21		
NORMAL MODE 53	OBSERVED=	0.0 CM-1	CALCULATED=	166.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	33.84	TH-3 32.68	TH-2 12.98	TH-5 10.05	TH-3 7.15	TH-4			
FORCE CONSTANTS-	96.70	T-OH							
OFF DIAGONAL-	NONE								
NORMAL MODE 54	OBSERVED=	0.0 CM-1	CALCULATED=	162.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	24.95	TH-5 22.78	TH-1 9.15	TH-4 7.31	C4CC 7.28	CO*C			
FORCE CONSTANTS-	60.66	T-OH 9.88	CCC 9.29	CCO 7.28	COC				
OFF DIAGONAL-	-1.67	SB21							
NORMAL MODE 55	OBSERVED=	0.0 CM-1	CALCULATED=	156.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	29.76	TH-4 25.74	TH-5 22.27	TH-3 7.20	TH-1				
FORCE CONSTANTS-	85.42	T-OH 5.68	CCC						
OFF DIAGONAL-	NONE								
NORMAL MODE 56	OBSERVED=	0.0 CM-1	CALCULATED=	155.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	54.36	TH-2 21.85	TH-1 15.09	TH-4					
FORCE CONSTANTS-	92.57	T-OH 5.98	CCC						
OFF DIAGONAL-	NONE								
NORMAL MODE 57	OBSERVED=	0.0 CM-1	CALCULATED=	151.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	30.93	TH-3 28.16	TH-4 9.27	TH-2 5.27	TH-2				
FORCE CONSTANTS-	90.93	T-OH 9.27	CCC						
OFF DIAGONAL-	NONE								
NORMAL MODE 58	OBSERVED=	0.0 CM-1	CALCULATED=	132.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	17.55	TH-5 12.90	CO*C 9.31	CCO* 7.36	TH-1 6.31	CCO* 5.46	TCC4		
FORCE CONSTANTS-	26.46	T-OH 22.04	CCO 12.90	COC 8.44	CCH 8.38	T-CC 7.60	CCC 5.95	T-CO	
OFF DIAGONAL-	3.71	BB43 -1.78	BB33						
NORMAL MODE 59	OBSERVED=	0.0 CM-1	CALCULATED=	86.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	21.55	C2CC 16.36	TCC5 11.51	TCC2 9.48	C3CC 8.09	C1CC			
FORCE CONSTANTS-	39.76	CCC 37.56	T-CC 20.84	CCO 5.72	CO				
OFF DIAGONAL-	-5.23	SB25 -4.11	SB21	-4.04	BB42	-1.62	BB34		
NORMAL MODE 60	OBSERVED=	0.0 CM-1	CALCULATED=	70.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	63.18	TCC5 5.55	CCO* 9.75	CCC					
FORCE CONSTANTS-	68.89	T-CC 11.72	CCO						
OFF DIAGONAL-	-1.53	BB34							
NORMAL MODE 61	OBSERVED=	0.0 CM-1	CALCULATED=	68.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	37.09	C3CC 14.40	TCC4 9.75	4CO* 9.72	C1CC 6.80	TCC2 5.45	O*CC 5.27	TCC5 5.01	C4CC
FORCE CONSTANTS-	37.09	T-CC 28.97	CCO 27.84	CCC					
OFF DIAGONAL-	-3.63	BB42 -2.48	SB25	-1.83	BB34	1.82	BB41		

2. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 5.44

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400									
MOLECULE 16 -6 NG-1237 BETA GLUCOSE-C-07									
PAGE 1									
NORMAL MODE 8	OBSERVED=	0.0 CM-1	CALCULATED=	1399.7 CM-1	ERROR=	0.0 CM-1	DR	0.0 PERCENT	
INTERNAL COORDINATES-	38.35 C2OH 37.29 C1OH								
FORCE CONSTANTS-	77.81 CCH 5.88 CCH			5.40 CCO					
OFF DIAGONAL-	6.64 SB28 2.65 BB35			-1.80 SB25	-1.65 SB27 -1.54 SB22				
NORMAL MODE 9	OBSERVED=	0.0 CM-1	CALCULATED=	1384.4 CM-1	ERROR=	0.0 CM-1	DR	0.0 PERCENT	
INTERNAL COORDINATES-	40.39 C3OH 14.69 C1OH								
FORCE CONSTANTS-	85.69 CCH 8.00 CCH								
OFF DIAGONAL-	4.54 SB28								
NORMAL MODE 10	OBSERVED=	0.0 CM-1	CALCULATED=	1381.2 CM-1	ERROR=	0.0 CM-1	DR	0.0 PERCENT	
INTERNAL COORDINATES-	41.21 C2OH 13.19 C1OH			14.33 C3OH					
FORCE CONSTANTS-	89.20 CCH 5.55 CCH								
OFF DIAGONAL-	3.85 SB28								
NORMAL MODE 11	OBSERVED=	0.0 CM-1	CALCULATED=	1374.6 CM-1	ERROR=	0.0 CM-1	DR	0.0 PERCENT	
INTERNAL COORDINATES-	92.18 C*CH								
FORCE CONSTANTS-	92.79 CCH								
OFF DIAGONAL-	2.11 SB28								
NORMAL MODE 12	OBSERVED=	0.0 CM-1	CALCULATED=	1296.2 CM-1	ERROR=	0.0 CM-1	DR	0.0 PERCENT	
INTERNAL COORDINATES-	48.33 C4OH 12.91 C4C5			12.58 C-CO9 8.04 C*CH					
FORCE CONSTANTS-	40.39 CCH 10.38 CCH			14.61 C5OH 7.09 CCH	6.64 CCH	5.88 CCO			
OFF DIAGONAL-	10.36 SB28 -5.21 SB26			-5.02 SB27 -3.84 SB21 -3.74 SB25	-2.93 SS18 2.88 BB36 -1.70 BB39 1.63 SB22				
NORMAL MODE 13	OBSERVED=	0.0 CM-1	CALCULATED=	1248.0 CM-1	ERROR=	0.0 CM-1	DR	0.0 PERCENT	
INTERNAL COORDINATES-	51.86 D*CI 19.57 C-C6			12.25 CCH 12.14 CCH	7.85 C1OH 6.27 CCO6				
FORCE CONSTANTS-	91.19 CCH 16.34 CCO			-6.65 SB28 -2.01 BB35 -1.72 SS19 -1.67 BB43 -1.60 SS20					
OFF DIAGONAL-	-15.85 SB27 -13.38 SB25								
NORMAL MODE 14	OBSERVED=	0.0 CM-1	CALCULATED=	1200.7 CM-1	ERROR=	0.0 CM-1	DR	0.0 PERCENT	
INTERNAL COORDINATES-	15.24 C4CH 10.71 C5O*			10.46 C-CO8 10.03 C-CO7 8.54 C-CO9 5.95 C9CC					
FORCE CONSTANTS-	45.15 CCH 23.47 CCH			20.22 CCH 15.24 CCH 7.71 CCH 5.95 CCH					
OFF DIAGONAL-	-14.27 SB25 -9.81 SB28			-7.95 SB27 6.19 BB34 4.61 BB29 -3.73 SB26	-2.60 BB35 -2.16 SS18 1.58 SB22				
NORMAL MODE 15	OBSERVED=	0.0 CM-1	CALCULATED=	1174.1 CM-1	ERROR=	0.0 CM-1	DR	0.0 PERCENT	
INTERNAL COORDINATES-	25.52 C5O* 16.16 C-CO8			12.65 C-CO6 6.79 C-CO7 5.27 HC5C 5.08 C5CH					
FORCE CONSTANTS-	66.72 CCH 20.83 CCH			12.79 CCH 9.64 CCO 7.30 CCH 5.36 CCH					
OFF DIAGONAL-	-14.25 SB27 -10.18 SB25			-3.10 SB28 -3.66 SB26 -3.19 SS18 2.62 BB29 2.55 BB34 1.54 BB33					
NORMAL MODE 16	OBSERVED=	0.0 CM-1	CALCULATED=	1154.3 CM-1	ERROR=	0.0 CM-1	DR	0.0 PERCENT	
INTERNAL COORDINATES-	28.25 C3C4 25.51 C4C5			13.81 C5C* 8.94 C2C3 7.71 HC3C 6.57 CC4H 6.18 CCO*	6.10 C-CO9 5.69 C-CO7				
FORCE CONSTANTS-	76.84 CCH 26.22 CCH			20.25 CCO 17.78 CCO					
OFF DIAGONAL-	-21.72 SB26 -13.74 SB22			-4.69 BB29 -3.71 SB25 -3.15 SB27 -3.07 BB43 -3.02 SS17 -2.64 SS18 -2.52 SB28					
NORMAL MODE 17	OBSERVED=	0.0 CM-1	CALCULATED=	1135.9 CM-1	ERROR=	0.0 CM-1	DR	0.0 PERCENT	
INTERNAL COORDINATES-	26.81 C-CO 22.67 C5C*			8.86 C4C5 6.24 CCO	6.11 C2C3 5.03 C-CO1				
FORCE CONSTANTS-	40.39 CCH 10.38 CCH			21.09 CCH 17.45 CCH	7.88 CCH				
OFF DIAGONAL-	-12.18 SB26 -7.00 SB28			-6.92 SB22 -4.95 SB27 -4.85 SB25	-3.59 SS18 2.59 BB29 -2.45 BB43 1.82 BB34				
NORMAL MODE 18	OBSERVED=	0.0 CM-1	CALCULATED=	1124.5 CM-1	ERROR=	0.0 CM-1	DR	0.0 PERCENT	
INTERNAL COORDINATES-	51.16 C-CO* 16.15 CCHB			14.25 CCH 10.22 CCH 8.83 HC5C 6.39 CCH	6.20 C5C* 5.10 C4C5				
FORCE CONSTANTS-	58.16 CCH 30.88 CCH			27.59 CCH 11.85 CCH 6.39 CCH					
OFF DIAGONAL-	-27.98 SB27 -6.51 SB28			-4.79 SB26 -3.97 SS18 -3.85 SB25	-3.49 SB21 -2.20 BB45				
NORMAL MODE 19	OBSERVED=	0.0 CM-1	CALCULATED=	1104.0 CM-1	ERROR=	0.0 CM-1	DR	0.0 PERCENT	
INTERNAL COORDINATES-	34.27 C1C2 18.19 C2C3			16.48 C-CO8 11.85 CCH2 9.30 C-CO7 7.52 C-CO6 7.46 HC2C 6.16 C4OH 6.07 C-CO9					
FORCE CONSTANTS-	55.57 CCH 42.72 CCH			26.37 CCH 14.30 CCH 6.50 CCH 6.16 CCH 5.60 CCH					
OFF DIAGONAL-	-20.41 SB26 -7.49 SB25			-7.15 SB28 -5.92 SS18 -5.22 SB22 4.85 BB29 -4.48 SB21 -4.03 SB27 -2.97 BB43					
NORMAL MODE 20	OBSERVED=	0.0 CM-1	CALCULATED=	1069.7 CM-1	ERROR=	0.0 CM-1	DR	0.0 PERCENT	
INTERNAL COORDINATES-	27.07 C-CO9 15.62 C1C2			11.04 C5O 10.57 C4OH 9.85 C-CO8 8.09 C2C3 5.38 C3C4					
FORCE CONSTANTS-	54.11 CCH 30.67 CCH			15.95 CCH 10.57 CCH 8.53 CCH 6.66 CCO					
OFF DIAGONAL-	-9.12 SB28 -8.86 SB26			-6.19 SB27 -4.75 SB22 -3.90 SB25	-3.09 SB24 2.46 BB29 -2.34 SB23 -1.58 BB36				
NORMAL MODE 21	OBSERVED=	0.0 CM-1	CALCULATED=	1037.5 CM-1	ERROR=	0.0 CM-1	DR	0.0 PERCENT	
INTERNAL COORDINATES-	44.65 C*CH 18.08 CCH			9.01 C5H					
FORCE CONSTANTS-	73.65 CCH 6.58 CCO								
OFF DIAGONAL-	7.64 SB27 -2.71 BB45								
NORMAL MODE 22	OBSERVED=	0.0 CM-1	CALCULATED=	1030.7 CM-1	ERROR=	0.0 CM-1	DR	0.0 PERCENT	
INTERNAL COORDINATES-	61.71 HCH 9.82 C5C*			6.99 CCH 10.23 C-CO*					
FORCE CONSTANTS-	61.71 HCH 11.78 CCH			10.63 CCH 10.01 CCH 7.13 CCO					
OFF DIAGONAL-	-5.60 SB26 5.01 SB27								
NORMAL MODE 23	OBSERVED=	0.0 CM-1	CALCULATED=	1015.9 CM-1	ERROR=	0.0 CM-1	DR	0.0 PERCENT	
INTERNAL COORDINATES-	38.13 C3C4 12.49 C-CO7			6.08 C2C3					
FORCE CONSTANTS-	50.34 CCH 19.91 CCH			15.82 CCO 8.76 CCH 8.60 CCH					
OFF DIAGONAL-	-12.15 SB21 -11.98 SB22			4.58 SB26 -3.53 SS18 3.02 BB43 2.96 SB25 -2.72 SB28 2.11 BB34 1.92 BB36					
NORMAL MODE 24	OBSERVED=	0.0 CM-1	CALCULATED=	999.7 CM-1	ERROR=	0.0 CM-1	DR	0.0 PERCENT	
INTERNAL COORDINATES-	20.52 C2C3 15.96 C1C2			8.90 C-CO1 7.49 C-CO8 7.23 C-CO6					
FORCE CONSTANTS-	42.89 CCH 27.58 CCH			16.01 CCO 11.75 CCH 7.64 CCH					
OFF DIAGONAL-	-11.54 SB22 -5.30 SB21			4.01 SB25 -3.94 SB24 3.54 BB34 -3.12 SB27 -2.82 SS18 -2.70 SB28 2.70 SB26					
NORMAL MODE 25	OBSERVED=	0.0 CM-1	CALCULATED=	983.9 CM-1	ERROR=	0.0 CM-1	DR	0.0 PERCENT	
INTERNAL COORDINATES-	17.57 C5H 12.98 C-CO*			10.16 CCH 9.21 C5C* 6.88 CCHB 5.91 CCH 5.55 C4C5					
FORCE CONSTANTS-	38.13 CCH 12.49 CCH			11.03 CCH 15.94 CCH					
OFF DIAGONAL-	9.60 SB27 -6.87 SB26			-3.22 SB21 -2.60 SB22 -2.19 BB45 2.11 SS18					
NORMAL MODE 26	OBSERVED=	0.0 CM-1	CALCULATED=	975.8 CM-1	ERROR=	0.0 CM-1	DR	0.0 PERCENT	
INTERNAL COORDINATES-	21.07 C1C2 7.67 CCH			5.68 C-CO1 5.24 C-CO7					
FORCE CONSTANTS-	21.07 CCH 21.55 CCH			21.04 CCH 12.28 CCH 10.17 CCH					
OFF DIAGONAL-	7.12 SB26 -6.35 SB22			-5.26 SB21 4.07 BB34 2.98 SB27 2.70 BB43 2.48 BB29 -2.21 SB25 -1.58 SB28					
NORMAL MODE 27	OBSERVED=	0.0 CM-1	CALCULATED=	963.5 CM-1	ERROR=	0.0 CM-1	DR	0.0 PERCENT	
INTERNAL COORDINATES-	13.65 C-CO* 12.53 CCH2			7.78 CCH 6.84 C5H 6.31 C-CO7 6.20 C4C5					
FORCE CONSTANTS-	29.70 CCH 26.78 CCH			21.90 CCH 8.83 CCH 6.72 CCO					
OFF DIAGONAL-	4.10 SB27 3.47 BB34			-3.20 SB26 -3.12 SB28 -1.99 BB45 -1.80 SB21					
NORMAL MODE 28	OBSERVED=	0.0 CM-1	CALCULATED=	953.1 CM-1	ERROR=	0.0 CM-1	DR	0.0 PERCENT	
INTERNAL COORDINATES-	18.78 CCH 13.64 HC4C			12.21 C-CO9 8.14 C-CO6 5.87 C-CO1 5.00 CCHB					
FORCE CONSTANTS-	33.10 CCH 30.06 CCH			23.67 CCH					
OFF DIAGONAL-	7.05 SB27 -3.50 SB24			-2.12 BB45 -1.69 SB28					
NORMAL MODE 29	OBSERVED=	0.0 CM-1	CALCULATED=	948.2 CM-1	ERROR=	0.0 CM-1	DR	0.0 PERCENT	
INTERNAL COORDINATES-	22.27 C5H 11.94 C5H			11.43 CCH 9.32 CCH					
FORCE CONSTANTS-	47.51 CCH 24.42 CCH			17.38 CCO 5.25 CCH					
OFF DIAGONAL-	2.85 BB34 2.79 SB27			2.69 SB26 -2.61 BB45 -1.57 SB28					
NORMAL MODE 30	OBSERVED=	0.0 CM-1	CALCULATED=	941.8 CM-1	ERROR=	0.0 CM-1	DR	0.0 PERCENT	
INTERNAL COORDINATES-	23.14 CCH 14.88 HC3C			6.82 CCH 6.14 CCH					
FORCE CONSTANTS-	42.14 CCH 29.71 CCH			13.99 CCH 8.74 CCH 6.36 CCH					
OFF DIAGONAL-	3.89 SB26 -3.63 SB21			-2.96 BB29 -2.71 SB27 -2.66 BB45 -2.28 SB28 -1.97 SB22					
NORMAL MODE 31	OBSERVED=	0.0 CM-1	CALCULATED=	938.6 CM-1	ERROR=	0.0 CM-1	DR	0.0 PERCENT	
INTERNAL COORDINATES-	34.33 CCH 7.88 CCH			14.83 CCH 5.55 C-CO8 5.26 CCH					
FORCE CONSTANTS-	56.58 CCH 24.38 CCH			9.05 CCH					
OFF DIAGONAL-	4.29 SB27 -2.87 BB45			-2.77 SB21					
NORMAL MODE 32	OBSERVED=	0.0 CM-1	CALCULATED=	932.4 CM-1	ERROR=	0.0 CM-1	DR	0.0 PERCENT	
INTERNAL COORDINATES-	57.43 CCH 17.02 HC2C			7.75 C-CO8					
FORCE CONSTANTS-	64.64 CCH 24.51 CCH			8.38 CCH					
OFF DIAGONAL-	-3.15 BB45 -2.32 SB22			-2.02 SB21 -1.91 BB29					
NORMAL MODE 33	OBSERVED=	0.0 CM-1	CALCULATED=	926.3 CM-1	ERROR=	0.0 CM-1	DR	0.0 PERCENT	
INTERNAL COORDINATES-	12.76 HC2C 11.57 CCH2			9.60 HC4C 7.67 CCH 6.36 CCH					
FORCE CONSTANTS-	48.40 CCH 22.66 CCH			12.81 CCH 10.98 CCH					
OFF DIAGONAL-	10.73 BB34 -5.98 BB29			-4.40 BB43 -2.79 SB22 -2.43 BB45 -1.54 SB24 1.52 SB25					
NORMAL MODE 34	OBSERVED=	0.0 CM-1	CALCULATED=	911.2 CM-1	ERROR=	0.0 CM-1	DR	0.0 PERCENT	
INTERNAL COORDINATES-	20.19 CCH 9.01 CCHB			7.73 CCH 6.84 CCH 5.72 CCH					
FORCE CONSTANTS-	48.15 CCH 31.53 CCH			7.35 CCH					
OFF DIAGONAL-	4.77 SB26 4.19 BB29			-2.72 BB45 -1.53 SB22					
NORMAL MODE 35	OBSERVED=	0.0 CM-1	CALCULATED=	903.5 CM-1	ERROR=	0.0 CM-1	DR	0.0 PERCENT	
INTERNAL COORDINATES-	27.92 CCH 8.53 CCHB			5.83 CCH 5.76 C4C5					
FORCE CONSTANTS-	52.28 CCH 24.21 CCH			9.04 CCH					
OFF DIAGONAL-	5.98 SB26 3.84 BB29			-2.55 SB21 -2.16 BB45					

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400									
MOLECULE 16 -6 NG-1237 BETA GLUCOSE-C-D7									
PAGE 2									
NORMAL MODE 36	OBSERVED=	0.0 CM-1	CALCULATED=	864.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	38.87	OC1H 27.07	CC1H	6.67 C1C2					
FORCE CONSTANTS-	34.73	UCH 31.14	CCH	10.93 CO	8.39 CC	7.44 CCO			
OFF DIAGONAL-	6.38	SB27 -4.45	SB26	-3.33 SB22	-2.62 BB45	-2.05 SB25	1.99 SS18	-1.89 BB29	-1.74 BB43
NORMAL MODE 37	OBSERVED=	0.0 CM-1	CALCULATED=	780.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	26.27	HC5C 16.44	C-0*	9.92 C5C1	9.77 CCHB	6.82 CASH			
FORCE CONSTANTS-	22.68	CCH 20.10	CO	11.41 CC	9.93 OCH				
OFF DIAGONAL-	11.07	SB26 -8.32	SB27	-3.36 SB21	2.53 SS18	-2.45 BB45	1.60 BB43		
NORMAL MODE 38	OBSERVED=	0.0 CM-1	CALCULATED=	767.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	19.31	CCHB 10.92	CCHA	9.17 OCO	9.00 C5O*	5.27 C5H			
FORCE CONSTANTS-	37.60	CCH 18.43	UCH	14.04 CO	7.81 CCO	9.17 OCO			
OFF DIAGONAL-	4.12	BB43 4.00	SB25	2.89 BB33	-2.60 SB27	-1.75 SB23	1.71 BB34	-1.66 SB24	
NORMAL MODE 39	OBSERVED=	0.0 CM-1	CALCULATED=	642.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	17.16	CCHA 17.14	CCO*	9.39 CCHH	9.28 CC4H	7.81 HC4C	7.23 C4C5	6.56 CCO*	5.13 HC3C
FORCE CONSTANTS-	53.11	CCH 30.72	CCO	10.51 CC					
OFF DIAGONAL-	-7.75	BB29 -6.22	BB34	4.44 BB43	2.68 SB21	1.87 SB25	-1.81 BB33	-1.61 SB22	
NORMAL MODE 40	OBSERVED=	0.0 CM-1	CALCULATED=	590.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	12.08	CCO* 10.48	CO*	9.68 O*CC	6.29 C-09	5.77 O9CC	5.26 C-07		
FORCE CONSTANTS-	35.26	CCO 16.68	CCO	10.48 CCH	8.63 CC	8.03 CCH	3.89 CC		
OFF DIAGONAL-	6.01	SB25 5.54	SB22	-1.28 SB27	-2.42 BB41	-2.36 SB21	2.21 SB24	-2.19 BB42	-2.05 BB34 1.76 BB43
NORMAL MODE 41	OBSERVED=	0.0 CM-1	CALCULATED=	547.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	8.78	CCO 8.75	OCO	8.44 O*CI	6.91 CCHB	6.53 O9CC	5.73 CCO7		
FORCE CONSTANTS-	34.73	CCO 20.22	CCH	16.59 CO	8.75 OCO	7.47 OCH			
OFF DIAGONAL-	5.49	BB43 5.34	SB24	-4.75 BB34	-4.49 SB27	-2.64 BB29	1.84 SB22	1.75 SB25	1.72 SS18
NORMAL MODE 42	OBSERVED=	0.0 CM-1	CALCULATED=	523.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	20.38	HC2C 19.10	CC3H	13.01 CCO9	11.64 O7CC	9.77 CC06	9.35 CCH2	8.65 CCO8	7.31 HC3C 5.23 CC1H
FORCE CONSTANTS-	68.21	CCH 54.04	CCO	10.69 BB34	-1.74 BB45	-1.55 SB21			
OFF DIAGONAL-	-23.70	BB34 -15.14	BB29						
NORMAL MODE 43	OBSERVED=	0.0 CM-1	CALCULATED=	488.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	10.83	O8CC 9.14	C4C5	6.98 CCH2	6.61 HC4C	5.73 CCO8			
FORCE CONSTANTS-	31.96	CCH 28.28	CCO	22.01 CC	10.54 CO				
OFF DIAGONAL-	-9.99	BB34 -6.68	BB29	6.10 BB43	3.27 SS18	3.00 SB21	2.24 SB25	-1.76 SB27	
NORMAL MODE 44	OBSERVED=	0.0 CM-1	CALCULATED=	436.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	12.10	O7CC 11.45	CC06	8.16 HC3C	7.53 C4O*	7.06 CC1H	6.97 CCH2	5.91 CCO*	5.01 CC4H
FORCE CONSTANTS-	53.28	CCO 31.89	CCH	7.92 CCH	5.25 CO	5.04 CC			
OFF DIAGONAL-	-10.23	BB34 -6.40	BB29	4.62 BB43	4.40 SB25	-1.91 SB26			
NORMAL MODE 45	OBSERVED=	0.0 CM-1	CALCULATED=	403.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	20.14	C2CC 11.30	CO*	10.74 CCO9	9.01 C3CC	6.25 C1CC			
FORCE CONSTANTS-	35.87	CCO 24.11	CCO	12.39 CCH	7.24 CO	6.03 CCH			
OFF DIAGONAL-	4.24	SB21 4.05	SB25	-1.88 BB42	-2.45 BB41	2.02 SB23			
NORMAL MODE 46	OBSERVED=	0.0 CM-1	CALCULATED=	368.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	13.56	O*CC 12.89	CCO*	12.52 O8CC	10.98 CCO8	8.56 C3CC	7.43 CCH2	7.00 HC4C	5.37 C1CC
FORCE CONSTANTS-	54.70	CCO 26.93	CCO	14.25 CCE	5.45 CC				
OFF DIAGONAL-	-7.20	BB34 5.60	SB21	-3.78 BB29	3.49 BB43	-1.82 BB42			
NORMAL MODE 47	OBSERVED=	0.0 CM-1	CALCULATED=	340.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	24.34	O9CC 8.32	CCO7	7.13 OCO	6.52 C2C3	5.94 CCO8	5.52 CCO9	5.30 C5O*	
FORCE CONSTANTS-	59.32	CCO 12.34	CCO	7.78 CCH	7.55 CO	7.13 OCO			
OFF DIAGONAL-	7.21	SB22 -7.11	BB34	-3.28 BB42	-2.89 SB21	2.81 BB43	-2.26 SB25	-1.57 BB29	-1.56 SB23
NORMAL MODE 48	OBSERVED=	0.0 CM-1	CALCULATED=	327.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	32.57	CCO7 15.19	CCO	11.24 CCO6	5.15 TH-2	5.10 TH-1			
FORCE CONSTANTS-	59.99	CCO 15.19	OCO	13.77 CCH	10.66 T-OH				
OFF DIAGONAL-	-7.94	BB34 3.24	SB22	-2.92 BB42	-2.67 SB24	-2.17 BB29	-1.52 SB21		
NORMAL MODE 49	OBSERVED=	0.0 CM-1	CALCULATED=	309.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	21.88	O8CC 12.08	O9CC	8.79 CCO8	8.38 O7CC	6.90 C3CC	5.63 CCO9	5.52 TH-3	
FORCE CONSTANTS-	75.26	CCO 11.31	T-OH	12.47 CCH	10.34 CCH				
OFF DIAGONAL-	-9.35	BB34 -3.63	BB42	-2.07 SB22	-1.80 SB26	1.52 BB43			
NORMAL MODE 50	OBSERVED=	0.0 CM-1	CALCULATED=	287.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	12.13	O7CC 12.13	CC08	11.17 CCO9	8.51 CCO6	8.09 CC3H	6.53 HC2C	5.99 CCH2	
FORCE CONSTANTS-	53.59	CCO 30.53	CCH	9.65 CCH					
OFF DIAGONAL-	-15.87	BB34 11.32	BB43	-6.92 BB29	-3.86 SB25	3.18 SB22	2.78 BB42	-2.08 SB21	1.60 BB45 -1.51 BB41
NORMAL MODE 51	OBSERVED=	0.0 CM-1	CALCULATED=	264.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	20.17	TH-5 10.60	CCO*	8.68 CCO*	5.56 CCO6				
FORCE CONSTANTS-	41.26	CCO 27.97	T-OH	12.88 CCH	5.05 CC				
OFF DIAGONAL-	-5.01	BB34 4.93	SB22	4.53 BB43	-2.19 BB33	-2.10 BB29	-1.96 SB26	-1.58 SB25	
NORMAL MODE 52	OBSERVED=	0.0 CM-1	CALCULATED=	247.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	22.80	TH-5 15.94	C4CC	15.05 TH-4	13.17 CCO*	6.11 TH-3			
FORCE CONSTANTS-	49.28	T-OH 19.62	CCO	16.53 CCC	5.25 CCH				
OFF DIAGONAL-	-3.18	BB34 2.49	SB21	-1.94 BB42					
NORMAL MODE 53	OBSERVED=	0.0 CM-1	CALCULATED=	226.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	36.80	TH-1 34.60	TH-2	16.38 TH-5	5.46 TH-3				
FORCE CONSTANTS-	94.95	T-OH							
OFF DIAGONAL-	NONE								
NORMAL MODE 54	OBSERVED=	0.0 CM-1	CALCULATED=	215.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	42.01	TH-1 21.34	TH-3	14.30 TH-2	6.16 TH-4				
FORCE CONSTANTS-	84.01	T-OH 9.21	CCO						
OFF DIAGONAL-	NONE								
NORMAL MODE 55	OBSERVED=	0.0 CM-1	CALCULATED=	213.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	36.17	TH-4 32.49	TH-2	5.10 TH-3					
FORCE CONSTANTS-	80.03	T-OH 12.48	CCO						
OFF DIAGONAL-	NONE								
NORMAL MODE 56	OBSERVED=	0.0 CM-1	CALCULATED=	210.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	47.92	TH-3 26.21	TH-4	6.75 TH-2	5.88 CCO8				
FORCE CONSTANTS-	82.69	T-OH 17.70	CCO						
OFF DIAGONAL-	-2.21	BB34							
NORMAL MODE 57	OBSERVED=	0.0 CM-1	CALCULATED=	198.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	31.88	TH-5 22.75	CCO*	19.83 C4CC					
FORCE CONSTANTS-	39.5	T-OH 9.18	CCO	21.35 CCH	10.13 CCH				
OFF DIAGONAL-	-4.66	BB34 -3.18	BB42	-2.68 BB33					
NORMAL MODE 58	OBSERVED=	0.0 CM-1	CALCULATED=	139.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	19.41	CO* 19.41	C4CC	8.25 TCC4	7.47 CCO*	6.12 TC01	5.93 CCH	5.47 OCO	5.01 C1CC
FORCE CONSTANTS-	24.44	CCO 19.54	CCO	14.45 CCH	10.11 T-CC	9.68 T-CC	8.41 CCH		
OFF DIAGONAL-	4.37	BB43 -1.97	SB25	1.66 BB41					
NORMAL MODE 59	OBSERVED=	0.0 CM-1	CALCULATED=	87.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	21.34	C2CC 18.81	TCC5	11.15 TCC6	9.18 C3CC	8.10 C1CC			
FORCE CONSTANTS-	39.55	T-CC 39.35	CCC	20.33 CCO	5.63 CO				
OFF DIAGONAL-	-5.16	SB25 -4.10	SB21	-3.97 BB42	2.39 BB41	-1.60 SB27	-1.58 BB34		
NORMAL MODE 60	OBSERVED=	0.0 CM-1	CALCULATED=	72.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	65.30	TCC5 5.48	C2CC	10.01 CCO					
FORCE CONSTANTS-	70.10	T-CC 10.73	CCC						
OFF DIAGONAL-	NONE								
NORMAL MODE 61	OBSERVED=	0.0 CM-1	CALCULATED=	69.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	15.13	TCC4 14.85	C3CC	10.27 CCO*	9.45 TCC3	8.64 C1CC	6.49 TCC2	5.57 O*CC	
FORCE CONSTANTS-	30.82	T-CC 30.82	CCC	28.39 CCH	5.00 T-CC				
OFF DIAGONAL-	-3.76	BB42 -2.57	SB25	-2.09 BB34	1.88 BB41				

2. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 0.0

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400										PAGE 1
MOLECULE 17 -6 NG-1237 BETA GLUCOSE-D12										
NORMAL MODE 8	OBSERVED=	0.0 CM-1	CALCULATED=	1270.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	38.42	O*CI 29.85 C-06	11.84 OCH	5.42 CCH	6.71 CCH	6.38 CCO6	5.80 C*CH			
FORCE CONSTANTS-	86.27	CO 23.93 CCO	11.04 OCH	5.42 CCH	5.15 CC					
OFF DIAGONAL-	16.70	SB25-15.54 SB27	-2.65 BB43	-1.93 SB26	1.84 BB34	-1.59 SB21	-1.59 SS19	-1.57 BB42	1.55 SB28	
NORMAL MODE 9	OBSERVED=	0.0 CM-1	CALCULATED=	1234.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	22.03	C-09 13.83 C50*	12.88 C4C5	8.75 C-07	7.60 HC4C	6.63 C*CH	5.37 OC4H			
FORCE CONSTANTS-	49.49	CO 23.90 CCH	17.59 CCO	16.28 CCH	CC 10.36	OCCH				
OFF DIAGONAL-	14.33	SB25-11.04 SB27	-9.98 SB26	5.35 BB34	-4.84 SS18	4.61 BB29	4.33 SB22	2.18 SB28	-1.78 SB21	
NORMAL MODE 10	OBSERVED=	0.0 CM-1	CALCULATED=	1195.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	28.95	C-08 16.62 C2C3	8.71 C4C5	8.14 C-07	7.49 OC3H	6.70 C-06	6.27 HC2C			
FORCE CONSTANTS-	50.18	CO 30.66 CCH	19.85 CCH	13.35 OCH	11.28 CCO	6.64 CCO				
OFF DIAGONAL-	12.97	SB26-12.61 SB27	-7.17 SB25	-6.58 SS18	4.07 SB28	4.03 BB29	-3.75 SB21	-2.13 BB43		
NORMAL MODE 11	OBSERVED=	0.0 CM-1	CALCULATED=	1174.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	30.93	C3C4 18.71 C2C3	12.11 C-07	11.56 HC3C	8.55 C-09	7.63 C-08	6.03 O*CI	5.82 CCO8	5.01 CC4H	
FORCE CONSTANTS-	52.12	CC 40.77 CO	17.17 CCH	15.32 CCH	8.54 OCH	5.49 OCH				
OFF DIAGONAL-	17.73	SB26 -8.97 SB27	-5.04 SB25	4.54 BB29	-4.48 SB22	-4.43 SS18	-4.36 SB21	3.28 SB28	-2.81 BB43	
NORMAL MODE 12	OBSERVED=	0.0 CM-1	CALCULATED=	1164.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	23.43	C5C1 11.33 C4C5	15.58 C50H	10.83 HC5C	8.20 C-09	6.30 C1C2	6.01 O9CC	5.74 C-06		
FORCE CONSTANTS-	53.19	CC 29.98 CCH	21.66 CCO	15.42 CCH	6.25 OCH					
OFF DIAGONAL-	15.61	SB22 -7.39 SB26	-6.49 SB27	-3.27 SB25	-1.92 BB43	1.75 SB23				
NORMAL MODE 13	OBSERVED=	0.0 CM-1	CALCULATED=	1155.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	27.03	C-0* 21.27 C5C*	13.02 OCHA	9.17 C-09	8.67 CCHB	7.44 OCHB	5.94 CCO*	5.73 C*OH		
FORCE CONSTANTS-	45.59	CC 23.54 OCH	22.28 CC	13.04 CCH	11.01 CCO	7.76 BCOH	5.72 CCC			
OFF DIAGONAL-	19.63	SB27 6.05 SB28	-5.83 SB26	-3.84 SB25	-3.82 SB22	-2.68 SS18	2.03 BB33	-1.60 SB21		
NORMAL MODE 14	OBSERVED=	0.0 CM-1	CALCULATED=	1131.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	44.79	C1C2 14.13 C10H	12.59 C-07	9.69 C4C5	7.67 C2C3	7.01 CC1H	6.45 O7CC			
FORCE CONSTANTS-	63.43	CC 20.77 CO	19.19 BCOH	18.61 CCH	12.65 CCO	7.63 OCH				
OFF DIAGONAL-	15.97	SB26-11.42 SB22	-9.36 SB27	-4.82 SS18	-3.18 SB21	3.07 BB29	-2.79 BB43	-2.48 BB34	-2.45 SB24	
NORMAL MODE 15	OBSERVED=	0.0 CM-1	CALCULATED=	1119.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	14.99	C50* 14.57 C10H	12.89 C-07	7.86 OCHA	7.82 CCHA	6.06 O*CI	5.77 C1C2	5.11 C-09		
FORCE CONSTANTS-	44.45	CC 19.06 BCOH	18.91 OCH	14.99 CCH	12.49 CC	8.86 CCO				
OFF DIAGONAL-	14.86	SB27 2.77 BB34	-2.54 SB23	-2.41 SB21	-2.34 SB22	-1.96 SS18	-1.92 SB25	-1.90 SB26	-1.54 BB43	
NORMAL MODE 16	OBSERVED=	0.0 CM-1	CALCULATED=	1097.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	16.01	C2OH 13.78 C3OH	7.77 C3C4	7.54 C-09	6.34 C10H	6.17 C2C3				
FORCE CONSTANTS-	36.13	BCOH 16.40 CO	15.91 CC	13.28 CCO	12.07 CCH	6.42 OCH				
OFF DIAGONAL-	6.54	SB22 -5.59 SB21	5.05 SB26	-4.71 BB36	4.42 BB34	2.83 BB43	-2.40 SB27	-2.07 SB25	-1.51 BB35	
NORMAL MODE 17	OBSERVED=	0.0 CM-1	CALCULATED=	1076.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	21.72	C3OH 12.59 C-07	11.40 CCH2	10.98 C10H	9.68 C2OH	6.62 C3C4	5.88 HC2C			
FORCE CONSTANTS-	43.85	BCOH 22.21 CCH	20.24 CO	10.18 CC	7.92 CCO	5.02 OCH				
OFF DIAGONAL-	9.11	SB28 4.84 BB34	-4.27 SB25	-3.44 BB36	2.18 BB29	-1.81 SB22	1.56 BB43	-1.55 SB21	-1.52 BB35	
NORMAL MODE 18	OBSERVED=	0.0 CM-1	CALCULATED=	1060.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	50.06	C*CH 13.00 C-0*	9.63 HCH	8.27 OCHB						
FORCE CONSTANTS-	56.20	BCOH 15.43 CO	15.24 OCH	9.63 HCH	7.21 CCH	6.60 CC				
OFF DIAGONAL-	8.83	SB28 -3.45 SB27	-2.45 SB26	-2.05 SB25	-1.88 BB35	-1.83 SB22				
NORMAL MODE 19	OBSERVED=	0.0 CM-1	CALCULATED=	1041.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	30.07	*CIH 10.71 OC1H	7.81 C*OH	6.54 *C5H						
FORCE CONSTANTS-	52.82	OCH 11.32 BCOH	9.27 CCH	7.77 CO	5.09 CCO					
OFF DIAGONAL-	4.13	SB27 -2.45 SB21	-1.95 BB45	1.61 BB34						
NORMAL MODE 20	OBSERVED=	0.0 CM-1	CALCULATED=	1029.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	52.60	HCH 8.70 C-0*	6.15 C4H	6.09 OCHA						
FORCE CONSTANTS-	52.00	HCH 13.08 C-0*	12.94 CCH	9.28 CO	5.17 BCOH					
OFF DIAGONAL-	6.21	SB27 -3.33 SB26	-1.70 SB28							
NORMAL MODE 21	OBSERVED=	0.0 CM-1	CALCULATED=	1027.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	14.14	*CIH 12.75 C2OH	11.78 OC1H	10.82 C10H	6.06 C5C1	5.90 C*OH				
FORCE CONSTANTS-	36.07	OCH 29.62 BCOH	14.49 CCH	9.81 CC	9.75 CO					
OFF DIAGONAL-	5.10	SB28 5.05 SB27	-4.47 SB26	-2.06 BB39	-1.76 BB45					
NORMAL MODE 22	OBSERVED=	0.0 CM-1	CALCULATED=	1021.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	16.96	C3C4 11.33 C4OH	7.74 C3OH	7.10 C-08	6.93 C-09	6.07 C*CH	5.72 OC2H	5.59 C2OH		
FORCE CONSTANTS-	24.30	CC 19.08 CO	15.22 CCH	14.37 OCH	14.01 BCOH	11.33 CCH	6.98 CCO			
OFF DIAGONAL-	6.14	SB28 -6.13 SB21	-4.40 SB22	4.32 SB27	2.02 BB34	1.53 BB43				
NORMAL MODE 23	OBSERVED=	0.0 CM-1	CALCULATED=	992.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	16.62	C-07 13.60 C-06	8.55 O*CI	7.68 C5C*	6.21 HC4C	5.68 OC4H	5.35 C10H			
FORCE CONSTANTS-	40.66	CO 19.73 CCH	16.80 OCH	15.76 CC	10.29 BCOH	6.14 CCO				
OFF DIAGONAL-	6.14	SB28 -5.53 SB26	-5.51 SB24	-2.72 SB22	1.58 SB21					
NORMAL MODE 24	OBSERVED=	0.0 CM-1	CALCULATED=	977.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	20.01	*C5H 17.20 OCHB	11.88 C5H	7.60 CCHA	6.25 C-0*					
FORCE CONSTANTS-	48.77	OCH 19.89 CCH	7.72 CCH	7.42 CCH						
OFF DIAGONAL-	8.32	SB26 7.57 SB27	-2.69 SB21	-2.26 BB45	-2.03 SB22	1.82 SS18	1.62 SB28			
NORMAL MODE 25	OBSERVED=	0.0 CM-1	CALCULATED=	971.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	12.98	C-08 8.21 C3OH	6.43 C2C3	6.41 HC2C	6.32 OC3H	6.30 OC2H	5.97 C-07			
FORCE CONSTANTS-	22.35	CO 17.96 CCH	16.60 OCH	15.97 BCOH	11.51 CC	7.53 CCO				
OFF DIAGONAL-	7.58	SB27 6.61 SB26	-6.59 SB28	3.95 BB34	-3.61 SS18	-3.04 SB21	-2.28 SB22	1.69 BB29		
NORMAL MODE 26	OBSERVED=	0.0 CM-1	CALCULATED=	966.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	11.17	C-08 11.09 C1C2	6.54 OC2H	6.17 C3C4	5.55 C-0*					
FORCE CONSTANTS-	25.66	CO 21.87 OCH	20.04 CCH	18.33 CC	12.36 CCO					
OFF DIAGONAL-	3.85	SB22 3.23 BB34	2.41 SS18	1.96 SB27	-1.86 BB29	-1.65 SB21				
NORMAL MODE 27	OBSERVED=	0.0 CM-1	CALCULATED=	955.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	17.75	C-09 8.72 *C5H	7.07 OC4H	6.52 HC3C	5.79 C-07					
FORCE CONSTANTS-	31.13	CO 28.05 OCH	22.12 CCH							
OFF DIAGONAL-	8.20	SB27 -3.27 SB28	2.51 SB26	1.91 BB29	-1.91 BB45	-1.79 SB21	-1.67 SB25			
NORMAL MODE 28	OBSERVED=	0.0 CM-1	CALCULATED=	947.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	19.22	OC4H 17.52 *C5H	9.35 C5H	7.85 C-09	5.71 C-08					
FORCE CONSTANTS-	44.33	OCH 19.17 CO	18.03 CCH	6.03 CC						
OFF DIAGONAL-	6.74	SB27 2.77 SB26	-2.41 BB45	1.99 BB29						
NORMAL MODE 29	OBSERVED=	0.0 CM-1	CALCULATED=	937.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	40.98	C*CH 8.78 HC4C	15.59 C1H	6.42 C-08	5.27 OC4H					
FORCE CONSTANTS-	3.73	BB29 2.68 SB27	17.58 CO	8.00 BCOH	5.01 CCO					
OFF DIAGONAL-			-2.52 SB28	-2.49 BB45	2.28 BB34	-1.82 SB24				
NORMAL MODE 30	OBSERVED=	0.0 CM-1	CALCULATED=	932.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	11.35	C-06 10.35 OC2H	1.78 HC3C	6.75 CCH3	5.58 OC4H	5.00 CC4H				
FORCE CONSTANTS-	32.40	CCH 30.40 CO	20.16 OCH	12.51 CCO						
OFF DIAGONAL-	5.33	BB34 -4.32 SB28	-3.94 BB29	-2.80 SB24	-2.58 BB43	-2.05 BB45				
NORMAL MODE 31	OBSERVED=	0.0 CM-1	CALCULATED=	912.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	19.50	HC2C 8.20 CCH2	8.07 CC4H	7.50 OC2H	5.95 CC1H					
FORCE CONSTANTS-	51.56	CCH 12.17 OCH	5.87 CC	5.46 CO	5.27 BCOH					
OFF DIAGONAL-	9.79	BB29 9.16 SB26	3.31 BB34	-2.77 BB45	-1.56 SB27					
NORMAL MODE 32	OBSERVED=	0.0 CM-1	CALCULATED=	883.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	31.29	OC3H 23.87 C3OH	8.57 CCH3	6.29 OC2H	6.26 C3C4	5.71 C2OH				
FORCE CONSTANTS-	46.26	CO 32.30 BCOH	11.88 CCH	7.74 CCH						
OFF DIAGONAL-	9.73	SB27 -5.76 SB28	-3.03 BB39	-2.53 BB29	-2.39 BB45	-1.89 SB22	-1.83 SB21			
NORMAL MODE 33	OBSERVED=	0.0 CM-1	CALCULATED=	881.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	39.87	OCHA 12.84 C3OH	14.55 CCH	12.18 CC	8.71 OC2H	8.47 C2C3	6.53 OCHB	5.69 C*OH		
FORCE CONSTANTS-	2.88	SB22 -2.28 SB21	2.15 BB39	2.00 BB36	-1.80 BB45	-1.55 SB27	-1.54 BB29			
NORMAL MODE 34	OBSERVED=	0.0 CM-1	CALCULATED=	874.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	21.42	OCHA 15.69 C2OH	12.83 OC2H	9.74 C*OH	9.02 OCCHB	7.61 C2C3	5.06 CCHA			
FORCE CONSTANTS-	44.48	OCH 25.76 BCOH	15.57 CCH	9.07 CC	6.42 CO					
OFF DIAGONAL-	2.14	SB22 -2.12 SB21	-2.09 SB27	-1.90 BB45	1.68 BB39					
NORMAL MODE 35	OBSERVED=	0.0 CM-1	CALCULATED=	829.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	25.34	OC1H 16.90 CC1H	14.56 C4OH	14.25 C10H	9.51 C1C2					
FORCE CONSTANTS-	33.26	OCH 26.91 CCH	15.36 BCOH	14.56 CCH	11.22 CC	6.16 CCO				
OFF DIAGONAL-	5.03	BB29 -4.01 SB22	-2.85 SB26	2.48 BB39	-2.17 BB45	1.83 BB34	-1.78 SB28			

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400									
MOLECULE 17 -6 NG-1237 BETA GLUCOSE-D12									
PAGE 2									
NORMAL MODE 36	OBSERVED=	0.0 CM-1	CALCULATED=	822.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	49.10	C4OH	9.23	OC4H	8.27	C4CS	5.95	OC1H	5.69
FORCE CONSTANTS-	49.10	COH	18.05	OGH	17.53	CCH	15.09	CC	6.09
OFF DIAGONAL-	-4.84	SB28	-4.22	SB21	-2.83	SB22	-2.82	BB36	2.56
								BB39	-2.52
								BB29	-2.06
								SB27	
NORMAL MODE 37	OBSERVED=	0.0 CM-1	CALCULATED=	779.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	32.17	HC2C	14.36	C-0*	12.38	CCBH	10.86	C5C*	
FORCE CONSTANTS-	49.11	CCH	18.47	CO	13.00	CC	10.86	OC*	
OFF DIAGONAL-	11.17	SB26	-7.98	SB27	-3.88	SB21	2.79	SS18	-2.14
								BB45	
NORMAL MODE 38	OBSERVED=	0.0 CM-1	CALCULATED=	757.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	29.33	CCBH	8.84	OCU	7.21	CCHA	7.03	C5O*	5.20
FORCE CONSTANTS-	29.86	CCH	19.16	OGH	12.87	CO	11.73	CCO	8.84
OFF DIAGONAL-	4.19	SB25	4.16	BB43	3.13	BB33	-1.98	SB27	-1.58
								SB24	1.57
								SB28	1.54
								BB34	
NORMAL MODE 39	OBSERVED=	0.0 CM-1	CALCULATED=	639.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	17.11	CCHA	16.62	CCO*	9.40	CCSH	9.16	CC4H	7.48
FORCE CONSTANTS-	53.15	CCH	29.99	CCO	10.82	CC	8.47	HC4C	7.37
OFF DIAGONAL-	-7.68	BB29	-6.26	BB34	4.33	BB43	2.72	SB21	-1.89
								BB33	-1.79
								SB22	1.72
								SB25	
NORMAL MODE 40	OBSERVED=	0.0 CM-1	CALCULATED=	544.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	9.25	CCO*	8.22	O1C1	7.92	OCO	6.48	CCBH	5.75
FORCE CONSTANTS-	35.12	CCO	15.38	CO	10.68	COC	8.91	CC	8.47
OFF DIAGONAL-	5.79	SB22	5.65	SB25	-2.84	SB27	-2.56	SB21	2.38
								SB24	-2.38
								BB41	-2.16
								BB42	-1.91
								BB34	1.55
								SB26	
NORMAL MODE 41	OBSERVED=	0.0 CM-1	CALCULATED=	586.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	11.76	4CO*	10.68	CO*C	9.29	O1CC	6.41	O9CC	5.76
FORCE CONSTANTS-	34.24	CCO	20.01	CCH	16.30	CO	7.92	OCO	7.58
OFF DIAGONAL-	5.36	BB43	4.91	SB24	-4.47	SB27	-4.24	BB34	-2.72
								BB29	2.42
								SB25	2.07
								SB22	1.79
								SS18	
NORMAL MODE 42	OBSERVED=	0.0 CM-1	CALCULATED=	521.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	19.13	HC2C	18.22	CC3H	13.45	CCO9	12.12	O7CC	10.42
FORCE CONSTANTS-	23.02	CCH	15.15	CC	10.51	BB43	-1.92	SB21	-1.73
OFF DIAGONAL-	-23.53	BB34	-14.45	BB29					
								BB45	
NORMAL MODE 43	OBSERVED=	0.0 CM-1	CALCULATED=	486.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	19.72	O8CC	8.55	C4C5	7.14	CCB	6.67	HC4C	6.25
FORCE CONSTANTS-	10.20	CCH	29.16	CCO	21.87	CC	10.19	CO	
OFF DIAGONAL-	-10.31	BB34	-6.74	BB29	6.05	BB43	3.28	SB21	3.21
								SS18	1.95
								SB25	-1.56
								SB27	
NORMAL MODE 44	OBSERVED=	0.0 CM-1	CALCULATED=	435.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	12.00	O7CC	11.79	CCO6	7.80	HC3C	7.28	CC1H	7.27
FORCE CONSTANTS-	53.69	CCO	31.86	CCH	6.70	CCC	5.51	CO	5.32
OFF DIAGONAL-	-10.48	BB34	-6.39	BB29	4.56	SB25	4.54	BB43	-1.95
								SB26	
NORMAL MODE 45	OBSERVED=	0.0 CM-1	CALCULATED=	398.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	20.49	C2CC	10.93	CCO9	10.51	CO1C	8.27	C3CC	7.24
FORCE CONSTANTS-	36.37	CCC	27.10	CCO	10.51	CO1C	6.65	CO	5.75
OFF DIAGONAL-	4.21	SB21	-4.10	BB42	3.91	SB25	-2.53	BB41	1.93
								SB23	-1.85
								BB36	
NORMAL MODE 46	OBSERVED=	0.0 CM-1	CALCULATED=	364.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	14.21	O1CC	13.87	O8CC	11.33	4CO*	10.80	CCO8	8.47
FORCE CONSTANTS-	14.21	CCO	20.12	CCH	11.68	CCC	6.11	CC	
OFF DIAGONAL-	-6.88	BB34	5.64	SB21	-3.61	BB29	3.20	BB43	-1.98
								BB42	
NORMAL MODE 47	OBSERVED=	0.0 CM-1	CALCULATED=	337.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	19.72	O9CC	12.77	CCO7	7.46	OCO	6.79	CCO8	6.58
FORCE CONSTANTS-	59.84	CCO	12.77	CCO7	7.59	CCH	7.46	OCO	7.38
OFF DIAGONAL-	7.44	SB22	-6.95	BB34	-3.32	BB42	-2.94	SB21	2.85
								BB43	-2.22
								SB25	-1.65
								SB23	
NORMAL MODE 48	OBSERVED=	0.0 CM-1	CALCULATED=	322.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	35.78	CCO7	15.68	OCO	10.40	CCO6			
FORCE CONSTANTS-	63.58	CCO	16.16	CCH	15.68	OCO	5.76	T-OH	
OFF DIAGONAL-	-9.03	BB34	2.84	SB22	-2.78	BB42	-2.71	SB24	-2.60
								BB29	
NORMAL MODE 49	OBSERVED=	0.0 CM-1	CALCULATED=	303.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	22.38	O8CC	13.85	O9CC	9.39	CCO8	8.32	O7CC	7.71
FORCE CONSTANTS-	80.62	CCO	11.02	CCC	10.81	CCH	5.58	T-OH	
OFF DIAGONAL-	-9.78	BB34	-3.99	BB42	-2.48	SB22	-2.01	SB26	
NORMAL MODE 50	OBSERVED=	0.0 CM-1	CALCULATED=	280.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	19.66	O7CC	11.63	CCO8	9.32	CCO9	8.36	CCO6	7.50
FORCE CONSTANTS-	32.57	CCO	28.67	CCH	11.57	CO	3.56	SB22	-3.53
OFF DIAGONAL-	-15.12	BB34	11.10	BB43	-6.42	BB29			
								SB25	-2.46
								SB21	2.39
								BB42	1.58
								BB45	
NORMAL MODE 51	OBSERVED=	0.0 CM-1	CALCULATED=	255.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	48.10	CCO	15.10	CCH	7.23	COC	7.14	CCO9	5.51
FORCE CONSTANTS-	6.20	SB22	6.19	BB43	-5.61	BB34	-2.62	SB26	-2.53
OFF DIAGONAL-								BB33	-2.42
								BB29	-1.95
								SB25	
NORMAL MODE 52	OBSERVED=	0.0 CM-1	CALCULATED=	231.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	34.86	CCO	18.30	C4CC	10.87	HC2C	5.28	CCHA	5.40
FORCE CONSTANTS-	41.98	CCO	29.42	CCC	15.59	T-OH	10.51	CCH	5.83
OFF DIAGONAL-	-6.73	BB34	-4.51	BB42	-2.93	BB33	1.71	SB21	
								T-CC	
NORMAL MODE 53	OBSERVED=	0.0 CM-1	CALCULATED=	166.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	35.42	TH-1	32.62	TH-2	12.05	TH-5	9.91	TH-3	6.80
FORCE CONSTANTS-	96.80	T-OH							
OFF DIAGONAL-	NONE								
NORMAL MODE 54	OBSERVED=	0.0 CM-1	CALCULATED=	161.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	24.38	TH-5	23.74	TH-1	11.42	TH-4	6.70	CO1C	6.13
FORCE CONSTANTS-	64.50	T-OH	8.76	CCO	8.46	CCC	6.70	COC	
OFF DIAGONAL-	-1.64	SB21							
NORMAL MODE 55	OBSERVED=	0.0 CM-1	CALCULATED=	156.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	29.09	TH-5	27.84	TH-4	21.37	TH-3	5.62	TH-1	5.32
FORCE CONSTANTS-	84.32	T-OH	6.20	CCC					
OFF DIAGONAL-	NONE								
NORMAL MODE 56	OBSERVED=	0.0 CM-1	CALCULATED=	155.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	92.52	TH-4	11.55	TH-1	14.94	TH-4			
FORCE CONSTANTS-	92.52	T-OH	6.00	CCO					
OFF DIAGONAL-	NONE								
NORMAL MODE 57	OBSERVED=	0.0 CM-1	CALCULATED=	131.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	15.43	TH-5	13.87	CO1C	9.11	CCO*	6.70	TH-1	6.10
FORCE CONSTANTS-	90.88	T-OH	9.31	CCO					
OFF DIAGONAL-	NONE								
NORMAL MODE 58	OBSERVED=	0.0 CM-1	CALCULATED=	151.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	26.31	TH-3	28.73	TH-4	5.38	TH-2			
FORCE CONSTANTS-	23.50	T-OH	22.03	CCO	13.87	COC	8.65	T-CC	8.56
OFF DIAGONAL-	3.79	BB43	-1.71	BB33				CCH	8.40
								CCC	6.41
								T-CO	
NORMAL MODE 59	OBSERVED=	0.0 CM-1	CALCULATED=	84.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	21.05	C2CC	18.16	TCC5	11.24	TCC	9.22	C3CC	7.86
FORCE CONSTANTS-	38.87	CCH	38.80	T-CC	20.43	CCO	6.42	CO	
OFF DIAGONAL-	-5.10	SB25	-3.94	BB42	-3.87	SB21	2.36	BB41	-1.60
								BB34	-1.58
								SB27	
NORMAL MODE 60	OBSERVED=	0.0 CM-1	CALCULATED=	70.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	5.43	TCC	10.83	CCC	10.50	CCO			
FORCE CONSTANTS-	68.99	T-CC							
OFF DIAGONAL-	NONE								
NORMAL MODE 61	OBSERVED=	0.0 CM-1	CALCULATED=	67.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	15.11	TCC4	14.51	C3CC	10.08	4CO*	9.26	TCC3	8.50
FORCE CONSTANTS-	35.44	T-CC	30.36	CCO	27.74	CCC	5.42	T-CO	
OFF DIAGONAL-	-3.69	BB42	-2.50	SB25	-2.01	BB34	1.84	BB41	

2. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 0.0

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400									
MOLECULE 18 -6 NG-1236 ALPHA GLUCOSE									
PAGE 1									
NORMAL MODE 8	OBSERVED=	1457.0	CM-1	CALCULATED=	1455.2	CM-1	ERROR=	1.8	CM-1 OR 0.1 PERCENT
INTERNAL COORDINATES-	67.91	C2OH							
FORCE CONSTANTS-	68.35	BCOH	6.57	CCH	6.05	CCO			
OFF DIAGONAL-	4.44	BB36	3.84	SB28	-1.77	SB25	1.68	BB34	
NORMAL MODE 9	OBSERVED=	1442.0	CM-1	CALCULATED=	1449.6	CM-1	ERROR=	-7.6	CM-1 OR -0.5 PERCENT
INTERNAL COORDINATES-	61.93	HCH	19.98	OCBH	19.15	OCMA			
FORCE CONSTANTS-	61.93	HCH	39.43	UCH					
OFF DIAGONAL-	-3.84	SB27							
NORMAL MODE 10	OBSERVED=	1427.0	CM-1	CALCULATED=	1422.5	CM-1	ERROR=	4.5	CM-1 OR 0.3 PERCENT
INTERNAL COORDINATES-	23.14	C3OH	19.88	C4OH	12.97	OC4H	6.97	HC4C	5.66
FORCE CONSTANTS-	43.34	BCOH	20.68	CCH	19.63	OCCH	7.51	CO	6.29
OFF DIAGONAL-	-5.31	SB27	-4.49	SB26	3.96	BB29	3.64	SB28	-3.03
									SB25 2.95 BB34 2.28 BB36 -1.77 BB43 -1.60 BB45
NORMAL MODE 11	OBSERVED=	1409.0	CM-1	CALCULATED=	1413.8	CM-1	ERROR=	-4.8	CM-1 OR -0.3 PERCENT
INTERNAL COORDINATES-	43.53	C3OH	9.49	OC3H	5.75	C2C3	5.37	OC4H	
FORCE CONSTANTS-	46.87	BCOH	24.80	UCH	16.09	CCH	6.21	CC	5.67
OFF DIAGONAL-	-4.95	SB27	4.05	SB28	-3.79	SB26	3.39	BB29	2.39
									BB36 -1.83 BB39 -1.60 BB45
NORMAL MODE 12	OBSERVED=	1408.8	CM-1	CALCULATED=	1408.8	CM-1	ERROR=	0.0	CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	54.76	C1OH	20.90	OC1H					
FORCE CONSTANTS-	57.10	BCOH	30.17	UCH	8.55	CCH			
OFF DIAGONAL-	4.75	SB28	-4.41	SB27	-3.06	BB39			
NORMAL MODE 13	OBSERVED=	1385.0	CM-1	CALCULATED=	1390.4	CM-1	ERROR=	-5.4	CM-1 OR -0.4 PERCENT
INTERNAL COORDINATES-	60.97	C'OH	8.99	C'CH	5.14	C1OH			
FORCE CONSTANTS-	68.14	BCOH	19.26	UCH	7.38	CCH	5.87	CC	
OFF DIAGONAL-	-3.92	SB26	-1.88	BB39	-1.86	SB27	1.82	SB28	
NORMAL MODE 14	OBSERVED=	1381.0	CM-1	CALCULATED=	1385.0	CM-1	ERROR=	-4.0	CM-1 OR -0.3 PERCENT
INTERNAL COORDINATES-	23.57	C'CH	18.90	C'OH	16.68	C1OH	14.28	OC1H	5.66
FORCE CONSTANTS-	51.06	UCH	41.85	BCOH					
OFF DIAGONAL-	-1.73	SB27	-2.04	BB45	2.07	BB37	-1.59	SB26	
NORMAL MODE 15	OBSERVED=	1375.0	CM-1	CALCULATED=	1372.2	CM-1	ERROR=	2.8	CM-1 OR 0.2 PERCENT
INTERNAL COORDINATES-	46.50	C4OH	14.57	C'CH	7.62	CC5H	7.27	HC4C	
FORCE CONSTANTS-	49.86	BCOH	24.44	CCH	23.01	OCCH			
OFF DIAGONAL-	4.33	BB29	-3.18	SB27	-2.18	BB36	-2.13	SB26	-1.88
									BB45
NORMAL MODE 16	OBSERVED=	1371.0	CM-1	CALCULATED=	1369.2	CM-1	ERROR=	1.8	CM-1 OR 0.1 PERCENT
INTERNAL COORDINATES-	15.00	OC2H	13.00	C3OH	12.71	OC3H	11.73	C4OH	11.48
FORCE CONSTANTS-	34.60	CCH	33.45	CCH	25.45	BCOH			
OFF DIAGONAL-	6.78	BB29	-5.25	SB27	3.03	BB34	-2.71	SB28	-2.70
									BB45
NORMAL MODE 17	OBSERVED=	1343.0	CM-1	CALCULATED=	1345.0	CM-1	ERROR=	-2.0	CM-1 OR -0.1 PERCENT
INTERNAL COORDINATES-	19.37	HC5C	15.82	CCHB	13.93	OC2H	7.28	HC2C	6.61
FORCE CONSTANTS-	57.85	CCH	27.89	UCH	6.15	BCOH			
OFF DIAGONAL-	12.61	BB29	-5.09	SB26	-3.60	BB45	-3.51	SB27	1.71
									BB34
NORMAL MODE 18	OBSERVED=	1328.0	CM-1	CALCULATED=	1326.9	CM-1	ERROR=	1.1	CM-1 OR 0.1 PERCENT
INTERNAL COORDINATES-	18.45	HC3C	9.62	CC4H	8.41	OC2H	6.96	HC2C	6.86
FORCE CONSTANTS-	27.40	CCH	29.94	UCH	8.63	CCH			
OFF DIAGONAL-	14.30	BB29	-9.81	SB26	-3.93	BB45	-3.15	SB27	
NORMAL MODE 19	OBSERVED=	1311.8	CM-1	CALCULATED=	1311.8	CM-1	ERROR=	0.0	CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	1.64	OC2H	10.75	C1OH	1.64	OC2H	10.75	C1OH	5.48
FORCE CONSTANTS-	50.26	CCH	23.00	UCH	13.67	CO	12.50	BCOH	
OFF DIAGONAL-	-3.29	SB28	-3.21	BB45	2.53	BB34	-2.24	SB26	-2.16
									SB25 1.71 BB29
NORMAL MODE 20	OBSERVED=	1298.0	CM-1	CALCULATED=	1298.8	CM-1	ERROR=	-0.8	CM-1 OR -0.1 PERCENT
INTERNAL COORDINATES-	18.20	OCMA	17.32	CCMA	14.68	OC4H	9.73	HC4C	8.94
FORCE CONSTANTS-	50.48	UCH	40.99	CCH	5.31	BCOH			
OFF DIAGONAL-	-3.58	BB45	-2.96	SB27	-2.04	BB29			
NORMAL MODE 21	OBSERVED=	1288.0	CM-1	CALCULATED=	1281.2	CM-1	ERROR=	6.8	CM-1 OR 0.5 PERCENT
INTERNAL COORDINATES-	12.79	OCMA	11.45	CCMA	10.06	OC1H	9.84	CC1H	9.03
FORCE CONSTANTS-	44.04	CCH	31.86	UCH	14.60	CO			
OFF DIAGONAL-	-3.18	BB45	2.90	BB29	2.69	BB34	-2.53	SB25	2.48
									SB27
NORMAL MODE 22	OBSERVED=	1270.0	CM-1	CALCULATED=	1268.7	CM-1	ERROR=	1.3	CM-1 OR 0.1 PERCENT
INTERNAL COORDINATES-	22.17	OC4H	10.86	CC1H	9.68	C'CH	8.17	OCMA	7.56
FORCE CONSTANTS-	32.26	UCH	39.20	UCH	7.73	CO			
OFF DIAGONAL-	-3.64	BB45	-3.63	BB29	2.89	SB27	2.58	BB34	
NORMAL MODE 23	OBSERVED=	1261.0	CM-1	CALCULATED=	1259.8	CM-1	ERROR=	1.2	CM-1 OR 0.1 PERCENT
INTERNAL COORDINATES-	48.86	UCH	40.10	CCH	14.38	CC4H	7.52	CC3H	6.08
FORCE CONSTANTS-	5.32	SB27	-4.80	BB29	3.65	BB34	-3.54	BB45	
OFF DIAGONAL-									
NORMAL MODE 24	OBSERVED=	1224.0	CM-1	CALCULATED=	1227.1	CM-1	ERROR=	-3.1	CM-1 OR -0.3 PERCENT
INTERNAL COORDINATES-	13.01	HC5C	1.97	OC4H	9.93	OCCH	1.79	C'CH	7.50
FORCE CONSTANTS-	42.58	CCH	36.87	UCH	9.84	CO	5.38	BCOH	5.19
OFF DIAGONAL-	-8.06	BB29	5.73	SB27	4.59	BB34	-3.22	SB25	-3.07
									BB45
NORMAL MODE 25	OBSERVED=	1203.0	CM-1	CALCULATED=	1191.5	CM-1	ERROR=	11.5	CM-1 OR 0.9 PERCENT
INTERNAL COORDINATES-	17.99	OC1	12.23	C5O*	10.03	OCCH	8.25	HC5C	7.98
FORCE CONSTANTS-	36.59	CO	31.79	CCH	26.89	UCH	9.16	CO	7.80
OFF DIAGONAL-	-5.84	SB25	-4.14	BB29	-2.53	SB26	-1.89	BB45	
NORMAL MODE 26	OBSERVED=	1147.0	CM-1	CALCULATED=	1142.6	CM-1	ERROR=	4.4	CM-1 OR 0.4 PERCENT
INTERNAL COORDINATES-	25.36	OC1	9.50	CC2H	7.10	C5O*	6.16	HC2C	6.12
FORCE CONSTANTS-	47.93	CCH	37.05	UCH	13.97	OCCH	9.71	UCH	7.31
OFF DIAGONAL-	-5.05	BB29	-2.83	SB27	2.70	BB34	-2.95	SB25	-1.75
									BB45 -1.59 SB22
NORMAL MODE 27	OBSERVED=	1126.0	CM-1	CALCULATED=	1134.3	CM-1	ERROR=	-8.3	CM-1 OR -0.7 PERCENT
INTERNAL COORDINATES-	29.30	C4OH	25.74	OCBH	21.68	CCH	13.82	CCO	9.87
FORCE CONSTANTS-	-8.40	SB25	3.81	SB27	-3.03	BB29	-2.93	SB28	-2.47
OFF DIAGONAL-									SB23 2.44 BB34 -1.53 SB22
NORMAL MODE 28	OBSERVED=	1118.0	CM-1	CALCULATED=	1122.6	CM-1	ERROR=	-4.6	CM-1 OR -0.4 PERCENT
INTERNAL COORDINATES-	32.04	C-O*	15.42	C-O*	8.78	C4C5	6.93	C5C*	5.75
FORCE CONSTANTS-	57.94	CO	21.47	CC	20.21	CCO	9.79	BCOH	9.37
OFF DIAGONAL-	-9.75	SB25	-8.62	SB28	-3.94	SB22	-2.96	SB26	1.93
									SB27 -1.91 SS18
NORMAL MODE 29	OBSERVED=	1109.0	CM-1	CALCULATED=	1106.5	CM-1	ERROR=	2.5	CM-1 OR 0.2 PERCENT
INTERNAL COORDINATES-	46.56	C4C5	14.89	C3C4	13.35	C2C3	7.81	C-O*	6.67
FORCE CONSTANTS-	78.77	CC	25.21	CC	15.66	CCO	6.47	CCC	6.39
OFF DIAGONAL-	-11.09	SB22	-4.65	SB21	-4.05	SB27	-3.67	SB25	-3.05
									SS18 -2.89 SS17 -1.95 SB26 -1.78 SB28
NORMAL MODE 30	OBSERVED=	1078.0	CM-1	CALCULATED=	1082.3	CM-1	ERROR=	-4.3	CM-1 OR -0.4 PERCENT
INTERNAL COORDINATES-	36.52	C-O*	26.70	C3C4	10.13	C-O*	8.88	OC1	8.68
FORCE CONSTANTS-	62.76	CO	36.31	CC	7.66	UCH			
OFF DIAGONAL-	-7.85	SS18	-6.09	SB27	-9.35	SB28	-2.91	SB22	-2.31
									SB21
NORMAL MODE 31	OBSERVED=	1072.0	CM-1	CALCULATED=	1066.3	CM-1	ERROR=	5.8	CM-1 OR 0.5 PERCENT
INTERNAL COORDINATES-	37.36	C1C2	22.21	C1C2	10.45	C-O*	10.01	C-O*	6.62
FORCE CONSTANTS-	68.34	CO	36.08	CC	8.23	BCOH	7.91	CCH	7.06
OFF DIAGONAL-	-7.49	SB28	-7.07	SB27	-5.52	SB26	-4.48	SS18	-4.46
									SB22 -4.23 SB25 -3.48 SB24 -1.58 BB34
NORMAL MODE 32	OBSERVED=	1065.0	CM-1	CALCULATED=	1061.8	CM-1	ERROR=	3.2	CM-1 OR 0.3 PERCENT
INTERNAL COORDINATES-	41.00	CC	20.79	C-O*	10.70	C2C3	5.77	OCCH	
FORCE CONSTANTS-	62.48	CC	27.17	CC	28.20	CCO	13.11	UCH	7.87
OFF DIAGONAL-	-16.48	SB22	-9.78	SB26	-9.44	SB28	-3.06	SB27	-2.90
									SB25 -2.76 BB34 -2.52 SB21 -1.54 SS17
NORMAL MODE 33	OBSERVED=	1053.0	CM-1	CALCULATED=	1044.6	CM-1	ERROR=	8.4	CM-1 OR 0.8 PERCENT
INTERNAL COORDINATES-	47.54	C-O*	10.94	C-O*	9.73	C-O*	8.04	C4OH	7.93
FORCE CONSTANTS-	79.32	CO	17.38	CC	18.36	CCCH	13.17	CCC	11.31
OFF DIAGONAL-	-10.26	SB28	-9.72	SB27	-9.35	SB25	-8.54	SB21	-5.53
									SS18 -3.33 BB34 -2.00 BB29 -1.86 BB36
NORMAL MODE 34	OBSERVED=	1019.0	CM-1	CALCULATED=	1017.2	CM-1	ERROR=	1.7	CM-1 OR 0.2 PERCENT
INTERNAL COORDINATES-	29.64	C5C*	20.61	C4C5	10.82	C5O*	10.08	C2C4	8.63
FORCE CONSTANTS-	63.04	CC	29.88	CC	14.75	CCO	12.11	CO	9.93
OFF DIAGONAL-	-23.35	SB21	-8.31	SS18	-7.61	SB22	-6.40	SB27	3.07
									SB25 1.98 SS17 -1.54 SB24
NORMAL MODE 35	OBSERVED=	997.0	CM-1	CALCULATED=	998.0	CM-1	ERROR=	-1.0	CM-1 OR -0.1 PERCENT
INTERNAL COORDINATES-	55.39	C-O*	16.70	C-O*	8.35	C-O*	7.95	C2C3	7.46
FORCE CONSTANTS-	55.39	CC	13.35	CCH	11.79	CO	11.09	CC	9.16
OFF DIAGONAL-	-7.62	SB26	-6.17	BB29	-4.53	SB25	-4.37	SB24	-3.52
									SB22 -3.34 SB21 -1.75 SB27 -1.74 SB26

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR MOLECULE 18										PAGE 2	
-6 NG=1236 ALPHA PROBLEM 400 GT											
NORMAL MODE 36	OBSERVED=	0.0 CM-1	CALCULATED=	961.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	28.95 C3C4	16.27 C-08	14.17 C-08	13.48 C5C1	7.81 C1C2						
FORCE CONSTANTS-	50.96 CC	36.16 CC	19.21 CCH	13.94 CCO							
OFF DIAGONAL-	-12.32 SB22	-6.38 SB26	5.31 SS18	-3.66 BB29	-3.25 SB25	-2.76 SB21	-2.40 SB28	-2.22 SB27			
NORMAL MODE 37	OBSERVED=	915.0 CM-1	CALCULATED=	904.0 CM-1	ERROR=	10.9 CM-1	OR	1.2 PERCENT			
INTERNAL COORDINATES-	25.85 C2C3	21.98 C-06	10.00 CCH2	9.66 CCO8	7.25 C1C2						
FORCE CONSTANTS-	35.04 CC	26.64 CC	22.95 CCH	17.22 CCO							
OFF DIAGONAL-	-9.72 SB22	-7.10 SB21	3.73 SB26	2.43 BB43	2.26 SS18	-2.12 SB24	-1.56 SB27	-1.53 BB29			
NORMAL MODE 38	OBSERVED=	837.0 CM-1	CALCULATED=	835.3 CM-1	ERROR=	1.6 CM-1	OR	0.2 PERCENT			
INTERNAL COORDINATES-	29.22 C5O1	17.52 CCHA	15.67 CCHB	12.40 C-01	6.59 C5C1						
FORCE CONSTANTS-	41.71 CO	39.33 CCH	8.08 CCO	7.44 CCH	7.01 CC						
OFF DIAGONAL-	-4.29 BB29	-2.84 SB23	-2.48 SB24	2.47 SB26	-2.01 SB25	2.00 SS18	-1.66 SB22				
NORMAL MODE 39	OBSERVED=	775.0 CM-1	CALCULATED=	760.2 CM-1	ERROR=	14.8 CM-1	OR	1.9 PERCENT			
INTERNAL COORDINATES-	13.44 C-04	9.83 C-06	7.70 CCO6	7.11 CCHH	6.74 C1C2	6.00 C2C3	5.64 C-0C				
FORCE CONSTANTS-	20.61 CCO	16.78 CC	13.29 CCH	12.78 CC	10.66 CCH	7.31 CCH					
OFF DIAGONAL-	6.03 BB43	5.23 SB25	-3.26 SB27	-2.61 BB34	2.57 SB22	-2.26 BB41	2.19 SB24	1.64 BB42	-1.63 SB26		
NORMAL MODE 40	OBSERVED=	620.0 CM-1	CALCULATED=	632.1 CM-1	ERROR=	-12.1 CM-1	OR	-1.9 PERCENT			
INTERNAL COORDINATES-	14.82 CCO8	11.81 CCO	9.04 CCO7	7.12 C-0C	6.71 CCO1	5.10 CCHB					
FORCE CONSTANTS-	36.94 CCO	20.49 CCH	11.81 CCO	10.43 CC	8.58 CCH	7.12 CCH					
OFF DIAGONAL-	-4.87 BB34	-3.99 BB29	3.94 BB43	3.15 SB25	2.88 SB24	1.95 SS18	-1.74 SB27	-1.73 SB26	1.68 SB22		
NORMAL MODE 41	OBSERVED=	605.0 CM-1	CALCULATED=	624.3 CM-1	ERROR=	-19.3 CM-1	OR	-3.2 PERCENT			
INTERNAL COORDINATES-	19.36 CCO*	16.45 O8CC	10.16 CCH5	8.24 HC4C	7.78 O9CC	5.75 C4CC					
FORCE CONSTANTS-	64.38 CCO	30.40 CCH	8.28 CCH								
OFF DIAGONAL-	-13.89 BB34	8.97 BB43	-6.84 BB29	3.71 SB25	-1.73 BB41						
NORMAL MODE 42	OBSERVED=	556.0 CM-1	CALCULATED=	556.3 CM-1	ERROR=	-0.3 CM-1	OR	-0.0 PERCENT			
INTERNAL COORDINATES-	18.08 UTCC	11.56 CCO9	6.44 C2C3	6.28 CCH3	5.93 C1C2	5.26 CCO8					
FORCE CONSTANTS-	45.81 CCO	24.34 CCH	15.85 CCH	10.27 CCH							
OFF DIAGONAL-	-10.68 BB34	6.87 BB43	-5.45 BB29	2.83 SS18	1.94 SB21	-1.80 SB22	-1.77 BB36	1.69 SB25	-1.63 SB27		
NORMAL MODE 43	OBSERVED=	539.0 CM-1	CALCULATED=	533.3 CM-1	ERROR=	5.7 CM-1	OR	1.1 PERCENT			
INTERNAL COORDINATES-	19.86 CCO	15.48 CCO	12.77 O8CC	8.99 C-09	6.71 CCO1	5.10 CCHB					
FORCE CONSTANTS-	42.47 CCO	15.48 CCO	13.18 CCO	11.86 CCH	6.87 CC	6.27 CCH					
OFF DIAGONAL-	6.07 SB25	-5.44 BB34	3.85 SB22	-3.07 SB21	-2.73 BB42	-2.18 SB27	1.94 SS18	-1.87 BB29	1.64 BB43		
NORMAL MODE 44	OBSERVED=	439.0 CM-1	CALCULATED=	453.2 CM-1	ERROR=	-14.2 CM-1	OR	-3.2 PERCENT			
INTERNAL COORDINATES-	10.20 C2C3	10.11 CCO*	8.93 C3CC	6.66 CCO6	6.19 CCH3	5.44 CCO9	5.22 HC5C				
FORCE CONSTANTS-	33.00 CCO	25.11 CCH	23.42 CCH	5.74 CC							
OFF DIAGONAL-	7.39 BB43	-5.37 BB34	-5.25 BB29	-1.56 BB41	1.52 SB22						
NORMAL MODE 45	OBSERVED=	422.0 CM-1	CALCULATED=	426.3 CM-1	ERROR=	-4.3 CM-1	OR	-1.0 PERCENT			
INTERNAL COORDINATES-	16.72 O9CC	13.15 O-0C	12.77 CCO	9.38 CCO7	8.26 CCO*	8.03 C1CC	5.07 C-0C				
FORCE CONSTANTS-	50.57 CCO	14.46 CCH	12.77 CCO	6.83 CC	6.07 CC	5.07 CCH					
OFF DIAGONAL-	6.31 SB22	4.80 SB25	-4.22 BB42	-3.97 SB21	-3.85 BB34	-1.53 SB27					
NORMAL MODE 46	OBSERVED=	404.0 CM-1	CALCULATED=	388.5 CM-1	ERROR=	15.5 CM-1	OR	3.8 PERCENT			
INTERNAL COORDINATES-	14.93 C2CC	12.36 O8CC	8.30 CCO	8.15 CCO8	6.77 C3CC	5.50 C1CC					
FORCE CONSTANTS-	42.47 CCO	27.20 CCH	8.30 CCO	6.80 CCH	6.79 CCH						
OFF DIAGONAL-	-5.39 BB34	-4.74 BB42	4.33 SB21	4.11 SB25	1.71 SB24	-1.60 BB41					
NORMAL MODE 47	OBSERVED=	361.0 CM-1	CALCULATED=	369.2 CM-1	ERROR=	-8.2 CM-1	OR	-2.3 PERCENT			
INTERNAL COORDINATES-	52.00 CCO	25.31 CCH	10.10 CCH	8.14 CCO8	6.49 CCO						
FORCE CONSTANTS-	52.00 CCO	25.31 CCH	10.10 CCH	8.14 CCO8	6.49 CCO						
OFF DIAGONAL-	-7.93 BB34	3.83 BB43	-3.50 SB26	-3.44 BB29	2.66 SB21	-2.14 BB33	1.55 SB24				
NORMAL MODE 48	OBSERVED=	327.0 CM-1	CALCULATED=	322.6 CM-1	ERROR=	4.4 CM-1	OR	1.3 PERCENT			
INTERNAL COORDINATES-	5.36 CCO8	10.73 CCO9	8.86 CCO*	6.95 C3C4	6.37 O7CC	5.55 CCO*					
FORCE CONSTANTS-	57.80 CCO	17.23 CC	11.61 CCH	6.56 CCH							
OFF DIAGONAL-	-8.41 BB34	5.32 SB21	3.52 BB43	2.57 SB22	-1.95 BB29						
NORMAL MODE 49	OBSERVED=	316.0 CM-1	CALCULATED=	312.8 CM-1	ERROR=	3.2 CM-1	OR	1.0 PERCENT			
INTERNAL COORDINATES-	22.95 CCO7	9.72 CCO9	8.46 O9CC	6.94 CCO*	6.14 CCO*	5.90 TH-2	5.29 O7CC				
FORCE CONSTANTS-	68.27 CCO	9.51 T-0H	7.74 CC	5.04 CO							
OFF DIAGONAL-	-5.29 BB34	4.58 SB22	-3.79 BB42								
NORMAL MODE 50	OBSERVED=	302.0 CM-1	CALCULATED=	304.3 CM-1	ERROR=	-2.3 CM-1	OR	-0.8 PERCENT			
INTERNAL COORDINATES-	27.57 O8CC	14.94 CCO8	14.63 O9CC	8.53 O7CC	6.40 TH-3	5.46 CCO*					
FORCE CONSTANTS-	67.27 CCO	13.72 T-0H	11.23 CCH	6.56 CCH							
OFF DIAGONAL-	-10.75 BB34	-3.19 BB42	1.65 SB25	-1.54 BB36							
NORMAL MODE 51	OBSERVED=	0.0 CM-1	CALCULATED=	257.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	59.36 CCO	18.95 O-0C	12.81 T-0H	8.03 CCH	7.32 O7CC	5.02 HC2C					
FORCE CONSTANTS-	59.36 CCO	18.95 O-0C	12.81 T-0H	8.03 CCH	7.32 O7CC	5.02 HC2C					
OFF DIAGONAL-	-8.95 BB34	7.14 BB43	-3.61 SB25	-3.26 BB33	-2.48 BB29	1.66 SB22					
NORMAL MODE 52	OBSERVED=	0.0 CM-1	CALCULATED=	237.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	59.71 TH-0	12.01 CCO	5.79 TH-4								
FORCE CONSTANTS-	76.40 T-0H										
OFF DIAGONAL-	NONE										
NORMAL MODE 53	OBSERVED=	0.0 CM-1	CALCULATED=	229.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	50.12 TH-1	26.63 TH-3	8.71 TH-4								
FORCE CONSTANTS-	93.96 T-0H										
OFF DIAGONAL-	NONE										
NORMAL MODE 54	OBSERVED=	0.0 CM-1	CALCULATED=	222.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	44.31 TH-4	19.28 TH-5	17.88 TH-1								
FORCE CONSTANTS-	89.52 T-0H	5.25 CCO									
OFF DIAGONAL-	NONE										
NORMAL MODE 55	OBSERVED=	0.0 CM-1	CALCULATED=	219.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	37.37 TH-3	28.77 TH-4	9.84 TH-1								
FORCE CONSTANTS-	83.12 T-0H	14.18 CCO									
OFF DIAGONAL-	-1.81 BB34										
NORMAL MODE 56	OBSERVED=	0.0 CM-1	CALCULATED=	213.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	69.27 TH-0	12.47 TH-3									
FORCE CONSTANTS-	83.64 T-0H	14.45 CCO									
OFF DIAGONAL-	NONE										
NORMAL MODE 57	OBSERVED=	0.0 CM-1	CALCULATED=	190.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	30.77 CCO*	15.07 TH-5	13.42 C4CC	8.50 C-0C	6.02 TCC5	5.92 CCO*					
FORCE CONSTANTS-	46.41 CCO	19.29 T-0H	15.19 CCH	8.50 CCH	8.37 T-CC	6.35 CCH					
OFF DIAGONAL-	-4.41 BB34	-3.19 BB42	-2.68 BB33								
NORMAL MODE 58	OBSERVED=	0.0 CM-1	CALCULATED=	131.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	20.32 C-0C	19.55 C4CC	8.66 TCC4	5.84 TCO1	5.45 C1CC	5.18 CCO					
FORCE CONSTANTS-	26.67 CCH	20.32 CCH	12.51 CCO	9.75 T-CC	9.63 T-CC	5.18 CCO					
OFF DIAGONAL-	-4.15 SB21	3.33 BB43	-2.24 BB37	2.11 BB41	2.07 SB22						
NORMAL MODE 59	OBSERVED=	0.0 CM-1	CALCULATED=	101.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	58.16 TCC5	8.34 C3CC	6.42 O9CC								
FORCE CONSTANTS-	67.27 T-CC	14.39 CCH	14.39 CCH								
OFF DIAGONAL-	-2.83 BB34	-2.80 SB25	-1.72 BB42								
NORMAL MODE 60	OBSERVED=	0.0 CM-1	CALCULATED=	82.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	43.93 C2C3	15.34 C-0C	7.82 C-0C	7.77 T-CC	6.93 TCC4	5.24 CCO8	5.17 O8CC				
FORCE CONSTANTS-	43.93 CCH	25.19 T-CC	19.59 CCO	8.02 CCH	5.53 T-CC						
OFF DIAGONAL-	-4.65 SB25	-4.27 BB42	-3.61 SB21	2.62 BB41	-1.54 SB27						
NORMAL MODE 61	OBSERVED=	0.0 CM-1	CALCULATED=	65.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	25.55 TCC5	13.92 C3CC	9.36 TCC4	7.17 TCC2	7.17 TCC3	5.80 CCO*					
FORCE CONSTANTS-	49.97 T-CC	22.02 CCO	21.54 CCH								
OFF DIAGONAL-	-2.59 BB42	-2.03 BB34	-1.63 SB25								

40. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 5.53

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR										PROBLEM	400	PAGE 1	
MOLECULE 19										-6	NG=1236	ALPHA	GG
NORMAL MODE 8		OBSERVED=	1457.0	CM-1	CALCULATED=		1455.2	CM-1	ERROR=	1.8	CM-1	OR	0.1 PERCENT
INTERNAL COORDINATES-		67.98	C2CH										
FORCE CONSTANTS-		68.42	BCOH	6.58	CCH	6.05	CCO						
OFF DIAGONAL-		4.45	BB36	3.84	SB28	1.77	SB25	1.68	BB34				
NORMAL MODE 9		OBSERVED=	1442.0	CM-1	CALCULATED=		1450.2	CM-1	ERROR=	-8.2	CM-1	OR	-0.6 PERCENT
INTERNAL COORDINATES-		60.52	HCH	20.63	CCHB	19.74	OCHA						
FORCE CONSTANTS-		60.52	HCH	40.55	OCH								
OFF DIAGONAL-		-4.23	SB27										
NORMAL MODE 10		OBSERVED=	1427.0	CM-1	CALCULATED=		1422.1	CM-1	ERROR=	4.9	CM-1	OR	0.3 PERCENT
INTERNAL COORDINATES-		25.02	C3OH	19.70	C4OH	12.48	OC4H	6.62	HC4C	5.45	CC5H		
FORCE CONSTANTS-		45.37	BCOH	19.81	CCH	19.00	OCH	7.22	CO	6.54	CC	5.76	CCO
OFF DIAGONAL-		-5.12	SB27	-4.59	SB26	3.82	BB29	3.68	SB28	-2.91	SB25	2.70	BB34
NORMAL MODE 11		OBSERVED=	1409.0	CM-1	CALCULATED=		1413.7	CM-1	ERROR=	-4.7	CM-1	OR	-0.3 PERCENT
INTERNAL COORDINATES-		41.32	C3OH	9.55	OC3H	5.75	OC4H	5.51	C2C3				
FORCE CONSTANTS-		45.09	BCOH	26.12	OCH	16.66	CCH	6.06	CC	5.87	CO		
OFF DIAGONAL-		-5.11	SB27	4.02	SB28	-3.87	SB26	3.57	BB29	2.27	BB36	-1.84	BB39
NORMAL MODE 12		OBSERVED=	0.0	CM-1	CALCULATED=		1408.8	CM-1	ERROR=	0.0	CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-		54.23	C1OH	20.80	OC1H								
FORCE CONSTANTS-		56.84	BCOH	30.22	OCH	8.73	CCH						
OFF DIAGONAL-		4.77	SB28	-4.46	SB27	-3.07	BB39						
NORMAL MODE 13		OBSERVED=	1385.0	CM-1	CALCULATED=		1396.1	CM-1	ERROR=	-11.1	CM-1	OR	-0.8 PERCENT
INTERNAL COORDINATES-		61.71	C1OH	8.79	CCHB	8.02	OC4H	7.04	CCHA	5.52	HCH		
FORCE CONSTANTS-		62.75	BCOH	20.89	CCH	11.26	OCH	5.52	HCH				
OFF DIAGONAL-		3.48	SB28	-2.90	SB26	-2.65	BB39	-2.60	SB27				
NORMAL MODE 14		OBSERVED=	1381.0	CM-1	CALCULATED=		1387.3	CM-1	ERROR=	-6.3	CM-1	OR	-0.4 PERCENT
INTERNAL COORDINATES-		41.25	C1OH	21.98	C1OH	16.43	OC1H	7.24	C4OH				
FORCE CONSTANTS-		60.24	OCH	30.29	BCOH								
OFF DIAGONAL-		-4.10	SB27	2.88	BB37	-2.36	BB45	-1.61	SB26				
NORMAL MODE 15		OBSERVED=	1375.0	CM-1	CALCULATED=		1371.0	CM-1	ERROR=	3.9	CM-1	OR	0.3 PERCENT
INTERNAL COORDINATES-		56.98	C4OH	7.46	C3OH	5.73	CC5H	5.54	HC3C	5.08	OC3H		
FORCE CONSTANTS-		65.52	BCOH	16.48	CCH	15.34	OCH						
OFF DIAGONAL-		-3.07	BB36	-2.63	SB28	2.52	BB29	-1.56	SB27				
NORMAL MODE 16		OBSERVED=	1371.0	CM-1	CALCULATED=		1365.8	CM-1	ERROR=	5.2	CM-1	OR	0.4 PERCENT
INTERNAL COORDINATES-		18.95	OC2H	12.71	HC2C	10.01	AC5H	8.24	HC4C	7.67	CC5H	7.29	OC3H
FORCE CONSTANTS-		43.15	CCH	37.30	OCH	14.03	BCOH	6.78	CO			6.89	C3OH
OFF DIAGONAL-		8.65	BB29	-6.77	SB27	-3.58	SB26	-3.31	BB45	2.91	BB34	-2.09	SB28
NORMAL MODE 17		OBSERVED=	1343.0	CM-1	CALCULATED=		1335.6	CM-1	ERROR=	7.4	CM-1	OR	0.5 PERCENT
INTERNAL COORDINATES-		16.05	C2CH	12.91	OC5H	12.93	OC2H	11.67	HC5C	7.55	HC3C	6.82	HC2C
FORCE CONSTANTS-		45.54	CCH	33.41	OCH	17.33	BCOH					5.83	CCHB
OFF DIAGONAL-		-6.02	SB27	5.02	BB29	-3.24	BB45	-2.16	SB26	-2.13	SB28		
NORMAL MODE 18		OBSERVED=	1328.0	CM-1	CALCULATED=		1328.5	CM-1	ERROR=	-0.5	CM-1	OR	-0.0 PERCENT
INTERNAL COORDINATES-		14.78	HC3C	11.68	CCHA	8.89	OCHA	7.26	CC4H	6.58	C1OH	6.41	HC5C
FORCE CONSTANTS-		57.44	CCH	28.44	OCH	7.67	BCOH	6.95	CC			6.29	OC1H
OFF DIAGONAL-		8.10	BB29	-6.64	SB26	-3.68	BB45	-2.33	SB27			6.10	OC3H
NORMAL MODE 19		OBSERVED=	0.0	CM-1	CALCULATED=		1312.1	CM-1	ERROR=	0.0	CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-		27.16	CCH2	12.94	CC1H	10.67	C1OH	10.56	OC2H	5.59	C-O6	5.02	HC2C
FORCE CONSTANTS-		42.64	CCH	21.43	OCH	14.46	CO	13.55	BCOH				
OFF DIAGONAL-		-3.35	SB28	-3.11	BB45	2.49	BB34	-2.25	SB26	-2.20	SB25		
NORMAL MODE 20		OBSERVED=	1298.0	CM-1	CALCULATED=		1294.1	CM-1	ERROR=	3.9	CM-1	OR	0.3 PERCENT
INTERNAL COORDINATES-		21.66	OC4H	16.16	OCHA	13.79	CCHA	11.25	HC4C	9.57	CC5H	6.88	OC3H
FORCE CONSTANTS-		61.26	OCH	36.04	CCH							5.32	OC4H
OFF DIAGONAL-		-3.91	BB45	1.86	BB34	-1.82	BB29	-1.52	SB27				
NORMAL MODE 21		OBSERVED=	1288.0	CM-1	CALCULATED=		1281.7	CM-1	ERROR=	6.3	CM-1	OR	0.5 PERCENT
INTERNAL COORDINATES-		10.97	CC1H	10.39	OC1H	9.83	CCBH	9.39	OCBH	9.11	CCH2	7.01	C-O6
FORCE CONSTANTS-		43.98	CCH	27.14	CO	15.54	CO					6.45	OC1
OFF DIAGONAL-		-3.00	BB45	2.95	BB34	-2.85	SB25	2.83	BB29	2.53	SB27		
NORMAL MODE 22		OBSERVED=	1270.0	CM-1	CALCULATED=		1268.9	CM-1	ERROR=	1.1	CM-1	OR	0.1 PERCENT
INTERNAL COORDINATES-		16.39	C5H	15.51	CC1H	13.32	OC4H	9.69	CCHB	8.45	OC4H	7.85	C1H
FORCE CONSTANTS-		50.77	OCH	37.17	CCH	5.80	CO						
OFF DIAGONAL-		-3.53	BB45	2.64	BB34	-1.83	BB29						
NORMAL MODE 23		OBSERVED=	1261.0	CM-1	CALCULATED=		1259.6	CM-1	ERROR=	1.4	CM-1	OR	0.1 PERCENT
INTERNAL COORDINATES-		27.47	OC3H	19.75	CC4H	7.51	C5H	6.16	OC4H	5.67	CC3H		
FORCE CONSTANTS-		46.15	OCH	40.70	CCH	5.60	CO						
OFF DIAGONAL-		7.40	SB27	-3.61	BB29	-3.48	BB45	3.17	BB34	-1.61	SB25	1.52	BB43
NORMAL MODE 24		OBSERVED=	1224.0	CM-1	CALCULATED=		1220.0	CM-1	ERROR=	-4.0	CM-1	OR	-0.3 PERCENT
INTERNAL COORDINATES-		14.43	OC4H	13.86	HC5C	8.46	CC5H	8.41	CC3H	7.14	OC3H		
FORCE CONSTANTS-		42.61	CCH	32.90	OCH	13.69	CO						
OFF DIAGONAL-		6.65	SB27	-4.12	BB29	-3.22	SB25	-2.98	BB45	2.28	BB34	1.70	BB43
NORMAL MODE 25		OBSERVED=	1203.0	CM-1	CALCULATED=		1181.3	CM-1	ERROR=	21.7	CM-1	OR	1.8 PERCENT
INTERNAL COORDINATES-		17.78	OC1H	12.57	HC5C	11.59	C5H	8.45	CC5H	7.38	OC2H	6.08	C2OH
FORCE CONSTANTS-		42.80	CCH	37.85	CO	16.29	OCH	9.42	CCO	7.76	BCOH	5.72	CC3H
OFF DIAGONAL-		-6.77	SB25	-5.11	SB26	-3.51	BB29	2.67	SB27	-2.44	BB45	5.04	OC4H
NORMAL MODE 26		OBSERVED=	1147.0	CM-1	CALCULATED=		1147.6	CM-1	ERROR=	-0.6	CM-1	OR	-0.0 PERCENT
INTERNAL COORDINATES-		17.59	C5C	13.27	OC1	12.85	C-O6	7.78	CCO	7.49	C4C5	5.96	OCHA
FORCE CONSTANTS-		41.62	CO	27.64	CC	17.01	CCH	13.33	OCH	13.13	C-CO	5.17	C-O7
OFF DIAGONAL-		-5.07	SB22	-3.12	SS18	-2.67	SB26	-2.32	SB25	-1.76	SB23	-1.65	SB28
NORMAL MODE 27		OBSERVED=	1126.0	CM-1	CALCULATED=		1140.5	CM-1	ERROR=	-14.5	CM-1	OR	-1.3 PERCENT
INTERNAL COORDINATES-		19.54	C5O	9.18	OCHA	7.38	OC1	6.16	C4C5	6.14	CC4H	5.80	CC4H
FORCE CONSTANTS-		35.72	CCH	31.00	CO	21.35	OCH	12.30	CC	9.69	CCO	5.79	OCBH
OFF DIAGONAL-		-6.20	BB29	-3.80	SB25	3.31	BB34	-3.24	SB22	-1.98	SB27	-1.91	BB43
NORMAL MODE 28		OBSERVED=	1118.0	CM-1	CALCULATED=		1122.0	CM-1	ERROR=	-4.0	CM-1	OR	-0.3 PERCENT
INTERNAL COORDINATES-		28.63	C-O7	16.30	C-O9	8.83	C2OH	7.75	C-O1	5.59	C5C1	5.54	C4C5
FORCE CONSTANTS-		32.72	CO	41.55	CCH	13.82	CCH	12.95	BCOH	9.83	OCH	8.95	CCH
OFF DIAGONAL-		-12.47	SB25	-9.30	SB28	8.54	SB27	-4.68	SB26	-4.28	SB22	-1.68	BB36
NORMAL MODE 29		OBSERVED=	1109.0	CM-1	CALCULATED=		1112.4	CM-1	ERROR=	-3.4	CM-1	OR	-0.3 PERCENT
INTERNAL COORDINATES-		25.99	C4C5	14.61	C-O7	10.93	C-O6	10.92	C5C	10.27	C3C4	7.95	C2C3
FORCE CONSTANTS-		55.31	CC	44.23	CCH	14.36	CO	9.40	OCH	8.91	CCC		
OFF DIAGONAL-		-8.80	SB22	-5.92	SB27	-5.44	SB25	-4.33	SB21	-4.01	SB26	-2.45	SS18
NORMAL MODE 30		OBSERVED=	1078.0	CM-1	CALCULATED=		1078.4	CM-1	ERROR=	-0.4	CM-1	OR	-0.0 PERCENT
INTERNAL COORDINATES-		44.23	C-O8	21.88	C3C4	11.52	OC1	7.70	C5C				
FORCE CONSTANTS-		61.56	CO	32.01	CC	9.45	CCH	7.81	CCH	7.44	OCH	7.23	CCC
OFF DIAGONAL-		-6.88	SS18	-6.13	SB27	-5.05	SB28	-3.91	SB25	-3.37	SB21	-2.97	SB22
NORMAL MODE 31		OBSERVED=	1072.0	CM-1	CALCULATED=		1063.3	CM-1	ERROR=	8.7	CM-1	OR	0.8 PERCENT
INTERNAL COORDINATES-		61.35	C1C2	18.37	C2C3	15.15	CCO	12.87	OCH	11.28	BCOH	9.43	CCH
FORCE CONSTANTS-		86.64	CC	23.79	CCH	15.15	CCO	12.87	OCH	11.28	BCOH	9.43	CCH
OFF DIAGONAL-		-16.83	SB22	-14.79	SB26	-7.15	SB27	-6.98	SS18	-5.46	SB28	-3.80	SB21
NORMAL MODE 32		OBSERVED=	1065.0	CM-1	CALCULATED=		1050.3	CM-1	ERROR=	14.7	CM-1	OR	1.4 PERCENT
INTERNAL COORDINATES-		33.62	C-O8	14.87	C3C4	12.24	C-O9	10.54	C5C	9.90	C4C5	9.74	C4CC
FORCE CONSTANTS-		52.46	CO	40.06	CCH	16.79	CCO	12.08	CCH	10.86	OCH	8.93	BCOH
OFF DIAGONAL-		-17.64	SB21	-8.80	SB27	-7.95	SS18	-6.50	SB28	-3.99	SB25	-1.72	SB26
NORMAL MODE 33		OBSERVED=	1053.0	CM-1	CALCULATED=		1047.8	CM-1	ERROR=	5.2	CM-1	OR	0.5 PERCENT
INTERNAL COORDINATES-		32.72	C-O9	12.49	C-O7	9.15	C2C3	7.61	C-O6	5.01	OC1		
FORCE CONSTANTS-		64.09	CO	14.66	CC	13.73	CCH	13.18	OCH	11.12	CCC	6.53	CCC
OFF DIAGONAL-		-7.23	SB25	-6.13	SB21	-4.42	SB28	-3.99	SS18	-3.98	SB27	-2.84	SB24
NORMAL MODE 34		OBSERVED=	1019.0	CM-1	CALCULATED=		1014.9	CM-1	ERROR=	4.1	CM-1	OR	0.4 PERCENT
INTERNAL COORDINATES-		21.52	C3C4	13.69	C-O8	10.93	C-O9	8.77	CC4H	6.54	C-O6	6.03	C-O8
FORCE CONSTANTS-		43.31	CO	30.57	CCH	28.86	CC	12.46	CCO	6.67	BCOH	5.89	HC4C
OFF DIAGONAL-		-7.31	SB22	-5.22	BB29	-5.12	SB28	-4.35	SB25	-2.83	SB26	-2.38	SB27
NORMAL MODE 35		OBSERVED=	997.0	CM-1	CALCULATED=		987.1	CM-1	ERROR=	9.9	CM-1	OR	1.0 PERCENT
INTERNAL COORDINATES-		18.53	C-O8	16.66	C-O7	15.16	C-O6	12.18	C3C4	10.42	C1C2	7.61	C2C3
FORCE CONSTANTS-		59.67	CO	34.29	CCH	16.54	CCH	10.95	CCO	10.20	BCOH	5.49	C3OH
OFF DIAGONAL-		-8.19	SB28	-7.16	SB22	-6.29	SB26	-3.91	SB24	-3.75	SB27	-2.48	SB25

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400				PAGE 2	
MOLECULE 19				GG	
NG=1236 ALPHA					
NORMAL MODE 36	OBSERVED=	0.0 CM-1	CALCULATED=	918.8 CM-1	ERROR= 0.0 CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	12.60	C-08 13.88 C4C5	10.15 CCO	8.39 CCH2	5.70 O'C1
FORCE CONSTANTS-	22.53	CO 33.88 CCH	16.21 CCH	6.09 CCH	5.82 CCO
OFF DIAGONAL-	-9.25	SB21 -6.25 SB27	6.17 SB26	-5.27 SB22	2.08 BB43
NORMAL MODE 37	OBSERVED=	915.0 CM-1	CALCULATED=	903.9 CM-1	ERROR= 11.0 CM-1 OR 1.2 PERCENT
INTERNAL COORDINATES-	15.88	C2C3 20.60 C-U6	9.83 CCH2	9.41 CCO8	6.26 C1C2
FORCE CONSTANTS-	35.17	CC 25.88 CO	23.31 CCH	17.00 CCO	
OFF DIAGONAL-	-9.75	SB22 -7.25 SB21	3.51 SB26	2.32 SS18	2.26 BB43 -2.16 SB24
NORMAL MODE 38	OBSERVED=	837.0 CM-1	CALCULATED=	847.4 CM-1	ERROR= -10.4 CM-1 OR -1.2 PERCENT
INTERNAL COORDINATES-	26.41	C5O* 17.11 CCH8	15.49 CCHA	6.91 O'C1	6.19 C5C1
FORCE CONSTANTS-	40.50	CO 36.44 CCH	13.37 CCH	8.20 CCO	8.11 CCH
OFF DIAGONAL-	-4.02	SB23 -2.73 SB25	-2.34 BB34	-2.15 SB24	-1.93 SB22 1.67 SS18
NORMAL MODE 39	OBSERVED=	775.0 CM-1	CALCULATED=	758.2 CM-1	ERROR= 16.8 CM-1 OR 2.2 PERCENT
INTERNAL COORDINATES-	11.11	CO'C 8.73 C-U6	7.16 CCH	6.80 C1CC	6.65 CCO6
FORCE CONSTANTS-	21.16	CCO 15.92 CO	14.02 CCH	11.17 CCH	11.11 CCH
OFF DIAGONAL-	-5.32	BB43 4.11 SB25	-2.94 SB27	2.31 SB24	-2.28 BB41 1.64 SS18 1.59 SB22
NORMAL MODE 40	OBSERVED=	620.0 CM-1	CALCULATED=	716.7 CM-1	ERROR= -96.7 CM-1 OR -15.6 PERCENT
INTERNAL COORDINATES-	18.67	CCO* 6.87 CCH5	6.70 O8CC	6.16 C4CC	5.67 CCO6
FORCE CONSTANTS-	47.06	CCO 23.45 CCH	7.92 CO	6.87 CC	6.56 CCH
OFF DIAGONAL-	-7.41	BB43 6.60 SB25	-6.55 BB34	-4.60 BB29	4.20 SB21 -2.47 SB27 -2.03 BB41 -1.62 SB22
NORMAL MODE 41	OBSERVED=	605.0 CM-1	CALCULATED=	594.1 CM-1	ERROR= 10.9 CM-1 OR 1.8 PERCENT
INTERNAL COORDINATES-	18.11	CCO 13.91 CCH7	10.15 CCO	7.39 CCH2	5.70 O'C1
FORCE CONSTANTS-	40.11	CCO 13.42 CC	13.04 CO	10.15 CCO	6.16 CCH
OFF DIAGONAL-	-4.09	SB24 3.01 SS18	-2.68 BB42	-2.60 BB34	2.17 BB43 -2.00 SB27 -1.94 SB23 -1.81 BB41 1.53 SB25
NORMAL MODE 42	OBSERVED=	556.0 CM-1	CALCULATED=	540.6 CM-1	ERROR= 15.4 CM-1 OR 2.8 PERCENT
INTERNAL COORDINATES-	17.88	O7CC 11.57 O'CC	11.38 CCO9	6.70 CCO	5.94 CCH3
FORCE CONSTANTS-	60.53	CCO 21.10 CCH	7.04 CC	6.80 CO	6.70 CCO
OFF DIAGONAL-	-11.18	BB34 5.53 BB43	-4.35 BB29	-3.78 SB21	3.45 SB25 -2.33 BB42 -1.55 BB36
NORMAL MODE 43	OBSERVED=	539.0 CM-1	CALCULATED=	530.5 CM-1	ERROR= 8.5 CM-1 OR 1.6 PERCENT
INTERNAL COORDINATES-	11.40	O9CC 10.70 C4C5	5.35 O8CC	5.31 HC4C	5.11 C4CC
FORCE CONSTANTS-	27.88	CCO 23.75 CCH	17.40 CCH	11.82 CO	5.84 CCH
OFF DIAGONAL-	-6.81	SB22 5.78 SB25	5.21 BB43	-4.73 BB34	4.20 SS18 -3.51 BB29 -2.95 SB21 -2.07 SB26 -1.98 SB27
NORMAL MODE 44	OBSERVED=	439.0 CM-1	CALCULATED=	510.6 CM-1	ERROR= -71.6 CM-1 OR -16.3 PERCENT
INTERNAL COORDINATES-	21.46	CCO* 18.23 CCO	11.56 CCO*	10.23 CCO9	7.38 O8CC
FORCE CONSTANTS-	63.52	CCO 18.23 CCO	16.77 CCH	10.23 CCO9	7.38 O8CC
OFF DIAGONAL-	-9.92	BB34 -3.84 SB22	3.37 BB43	-2.93 BB42	2.68 SB24 -1.94 BB29 1.91 SB25 1.73 SB21 -1.54 BB41
NORMAL MODE 45	OBSERVED=	422.0 CM-1	CALCULATED=	431.6 CM-1	ERROR= -9.6 CM-1 OR -2.3 PERCENT
INTERNAL COORDINATES-	11.95	O9CC 11.34 C2CC	9.84 C1CC	8.48 CCO*	6.12 CCO
FORCE CONSTANTS-	5.30	CCO 11.34 C2CC	9.84 C1CC	8.48 CCO*	6.12 CCO
OFF DIAGONAL-	-5.30	SB22 3.11 BB43	2.36 SB25	-1.98 BB41	-1.91 BB29
NORMAL MODE 46	OBSERVED=	404.0 CM-1	CALCULATED=	400.3 CM-1	ERROR= 3.7 CM-1 OR 0.9 PERCENT
INTERNAL COORDINATES-	18.41	C3C 10.49 O'CC	13.13 CCO	12.59 CCO	6.50 O8CC
FORCE CONSTANTS-	36.84	CCO 34.34 CCH	12.55 CCO		6.01 O9CC
OFF DIAGONAL-	-5.39	BB42 5.00 SB21	4.05 SB25	-1.74 BB41	
NORMAL MODE 47	OBSERVED=	361.0 CM-1	CALCULATED=	355.2 CM-1	ERROR= 5.8 CM-1 OR 1.6 PERCENT
INTERNAL COORDINATES-	24.06	CCO8 14.18 CCO*	11.90 CCO7	5.29 C1CC	5.28 HC4C
FORCE CONSTANTS-	69.21	CCO 23.50 CCH	10.92 CCH	5.44 CC	
OFF DIAGONAL-	-13.81	BB34 -4.41 BB29	3.90 BB43	3.17 SB21	-1.85 SB26
NORMAL MODE 48	OBSERVED=	327.0 CM-1	CALCULATED=	319.6 CM-1	ERROR= 7.4 CM-1 OR 2.3 PERCENT
INTERNAL COORDINATES-	23.53	O7CC 20.02 CCO7	11.08 CCO9	8.25 TH-2	6.12 C3C4
FORCE CONSTANTS-	65.01	CCO 10.74 CCH	10.15 CCO	5.56 CCO	5.43 CCH
OFF DIAGONAL-	-6.43	BB34 3.36 SB22	-3.37 BB42		
NORMAL MODE 49	OBSERVED=	316.0 CM-1	CALCULATED=	313.4 CM-1	ERROR= 2.6 CM-1 OR 1.1 PERCENT
INTERNAL COORDINATES-	18.41	O8C 20.71 CCO8	9.84 O9CC	9.23 CCO*	7.38 TH-3
FORCE CONSTANTS-	85.71	CCO 10.59 T-UH	6.34 CCH	6.13 CC	
OFF DIAGONAL-	-6.89	BB34 -4.73 BB42	-2.17 SB21	-1.92 SB26	-1.89 BB36 1.51 BB41 -1.51 BB43
NORMAL MODE 50	OBSERVED=	302.0 CM-1	CALCULATED=	275.8 CM-1	ERROR= 26.2 CM-1 OR 8.7 PERCENT
INTERNAL COORDINATES-	23.92	CCO 14.99 C4CC	11.52 TH-3	10.50 O9CC	5.14 TH-4
FORCE CONSTANTS-	55.92	CCO 19.09 T-OH	17.13 CCH	10.03 CCH	
OFF DIAGONAL-	-7.07	BB34 -3.39 BB42	-2.67 BB33	-2.07 SB25	1.64 SB22
NORMAL MODE 51	OBSERVED=	0.0 CM-1	CALCULATED=	263.9 CM-1	ERROR= 0.0 CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	21.61	CCO6 10.03 O'CC	8.13 TH-5	6.57 CCH2	6.39 CCO8
FORCE CONSTANTS-	54.66	CCO 19.92 CCH	13.44 T-OH	10.60 CCH	
OFF DIAGONAL-	-6.87	BB34 6.36 BB43	-3.63 BB33	-3.07 SB25	-1.66 BB29 1.60 SB22
NORMAL MODE 52	OBSERVED=	0.0 CM-1	CALCULATED=	247.3 CM-1	ERROR= 0.0 CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	31.60	TH-1 9.01 CCO*	6.77 CCO*	6.17 CCO9	
FORCE CONSTANTS-	39.73	T-OH 19.10 CCO	9.82 CCH	6.17 CCO9	
OFF DIAGONAL-	-4.31	BB43 -3.40 BB34	3.19 SB22	-2.12 BB33	-1.74 SB26
NORMAL MODE 53	OBSERVED=	0.0 CM-1	CALCULATED=	225.8 CM-1	ERROR= 0.0 CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	23.36	TH-3 32.51 TH-4	10.01 TH-5		
FORCE CONSTANTS-	93.84	T-OH			
OFF DIAGONAL-	NONE				
NORMAL MODE 54	OBSERVED=	0.0 CM-1	CALCULATED=	223.7 CM-1	ERROR= 0.0 CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	34.67	TH-1 23.31 TH-5	12.34 TH-4	9.38 TH-3	5.27 CCO*
FORCE CONSTANTS-	82.76	T-OH 10.47 CCO			
OFF DIAGONAL-	NONE				
NORMAL MODE 55	OBSERVED=	0.0 CM-1	CALCULATED=	214.6 CM-1	ERROR= 0.0 CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	36.40	TH-4 17.56 TH-2	11.14 TH-5	8.47 TH-3	6.02 TH-1
FORCE CONSTANTS-	79.59	T-OH 17.01 CCO			
OFF DIAGONAL-	-2.13	BB34			
NORMAL MODE 56	OBSERVED=	0.0 CM-1	CALCULATED=	213.1 CM-1	ERROR= 0.0 CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	58.84	TH-2 9.92 TH-3	7.38 TH-4	5.56 TH-5	
FORCE CONSTANTS-	82.87	T-OH 14.82 CCO			
OFF DIAGONAL-	-1.80	BB34			
NORMAL MODE 57	OBSERVED=	0.0 CM-1	CALCULATED=	209.3 CM-1	ERROR= 0.0 CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	23.22	TH-5 19.73 TH-1	13.72 TH-3	6.15 C4CC	5.71 CCO*
FORCE CONSTANTS-	56.99	T-OH 19.10 CCO	9.99 CCH	5.34 CCH	
OFF DIAGONAL-	2.31	BB43 -1.81 BB34	1.52 SB21		
NORMAL MODE 58	OBSERVED=	0.0 CM-1	CALCULATED=	132.0 CM-1	ERROR= 0.0 CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	23.55	CO 0.0 CM-1	10.42 TH-4	7.75 C1CC	6.89 TCO1
FORCE CONSTANTS-	23.55	CCO 19.58 CCH	14.84 CCO	11.25 T-CC	10.59 T-CC
OFF DIAGONAL-	4.08	BB43 2.49 BB41	-2.44 BB37	-1.99 SB21	
NORMAL MODE 59	OBSERVED=	0.0 CM-1	CALCULATED=	88.0 CM-1	ERROR= 0.0 CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	28.77	TCC5 17.70 C2CC	8.66 TCC2	7.06 C1CC	6.18 C3CC
FORCE CONSTANTS-	44.93	T-CC 33.14 CCH	16.44 CCO		
OFF DIAGONAL-	-3.95	SB25 -3.25 BB42	-2.95 SB21	1.89 BB41	
NORMAL MODE 60	OBSERVED=	0.0 CM-1	CALCULATED=	76.6 CM-1	ERROR= 0.0 CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	47.95	TCC5 11.77 C3CC	8.07 TCC2	7.18 C2CC	
FORCE CONSTANTS-	59.60	T-CC 23.42 CCH	11.04 CCO		
OFF DIAGONAL-	-2.35	SB21 -2.19 BB42	-2.15 SB25		
NORMAL MODE 61	OBSERVED=	0.0 CM-1	CALCULATED=	70.0 CM-1	ERROR= 0.0 CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	14.24	TCC4 11.96 C1CC	10.29 CCO	7.77 TCC5	7.70 TCC3
FORCE CONSTANTS-	39.33	T-CC 31.36 CCH	23.16 CCH	6.11 T-CC	6.11 T-CC
OFF DIAGONAL-	-3.30	BB42 -2.88 BB34	-2.38 SB25	1.64 BB41	

40. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 11.39

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400	MOLECULE 20	-6	NG=1236	ALPHA	GLUCOSE	TG	PAGE 1
NORMAL MODE 8	OBSERVED=	1457.0	CM-1	CALCULATED=	1455.2	CM-1	ERROR= 1.8 CM-1 OR 0.1 PERCENT
INTERNAL COORDINATES-	67.81 C2OH						
FORCE CONSTANTS-	68.26 BCOH 6.61 CCH			6.07 CCO			
OFF DIAGONAL-	4.44 BB36 3.85 SB28			-1.79 SB25 1.69 BB34			
NORMAL MODE 9	OBSERVED=	1442.0	CM-1	CALCULATED=	1449.5	CM-1	ERROR= -7.5 CM-1 OR -0.5 PERCENT
INTERNAL COORDINATES-	58.29 HCH 22.20 OCHA			20.72 OCHB			
FORCE CONSTANTS-	58.29 HCH 43.08 OCH						
OFF DIAGONAL-	-4.47 SB27						
NORMAL MODE 10	OBSERVED=	1427.0	CM-1	CALCULATED=	1432.3	CM-1	ERROR= -5.3 CM-1 OR -0.4 PERCENT
INTERNAL COORDINATES-	9.67 CCHA 8.94 CC4H			8.47 C1OH 7.91 HC4C 7.35 C5O1			
FORCE CONSTANTS-	34.11 CCH 27.99 OCH			19.16 BCOH 11.84 CO 6.79 CCO			
OFF DIAGONAL-	-8.57 SB27 6.70 BB34			-5.90 SB26 5.31 RH29 -4.45 SB25			
NORMAL MODE 11	OBSERVED=	1409.0	CM-1	CALCULATED=	1416.4	CM-1	ERROR= -7.4 CM-1 OR -0.5 PERCENT
INTERNAL COORDINATES-	62.18 C3OH 7.92 C2C3			19.18 BC3H			
FORCE CONSTANTS-	69.90 BCOH 9.10 OCH			9.01 CC 8.47 CCH			
OFF DIAGONAL-	4.03 SB28 3.82 BB36			-3.79 SB26 -2.16 SB27 -1.66 BB39			
NORMAL MODE 12	OBSERVED=	1408.9	CM-1	CALCULATED=	1408.9	CM-1	ERROR= 0.0 CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	56.33 C1OH 21.67 OC1H			5.53 C1H			
FORCE CONSTANTS-	57.88 BCOH 30.77 UCH			7.40 CCH			
OFF DIAGONAL-	4.71 SB28 -4.32 SB27			-3.04 BB39			
NORMAL MODE 13	OBSERVED=	1385.0	CM-1	CALCULATED=	1402.1	CM-1	ERROR= -17.1 CM-1 OR -1.2 PERCENT
INTERNAL COORDINATES-	19.46 C4OH 19.45 C1OH			11.01 OC4H 5.86 CC4H 5.84 OC3H			
FORCE CONSTANTS-	42.19 BCOH 24.20 CCH			22.75 OCH 5.18 CO			
OFF DIAGONAL-	-5.58 SB26 -5.39 SB27			4.55 SB28 4.50 BB29 -2.36 BB39			
NORMAL MODE 14	OBSERVED=	1381.0	CM-1	CALCULATED=	1384.7	CM-1	ERROR= -3.7 CM-1 OR -0.3 PERCENT
INTERNAL COORDINATES-	43.07 C1H 21.48 C1OH			17.92 OC1H 8.12 C1OH			
FORCE CONSTANTS-	63.41 OCH 31.36 BCOH						
OFF DIAGONAL-	-4.08 SB27 2.66 BB37			-2.38 BB45 1.64 BB39 -1.62 SB26			
NORMAL MODE 15	OBSERVED=	1375.0	CM-1	CALCULATED=	1370.5	CM-1	ERROR= 4.5 CM-1 OR 0.3 PERCENT
INTERNAL COORDINATES-	49.50 C4OH 10.76 C3OH			8.37 OC3H 7.41 HC3C			
FORCE CONSTANTS-	68.41 BCOH 17.63 CCH			16.70 OCH			
OFF DIAGONAL-	2.94 BB29 -2.87 SB28			-2.84 BB36 -1.93 SB27 1.86 BB34			
NORMAL MODE 16	OBSERVED=	1371.0	CM-1	CALCULATED=	1367.0	CM-1	ERROR= 4.0 CM-1 OR 0.3 PERCENT
INTERNAL COORDINATES-	71.21 C1OH 12.91 C5H			5.61 HC4C 5.56 HC2C			
FORCE CONSTANTS-	41.98 HCCH 27.85 OCH			25.96 CCH			
OFF DIAGONAL-	5.40 BB29 -4.69 SB27			2.46 BB34 -2.19 BB45 -1.78 SB28			
NORMAL MODE 17	OBSERVED=	1343.0	CM-1	CALCULATED=	1347.6	CM-1	ERROR= -4.6 CM-1 OR -0.3 PERCENT
INTERNAL COORDINATES-	15.15 OC2H 11.70 HC5C			9.77 HC2C 9.76 CCHA 8.76 C1OH			
FORCE CONSTANTS-	49.39 CCH 29.19 OCH			13.15 BCOH 6.03 CC5H 5.98 OCHA			
OFF DIAGONAL-	10.72 BB29 -3.31 BB45			-3.29 SB27 -2.96 SB26 2.42 BB34 -2.28 SB28			
NORMAL MODE 18	OBSERVED=	1328.0	CM-1	CALCULATED=	1324.9	CM-1	ERROR= 3.1 CM-1 OR 0.2 PERCENT
INTERNAL COORDINATES-	20.00 HC3C 10.97 CC4H			9.75 OC2H 8.91 OC3H 8.57 HC4C			
FORCE CONSTANTS-	67.67 CCH 26.67 OCH			3.47 CC			
OFF DIAGONAL-	14.92 BB29 -9.88 SB26			-4.15 BB45 -2.40 SB27			
NORMAL MODE 19	OBSERVED=	1313.3	CM-1	CALCULATED=	1313.3	CM-1	ERROR= 0.0 CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	19.39 CCH2 13.37 CC1H			10.06 C1OH 9.35 OC2H 8.85 C5H			
FORCE CONSTANTS-	44.41 CCH 30.23 OCH			14.48 BCOH 7.28 OC1H 5.08 CCHB			
OFF DIAGONAL-	-3.18 BB45 2.62 BB34			-2.58 SB28			
NORMAL MODE 20	OBSERVED=	1298.0	CM-1	CALCULATED=	1295.5	CM-1	ERROR= 2.5 CM-1 OR -0.6 PERCENT
INTERNAL COORDINATES-	20.28 CCHB 12.59 OCHB			9.87 C1OH 10.72 CO			
FORCE CONSTANTS-	48.91 BCOH 24.91 CCH			11.75 BCOH			
OFF DIAGONAL-	3.21 BB34 -2.88 BB45			-1.75 SB28			
NORMAL MODE 21	OBSERVED=	1288.0	CM-1	CALCULATED=	1290.9	CM-1	ERROR= -2.9 CM-1 OR -0.2 PERCENT
INTERNAL COORDINATES-	20.19 OC4H 16.28 C5H			7.92 HC4C 7.51 OCHB 6.11 OCHA			
FORCE CONSTANTS-	59.96 OCH 32.35 CCH			6.24 CO			
OFF DIAGONAL-	-3.67 BB45 -2.89 BB29			2.04 BB34			
NORMAL MODE 22	OBSERVED=	1270.0	CM-1	CALCULATED=	1272.0	CM-1	ERROR= -2.0 CM-1 OR -0.2 PERCENT
INTERNAL COORDINATES-	24.33 CC1H 8.75 OC4H			8.51 C5H 7.89 C1H 6.72 OC1H			
FORCE CONSTANTS-	46.01 CCH 33.91 OCH			11.96 CO			
OFF DIAGONAL-	4.47 BB34 -3.38 BB45			-2.39 SB25			
NORMAL MODE 23	OBSERVED=	1261.0	CM-1	CALCULATED=	1259.6	CM-1	ERROR= 1.4 CM-1 OR 0.1 PERCENT
INTERNAL COORDINATES-	28.14 OC3H 20.16 CC4H			6.27 CC3H 5.94 C5H 5.67 OC4H			
FORCE CONSTANTS-	47.81 OCH 38.55 CCH			3.49 BB45 3.28 BB34 -1.61 SB25			
OFF DIAGONAL-	6.87 SB27 -4.25 BB29						
NORMAL MODE 24	OBSERVED=	1224.0	CM-1	CALCULATED=	1226.0	CM-1	ERROR= -2.0 CM-1 OR -0.2 PERCENT
INTERNAL COORDINATES-	45.29 OCH 39.05 CCH			16.84 HC3C 9.58 CC5H 7.23 CC3H			
FORCE CONSTANTS-	48.29 CCH 39.05 CCH			9.99 CO 6.74 OC3H 6.29 OCHB			
OFF DIAGONAL-	-6.81 BB29 4.94 SB27			3.06 BB34 -3.02 BB45 -2.79 SB25			
NORMAL MODE 25	OBSERVED=	1203.0	CM-1	CALCULATED=	1194.4	CM-1	ERROR= 8.6 CM-1 OR 0.7 PERCENT
INTERNAL COORDINATES-	20.85 OC1C 18.32 C5O1			9.00 OCHA 7.70 OC2H 7.11 CC5H			
FORCE CONSTANTS-	42.63 CO 29.35 CCH			26.35 OCH 9.41 CCO 6.69 BCOH			
OFF DIAGONAL-	-6.54 SB25 -3.30 BB29			-1.91 BB45			
NORMAL MODE 26	OBSERVED=	1147.0	CM-1	CALCULATED=	1143.4	CM-1	ERROR= 3.6 CM-1 OR 0.3 PERCENT
INTERNAL COORDINATES-	18.33 OC1C 11.90 C5O1			9.43 CCH2 8.30 CC4H 8.24 HC4C			
FORCE CONSTANTS-	47.45 CCH 43.52 CO			10.60 OCH 7.21 CCO			
OFF DIAGONAL-	-7.73 BB29 4.02 BB34			-2.96 SB27 -2.20 BB43 -2.18 BB45			
NORMAL MODE 27	OBSERVED=	1126.0	CM-1	CALCULATED=	1126.6	CM-1	ERROR= -0.4 CM-1 OR -0.0 PERCENT
INTERNAL COORDINATES-	14.53 C-O7 11.26 C-U9			9.99 C2OH 8.63 C-O8 5.18 O9CC			
FORCE CONSTANTS-	45.64 CO 18.93 CCO			15.33 CCH 14.78 BCOH 9.77 CCH			
OFF DIAGONAL-	-13.07 SB25 11.14 SB27			-8.68 SB28 2.65 BB43 -1.79 BB36			
NORMAL MODE 28	OBSERVED=	1118.0	CM-1	CALCULATED=	1115.0	CM-1	ERROR= 3.0 CM-1 OR 0.3 PERCENT
INTERNAL COORDINATES-	29.45 C-O7 13.65 C-U6			12.26 C2C3 9.65 C-O9 8.30 C5C1			
FORCE CONSTANTS-	63.51 CO 18.08 CC			12.90 CCC 12.86 CCO 11.72 OCH			
OFF DIAGONAL-	-8.94 SB25 -5.27 SB27			-3.15 SB28 -3.08 SB21 -2.13 SB22			
NORMAL MODE 29	OBSERVED=	1109.0	CM-1	CALCULATED=	1109.8	CM-1	ERROR= 0.8 CM-1 OR 0.7 PERCENT
INTERNAL COORDINATES-	49.21 C4C 34.62 C5C1			7.10 C-O8 6.30 CCH 6.30 OCH			
FORCE CONSTANTS-	84.04 CO 18.39 CC			12.42 CCO 6.30 CCH 6.30 OCH			
OFF DIAGONAL-	-14.45 SB22 -8.57 SB26			-3.46 SS18 -3.21 SB27 -2.65 SS17			
NORMAL MODE 30	OBSERVED=	1078.0	CM-1	CALCULATED=	1079.6	CM-1	ERROR= -1.6 CM-1 OR -0.1 PERCENT
INTERNAL COORDINATES-	32.97 C-O8 24.88 C3C4			18.60 C-O7 5.23 OC1C			
FORCE CONSTANTS-	63.19 CO 33.95 CC			12.82 CCO 6.56 CCH 6.25 CCC			
OFF DIAGONAL-	-6.74 SS18 -6.19 SB25			-5.72 SB21 -5.22 SB28 -3.24 SB27			
NORMAL MODE 31	OBSERVED=	1072.0	CM-1	CALCULATED=	1063.5	CM-1	ERROR= 8.5 CM-1 OR 0.8 PERCENT
INTERNAL COORDINATES-	56.55 C1C2 19.32 C2C3			8.79 C-O6 7.03 C-O8 6.78 C1OH			
FORCE CONSTANTS-	81.71 CO 28.74 CC			14.39 CCO 11.20 BCOH 11.19 OCH			
OFF DIAGONAL-	-14.80 SB22 -11.68 SB26			-7.24 SS18 -6.84 SB27 -5.67 SB28			
NORMAL MODE 32	OBSERVED=	1065.0	CM-1	CALCULATED=	1057.4	CM-1	ERROR= 7.6 CM-1 OR 0.7 PERCENT
INTERNAL COORDINATES-	41.51 C-O8 11.09 C3C4			9.76 C-O8 9.48 C-O8 8.82 C1C2			
FORCE CONSTANTS-	60.85 CO 24.03 CC			9.54 OCH 9.40 CO 8.35 CCH			
OFF DIAGONAL-	-5.03 SB22 -4.41 SB21			-3.88 SB28 -3.67 SB27 -3.02 SS18			
NORMAL MODE 33	OBSERVED=	1053.0	CM-1	CALCULATED=	1040.1	CM-1	ERROR= 12.9 CM-1 OR 1.2 PERCENT
INTERNAL COORDINATES-	10.91 C-O7 17.94 C3C4			10.93 CCO 7.98 C5C1 7.03 C-O8 6.95 OC4H			
FORCE CONSTANTS-	56.23 CO 35.75 CC			16.88 CCC 15.98 CCH 12.18 BCOH			
OFF DIAGONAL-	-14.07 SB21 -9.44 SB28			-9.34 SB27 -6.64 SB25 -5.94 SS18			
NORMAL MODE 34	OBSERVED=	1019.0	CM-1	CALCULATED=	1011.4	CM-1	ERROR= 7.6 CM-1 OR 0.8 PERCENT
INTERNAL COORDINATES-	18.28 C-O7 10.40 C-O7			10.10 C5C1 7.60 C-O9			
FORCE CONSTANTS-	57.00 CO 28.69 CCH			14.95 CC 8.28 CCO 6.92 CCC			
OFF DIAGONAL-	-7.13 SB21 -4.51 BB29			-3.93 SB27 -2.13 SB28			
NORMAL MODE 35	OBSERVED=	997.0	CM-1	CALCULATED=	981.7	CM-1	ERROR= 15.3 CM-1 OR 1.5 PERCENT
INTERNAL COORDINATES-	19.08 C1C2 14.50 C-O6			12.06 C2C3 10.07 C-O7 9.26 C5O1			
FORCE CONSTANTS-	67.29 CO 17.46 CC			12.12 CCH 10.05 CCH 7.77 BCOH			
OFF DIAGONAL-	-7.48 SB24 -6.09 SB28			-5.90 SB21 -2.93 SB25 -2.97 SB22			

40. EXPERIMENTAL FREQUENCIES AVERAGE ERROR = 8.42

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400				PAGE 1	
MOLECULE 21 -6 NG-1237 BETA GLUCOSE GT					
NORMAL MODE 8	OBSERVED=	1449.0 CM-1	CALCULATED=	1449.7 CM-1	ERROR= -0.7 CM-1 OR -0.0 PERCENT
INTERNAL COORDINATES-	62.32 HCH 19.89 OCHB		18.81 OCHA		
FORCE CONSTANTS-	62.32 HCH 39.08 OCH				
OFF DIAGONAL-	-3.82 SB27				
NORMAL MODE 9	OBSERVED=	1415.0 CM-1	CALCULATED=	1421.7 CM-1	ERROR= -6.7 CM-1 OR -0.5 PERCENT
INTERNAL COORDINATES-	32.35 C1H 17.29 OC1H		13.42 C1OH 9.04 C2OH 8.13 C1H 5.71 OC2H		
FORCE CONSTANTS-	57.05 OCH 22.61 BCOH		13.86 CCH 7.48 CO 5.58 CCO		
OFF DIAGONAL-	-9.45 SB27 3.63 SB28		2.97 BB29 -2.59 BB45 -2.52 SB25		2.38 BB34 -2.04 BB43 -1.97 BB39
NORMAL MODE 10	OBSERVED=	0.0 CM-1	CALCULATED=	1410.5 CM-1	ERROR= -5.0 CM-1 OR -0.0 PERCENT
INTERNAL COORDINATES-	18.41 OCH 31.97 OCH		11.17 CCOH 8.71 OC3H 6.90 HC3C 5.08 C1H 5.05 C-O9		
FORCE CONSTANTS-	46.90 OCH 38.51 CCH		10.91 CO		
OFF DIAGONAL-	-10.07 SB27 7.90 BB29		-5.06 SB26		4.62 BB34 -3.42 SB25 -3.29 BB45 1.70 SB28
NORMAL MODE 11	OBSERVED=	1402.0 CM-1	CALCULATED=	1407.2 CM-1	ERROR= -5.2 CM-1 OR -0.4 PERCENT
INTERNAL COORDINATES-	25.73 C1H 24.45 C1OH		12.52 C2OH 10.93 OC1H		
FORCE CONSTANTS-	45.80 OCH 37.70 BCOH		7.77 CCH		
OFF DIAGONAL-	2.20 SB28 -2.03 BB45		-1.82 SB26		
NORMAL MODE 12	OBSERVED=	0.0 CM-1	CALCULATED=	1395.5 CM-1	ERROR= 0.0 CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	70.85 C*OH 7.08 CCHB		6.58 OCHA		
FORCE CONSTANTS-	72.05 BCOH 13.88 CCH		9.28 OCH		
OFF DIAGONAL-	-3.51 SB26 2.87 SB28		2.73 BB29		-2.00 BB39 -1.62 SB27
NORMAL MODE 13	OBSERVED=	1387.0 CM-1	CALCULATED=	1393.7 CM-1	ERROR= -6.7 CM-1 OR -0.5 PERCENT
INTERNAL COORDINATES-	63.63 C3OH 13.20 OC3H				
FORCE CONSTANTS-	67.95 BCOH 16.81 OCH		8.47 CCH		
OFF DIAGONAL-	-4.65 SB28 -3.29 SB27		-3.16 SB26		-2.75 BB39
NORMAL MODE 14	OBSERVED=	1375.0 CM-1	CALCULATED=	1388.2 CM-1	ERROR= -13.2 CM-1 OR -1.0 PERCENT
INTERNAL COORDINATES-	41.35 C1OH 10.64 C2OH		8.03 OCH		
FORCE CONSTANTS-	70.48 BCOH 10.64 CCH		-1.71 SB27		-1.60 BB39
OFF DIAGONAL-	3.20 SB28 -2.57 SB26				
NORMAL MODE 15	OBSERVED=	1369.0 CM-1	CALCULATED=	1367.0 CM-1	ERROR= 2.0 CM-1 OR 0.1 PERCENT
INTERNAL COORDINATES-	20.48 C2OH 17.09 C3OH		6.35 HC2C 6.15 OC2H 6.06 CC4H 5.55 C5H 5.54 OC3H 5.35 CC3H		
FORCE CONSTANTS-	38.56 BCOH 30.27 CCH		21.01 OCH		
OFF DIAGONAL-	6.39 BB29 -3.70 SB27		3.16 BB34 -2.82 SB28 -2.11 BB36 -1.98 BB45 1.87 SB26 1.82 BB39		
NORMAL MODE 16	OBSERVED=	1351.0 CM-1	CALCULATED=	1345.7 CM-1	ERROR= 5.3 CM-1 OR 0.4 PERCENT
INTERNAL COORDINATES-	14.58 CCHB 14.35 HC5C		10.55 OCHB 6.73 C5H 6.29 OC2H 5.86 CC3H		
FORCE CONSTANTS-	49.34 CCH 32.83 CCH		9.40 BCOH		
OFF DIAGONAL-	11.17 BB29 -3.81 SB27		-3.61 SB26		-3.44 BB45 1.51 BB34
NORMAL MODE 17	OBSERVED=	1343.0 CM-1	CALCULATED=	1327.6 CM-1	ERROR= 15.4 CM-1 OR 1.1 PERCENT
INTERNAL COORDINATES-	14.85 HC3C 12.77 CC4H		6.65 CCHB 6.58 HC4C 5.60 CCH2 5.23 OC2H 5.15 OCHB 5.04 HC5C		
FORCE CONSTANTS-	62.59 CCH 17.54 OCH		10.44 BCOH		
OFF DIAGONAL-	13.82 BB29 -7.25 SB26		-3.48 BB45 -2.69 SB27		
NORMAL MODE 18	OBSERVED=	1308.0 CM-1	CALCULATED=	1308.7 CM-1	ERROR= -0.7 CM-1 OR -0.0 PERCENT
INTERNAL COORDINATES-	11.40 C5H 9.90 CCHA		8.19 CC2C 8.09 C4OH 7.81 OC4H 7.30 CCHB 6.84 HC2C 5.24 CC1H 5.14 OCHB		
FORCE CONSTANTS-	44.93 CCH 8.57 CCH		4.44 HC3C		
OFF DIAGONAL-	-4.44 SB27 -3.42 SB26		-3.21 BB45 3.08 BB29		
NORMAL MODE 19	OBSERVED=	0.0 CM-1	CALCULATED=	1296.4 CM-1	ERROR= 6.0 CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	64.03 CCH 21.18 OCH		7.32 CCH		
FORCE CONSTANTS-	8.42 BB29 -6.10 SB26		-3.59 BB45		
NORMAL MODE 20	OBSERVED=	1283.0 CM-1	CALCULATED=	1283.1 CM-1	ERROR= -0.1 CM-1 OR -0.0 PERCENT
INTERNAL COORDINATES-	25.32 CCHA 17.60 C4OH		15.84 OCHA 11.36 CC3H 6.87 C5H		
FORCE CONSTANTS-	39.43 CCH 26.27 OCH		17.60 COH		
OFF DIAGONAL-	-2.68 BB45				
NORMAL MODE 21	OBSERVED=	1270.0 CM-1	CALCULATED=	1272.2 CM-1	ERROR= -2.2 CM-1 OR -0.2 PERCENT
INTERNAL COORDINATES-	22.58 OC3H 14.43 OC2H		10.99 CC3H 8.29 CC4H 8.17 OC4H		
FORCE CONSTANTS-	49.42 OCH 28.40 CC1H		11.40 CO		
OFF DIAGONAL-	8.11 SB27 -3.12 BB45		-2.85 BB29 -2.56 SB25 -2.49 SB26 1.79 BB34 1.54 BB43		
NORMAL MODE 22	OBSERVED=	1263.0 CM-1	CALCULATED=	1260.7 CM-1	ERROR= 2.3 CM-1 OR 0.2 PERCENT
INTERNAL COORDINATES-	13.42 OC4H 13.33 OC2H		10.37 C4OH 8.28 OC1C 6.17 C-O6 5.57 HC3C 5.08 CC3H		
FORCE CONSTANTS-	32.59 CCH 25.93 CCH		19.09 CO 7.75 OCH		
OFF DIAGONAL-	-4.58 SB27 -4.31 BB29		4.04 SB25 19.35 BB34 -2.30 BB45		
NORMAL MODE 23	OBSERVED=	1250.0 CM-1	CALCULATED=	1253.8 CM-1	ERROR= -3.8 CM-1 OR -0.3 PERCENT
INTERNAL COORDINATES-	39.11 OCH 28.04 CCH		15.74 HC5C 6.91 CCHB 5.69 C5O*		
FORCE CONSTANTS-	39.11 OCH 28.04 CCH		9.33 CO		
OFF DIAGONAL-	6.71 SB27 -5.07 BB29		2.63 BB34 -2.63 BB45 -1.91 SB25		
NORMAL MODE 24	OBSERVED=	1222.0 CM-1	CALCULATED=	1222.3 CM-1	ERROR= -0.3 CM-1 OR -0.0 PERCENT
INTERNAL COORDINATES-	17.78 OC1C 14.55 C-O6		8.52 HC5C 7.25 HC5C 7.14 OC3H 6.18 CCH2 6.13 OC4H 5.85 CC3H		
FORCE CONSTANTS-	37.60 CO 36.15 CCH		20.76 CCH 10.73 CCO		
OFF DIAGONAL-	-5.99 BB29 -5.73 SB25		5.13 BB34 -2.30 BB45		
NORMAL MODE 25	OBSERVED=	1202.0 CM-1	CALCULATED=	1194.3 CM-1	ERROR= 7.7 CM-1 OR 0.6 PERCENT
INTERNAL COORDINATES-	14.49 C-O6 14.03 O*CI		8.97 OC2H 8.92 CC1H 8.86 OC1H 7.90 HC4C 6.75 CC4H		
FORCE CONSTANTS-	38.21 CO 31.86 CCH		25.36 OCH		
OFF DIAGONAL-	-5.11 BB29 -4.64 SB25		-2.50 SB28 2.28 BB34 -2.14 BB45 -1.71 SB27		
NORMAL MODE 26	OBSERVED=	1152.0 CM-1	CALCULATED=	1161.0 CM-1	ERROR= -9.0 CM-1 OR -0.8 PERCENT
INTERNAL COORDINATES-	13.58 OCHB 12.01 C5O*		9.27 OCHA 6.38 HC5C 5.11 CC1H		
FORCE CONSTANTS-	33.25 OCH 29.79 CCH		20.46 CCH 11.48 BCOH		
OFF DIAGONAL-	-6.87 SB25 6.25 SB27		-5.45 BB29 3.65 BB34 -2.75 SB28		
NORMAL MODE 27	OBSERVED=	1126.0 CM-1	CALCULATED=	1128.6 CM-1	ERROR= -2.6 CM-1 OR -0.2 PERCENT
INTERNAL COORDINATES-	12.84 C5O 21.46 C4C5		12.08 CCH 10.36 CCH 6.92 C-O4 6.76 OC6B 6.20 O*CI 5.12 C3C4		
FORCE CONSTANTS-	36.93 CCH 18.93 CCO		12.89 CO 13.05 OCH 6.13 CCH 1.52 SB24		
OFF DIAGONAL-	-12.34 SB22 -5.19 SB26		-2.34 SB23 -1.97 SS18 -1.77 SS17		
NORMAL MODE 28	OBSERVED=	1116.0 CM-1	CALCULATED=	1114.9 CM-1	ERROR= 1.1 CM-1 OR 0.1 PERCENT
INTERNAL COORDINATES-	17.19 C5O 13.81 C5C*		9.64 CC1H 8.37 OC1H 9.00 CC4H 6.84 HC4C 6.85 C-O7 6.77 CCH2		
FORCE CONSTANTS-	41.63 CCH 31.74 CO		17.95 OCH 17.33 CC 17.26 CCO 6.15 CCC		
OFF DIAGONAL-	-8.20 BB29 -7.44 SB25		-5.82 SB27 -3.51 BB43 -2.96 SB26 -2.70 SB22 -2.35 BB45 -1.99 SB28 1.93 BB34		
NORMAL MODE 29	OBSERVED=	1097.0 CM-1	CALCULATED=	1107.9 CM-1	ERROR= -10.9 CM-1 OR -1.0 PERCENT
INTERNAL COORDINATES-	20.63 C5O 17.07 C-O7		15.39 C-O9 7.63 C-O8 6.87 C1C2 6.42 C3C4 5.68 C4C5 5.51 C-O6		
FORCE CONSTANTS-	67.56 CO 22.72 CC		7.84 OCH 6.82 CCO 5.16 CCH		
OFF DIAGONAL-	-5.96 SS18 -4.80 SB28		-4.54 SB25		
NORMAL MODE 30	OBSERVED=	1079.0 CM-1	CALCULATED=	1086.0 CM-1	ERROR= -7.0 CM-1 OR -0.6 PERCENT
INTERNAL COORDINATES-	37.71 C3C4 24.64 C-U*		19.56 C2C3 8.51 C-O7 5.47 C2OH		
FORCE CONSTANTS-	63.85 CO 35.45 CO		12.12 CCO 7.70 BCOH 7.27 CCC		
OFF DIAGONAL-	-9.21 SB22 -4.72 SB28		-4.48 SB27 -4.05 SB25 -3.65		6.22 OCH -6.11 CCH SB26 -2.58 SB21 -2.32 BB34 -2.31 SS17 -1.77 SS18
NORMAL MODE 31	OBSERVED=	1069.0 CM-1	CALCULATED=	1064.9 CM-1	ERROR= 4.1 CM-1 OR 0.4 PERCENT
INTERNAL COORDINATES-	35.69 C5O 21.43 C2C3		16.13 C-O7 10.36 C2OH		
FORCE CONSTANTS-	39.79 CCH 28.94 CCH		10.09 CO 8.73 BCOH 6.78 CCC 6.18 OCH		
OFF DIAGONAL-	-7.78 SB28 -6.14 SB27		-5.14 SB22 -4.33 SB21 -2.93 SB25 -2.75 SS18 -1.60 SB24		
NORMAL MODE 32	OBSERVED=	1050.0 CM-1	CALCULATED=	1058.3 CM-1	ERROR= -8.3 CM-1 OR -0.8 PERCENT
INTERNAL COORDINATES-	10.09 C5O 27.99 C1C2		13.08 CCH 10.36 C2OH 9.77 C3OH 7.42 C2C3 6.73 OC3H 5.84 O*CC		
FORCE CONSTANTS-	56.64 CCH 44.73 CC		14.63 CCO 13.43 BCOH 12.84 OCH 12.14 CCC 11.74 CCH		
OFF DIAGONAL-	-12.25 SB27 -10.07 SB28		-8.55 SB25 -7.94 SB21 -6.86 SS18 -6.47 SB22 -3.41 BB34 -2.71 BB36 -2.52 BB29		
NORMAL MODE 33	OBSERVED=	1024.0 CM-1	CALCULATED=	1039.3 CM-1	ERROR= -15.3 CM-1 OR -1.5 PERCENT
INTERNAL COORDINATES-	30.72 C-O9 20.64 C1C2		14.41 C-O8 14.40 C-O7 6.62 C4OH		
FORCE CONSTANTS-	71.37 CO 29.61 CC		9.85 CCH 8.37 CCO 6.88 OCH		
OFF DIAGONAL-	-10.91 SB28 -9.43 SB27		-5.68 SS18 -5.16 SB22 -3.62 SB21 -2.84 SB25 -1.97 SB24 -1.85 BB29		
NORMAL MODE 34	OBSERVED=	1012.0 CM-1	CALCULATED=	1015.8 CM-1	ERROR= -3.8 CM-1 OR -0.4 PERCENT
INTERNAL COORDINATES-	38.53 C4C5 25.42 C-O9		20.20 C4OH 9.87 C-O*		
FORCE CONSTANTS-	51.33 CC 42.12 CO		20.20 CCO 10.22 OCH 9.61 CCC 7.63 CCO		
OFF DIAGONAL-	-16.59 SB21 -9.94 SB28		-9.69 SB27 -8.55 SS18 -4.29 SB22 1.64 SB25 1.54 SB26		
NORMAL MODE 35	OBSERVED=	1006.0 CM-1	CALCULATED=	988.1 CM-1	ERROR= 17.9 CM-1 OR 1.8 PERCENT
INTERNAL COORDINATES-	25.43 C2C2 35.93 C1C2		9.80 C-O9 9.28 C-O6 8.97 C-O7 6.56 CCO8 6.19 O*CI		
FORCE CONSTANTS-	44.53 CCH 28.94 CCH		21.00 CCO 11.03 CCH		
OFF DIAGONAL-	-13.45 SB22 -6.03 SB21		-3.95 SB24 -3.61 SB27 -2.42 SB26 2.22 BB34 -2.06 BB29 2.02 SS18		

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400										PAGE 2
MOLECULE 21		-6 NG=1237		BETA GLUCOSE		GT				
NORMAL MODE 36		OBSERVED=	992.0 CM-1	CALCULATED=		972.5 CM-1	ERROR=	-20.5 CM-1	OR -2.1 PERCENT	
INTERNAL COORDINATES-		26.85 C3C4	16.99 C-08	16.08 C-07		13.38 C-07	0.17 C1G2	5.77 HC4C		
FORCE CONSTANTS-		49.02 CC	36.29 CC	19.90 CCH		15.49 CCO				
OFF DIAGONAL-		-12.54 SB22	6.06 SS18	-5.50 SB26		-4.14 SB25	-3.89 SB21	-3.86 BB29	-1.95 SB28	
NORMAL MODE 37		OBSERVED=	913.0 CM-1	CALCULATED=		951.3 CM-1	ERROR=	-38.3 CM-1	OR -4.2 PERCENT	
INTERNAL COORDINATES-		17.28 C-06	17.28 C5C1	12.24 O1C1		7.39 C1C2				
FORCE CONSTANTS-		43.09 CO	25.59 CC	13.45 CCO		8.57 CCH	6.49 CCC	5.28 CCH		
OFF DIAGONAL-		-7.77 SB24	-6.00 SB21	5.99 SB27		-5.87 SB22	3.56 SS18	-2.15 SB25	2.06 BB43	
NORMAL MODE 38		OBSERVED=	898.0 CM-1	CALCULATED=		874.5 CM-1	ERROR=	23.5 CM-1	OR 2.6 PERCENT	
INTERNAL COORDINATES-		19.80 C5O1	17.61 CCHA	15.84 CCHB		9.12 OCO	6.46 C5C1	5.11 OCHA		
FORCE CONSTANTS-		38.88 CCH	24.71 CO	10.96 CCH		9.12 OCO	8.01 CC	6.02 CCO		
OFF DIAGONAL-		-3.97 BB29	-3.86 SB23	-2.73 SB27		1.98 BB34	1.93 SB26	-1.91 SB24	1.86 SS18	
NORMAL MODE 39		OBSERVED=	714.0 CM-1	CALCULATED=		649.6 CM-1	ERROR=	64.4 CM-1	OR 9.0 PERCENT	
INTERNAL COORDINATES-		15.76 OBCC	12.94 CC01	8.35 CCO9		7.55 CC5H	7.20 U9CC	6.45 O7CC	5.48 CC01	
FORCE CONSTANTS-		68.13 CCO	30.38 CCH	6.46 CCG					5.36 HC4C	
OFF DIAGONAL-		-16.06 BB34	8.50 BB43	-6.93 BB29		3.66 SB25	-2.16 BB41	-1.96 BB42	5.07 HC3C	
NORMAL MODE 40		OBSERVED=	632.0 CM-1	CALCULATED=		640.6 CM-1	ERROR=	-8.6 CM-1	OR -1.4 PERCENT	
INTERNAL COORDINATES-		7.85 HC2C	7.15 OCU	6.94 CCHB		6.87 CC3H	6.85 CCO9	6.08 O7CC	5.33 HC5C	
FORCE CONSTANTS-		40.54 CCH	31.18 CCO	6.35 CCH		7.44 CO	7.15 OCO			
OFF DIAGONAL-		-10.17 BB34	9.35 BB43	-8.42 BB29		4.01 SB25	3.76 SB24	-3.65 SB27	2.51 BB42	
NORMAL MODE 41		OBSERVED=	593.0 CM-1	CALCULATED=		599.9 CM-1	ERROR=	-6.9 CM-1	OR -1.2 PERCENT	
INTERNAL COORDINATES-		19.02 CO7C	10.58 O1CC	9.18 C-07		6.01 CCO6	5.94 CCO1	5.50 C-09		
FORCE CONSTANTS-		35.66 CCO	19.30 CO	14.00 CCH		11.80 CC	7.12 CCC			
OFF DIAGONAL-		7.98 SB25	6.16 SB22	-2.92 SB27		-2.40 BB41	-2.21 SB23	2.20 SS18	2.15 BB43	
NORMAL MODE 42		OBSERVED=	574.0 CM-1	CALCULATED=		580.3 CM-1	ERROR=	-6.3 CM-1	OR -1.1 PERCENT	
INTERNAL COORDINATES-		12.01 CCO6	11.06 CCO8	8.57 CCH2		8.20 CCO1	7.93 OCO		6.41 O1CC	
FORCE CONSTANTS-		54.94 CCO	34.88 CCH	7.93 OCO		7.46 CO			5.39 CC3H	
OFF DIAGONAL-		-15.12 BB34	7.66 BB43	-7.54 BB29		3.52 SB24	-2.56 SB25			
NORMAL MODE 43		OBSERVED=	519.0 CM-1	CALCULATED=		503.5 CM-1	ERROR=	15.5 CM-1	OR 3.0 PERCENT	
INTERNAL COORDINATES-		13.11 CCO1	6.15 HC5C	5.22 C3CC		5.10 O1C1				
FORCE CONSTANTS-		30.51 CCO	23.49 CCH	14.84 CCO		7.44 CO	6.48 CC	6.01 CCH	1.98 SS18	
OFF DIAGONAL-		-8.44 BB34	7.69 BB43	-5.77 BB29		-3.70 SB27	2.80 SB24	2.35 SB25	1.63 BB42	
NORMAL MODE 44		OBSERVED=	454.0 CM-1	CALCULATED=		436.1 CM-1	ERROR=	17.9 CM-1	OR 3.9 PERCENT	
INTERNAL COORDINATES-		14.87 C1CC	9.29 CCO1	8.74 C4C5		7.88 O1CC	6.45 CCO8			
FORCE CONSTANTS-		35.56 CCO	18.12 CCH	17.86 CCO		8.77 CO	6.44 CCH			
OFF DIAGONAL-		5.00 SB22	5.00 SB25	3.20 BB43		2.16 SB21	-1.86 BB42	1.78 SS18	-1.70 SB26	
NORMAL MODE 45		OBSERVED=	425.0 CM-1	CALCULATED=		411.8 CM-1	ERROR=	13.2 CM-1	OR 3.1 PERCENT	
INTERNAL COORDINATES-		16.62 C2CC	11.97 C3CC	10.50 CCH2		9.87 CCO9				
FORCE CONSTANTS-		32.51 CCO	23.89 CCO	10.50 CCH		7.64 CC	7.27 CO	5.27 CCH	1.53 SB23	
OFF DIAGONAL-		3.40 SB25	-3.00 BB42	2.19 BB43		-2.09 BB41	2.07 SB22	1.82 SB21		
NORMAL MODE 46		OBSERVED=	401.0 CM-1	CALCULATED=		406.5 CM-1	ERROR=	-5.5 CM-1	OR -1.4 PERCENT	
INTERNAL COORDINATES-		13.55 O7CC	13.09 CCO1	7.98 OBCC						
FORCE CONSTANTS-		52.46 CCO	28.51 CCH	7.85 CCO						
OFF DIAGONAL-		-10.95 BB34	-6.20 BB29	5.94 BB43						
NORMAL MODE 47		OBSERVED=	347.0 CM-1	CALCULATED=		352.6 CM-1	ERROR=	-5.6 CM-1	OR -1.6 PERCENT	
INTERNAL COORDINATES-		23.63 O9CC	11.15 OBCC	10.77 O1CC		9.38 CCO7				
FORCE CONSTANTS-		62.58 CCO	11.39 CCH	10.77 CCO		7.44 CO	6.52 CCC			
OFF DIAGONAL-		-8.59 BB34	-2.57 BB42	2.33 BB43		2.22 SB22	-2.14 BB29			
NORMAL MODE 48		OBSERVED=	327.0 CM-1	CALCULATED=		329.0 CM-1	ERROR=	-2.0 CM-1	OR -0.6 PERCENT	
INTERNAL COORDINATES-		27.90 CCO7	12.35 CCO8	11.06 CCO1		10.93 OCO	6.41 CCO6			
FORCE CONSTANTS-		65.91 CCO	15.64 CCH	10.93 CCO		10.12 T-OH				
OFF DIAGONAL-		9.95 BB34	-2.17 BB42	-2.02 BB29		1.96 SB21				
NORMAL MODE 49		OBSERVED=	309.0 CM-1	CALCULATED=		312.2 CM-1	ERROR=	-3.2 CM-1	OR -1.0 PERCENT	
INTERNAL COORDINATES-		19.19 CCO6	6.85 CCO1	6.64 O9CC		6.48 OCO	5.52 CCO9	5.46 O7CC	5.20 C4CC	
FORCE CONSTANTS-		52.78 CCO	16.41 CC	6.96 CCO		6.84 T-OH	6.48 OCO			
OFF DIAGONAL-		6.39 SB21	-3.93 BB34	-2.77 BB42		2.48 SB22	-1.90 SB26			
NORMAL MODE 50		OBSERVED=	289.0 CM-1	CALCULATED=		304.1 CM-1	ERROR=	-15.1 CM-1	OR -5.2 PERCENT	
INTERNAL COORDINATES-		26.51 OBCC	13.60 CCO8	9.66 O9CC		8.80 TH-3	6.60 O7CC	5.07 CCO1		
FORCE CONSTANTS-		72.40 CCO	12.75 CCH	11.92 T-OH		6.56 CCC				
OFF DIAGONAL-		-11.27 BB34	3.65 BB43	-2.98 SB21		-2.06 BB42	-1.80 BB29	1.58 SB22		
NORMAL MODE 51		OBSERVED=	274.0 CM-1	CALCULATED=		295.2 CM-1	ERROR=	-21.2 CM-1	OR -7.7 PERCENT	
INTERNAL COORDINATES-		19.55 O7CC	19.22 CCO9	6.17 CCO8		5.26 TH-4				
FORCE CONSTANTS-		57.39 CCO	19.12 CCH	8.49 CCO		6.76 T-OH				
OFF DIAGONAL-		-12.01 BB34	8.21 BB43	-4.18 BB29		4.09 SB22	-1.95 SB25	-1.82 SB21	-1.78 BB36	
NORMAL MODE 52		OBSERVED=	250.0 CM-1	CALCULATED=		232.1 CM-1	ERROR=	17.9 CM-1	OR 7.2 PERCENT	
INTERNAL COORDINATES-		12.83 TH-1	20.94 TH-6	19.38 TH-2		13.29 TH-3	5.51 CCO1			
FORCE CONSTANTS-		86.84 T-OH	8.35 CCO							
OFF DIAGONAL-		NONE								
NORMAL MODE 53		OBSERVED=	227.0 CM-1	CALCULATED=		226.7 CM-1	ERROR=	0.3 CM-1	OR 0.1 PERCENT	
INTERNAL COORDINATES-		86.96 TH-5								
FORCE CONSTANTS-		88.72 T-OH								
OFF DIAGONAL-		NONE								
NORMAL MODE 54		OBSERVED=	0.0 CM-1	CALCULATED=		218.2 CM-1	ERROR=	0.0 CM-1	OR 0.0 PERCENT	
INTERNAL COORDINATES-		40.10 TH-4	20.90 TH-2	17.54 TH-1		7.85 TH-3				
FORCE CONSTANTS-		87.21 T-OH	7.84 CCO							
OFF DIAGONAL-		NONE								
NORMAL MODE 55		OBSERVED=	0.0 CM-1	CALCULATED=		215.7 CM-1	ERROR=	0.0 CM-1	OR 0.0 PERCENT	
INTERNAL COORDINATES-		39.89 TH-2	33.98 TH-1	11.84 TH-3						
FORCE CONSTANTS-		86.78 T-OH	9.70 CCO							
OFF DIAGONAL-		NONE								
NORMAL MODE 56		OBSERVED=	0.0 CM-1	CALCULATED=		210.8 CM-1	ERROR=	0.0 CM-1	OR 0.0 PERCENT	
INTERNAL COORDINATES-		53.17 TH-3	18.41 TH-6	9.09 TH-2		6.41 CCO8				
FORCE CONSTANTS-		82.87 T-OH	17.56 CCO							
OFF DIAGONAL-		-2.20 BB34								
NORMAL MODE 57		OBSERVED=	0.0 CM-1	CALCULATED=		193.3 CM-1	ERROR=	0.0 CM-1	OR 0.0 PERCENT	
INTERNAL COORDINATES-		35.79 CCO	15.50 CO1C	12.85 CCH		8.47 TH-3	5.08 T-CC	6.17 CCH		
FORCE CONSTANTS-		49.77 CCO	13.31 T-OH	12.50 CCO		12.50 CCO	5.90 T-CC			
OFF DIAGONAL-		-4.07 BB42	-4.03 BB34	-2.46 BB33						
NORMAL MODE 58		OBSERVED=	0.0 CM-1	CALCULATED=		149.3 CM-1	ERROR=	0.0 CM-1	OR 0.0 PERCENT	
INTERNAL COORDINATES-		24.00 C4CC	15.34 CO1C	6.94 CCO1		6.42 TCC4	5.62 TCO1	5.34 CCO6		
FORCE CONSTANTS-		29.25 CCO	20.86 CCO	15.34 CCO		9.54 T-CO	7.56 T-CC	6.79 CCH		
OFF DIAGONAL-		-3.97 SB21	3.77 BB43	-2.78 BB42		-2.21 SB25	2.09 SB22	-1.86 BB34		
NORMAL MODE 59		OBSERVED=	0.0 CM-1	CALCULATED=		98.4 CM-1	ERROR=	0.0 CM-1	OR 0.0 PERCENT	
INTERNAL COORDINATES-		54.69 TCC5	9.39 C3CC	6.31 O9CC		5.12 TCC2				
FORCE CONSTANTS-		63.81 T-CC	18.03 CCO	17.81 CCC						
OFF DIAGONAL-		-3.33 SB25	-2.71 BB34	-2.48 BB42		-2.13 SB21				
NORMAL MODE 60		OBSERVED=	0.0 CM-1	CALCULATED=		83.8 CM-1	ERROR=	0.0 CM-1	OR 0.0 PERCENT	
INTERNAL COORDINATES-		21.51 C2CC	16.37 C1CC	10.17 TCC4		7.93 TCC1	6.48 TCC5	5.97 TCC2	5.05 CCO8	
FORCE CONSTANTS-		42.33 CCO	30.57 T-CC	20.43 CCO						
OFF DIAGONAL-		-4.50 SB25	-4.31 BB42	-3.34 SB21		2.37 BB41				
NORMAL MODE 61		OBSERVED=	0.0 CM-1	CALCULATED=		65.6 CM-1	ERROR=	0.0 CM-1	OR 0.0 PERCENT	
INTERNAL COORDINATES-		22.43 TCC5	24.55 C3CC	21.84 CCO						
FORCE CONSTANTS-		49.76 T-CC	22.92 CCO	21.84 CCO						
OFF DIAGONAL-		-2.41 BB42	-2.03 BB34	-1.83 SB25						

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400										PAGE 1	
MOLECULE 22 -6 NG=1237 BETA GLUCOSE 400 GG											
NORMAL MODE 8	OBSERVED=	1449.0 CM-1	CALCULATED=	1450.1 CM-1	ERROR=	-1.1 CM-1	OR	-0.1 PERCENT			
INTERNAL COORDINATES-	61.32	HCH 20.28	OCBH	19.71	OCBA						
FORCE CONSTANTS-	57.44	OCB 36.82	CCH	10.26	CO						
OFF DIAGONAL-	-4.13	SB27									
NORMAL MODE 9	OBSERVED=	1415.0 CM-1	CALCULATED=	1421.7 CM-1	ERROR=	-6.7 CM-1	OR	-0.5 PERCENT			
INTERNAL COORDINATES-	32.72	C1H 17.51	OC1H	13.38	C1OH	8.95	C2OH	8.15	CC1H	5.63	OC2H
FORCE CONSTANTS-	57.44	OCB 22.47	BCOH	13.76	CCH	7.42	CO	3.56	CCO		
OFF DIAGONAL-	-9.47	SB27	3.61	SB28	2.93	BB29	-2.60	BB45	-2.50	SB25	2.37
NORMAL MODE 10	OBSERVED=	0.0 CM-1	CALCULATED=	1410.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	17.64	OC4H	11.08	HC4C	10.28	CC5H	8.94	OC3H	6.97	C1H	6.71
FORCE CONSTANTS-	45.87	OCB 36.82	CCH	10.26	CO						
OFF DIAGONAL-	-9.73	SB27	7.73	BB29	-5.18	SB26	4.24	BB34	-3.24	SB25	-3.21
NORMAL MODE 11	OBSERVED=	1402.0 CM-1	CALCULATED=	1407.1 CM-1	ERROR=	-5.1 CM-1	OR	-0.4 PERCENT			
INTERNAL COORDINATES-	24.99	C1OH	23.17	C1H	11.63	C2OH	9.51	OC1H			
FORCE CONSTANTS-	43.07	OCB 37.37	BCOH	9.70	CCH	5.58	HCH	5.27	CO		
OFF DIAGONAL-	-2.28	SB28	-2.00	BB45	-1.89	SB26					
NORMAL MODE 12	OBSERVED=	0.0 CM-1	CALCULATED=	1394.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	45.98	C3OH	16.49	C1OH	11.59	OC3C					
FORCE CONSTANTS-	66.66	BCOH	16.46	UCH	10.49	CCH					
OFF DIAGONAL-	4.67	SB28	-3.45	SB27	-2.73	SB26	-2.66	BB39			
NORMAL MODE 13	OBSERVED=	1387.0 CM-1	CALCULATED=	1392.0 CM-1	ERROR=	-5.0 CM-1	OR	-0.4 PERCENT			
INTERNAL COORDINATES-	52.43	C1UH	16.56	C3UH	7.51	OC4H					
FORCE CONSTANTS-	76.72	BCOH	10.42	UCH	8.52	CCH					
OFF DIAGONAL-	3.11	SB28	-1.91	BB39							
NORMAL MODE 14	OBSERVED=	1375.0 CM-1	CALCULATED=	1387.7 CM-1	ERROR=	-12.7 CM-1	OR	-0.9 PERCENT			
INTERNAL COORDINATES-	36.49	C1UH	33.63	C2OH	11.68	HC2C	7.26	HC2C	6.60	CC3H	5.38
FORCE CONSTANTS-	74.98	BCOH	10.88	CCH	8.70	UCH	5.20	CC			
OFF DIAGONAL-	3.17	SB28	-2.95	SB26	-1.81	BB29	-1.61	BB39			
NORMAL MODE 15	OBSERVED=	1369.0 CM-1	CALCULATED=	1365.5 CM-1	ERROR=	3.5 CM-1	OR	0.3 PERCENT			
INTERNAL COORDINATES-	21.07	C2OH	16.04	C3OH	7.42	OC2H	7.26	HC2C	6.60	CC3H	5.38
FORCE CONSTANTS-	39.21	BCOH	30.83	CCH	20.23	UCH	3.22	BB34	-3.05	SB28	-2.24
OFF DIAGONAL-	6.14	BB29	-3.94	SB27	-3.05	SB28	-2.24	BB36	1.99	BB39	-1.98
NORMAL MODE 16	OBSERVED=	1351.0 CM-1	CALCULATED=	1345.1 CM-1	ERROR=	5.9 CM-1	OR	0.4 PERCENT			
INTERNAL COORDINATES-	15.44	HC5C	14.89	CCHB	12.12	OCBH	11.68	CCH	10.22	CO	9.87
FORCE CONSTANTS-	45.98	C1H	30.47	BCOH	5.89	CCH	5.89	HCH	5.27	CO	
OFF DIAGONAL-	-6.84	SB27	-3.20	BB45	2.06	BB30	-2.01	SB28	1.81	BB29	
NORMAL MODE 17	OBSERVED=	1343.0 CM-1	CALCULATED=	1332.0 CM-1	ERROR=	11.0 CM-1	OR	0.8 PERCENT			
INTERNAL COORDINATES-	18.57	HC3H	15.32	CC4H	6.87	OC2H	5.84	CC2H	5.79	CC4H	
FORCE CONSTANTS-	62.92	CCH	18.48	UCH	9.65	BCOH	-3.54	BB45	-2.74	SB27	2.03
OFF DIAGONAL-	12.52	BB29	-6.76	SB26	-3.54	BB45	-2.74	SB27	2.03	BB34	
NORMAL MODE 18	OBSERVED=	1338.0 CM-1	CALCULATED=	1304.9 CM-1	ERROR=	33.1 CM-1	OR	0.2 PERCENT			
INTERNAL COORDINATES-	13.84	CC2H	9.68	HC2C	9.03	OC4H	8.75	C5H	7.88	CC4H	7.80
FORCE CONSTANTS-	51.33	CCH	27.59	UCH	7.80	CO	6.93	BCOH	6.17	CO	
OFF DIAGONAL-	6.57	BB29	-5.07	SB26	-3.32	BB45	-2.87	SB27	1.88	BB34	
NORMAL MODE 19	OBSERVED=	0.0 CM-1	CALCULATED=	1295.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	14.35	C4OH	13.21	C5H	10.08	OC4H	8.65	CC2H	8.34	HC3C	6.59
FORCE CONSTANTS-	47.82	CCH	30.70	UCH	14.35	COH					
OFF DIAGONAL-	3.90	BB29	-3.59	SB26	-3.30	BB45					
NORMAL MODE 20	OBSERVED=	1283.0 CM-1	CALCULATED=	1290.1 CM-1	ERROR=	-7.1 CM-1	OR	-0.5 PERCENT			
INTERNAL COORDINATES-	20.52	UCHB	17.78	CCHB	11.62	OCBA	7.40	C5H	6.45	CC4H	
FORCE CONSTANTS-	45.98	CCH	30.47	BCOH	5.89	CCH					
OFF DIAGONAL-	-3.16	BB45	-2.52	SB27	1.56	BB34					
NORMAL MODE 21	OBSERVED=	1270.0 CM-1	CALCULATED=	1272.0 CM-1	ERROR=	-2.9 CM-1	OR	-0.2 PERCENT			
INTERNAL COORDINATES-	13.59	OC2H			11.13	CC5H	8.80	C4OH	5.31	CC4H	
FORCE CONSTANTS-	42.87	UCH	24.17	CCH	12.88	CO	6.80	COH			
OFF DIAGONAL-	7.82	SB27	-2.74	SB25	-2.66	BB45	-2.19	BB29	1.85	BB34	1.79
NORMAL MODE 22	OBSERVED=	1263.0 CM-1	CALCULATED=	1261.4 CM-1	ERROR=	1.6 CM-1	OR	0.1 PERCENT			
INTERNAL COORDINATES-	20.85	C4OH	13.92	OC2H	6.57	CC3H	5.88	C1H	5.71	C5H	5.28
FORCE CONSTANTS-	28.62	UCH	23.03	CCH	20.85	COH	13.89	CO	6.66	CCO	5.36
OFF DIAGONAL-	4.03	SB27	-3.10	SB25	-2.68	BB29	2.66	BB34	-2.03	BB45	-1.66
NORMAL MODE 23	OBSERVED=	1250.0 CM-1	CALCULATED=	1252.4 CM-1	ERROR=	-2.4 CM-1	OR	-0.2 PERCENT			
INTERNAL COORDINATES-	10.50	CC4H	9.99	HC5C	9.60	OC4H	9.23	OC3H	8.67	C5H	6.41
FORCE CONSTANTS-	36.98	CCH	33.83	UCH	16.48	CO	5.96	COH			
OFF DIAGONAL-	6.31	SB27	-2.88	BB45	-2.51	SB25	2.31	BB34	-2.19	BB29	
NORMAL MODE 24	OBSERVED=	1222.0 CM-1	CALCULATED=	1216.2 CM-1	ERROR=	5.8 CM-1	OR	0.5 PERCENT			
INTERNAL COORDINATES-	16.45	C1H	16.41	C-06	8.89	HC5C	8.42	HC2C	7.74	OC4H	
FORCE CONSTANTS-	39.93	CCH	39.03	CCH	18.19	UCH	9.70	CO			
OFF DIAGONAL-	-6.00	SB25	-3.66	BB29	3.25	BB34	-2.37	BB45	-2.06	SB26	
NORMAL MODE 25	OBSERVED=	1202.0 CM-1	CALCULATED=	1192.8 CM-1	ERROR=	9.2 CM-1	OR	0.8 PERCENT			
INTERNAL COORDINATES-	15.42	C1H	11.29	C-06	9.74	CC1H	9.32	OC1H	8.96	OC2H	7.22
FORCE CONSTANTS-	35.40	CCH	30.70	UCH	26.04	UCH					
OFF DIAGONAL-	-5.05	BB29	-4.60	SB25	-2.23	BB45	1.73	BB34	-1.63	SB28	
NORMAL MODE 26	OBSERVED=	1152.0 CM-1	CALCULATED=	1157.5 CM-1	ERROR=	-5.5 CM-1	OR	-0.5 PERCENT			
INTERNAL COORDINATES-	21.62	C5C	10.87	HC5C	7.97	C5C	7.03	OCBH	6.12	CCO*	5.79
FORCE CONSTANTS-	35.78	CCH	31.32	CO	18.97	UCH	14.29	UCH	11.87	CC	
OFF DIAGONAL-	-10.11	SB25	8.43	SB27	-7.47	SB26	-4.73	BB29	-3.87	SB22	-2.20
NORMAL MODE 27	OBSERVED=	1126.0 CM-1	CALCULATED=	1127.7 CM-1	ERROR=	-1.7 CM-1	OR	-0.1 PERCENT			
INTERNAL COORDINATES-	44.10	C5C	17.36	C-0*	14.67	C4C5	11.40	OC4H	6.25	CCO*	6.17
FORCE CONSTANTS-	62.91	CC	28.76	CO	14.38	UCH	10.00	CCH	9.30	UCH	7.12
OFF DIAGONAL-	-13.01	SB22	-11.92	SB26	-4.97	SB28	-4.76	SB27	-4.28	SS18	-3.20
NORMAL MODE 28	OBSERVED=	1116.0 CM-1	CALCULATED=	1118.6 CM-1	ERROR=	-2.6 CM-1	OR	-0.2 PERCENT			
INTERNAL COORDINATES-	17.75	C5O	10.94	OC1H	9.07	CC1H	9.83	CC2H	7.47	CC4H	6.34
FORCE CONSTANTS-	42.36	CCH	27.77	CO	26.93	UCH	12.22	CO	8.35	CC	
OFF DIAGONAL-	-9.20	BB29	-6.55	SB25	4.12	BB34	-3.50	SB27	-2.35	BB43	-2.34
NORMAL MODE 29	OBSERVED=	1097.0 CM-1	CALCULATED=	1107.3 CM-1	ERROR=	-10.3 CM-1	OR	-0.9 PERCENT			
INTERNAL COORDINATES-	21.09	C5O	16.80	C-09	12.93	UCH	8.98	CCH	6.45	CCO	5.92
FORCE CONSTANTS-	45.98	CCH	30.47	BCOH	5.89	CCH	5.89	HCH	5.27	CO	
OFF DIAGONAL-	-4.95	SB25	-4.64	SB28	-4.37	SS18	2.03	SB27	-1.64	BB29	
NORMAL MODE 30	OBSERVED=	1079.0 CM-1	CALCULATED=	1078.8 CM-1	ERROR=	0.2 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	31.54	C2C	29.69	C3C4	17.07	C-07	9.32	C2OH	5.46	C-08	5.22
FORCE CONSTANTS-	69.10	CC	27.81	CO	12.74	UCH	12.10	BCOH	9.99	CCCH	6.90
OFF DIAGONAL-	-9.34	SB22	-6.45	SB28	-6.17	SB27	-3.92	SB26	-3.34	SB25	-3.13
NORMAL MODE 31	OBSERVED=	1069.0 CM-1	CALCULATED=	1059.1 CM-1	ERROR=	9.9 CM-1	OR	0.9 PERCENT			
INTERNAL COORDINATES-	43.15	C-08	23.76	C1C2	22.57	C2C3	11.58	C3OH	8.65	OC3H	8.08
FORCE CONSTANTS-	53.52	CC	50.00	CO	16.06	UCH	14.09	BCOH	12.41	UCH	10.75
OFF DIAGONAL-	-11.61	SB27	-9.65	SB28	-9.15	SB21	-8.14	SB22	-8.13	SS18	-6.07
NORMAL MODE 32	OBSERVED=	1050.0 CM-1	CALCULATED=	1050.2 CM-1	ERROR=	-0.2 CM-1	OR	-0.0 PERCENT			
INTERNAL COORDINATES-	25.64	C-07	18.40	C1C2	12.91	C-0*	11.70	C3C4	5.44	CC3H	
FORCE CONSTANTS-	45.51	CO	34.91	CC	15.60	CCH	11.24	UCH	9.86	CCO	6.63
OFF DIAGONAL-	-8.81	SB21	-6.83	SB27	-6.81	SB22	-4.89	SS18	-4.24	SB28	-2.65
NORMAL MODE 33	OBSERVED=	1024.0 CM-1	CALCULATED=	1032.3 CM-1	ERROR=	-8.1 CM-1	OR	-0.8 PERCENT			
INTERNAL COORDINATES-	48.82	C-09	22.19	C4OH	11.77	C4C5	9.37	C4C5	6.96	C3CC	6.81
FORCE CONSTANTS-	63.45	CO	30.60	CC	22.19	UCH	11.74	CC2	8.64	CCO	8.04
OFF DIAGONAL-	-15.43	SB28	-9.32	SB27	-8.82	SB21	-7.01	SS18	-6.32	SB25	-2.66
NORMAL MODE 34	OBSERVED=	1012.0 CM-1	CALCULATED=	1008.3 CM-1	ERROR=	3.7 CM-1	OR	0.4 PERCENT			
INTERNAL COORDINATES-	55.50	C-04	18.13	C3C4	18.66	CCH	8.77	COH	6.47	C4C5	5.91
FORCE CONSTANTS-	55.50	CC	37.03	CC	-6.07	SB28	-4.70	SB27	-2.76	SB25	-2.54
OFF DIAGONAL-	-7.12	SB26	-6.37	SB22	-6.07	SB28	-4.70	SB27	-2.76	SB25	-2.54
NORMAL MODE 35	OBSERVED=	1006.0 CM-1	CALCULATED=	988.5 CM-1	ERROR=	17.5 CM-1	OR	1.7 PERCENT			
INTERNAL COORDINATES-	25.00	C2C3	11.42	C1C2	10.72	C-09	9.11	C-06	9.05	C-07	6.50
FORCE CONSTANTS-	40.00	CC	36.20	CC	21.21	UCH	10.66	CCH	10.06	UCH	
OFF DIAGONAL-	-13.64	SB22	-6.05	SB21	-4.88	SB24	-3.85	SB27	-2.15	SB26	2.12

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400									
MOLECULE 22 -6 NG=1237 BETA GLUCOSE GG									
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NORMAL MODE 36	OBSERVED=	952.0 CM-1	CALCULATED=	967.0 CM-1	ERROR=	-15.0 CM-1	OR	-1.6 PERCENT	
INTERNAL COORDINATES-	21.63	C-06 16.41 C-U8	15.96 C1C2	6.33 C-01	5.17 C-07	5.18 C-06			
FORCE CONSTANTS-	51.95	CC 21.07 CC	11.02 CCO	7.30 CCH	6.91 CCH				
OFF DIAGONAL-	-6.44	SB22 4.43 SS18	-3.98 SB24	2.79 SB27	-1.72 SB21	-1.62 SB26			
NORMAL MODE 37	OBSERVED=	913.0 CM-1	CALCULATED=	904.5 CM-1	ERROR=	8.5 CM-1	OR	0.9 PERCENT	
INTERNAL COORDINATES-	28.12	C5C1 19.42 C-U*	8.11 CCH8	6.27 C5D1	5.87 C4C5	5.78 HC5C			
FORCE CONSTANTS-	30.66	CC 30.98 CC	17.47 CCH	7.46 CCO					
OFF DIAGONAL-	-7.58	SB26 -6.49 SB21	6.30 SS18	-6.05 SB22	-3.56 SB25	-3.04 SB27			
NORMAL MODE 38	OBSERVED=	898.0 CM-1	CALCULATED=	891.3 CM-1	ERROR=	6.7 CM-1	OR	0.8 PERCENT	
INTERNAL COORDINATES-	15.97	C5D1 13.42 CCHA	12.12 CCH8	11.45 C4C5	8.85 CCO	5.60 C-01	5.08 C-0*		
FORCE CONSTANTS-	30.66	CC 29.20 CC	14.03 CC	13.38 CCH	8.85 CCO	8.21 CCO			
OFF DIAGONAL-	-5.05	SB21 -4.82 SB24	-3.33 SB23	-2.41 SB27	-2.28 SS18	2.11 SB25	-1.94 SB22	1.68 BB43	
NORMAL MODE 39	OBSERVED=	714.0 CM-1	CALCULATED=	723.0 CM-1	ERROR=	-9.0 CM-1	OR	-1.3 PERCENT	
INTERNAL COORDINATES-	18.99	CCO* 7.63 CCO*	6.82 CCH8	6.70 CCH5	5.82 CCH	5.63 C4C5	5.30 C4CC		
FORCE CONSTANTS-	40.74	CCO 27.52 CCH	8.71 CC	5.76 CCH	5.20 CCO				
OFF DIAGONAL-	-7.84	BB43 -7.50 BB34	5.01 SB25	-4.80 BB29	4.07 SB21	-2.01 SB27	-1.72 BB41		
NORMAL MODE 40	OBSERVED=	632.0 CM-1	CALCULATED=	623.1 CM-1	ERROR=	8.9 CM-1	OR	1.4 PERCENT	
INTERNAL COORDINATES-	12.60	C0C6 8.81 C0*C	6.94 CCH3	6.77 HC2C	6.49 CCO9	5.73 C-06			
FORCE CONSTANTS-	42.03	CCO 21.75 CCH	12.21 CCO	8.81 CCH	5.07 CCH				
OFF DIAGONAL-	-7.28	BB34 6.69 BB43	6.59 SB25	-4.94 BB29	-2.85 SB27	1.96 SB24	-1.71 BB41		
NORMAL MODE 41	OBSERVED=	593.0 CM-1	CALCULATED=	600.4 CM-1	ERROR=	-7.4 CM-1	OR	-1.2 PERCENT	
INTERNAL COORDINATES-	14.92	OCO 10.57 C9CC	9.21 CCO6	8.04 C4CC	7.92 CCO*	7.34 C07C	7.33 CCO9	5.53 CCO7	
FORCE CONSTANTS-	58.19	CCO 17.91 CCH	14.92 CCO	9.31 CCH	7.46 CCH	6.26 CCO			
OFF DIAGONAL-	-10.80	BB34 -4.96 BB42	4.93 SB24	-4.49 SB21	4.45 BB43	-2.33 SB25	-2.23 BB29	2.02 SB22	-1.74 BB41
NORMAL MODE 42	OBSERVED=	574.0 CM-1	CALCULATED=	582.5 CM-1	ERROR=	-8.5 CM-1	OR	-1.5 PERCENT	
INTERNAL COORDINATES-	19.64	C0CC 13.71 CCO*	6.14 C-07	5.37 HC4C	5.02 CCH				
FORCE CONSTANTS-	40.61	CCO 21.77 CCH	6.11 CCH	5.84 CCH	5.02 CCH				
OFF DIAGONAL-	-8.72	BB34 6.28 SB25	5.78 BB43	-4.88 BB29	3.93 SB22	-2.81 SB27	-1.62 BB41		
NORMAL MODE 43	OBSERVED=	519.0 CM-1	CALCULATED=	524.1 CM-1	ERROR=	-5.1 CM-1	OR	-1.0 PERCENT	
INTERNAL COORDINATES-	9.61	C0C* 9.33 C4C5	6.28 CCH8	5.73 C3C4	5.23 CCH2				
FORCE CONSTANTS-	33.88	CCO 23.42 CCH	17.24 CCH	16.58 CCH					
OFF DIAGONAL-	-6.98	BB34 5.32 BB43	4.29 SS18	3.73 SB21	-3.30 BB29	1.86 SB25	-1.65 SB27		
NORMAL MODE 44	OBSERVED=	454.0 CM-1	CALCULATED=	459.5 CM-1	ERROR=	-5.5 CM-1	OR	-1.2 PERCENT	
INTERNAL COORDINATES-	10.61	C0CC 9.37 CCO6	9.86 CCH1	5.30 CCH2	5.15 CCO9				
FORCE CONSTANTS-	42.28	CCO 25.10 CCH	9.30 CCH	8.51 CCH	7.38 CCO				
OFF DIAGONAL-	-7.89	BB34 5.94 BB43	-5.41 BB29	3.45 SB25	-2.11 SB26	-1.61 SB27	1.53 SS18		
NORMAL MODE 45	OBSERVED=	425.0 CM-1	CALCULATED=	414.4 CM-1	ERROR=	10.6 CM-1	OR	2.5 PERCENT	
INTERNAL COORDINATES-	20.06	C2CC 11.54 C0*C	10.73 C1CC	9.63 CCO9	5.70 C3CC	5.25 CCO8			
FORCE CONSTANTS-	36.90	CCO 20.82 CCO	11.54 CCO	6.55 CCO	5.64 CCH	5.47 CCH			
OFF DIAGONAL-	4.09	SB21 2.90 SB25	-2.88 BB42	2.29 BB43	-2.27 BB41	1.70 SB23			
NORMAL MODE 46	OBSERVED=	401.0 CM-1	CALCULATED=	388.6 CM-1	ERROR=	12.4 CM-1	OR	3.1 PERCENT	
INTERNAL COORDINATES-	17.22	C0CC 16.13 CCO*	13.53 C3CC	8.69 CCH8	6.19 C1CC				
FORCE CONSTANTS-	52.44	CCO 20.54 CCH	10.11 CCH	5.84 CCH	5.02 CCH				
OFF DIAGONAL-	6.13	SB21 -4.67 BB34	3.36 SB25	3.03 BB43	-3.02 BB42	-1.87 BB41	-1.60 BB29		
NORMAL MODE 47	OBSERVED=	347.0 CM-1	CALCULATED=	346.8 CM-1	ERROR=	0.2 CM-1	OR	0.1 PERCENT	
INTERNAL COORDINATES-	26.49	C0CC 15.04 CCO7	9.83 CCO8	7.73 CCH					
FORCE CONSTANTS-	67.37	CCO 10.60 CCH	8.75 CC	7.72 CCO					
OFF DIAGONAL-	-8.58	BB34 5.05 SB22	-3.11 SB25	2.82 BB43	-2.63 BB42	-2.32 BB29	-2.09 SB21		
NORMAL MODE 48	OBSERVED=	327.0 CM-1	CALCULATED=	333.4 CM-1	ERROR=	-6.4 CM-1	OR	-1.9 PERCENT	
INTERNAL COORDINATES-	8.97	CCO 15.54 CCO	11.24 CCH8	7.44 CCO6					
FORCE CONSTANTS-	51.08	CCO 15.54 CCO	13.65 CCH	8.48 CC	8.07 T-OH	5.85 CCH			
OFF DIAGONAL-	-6.94	BB34 5.31 SB22	-2.63 BB29	-2.50 SB24	2.40 BB43	-2.20 SB21	-1.80 BB42		
NORMAL MODE 49	OBSERVED=	309.0 CM-1	CALCULATED=	313.7 CM-1	ERROR=	-4.7 CM-1	OR	-1.5 PERCENT	
INTERNAL COORDINATES-	21.16	C0CC 11.72 CCO8	11.35 C07C	10.42 CCO7	9.50 CCO9	6.23 CCO9	6.18 CCO6	5.84 TH-3	
FORCE CONSTANTS-	82.77	CCO 12.97 T-OH	7.33 CCH	5.84 CCH					
OFF DIAGONAL-	-8.69	BB34 -4.48 BB42	-3.18 SB22	1.71 BB41	-1.68 SB26				
NORMAL MODE 50	OBSERVED=	289.0 CM-1	CALCULATED=	297.6 CM-1	ERROR=	-8.6 CM-1	OR	-3.0 PERCENT	
INTERNAL COORDINATES-	21.26	C0CC 12.30 CCO8	11.84 CCO9	9.48 CCO6	5.43 CCH3				
FORCE CONSTANTS-	58.15	CCO 20.00 CCH	8.29 CCO	5.84 CCH	5.43 T-OH				
OFF DIAGONAL-	-12.79	BB34 6.41 BB43	4.88 SB22	-4.34 BB29	-2.59 SB21	-2.35 SB25			
NORMAL MODE 51	OBSERVED=	274.0 CM-1	CALCULATED=	277.6 CM-1	ERROR=	-3.6 CM-1	OR	-1.3 PERCENT	
INTERNAL COORDINATES-	20.38	CCO 22.91 TH-5	7.81 CCH	7.93 CCH					
FORCE CONSTANTS-	50.37	CCO 22.91 T-OH	9.44 CCH	8.58 CCH					
OFF DIAGONAL-	-5.69	BB34 3.07 SB22	-2.48 BB33	-2.18 BB42					
NORMAL MODE 52	OBSERVED=	250.0 CM-1	CALCULATED=	260.4 CM-1	ERROR=	-10.4 CM-1	OR	-4.2 PERCENT	
INTERNAL COORDINATES-	16.35	C4CC 11.72 TH-4	10.00 CCO8	9.66 CCO*	8.49 CCO9	5.19 TH-3	5.01 TCC		
FORCE CONSTANTS-	29.16	CCO 17.40 CCH	17.02 T-OH	9.66 CCH	8.32 CCH	7.00 T-CC	6.13 CCH		
OFF DIAGONAL-	4.07	SB21 -3.82 BB34	3.51 BB43	-2.15 SB26					
NORMAL MODE 53	OBSERVED=	227.0 CM-1	CALCULATED=	226.6 CM-1	ERROR=	0.4 CM-1	OR	0.2 PERCENT	
INTERNAL COORDINATES-	38.14	TH-1 36.20 TH-2	9.84 TH-5	7.71 TH-3					
FORCE CONSTANTS-	95.78	T-CH							
OFF DIAGONAL-	NONE								
NORMAL MODE 54	OBSERVED=	0.0 CM-1	CALCULATED=	216.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	34.08	TH-1 24.56 TH-3	16.41 TH-4	7.28 TH-2					
FORCE CONSTANTS-	84.34	T-OH 8.46 CCO							
OFF DIAGONAL-	NONE								
NORMAL MODE 55	OBSERVED=	0.0 CM-1	CALCULATED=	214.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	39.81	TH-1 32.75 TH-4	7.28 TH-1						
FORCE CONSTANTS-	83.10	T-OH 11.58 CCO							
OFF DIAGONAL-	NONE								
NORMAL MODE 56	OBSERVED=	0.0 CM-1	CALCULATED=	211.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	54.54	TH-1 39.39 TH-1	8.61 CCO*	6.99 C4CC					
FORCE CONSTANTS-	68.84	T-OH 15.45 CCO	7.92 CCH						
OFF DIAGONAL-	-1.93	BB34							
NORMAL MODE 57	OBSERVED=	0.0 CM-1	CALCULATED=	210.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	44.75	TH-3 26.09 TH-4	7.14 TH-2	5.67 CCO8					
FORCE CONSTANTS-	81.81	T-OH 18.18 CCO							
OFF DIAGONAL-	-2.31	BB34							
NORMAL MODE 58	OBSERVED=	0.0 CM-1	CALCULATED=	141.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	18.10	C0*C 11.52 C4CC	7.92 TCC4	6.52 CCO*	5.92 TCO1	5.79 CCO*	5.18 CCO		
FORCE CONSTANTS-	23.50	CCO 18.10 CCH	16.72 CCH	9.68 T-CC	9.50 T-CC	8.32 CCH	5.18 CCO		
OFF DIAGONAL-	4.64	BB43 -1.95 SB25	1.67 BB41						
NORMAL MODE 59	OBSERVED=	0.0 CM-1	CALCULATED=	89.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	20.85	C2CC 20.07 TCC5	10.49 TCC2	8.23 C1CC	8.23 C3CC				
FORCE CONSTANTS-	40.53	T-CC 38.63 CCO	20.10 CCO	2.32 BB41	-1.59 BB34				
OFF DIAGONAL-	-5.00	SB25 -4.12 SB21	-3.91 BB42						
NORMAL MODE 60	OBSERVED=	0.0 CM-1	CALCULATED=	74.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	39.81	TCC 6.46 C3CC	6.46 C3CC						
FORCE CONSTANTS-	67.73	T-CC 15.49 CCH	8.95 CCO						
OFF DIAGONAL-	-1.60	BB42							
NORMAL MODE 61	OBSERVED=	0.0 CM-1	CALCULATED=	70.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	15.66	TCC 11.16 CCO*	10.94 C3CC	10.74 C1CC	8.89 TCC3	5.21 TCO2	5.12 CCO*		
FORCE CONSTANTS-	33.67	T-CC 33.54 CCO	25.47 CCH	5.89 T-CC					
OFF DIAGONAL-	-3.68	BB42 -2.84 BB34	-2.58 SB25	1.80 BB41					

43. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 6.39

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400									
MOLECULE 23 -6 NG=1237 BETA GLUCOSE TG									
PAGE 1									
NORMAL MODE 8 OBSERVED= 1449.0 CM-1 CALCULATED= 1449.4 CM-1 ERROR= -0.4 CM-1 OR -0.0 PERCENT									
INTERNAL COORDINATES-	59.77	HCH	21.48	OC4A	19.84	OC4B			
FORCE CONSTANTS-	59.77	HCH	41.45	UCH					
OFF DIAGONAL-	-4.17	SB27							
NORMAL MODE 9 OBSERVED= 1415.0 CM-1 CALCULATED= 1422.0 CM-1 ERROR= -7.0 CM-1 OR -0.5 PERCENT									
INTERNAL COORDINATES-	9.73	OC4H	9.19	HC4C	9.05	C5H	7.82	C5H	7.45
FORCE CONSTANTS-	38.67	UCH	36.82	CCH	10.34	CO	9.37	BCOH	6.61
OFF DIAGONAL-	-9.96	SB27	6.72	BB29	6.40	BB34	-5.01	SB26	-4.06
NORMAL MODE 10 OBSERVED= 0.0 CM-1 CALCULATED= 1421.5 CM-1 ERROR= 0.0 CM-1 OR 0.0 PERCENT									
INTERNAL COORDINATES-	28.38	C1H	15.87	OC1H	11.76	C1OH	6.14	C1H	5.49
FORCE CONSTANTS-	52.30	UCH	19.34	BCOH	19.01	CCH	9.50	CO	5.98
OFF DIAGONAL-	-5.66	SB27	3.69	BB34	3.22	SB28	-3.18	SB25	3.17
NORMAL MODE 11 OBSERVED= 1402.0 CM-1 CALCULATED= 1407.5 CM-1 ERROR= -5.5 CM-1 OR -0.4 PERCENT									
INTERNAL COORDINATES-	29.13	C1H	20.99	C1OH	14.03	C2OH	13.47	OC1H	6.53
FORCE CONSTANTS-	51.71	UCH	35.11	BCOH	6.42	CCH			
OFF DIAGONAL-	-2.18	BB45	2.11	SB28	-1.88	SB26			
NORMAL MODE 12 OBSERVED= 0.0 CM-1 CALCULATED= 1397.1 CM-1 ERROR= 0.0 CM-1 OR 0.0 PERCENT									
INTERNAL COORDINATES-	35.39	C3OH	19.04	OC3H	9.28	C1OH	6.25	HC3C	
FORCE CONSTANTS-	49.56	BCOH	24.88	UCH	18.05	CCH			
OFF DIAGONAL-	5.08	SB28	-4.93	SB27	-4.63	SB26	3.59	BB29	-2.67
NORMAL MODE 13 OBSERVED= 1387.0 CM-1 CALCULATED= 1390.8 CM-1 ERROR= -3.8 CM-1 OR -0.3 PERCENT									
INTERNAL COORDINATES-	26.11	C3OH	21.14	C1UH	17.58	C1OH	15.29	C2OH	
FORCE CONSTANTS-	80.12	BCOH	8.90	UCH	5.22	CCH			
OFF DIAGONAL-	3.00	SB28	-1.73	BB39					
NORMAL MODE 14 OBSERVED= 1375.0 CM-1 CALCULATED= 1386.9 CM-1 ERROR= -11.9 CM-1 OR -0.9 PERCENT									
INTERNAL COORDINATES-	33.00	C1OH	22.04	C1OH	19.95	C2OH			
FORCE CONSTANTS-	76.24	BCOH	11.00	UCH	8.04	CCH			
OFF DIAGONAL-	2.10	SB28	-2.01	SB26	-1.55	SB27			
NORMAL MODE 15 OBSERVED= 1369.0 CM-1 CALCULATED= 1372.7 CM-1 ERROR= -3.7 CM-1 OR -0.3 PERCENT									
INTERNAL COORDINATES-	17.81	C3OH	14.54	C2UH	14.16	C1OH	6.44	HC5C	5.85
FORCE CONSTANTS-	44.40	BCOH	26.29	CCH	16.01	UCH			
OFF DIAGONAL-	5.71	BB29	-3.93	SB27	3.13	BB34	-2.76	SB28	1.52
NORMAL MODE 16 OBSERVED= 1351.0 CM-1 CALCULATED= 1355.1 CM-1 ERROR= -4.1 CM-1 OR -0.3 PERCENT									
INTERNAL COORDINATES-	12.28	C2OH	10.28	OC2H	9.99	CC3H	7.11	CCH	6.24
FORCE CONSTANTS-	46.39	CCH	22.07	CCH	19.22	BCOH			
OFF DIAGONAL-	10.12	BB29	-4.56	SB27	3.48	BB34	-2.76	BB45	-1.89
NORMAL MODE 17 OBSERVED= 1343.0 CM-1 CALCULATED= 1326.6 CM-1 ERROR= 16.4 CM-1 OR 1.2 PERCENT									
INTERNAL COORDINATES-	14.15	HC3C	12.75	CC4H	8.10	HC4C	7.87	HC5C	6.35
FORCE CONSTANTS-	64.91	CCH	17.05	UCH	8.12	BCOH			
OFF DIAGONAL-	13.89	BB29	-7.19	SB26	-3.61	BB45	-1.69	SB27	
NORMAL MODE 18 OBSERVED= 1308.0 CM-1 CALCULATED= 1318.1 CM-1 ERROR= -10.1 CM-1 OR -0.8 PERCENT									
INTERNAL COORDINATES-	26.87	CCHB	22.88	OCBH	16.54	C5H	8.72	HC5C	
FORCE CONSTANTS-	44.33	UCH	44.27	CCH					
OFF DIAGONAL-	-3.63	BB45	3.27	BB34	-2.92	SB27			
NORMAL MODE 19 OBSERVED= 0.0 CM-1 CALCULATED= 1303.7 CM-1 ERROR= 0.0 CM-1 OR 0.0 PERCENT									
INTERNAL COORDINATES-	13.00	CC2H	11.01	HC2C	8.25	CC5H	7.93	C5H	7.54
FORCE CONSTANTS-	59.40	CCH	24.00	UCH	7.41	CO	6.72	COH	6.08
OFF DIAGONAL-	9.05	BB29	-5.91	SB26	-3.36	BB45			
NORMAL MODE 20 OBSERVED= 1283.0 CM-1 CALCULATED= 1294.9 CM-1 ERROR= -11.9 CM-1 OR -0.9 PERCENT									
INTERNAL COORDINATES-	17.97	C4OH	14.07	C5H	9.33	OC4H	8.99	CC5H	8.32
FORCE CONSTANTS-	43.89	CCH	31.72	UCH	17.97	COH			
OFF DIAGONAL-	-3.16	BB45	2.71	BB29	-2.27	SB26			
NORMAL MODE 21 OBSERVED= 1270.0 CM-1 CALCULATED= 1272.7 CM-1 ERROR= -2.7 CM-1 OR -0.2 PERCENT									
INTERNAL COORDINATES-	24.35	OC3H	12.25	OC2H	9.35	CC3H	7.69	CC4H	7.43
FORCE CONSTANTS-	46.75	UCH	22.62	CCH	10.03	CO	7.69	COH	
OFF DIAGONAL-	8.23	SB27	-3.45	BB29	-2.74	BB45	-2.42	SB25	2.21
NORMAL MODE 22 OBSERVED= 1263.0 CM-1 CALCULATED= 1263.1 CM-1 ERROR= -0.1 CM-1 OR -0.0 PERCENT									
INTERNAL COORDINATES-	15.50	C4OH	15.05	OC2H	9.11	OC1C	8.96	OC4H	6.90
FORCE CONSTANTS-	27.06	UCH	23.52	CCH	20.58	CO	15.50	COH	7.76
OFF DIAGONAL-	-4.18	SB25	3.84	SB27	-3.33	BB29	3.09	BB34	-2.02
NORMAL MODE 23 OBSERVED= 1250.0 CM-1 CALCULATED= 1246.2 CM-1 ERROR= 3.8 CM-1 OR 0.3 PERCENT									
INTERNAL COORDINATES-	14.30	C4OH	12.15	C5H	7.76	CC4H	6.51	OC3H	5.86
FORCE CONSTANTS-	33.10	CCH	29.94	CCH	15.17	CO	15.30	COH	
OFF DIAGONAL-	6.49	SB27	-3.85	BB29	-2.47	BB45	-2.41	SB25	1.68
NORMAL MODE 24 OBSERVED= 1222.0 CM-1 CALCULATED= 1215.2 CM-1 ERROR= 6.8 CM-1 OR 0.5 PERCENT									
INTERNAL COORDINATES-	18.14	C5H	14.87	C-06	7.40	OC5H	7.42	HC2C	6.89
FORCE CONSTANTS-	38.31	CO	35.66	CCH	26.08	UCH	8.00	CCO	
OFF DIAGONAL-	-4.97	SB25	-4.60	BB29	3.60	BB34	-2.43	BB45	
NORMAL MODE 25 OBSERVED= 1202.0 CM-1 CALCULATED= 1190.7 CM-1 ERROR= 11.3 CM-1 OR 0.9 PERCENT									
INTERNAL COORDINATES-	19.44	CC1H	9.21	C-06	9.06	OC1C	8.67	OC2H	8.59
FORCE CONSTANTS-	32.51	UCH	31.62	CC	29.91	CCH			
OFF DIAGONAL-	-5.28	BB29	-4.34	SB25	-2.12	BB45	2.08	SB27	1.80
NORMAL MODE 26 OBSERVED= 1152.0 CM-1 CALCULATED= 1161.6 CM-1 ERROR= -9.6 CM-1 OR -0.8 PERCENT									
INTERNAL COORDINATES-	21.84	C5C1	10.86	OC4A	6.62	4C01	5.58	HC5C	
FORCE CONSTANTS-	30.03	CO	28.07	CCH	21.27	UCH	16.42	CCO	9.53
OFF DIAGONAL-	-8.82	SB25	8.09	SB27	-5.67	BB29	2.71	BB34	-1.59
NORMAL MODE 27 OBSERVED= 1126.0 CM-1 CALCULATED= 1115.2 CM-1 ERROR= 10.8 CM-1 OR 1.0 PERCENT									
INTERNAL COORDINATES-	13.22	C-07	11.62	CC1H	11.29	OC1H	9.12	CC2H	8.34
FORCE CONSTANTS-	28.48	UCH	26.52	CC	16.58	CC	16.11	OC4H	6.49
OFF DIAGONAL-	-10.20	BB29	-6.90	SB25	3.61	BB34	-2.97	BB45	-2.62
NORMAL MODE 28 OBSERVED= 1116.0 CM-1 CALCULATED= 1102.4 CM-1 ERROR= 13.6 CM-1 OR 1.2 PERCENT									
INTERNAL COORDINATES-	21.75	C5C1	14.87	C-08	10.67	C5OH	8.81	C-07	6.95
FORCE CONSTANTS-	52.00	CO	30.82	CC	12.95	CCH	8.42	UCH	
OFF DIAGONAL-	-5.57	SB28	-4.96	SS18	-4.09	SB22	-2.40	SB26	1.87
NORMAL MODE 29 OBSERVED= 1097.0 CM-1 CALCULATED= 1097.4 CM-1 ERROR= -0.4 CM-1 OR -0.0 PERCENT									
INTERNAL COORDINATES-	24.13	C4C3	22.91	C3C4	19.98	C5OH	12.55	C5C1	6.45
FORCE CONSTANTS-	67.26	CC	29.99	CC	16.17	CCO	10.13	UCH	8.79
OFF DIAGONAL-	-13.25	SB22	-7.61	SB26	-3.88	SB27	-3.88	BB34	-2.82
NORMAL MODE 30 OBSERVED= 1079.0 CM-1 CALCULATED= 1076.5 CM-1 ERROR= 2.5 CM-1 OR 0.2 PERCENT									
INTERNAL COORDINATES-	24.54	C-07	20.71	C2C3	11.44	C-08	8.93	C3C4	8.81
FORCE CONSTANTS-	49.71	CO	33.68	CC	16.66	CCO	13.75	CCH	11.48
OFF DIAGONAL-	-8.30	SB28	-6.56	SB25	-6.15	SB22	-4.42	SB27	-3.51
NORMAL MODE 31 OBSERVED= 1069.0 CM-1 CALCULATED= 1059.8 CM-1 ERROR= 9.2 CM-1 OR 0.9 PERCENT									
INTERNAL COORDINATES-	46.32	C-08	20.15	C-08	14.71	C3C4	6.88	C-06	6.30
FORCE CONSTANTS-	79.11	CO	23.62	CC	9.88	BCOH	8.48	CO	8.49
OFF DIAGONAL-	-9.78	SB28	-9.33	SB27	-5.21	SS18	-4.45	SB25	-4.27
NORMAL MODE 32 OBSERVED= 1050.0 CM-1 CALCULATED= 1057.3 CM-1 ERROR= -7.3 CM-1 OR -0.7 PERCENT									
INTERNAL COORDINATES-	28.51	C2C3	27.57	C1C2	24.51	C-08	16.03	C-08	5.40
FORCE CONSTANTS-	56.48	CO	46.95	CC	11.14	CCO	8.97	BCOH	6.69
OFF DIAGONAL-	-8.10	SB22	-7.66	SB27	-6.41	SB28	-5.89	SB21	-5.25
NORMAL MODE 33 OBSERVED= 1024.0 CM-1 CALCULATED= 1032.0 CM-1 ERROR= -18.0 CM-1 OR -1.8 PERCENT									
INTERNAL COORDINATES-	11.87	C3C4	21.04	C-07	9.50	UCH	4.35	C4C1	
FORCE CONSTANTS-	36.15	CC	33.73	CC	16.35	UCH	12.62	CCH	11.26
OFF DIAGONAL-	-11.91	SB21	-8.15	SB22	-6.29	SB27	-4.28	SB28	-2.91
NORMAL MODE 34 OBSERVED= 1012.0 CM-1 CALCULATED= 1032.0 CM-1 ERROR= -20.0 CM-1 OR -2.0 PERCENT									
INTERNAL COORDINATES-	49.89	C-09	21.80	C4OH	11.29	C4C5	6.95	C-08	6.77
FORCE CONSTANTS-	65.97	CO	26.17	CC	21.80	COH	10.98	CCC	9.91
OFF DIAGONAL-	-15.82	SB28	-9.24	SB27	-8.34	SB21	-6.32	SB25	-6.25
NORMAL MODE 35 OBSERVED= 1006.0 CM-1 CALCULATED= 986.1 CM-1 ERROR= 19.9 CM-1 OR 2.0 PERCENT									
INTERNAL COORDINATES-	23.30	C1C2	17.00	C2C3	12.76	C-09	11.08	C-07	6.38
FORCE CONSTANTS-	45.44	CC	36.36	CC	20.43	CCO	10.87	UCH	8.34
OFF DIAGONAL-	-14.95	SB22	-5.56	SB21	-3.71	SB27	-3.20	SB26	-3.07

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400				PAGE 2	
MOLECULE 23		-6 NG=1237 BETA GLUCOSE TG			
NORMAL MODE 36	OBSERVED= 952.0 CM-1	CALCULATED= 977.6 CM-1	ERROR= -25.6 CM-1	DR	-2.7 PERCENT
INTERNAL COORDINATES-	23.18 C5C* 22.12 C-08	11.61 C4C5 10.05 C3C4	7.43 C2C3		
FORCE CONSTANTS-	55.21 CC 26.22 CC	16.78 CCO 15.19 CCH			
OFF DIAGONAL-	-13.27 SB22 -6.36 SB26	-5.06 SB21 3.67 SS18	-2.66 BB29		
NORMAL MODE 37	OBSERVED= 913.0 CM-1	CALCULATED= 942.1 CM-1	ERROR= -29.1 CM-1	OR	-3.2 PERCENT
INTERNAL COORDINATES-	25.10 C-06 16.36 O* C1	14.84 C5C 8.46 OCO	5.10 CCO7		
FORCE CONSTANTS-	48.85 CC 19.91 CC	10.32 CCO 9.45 CCH	8.46 OCO	6.53 CCC	6.46 CCH
OFF DIAGONAL-	-11.16 SB24 -5.18 SB21	4.87 SB27 -3.74 SB22	-2.94 SB23	2.12 SS18	1.98 BB43
NORMAL MODE 38	OBSERVED= 898.0 CM-1	CALCULATED= 849.2 CM-1	ERROR= 48.8 CM-1	OR	5.3 PERCENT
INTERNAL COORDINATES-	23.39 CCHB 20.70 CCHA	18.92 C4C5 8.02 C5CH	9.91 CCH		
FORCE CONSTANTS-	65.29 CCH 22.45 CC	12.23 CCO			
OFF DIAGONAL-	-8.42 BB29 -5.48 SB22	-2.64 SB21			
NORMAL MODE 39	OBSERVED= 714.0 CM-1	CALCULATED= 678.4 CM-1	ERROR= 35.6 CM-1	UR	5.0 PERCENT
INTERNAL COORDINATES-	46.66 OCO 7.29 C-06	9.89 CCO* 5.55 C* C			
FORCE CONSTANTS-	22.79 CCO 19.35 CO	16.66 OCO 8.70 OCH	7.32 CCH	5.55 COC	
OFF DIAGONAL-	7.51 SB24 -6.50 SB27	6.28 SB25 4.70 BB43	4.02 SB22	1.76 SS18	-1.66 BB34
NORMAL MODE 40	OBSERVED= 632.0 CM-1	CALCULATED= 623.6 CM-1	ERROR= 8.4 CM-1	OR	1.3 PERCENT
INTERNAL COORDINATES-	5.47 O* C2 14.33 CCG9	9.88 HC2C 8.73 CC3H	7.73 CCO8	7.70 CCO8	7.48 C4CC
FORCE CONSTANTS-	59.51 CCO 40.01 CCH	16.18 *CCC			5.53 HC3C
OFF DIAGONAL-	-17.99 BB34 10.36 BB43	-9.13 BB29 -1.91 BB41			
NORMAL MODE 41	OBSERVED= 593.0 CM-1	CALCULATED= 603.6 CM-1	ERROR= -10.6 CM-1	OR	-1.8 PERCENT
INTERNAL COORDINATES-	14.82 CCO6 11.86 C* C	10.16 CCO7 8.32 C-07	7.48 CCO1	6.58 O* CC	5.83 C1C2
FORCE CONSTANTS-	50.25 CCO 17.45 CO	11.86 COC 9.56 CC	5.80 CCH		
OFF DIAGONAL-	5.97 SB25 -4.75 BB34	3.31 SB22 2.99 BB43	-2.96 SB27	-2.77 BB42	-2.66 SB23
NORMAL MODE 42	OBSERVED= 574.0 CM-1	CALCULATED= 561.3 CM-1	ERROR= 12.7 CM-1	OR	2.2 PERCENT
INTERNAL COORDINATES-	13.98 UBCC 9.64 C4C1	6.88 CCH2 6.57 HC4C	6.37 C4CC	5.76 HC3C	5.43 CC1H
FORCE CONSTANTS-	33.03 O* CC 4.74 CCH	7.58 CCH			5.38 O* CC
OFF DIAGONAL-	-13.51 BB34 10.91 BB43	-9.25 BB29 2.94 BB42	2.49 SB25		
NORMAL MODE 43	OBSERVED= 519.0 CM-1	CALCULATED= 500.5 CM-1	ERROR= 18.5 CM-1	OR	3.6 PERCENT
INTERNAL COORDINATES-	16.75 CCO* 8.51 O* CC	8.19 C4C5 8.37 HC5C	5.88 C3C4		
FORCE CONSTANTS-	17.84 CCO 26.72 CC	17.95 CCH 8.14 CO			
OFF DIAGONAL-	-7.95 BB34 5.16 BB43	4.29 SB21 -3.84 BB29	3.15 SS18	3.04 SB22	2.91 SB25
NORMAL MODE 44	OBSERVED= 454.0 CM-1	CALCULATED= 451.7 CM-1	ERROR= 2.3 CM-1	OR	0.5 PERCENT
INTERNAL COORDINATES-	16.47 C1C2 12.29 CCG*	9.62 C2CC 6.33 CCO8			
FORCE CONSTANTS-	31.15 CCO 27.86 CCC	15.11 CCO 8.51 CC			
OFF DIAGONAL-	5.35 SB21 5.07 SB25	2.93 BB43 -2.74 BB42	-1.94 BB41	1.53 SB24	
NORMAL MODE 45	OBSERVED= 425.0 CM-1	CALCULATED= 407.9 CM-1	ERROR= 17.1 CM-1	OR	4.0 PERCENT
INTERNAL COORDINATES-	12.93 CCO9 10.43 CCO	9.67 O* CC 8.62 C4CC	6.50 CCH2	6.06 CC1H	
FORCE CONSTANTS-	47.05 CCO 31.67 CCH	10.87 CCO 10.43 OCO			
OFF DIAGONAL-	-10.73 BB34 -7.07 BB29	7.00 BB43 -2.93 SB22	1.56 BB42		
NORMAL MODE 46	OBSERVED= 401.0 CM-1	CALCULATED= 401.7 CM-1	ERROR= -0.7 CM-1	OR	-0.2 PERCENT
INTERNAL COORDINATES-	13.75 C3CC 12.77 C2CC	9.92 C* C 8.29 O* CC	7.11 O8CC	5.29 O* CC	
FORCE CONSTANTS-	28.66 CCO 26.74 CCH	9.92 COC 8.86 CC	5.79 CC	5.58 CCH	
OFF DIAGONAL-	4.38 SB21 5.07 SB25	-2.60 BB42 2.14 BB43	2.13 SB23	-1.83 BB41	1.65 SB22
NORMAL MODE 47	OBSERVED= 347.0 CM-1	CALCULATED= 352.6 CM-1	ERROR= -5.6 CM-1	OR	-1.6 PERCENT
INTERNAL COORDINATES-	52.43 O* CC 14.92 C* CC	5.06 UBCC			
FORCE CONSTANTS-	67.92 CCO 10.19 CCH	7.24 CCH			
OFF DIAGONAL-	-7.46 BB34 4.99 SB22	-2.84 BB42 -1.81 BB29	1.80 BB43		
NORMAL MODE 48	OBSERVED= 327.0 CM-1	CALCULATED= 335.5 CM-1	ERROR= -8.5 CM-1	OR	-2.6 PERCENT
INTERNAL COORDINATES-	29.04 CCO7 17.38 C4C1	12.30 CCO8 5.98 O* C1	5.03 CCO*		
FORCE CONSTANTS-	71.39 CCO 11.36 CCH	10.54 CO 7.57 CCC	5.16 T-OH		
OFF DIAGONAL-	-9.81 BB34 -2.62 BB42	2.31 SB22 -2.00 BB29	-1.96 SB27		
NORMAL MODE 49	OBSERVED= 309.0 CM-1	CALCULATED= 318.5 CM-1	ERROR= -9.5 CM-1	OR	-3.1 PERCENT
INTERNAL COORDINATES-	23.73 CCO6 17.79 OCO	8.64 CCO9 8.06 CCO7	6.37 TH-1	6.07 C2C3	
FORCE CONSTANTS-	53.44 CCO 17.79 CCO	10.82 T-OH 8.65 CC	6.81 CO		
OFF DIAGONAL-	-4.12 BB42 -3.29 BB34	1.83 SB24			
NORMAL MODE 50	OBSERVED= 289.0 CM-1	CALCULATED= 302.5 CM-1	ERROR= -13.5 CM-1	OR	-4.7 PERCENT
INTERNAL COORDINATES-	21.58 UBCC 20.20 CCO8	10.53 TH-3 7.42 O* CC	5.26 C1CC	5.26 CCO6	
FORCE CONSTANTS-	9.71 CCO 12.26 T-OH	11.16 CCH 9.41 CCC	6.48 CC		
OFF DIAGONAL-	-10.05 BB34 6.73 BB43	4.42 SB22 -3.99 SB21	-1.94 BB42	-1.76 BB29	
NORMAL MODE 51	OBSERVED= 274.0 CM-1	CALCULATED= 295.6 CM-1	ERROR= -21.6 CM-1	OR	-7.9 PERCENT
INTERNAL COORDINATES-	52.43 O* CC 14.92 C* CC	8.04 O* CC			
FORCE CONSTANTS-	60.46 CCO 23.20 CCH	6.03 CCH			
OFF DIAGONAL-	-13.86 BB34 8.80 BB43	-5.03 BB29 3.08 SB22	-3.00 SB25	-2.05 BB36	-1.86 SB21
NORMAL MODE 52	OBSERVED= 250.0 CM-1	CALCULATED= 242.4 CM-1	ERROR= 7.6 CM-1	OR	3.0 PERCENT
INTERNAL COORDINATES-	34.80 TH-9 9.79 C4CC	9.33 CCO1			
FORCE CONSTANTS-	67.70 T-OH 15.82 CCO	10.73 CCC			
OFF DIAGONAL-	-2.91 BB34				
NORMAL MODE 53	OBSERVED= 227.0 CM-1	CALCULATED= 218.2 CM-1	ERROR= 0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	42.05 TH-4 21.30 TH-1	12.68 TH-3 12.63 TH-2			
FORCE CONSTANTS-	96.83 T-OH				
OFF DIAGONAL-	NONE				
NORMAL MODE 54	OBSERVED= 0.0 CM-1	CALCULATED= 227.0 CM-1	ERROR= 0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	25.47 TH-1 25.23 TH-2	16.64 TH-4 15.62 TH-3	13.87 TH-5		
FORCE CONSTANTS-	88.86 T-OH 6.62 CCO				
OFF DIAGONAL-	NONE				
NORMAL MODE 55	OBSERVED= 0.0 CM-1	CALCULATED= 215.2 CM-1	ERROR= 0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	41.65 TH-2 37.13 TH-1				
FORCE CONSTANTS-	87.17 T-OH 9.85 CCO				
OFF DIAGONAL-	NONE				
NORMAL MODE 56	OBSERVED= 0.0 CM-1	CALCULATED= 210.8 CM-1	ERROR= 0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	52.43 TH-9 22.17 TH-4	7.40 TH-2 6.15 CCO8			
FORCE CONSTANTS-	83.19 T-OH 17.52 CCO				
OFF DIAGONAL-	-2.14 BB34				
NORMAL MODE 57	OBSERVED= 0.0 CM-1	CALCULATED= 194.0 CM-1	ERROR= 0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	24.05 TH-9 23.52 C4CC	13.46 TCC5 5.21 CO* C			
FORCE CONSTANTS-	26.87 CCC 26.25 T-OH	14.98 T-CC 13.82 CCO	5.36 T-CO	5.21 CCO	
OFF DIAGONAL-	-1.68 BB42 1.61 BB43				
NORMAL MODE 58	OBSERVED= 0.0 CM-1	CALCULATED= 147.5 CM-1	ERROR= 0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	30.70 CCO1 22.34 C* C	9.57 CCO* 5.95 TCC4			
FORCE CONSTANTS-	48.68 CCO 22.34 CCO	8.64 CCH 6.94 T-CC	6.79 CCC	5.59 T-CO	
OFF DIAGONAL-	-8.93 BB34 -3.98 SB25	-1.96 BB42 1.73 BB43			
NORMAL MODE 59	OBSERVED= 0.0 CM-1	CALCULATED= 92.4 CM-1	ERROR= 0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	39.25 TCC5 13.09 C1CC	10.89 TCC4 8.11 C2CC			
FORCE CONSTANTS-	56.06 T-CC 12.86 CCO	18.31 CCO			
OFF DIAGONAL-	-3.42 SB25 -2.79 BB42	-2.20 SB21 1.67 BB41			
NORMAL MODE 60	OBSERVED= 0.0 CM-1	CALCULATED= 83.6 CM-1	ERROR= 0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	18.40 C3CC 17.32 C2CC	10.99 TCC5 6.47 CCO9	5.17 TCC3		
FORCE CONSTANTS-	36.56 CCC 34.68 T-CC	23.05 CCO			
OFF DIAGONAL-	-4.19 SB25 -3.94 BB42	2.07 BB41 -1.60 BB34			
NORMAL MODE 61	OBSERVED= 0.0 CM-1	CALCULATED= 65.1 CM-1	ERROR= 0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	28.63 TCC5 9.67 TCC4	8.79 CCO1			
FORCE CONSTANTS-	48.31 T-CC 22.01 CCO	19.64 CCC			
OFF DIAGONAL-	-2.83 BB34 -2.59 BB42	-1.95 SB25			

43. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 11.28

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR GALACTOSE	PROBLEM 400	PAGE 1
MOLECULE 24	GT	
NORMAL MODE 8 OBSERVED= 1487.0 CM-1	CALCULATED= 1455.5 CM-1	ERROR= 31.5 CM-1 OR 2.1 PERCENT
INTERNAL COORDINATES- 67.25 C2OH 5.25 CC3H		
FORCE CONSTANTS- 67.99 HCOH 5.26 CCH	6.09 CCO	
OFF DIAGONAL- 4.46 BB36 3.83 SB28	1.77 BB34 -1.77 SB25	
NORMAL MODE 9 OBSERVED= 1454.0 CM-1	CALCULATED= 1449.7 CM-1	ERROR= 4.3 CM-1 OR 0.3 PERCENT
INTERNAL COORDINATES- 61.81 HCH 20.01 OCHB		
FORCE CONSTANTS- 61.81 HCH 39.42 OCH	18.99 OCHA	
OFF DIAGONAL- -3.88 SB27		
NORMAL MODE 10 OBSERVED= 1434.0 CM-1	CALCULATED= 1430.0 CM-1	ERROR= 3.9 CM-1 OR 0.3 PERCENT
INTERNAL COORDINATES- 53.89 C3OH 9.05 C4OH	8.00 C2C3 5.17 OC3H	
FORCE CONSTANTS- 64.27 BCOH 12.60 CCH	9.63 CC 7.51 OCH	
OFF DIAGONAL- 4.63 SB28 4.19 BB36	-2.95 SB26 -2.15 SB27 -1.74 SB21 -1.61 SB22 -1.61 BB39	
NORMAL MODE 11 OBSERVED= 1407.0 CM-1	CALCULATED= 1409.6 CM-1	ERROR= 0.0 CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES- 45.61 C1OH 23.57 OC1H	8.81 C1H	
FORCE CONSTANTS- 50.90 BCOH 37.12 OCH	8.23 CCH	
OFF DIAGONAL- -4.97 SB27 4.48 SB28	-3.01 BB39 -1.72 BB45	
NORMAL MODE 12 OBSERVED= 1407.0 CM-1	CALCULATED= 1407.8 CM-1	ERROR= 0.0 CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES- 34.28 C4OH 17.26 OC4H	7.89 C3OH 7.43 C1OH	
FORCE CONSTANTS- 59.28 BCOH 23.63 CCH	17.69 CCH	
OFF DIAGONAL- -5.15 SB27 4.82 SB28	-2.28 BB39 -1.63 BB45	
NORMAL MODE 13 OBSERVED= 1404.0 CM-1	CALCULATED= 1392.1 CM-1	ERROR= 11.9 CM-1 OR 0.8 PERCENT
INTERNAL COORDINATES- 52.23 C1CH 13.88 C1H	9.63 C1OH 5.96 CCHA	
FORCE CONSTANTS- 63.14 BCOH 22.52 OCH	9.20 CC 6.14 CC	
OFF DIAGONAL- -3.64 SB26 -2.03 SB27		
NORMAL MODE 14 OBSERVED= 1381.0 CM-1	CALCULATED= 1384.7 CM-1	ERROR= -3.7 CM-1 OR -0.3 PERCENT
INTERNAL COORDINATES- 31.31 C1H 28.00 C1OH	16.46 C1OH 12.18 OC1H	
FORCE CONSTANTS- 48.23 OCH 46.00 BCOH		
OFF DIAGONAL- -3.34 SB27 -1.93 BB45	1.83 BB37	
NORMAL MODE 15 OBSERVED= 1375.0 CM-1	CALCULATED= 1361.8 CM-1	ERROR= 13.2 CM-1 OR 1.0 PERCENT
INTERNAL COORDINATES- 25.17 OC2H 16.60 HC2C	9.46 OC3H 6.91 CC3H 5.64 C3OH 5.44 C5H 5.30 HC5C	
FORCE CONSTANTS- 44.38 UCH 39.68 CCH	9.79 BCOH 6.53 CO	
OFF DIAGONAL- 7.37 BB29 -6.59 SB27	-3.39 BB45 -1.96 SB26 1.93 BB34 -1.65 SB25 -1.59 SB28	
NORMAL MODE 16 OBSERVED= 1358.0 CM-1	CALCULATED= 1356.6 CM-1	ERROR= 1.4 CM-1 OR 0.1 PERCENT
INTERNAL COORDINATES- 15.45 C5H 12.72 HC5C	12.37 C4OH 11.82 CCHB 8.61 OC2H 7.36 HC2C 5.75 OCHB	
FORCE CONSTANTS- 41.5 CCH 38.28 OCH	14.64 BCOH	
OFF DIAGONAL- 8.21 BB29 -5.46 SB27	-3.18 BB45 -2.67 SB26	
NORMAL MODE 17 OBSERVED= 1332.0 CM-1	CALCULATED= 1334.6 CM-1	ERROR= -2.6 CM-1 OR -0.2 PERCENT
INTERNAL COORDINATES- 19.08 C4CH 14.92 C5H	11.24 CCHH 5.55 OC3H 5.43 C1OH 5.34 HC3C	
FORCE CONSTANTS- 49.79 CCH 25.63 BCOH	18.80 OCH 7.90 CO	
OFF DIAGONAL- 4.95 BB29 -4.69 SB27	-3.90 SB28 -2.84 BB45 -2.66 SB26 -1.66 SB25	
NORMAL MODE 18 OBSERVED= 1318.0 CM-1	CALCULATED= 1318.5 CM-1	ERROR= 0.0 CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES- 14.38 HC3C 13.86 OC3H	9.97 CCH2 9.87 CC1H 7.31 HC2C 5.31 OC1H 5.00 C1OH	
FORCE CONSTANTS- 51.74 CCH 24.80 OCH	12.44 BCOH 9.96 CO	
OFF DIAGONAL- -3.31 BB45 -2.81 SB26	-2.29 SB28 1.72 BB29 1.52 BB34	
NORMAL MODE 19 OBSERVED= 1310.0 CM-1	CALCULATED= 1305.5 CM-1	ERROR= 4.5 CM-1 OR 0.3 PERCENT
INTERNAL COORDINATES- 19.50 OC3H 16.77 CCH2	15.81 OC2H 10.70 HC3C 5.66 C1OH	
FORCE CONSTANTS- 46.40 OCH 43.46 CCH	7.48 BCOH 5.65 CO	
OFF DIAGONAL- -3.67 BB45 -2.00 SB27	-1.99 SB28 -1.72 BB43	
NORMAL MODE 20 OBSERVED= 1305.0 CM-1	CALCULATED= 1285.9 CM-1	ERROR= 19.1 CM-1 OR 1.5 PERCENT
INTERNAL COORDINATES- 17.24 OC4H 14.53 CC1H	11.69 OC1H 7.80 C5H 5.46 CCH2	
FORCE CONSTANTS- 42.74 UCH 34.96 CCH	10.97 CO	
OFF DIAGONAL- 3.35 BB34 -3.16 BB45	-2.17 SB25	
NORMAL MODE 21 OBSERVED= 1280.0 CM-1	CALCULATED= 1278.6 CM-1	ERROR= 1.4 CM-1 OR 0.1 PERCENT
INTERNAL COORDINATES- 46.28 C1CH 41.11 CCHA	9.93 OC4H 5.53 C5H	
FORCE CONSTANTS- 44.2 OCH 5.88 CCH		
OFF DIAGONAL- -3.55 BB45 -3.01 SB26		
NORMAL MODE 22 OBSERVED= 1273.0 CM-1	CALCULATED= 1275.4 CM-1	ERROR= -2.4 CM-1 OR -0.2 PERCENT
INTERNAL COORDINATES- 16.83 C5H 16.72 OC4H	15.89 C5H 10.69 CC1H	
FORCE CONSTANTS- 43.95 OCH 36.90 CCH	8.27 CO	
OFF DIAGONAL- 3.71 SB27 -3.33 BB45	1.84 BB34	
NORMAL MODE 23 OBSERVED= 1246.0 CM-1	CALCULATED= 1245.7 CM-1	ERROR= 0.3 CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES- 26.13 CC4H 16.44 HC4C	8.46 C5H 6.28 C3OH 6.26 HC5C	
FORCE CONSTANTS- 62.55 CCH 19.86 OCH	8.41 BCOH 5.40 CO	
OFF DIAGONAL- -3.58 BB45 3.42 SB27	3.30 BB34 -2.69 BB29 -1.97 SB26 -1.85 SB25	
NORMAL MODE 24 OBSERVED= 1230.0 CM-1	CALCULATED= 1229.3 CM-1	ERROR= 0.7 CM-1 OR 0.1 PERCENT
INTERNAL COORDINATES- 18.09 OCHB 17.24 HC5C	10.96 C5H 8.55 CC4H 7.26 C4C5 7.09 CCHB 6.89 HC4C 5.41 OC3H	
FORCE CONSTANTS- 56.82 CCH 30.07 OCH	13.66 CC 5.60 CCO	
OFF DIAGONAL- -9.02 SB26 -6.04 BB29	-3.58 BB45 3.34 BB34 -2.66 SB22 -2.11 BB43 1.94 SB27 1.88 BB33	
NORMAL MODE 25 OBSERVED= 1212.0 CM-1	CALCULATED= 1212.4 CM-1	ERROR= 0.0 CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES- 20.80 CC3H 12.51 HC3C	10.34 C2OH 8.92 C4C5 8.92 C3C4 5.83 OC2H	
FORCE CONSTANTS- 41.98 CCH 31.24 CCH2	14.82 CCH 12.04 CO 11.85 BCOH	
OFF DIAGONAL- -9.25 SB26 5.91 SB27	-4.94 SB25 -4.22 BB29 -4.14 SB22 3.30 BB34 -2.40 SB28 -2.39 BB45 2.15 BB33	
NORMAL MODE 26 OBSERVED= 1152.0 CM-1	CALCULATED= 1166.2 CM-1	ERROR= -14.2 CM-1 OR -1.2 PERCENT
INTERNAL COORDINATES- 11.27 C19 C5O	11.66 C1H 8.14 C3C4 6.48 CCH2 5.40 OC2H 5.16 OC1H	
FORCE CONSTANTS- 59.78 CO 20.86 CC	19.40 OCH 16.46 CCH 14.84 CCO	
OFF DIAGONAL- -7.94 SB25 -6.91 SB26	-5.49 SB27 -3.23 SS18 -2.48 SB22 -2.02 BB43 -1.98 SB21 -1.80 SB28 -1.75 SB24	
NORMAL MODE 27 OBSERVED= 1135.0 CM-1	CALCULATED= 1138.4 CM-1	ERROR= -3.4 CM-1 OR -0.3 PERCENT
INTERNAL COORDINATES- 14.54 OCHB 9.98 C5C	9.83 CCO1 9.05 C4C5 8.11 OC1 6.33 OCHA 6.23 C-OB 5.99 C-OC 5.41 C-OT	
FORCE CONSTANTS- 27.74 CO 24.31 OCH	21.89 CC 15.90 CCO 9.51 CCH 5.99 CCO	
OFF DIAGONAL- -6.59 SB22 -3.86 SB25	-3.17 SB23	
NORMAL MODE 28 OBSERVED= 1110.0 CM-1	CALCULATED= 1113.1 CM-1	ERROR= -3.1 CM-1 OR -0.3 PERCENT
INTERNAL COORDINATES- C-09 17.64 C-07 14.98 C3C4 7.24 C-08 6.82 OC3H 6.08 C2CC 6.00 C-0* 5.26 CC4H 5.04 C5H		
FORCE CONSTANTS- 59.98 CO 19.53 CC	15.54 OCH 14.94 CCO 11.91 CCH 11.72 CCH 9.42 BCOH	
OFF DIAGONAL- -11.84 SB25 -8.43 SB28	-6.31 SS18 -5.77 SB21 -4.16 SB26 -2.99 SB27 -2.14 BB34 1.81 SB22	
NORMAL MODE 29 OBSERVED= 1103.0 CM-1	CALCULATED= 1106.1 CM-1	ERROR= -3.1 CM-1 OR -0.3 PERCENT
INTERNAL COORDINATES- 17.15 C3C4 10.58 C-07 10.37 C2C3 7.17 C2OH 6.04 C1C2 5.87 C5O*		
FORCE CONSTANTS- 49.8 CCH 25.98 CO 14.96 CCH	12.00 CCH 8.23 OCH 7.68 BCOH	
OFF DIAGONAL- -9.97 SB22 4.43 SB26	-3.84 SB25 3.92 SB27 -2.70 SB28 1.78 BB43 -1.63 SS17	
NORMAL MODE 30 OBSERVED= 1078.0 CM-1	CALCULATED= 1090.8 CM-1	ERROR= -12.8 CM-1 OR -1.2 PERCENT
INTERNAL COORDINATES- 10.78 C-08 20.70 C-08 13.33 C-08 8.57 C5C	6.26 C-06	
FORCE CONSTANTS- 76.66 CO 27.19 CC	5.58 BCOH	
OFF DIAGONAL- -7.48 SS18 -6.88 SB28	-3.98 SB25 -3.34 SB27	
NORMAL MODE 31 OBSERVED= 1065.0 CM-1	CALCULATED= 1071.8 CM-1	ERROR= -6.8 CM-1 OR -0.6 PERCENT
INTERNAL COORDINATES- 43.16 C-0* 17.52 C-08 10.09 C1C2 8.11 C-06 5.36 OC1 6.33 OCHA 6.23 C-OB 5.99 C-OC 5.41 C-OT		
FORCE CONSTANTS- 76.79 CO 17.19 CC	10.09 CCH 9.81 BCOH 7.84 CCO 7.72 CCH 7.27 OCH	
OFF DIAGONAL- -9.19 SB28 -8.23 SB25	-5.60 SB27 -3.38 SB24 -2.92 SB26 -2.85 SS18	
NORMAL MODE 32 OBSERVED= 1040.0 CM-1	CALCULATED= 1051.6 CM-1	ERROR= -11.6 CM-1 OR -1.1 PERCENT
INTERNAL COORDINATES- 51.94 C1C2 12.44 C-06 11.37 C-0* 7.36 C1OH 6.23 C5C	5.77 C2C3 5.75 CCO1 5.53 C5O*	
FORCE CONSTANTS- 64.43 CC 30.29 CO 10.26 CCH 12.17 OCH 11.31 CCH 7.78 BCOH		
OFF DIAGONAL- -16.18 SB22 -11.50 SB26	-5.27 SB27 -4.44 SB21 -4.23 SB28 -4.14 SS18 -3.02 BB34 -2.08 SB24 -1.57 BB43	
NORMAL MODE 33 OBSERVED= 1030.0 CM-1	CALCULATED= 1037.1 CM-1	ERROR= 0.0 CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES- 23.68 C-0* 22.87 C-09 18.29 C5C 13.29 C4C5 9.18 OC1 6.27 C3O*	6.03 C3C4	
FORCE CONSTANTS- 69.05 CO 39.62 CC	10.04 CCH 8.86 OCH 7.96 BCOH	
OFF DIAGONAL- -12.95 SB21 -10.66 SS18	10.19 SB27 -6.66 SB28 -3.45 SB26 -2.06 SB24	
NORMAL MODE 34 OBSERVED= 997.0 CM-1	CALCULATED= 987.5 CM-1	ERROR= 9.5 CM-1 OR 0.9 PERCENT
INTERNAL COORDINATES- 34.22 C3C4 25.79 C-06 21.46 C5C 7.26 C5H 6.05 C-0*		
FORCE CONSTANTS- 34.22 CC 30.19 CCH	21.46 C5C 7.26 C5H 6.05 C-0*	
OFF DIAGONAL- -7.85 SB22 -6.60 SB21	6.18 SB26 -3.39 SB25 -2.97 BB29 2.77 BB43	
NORMAL MODE 35 OBSERVED= 970.0 CM-1	CALCULATED= 979.2 CM-1	ERROR= -9.2 CM-1 OR -0.9 PERCENT
INTERNAL COORDINATES- 23.22 C-08 19.07 C5C 10.37 C-0* 8.66 C3C4 6.50 C-07 5.96 C1C2 5.02 C-0*		
FORCE CONSTANTS- 53.29 CO 39.38 CC	23.49 CCH 8.90 CCO 7.50 BCOH	
OFF DIAGONAL- -7.32 SB22 -6.72 SB28	-6.11 SB26 -5.16 SB27 -4.29 SB25 -2.90 SB24 -2.71 SB21 -2.39 BB34 -1.90 BB29	

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400									
MOLECULE 24 -6 NG-1235 ALPHA GALACTOSE GT									
PAGE 2									
NORMAL MODE 36 OBSERVED= 955.0 CM-1 CALCULATED= 921.9 CM-1 ERROR= 33.1 CM-1 OR 3.5 PERCENT									
INTERNAL COORDINATES-	16.64	C4C5	11.71	C-06	10.71	C-09	9.37	C2C3	
FORCE CONSTANTS-	30.25	CCH	29.45	CC	27.77	CO	10.17	CCO	5.01 CCC
OFF DIAGONAL-	8.68	S826	-7.77	S821	-5.42	S822	-4.14	S825	2.96 BB43 2.63 SS18 -2.54 BB29 -2.18 SB24
NORMAL MODE 37 OBSERVED= 886.0 CM-1 CALCULATED= 862.9 CM-1 ERROR= 23.1 CM-1 OR 2.6 PERCENT									
INTERNAL COORDINATES-	21.90	C-09	14.08	C2C3	8.38	C3C4	8.05	C-06	7.02 HC3C
FORCE CONSTANTS-	34.93	CO	26.14	CC	21.10	CCH	11.00	CCO	6.31 CCH
OFF DIAGONAL-	-9.11	S821	-6.51	S822	5.36	S826	-3.64	S827	2.76 BB43 2.01 SS18
NORMAL MODE 38 OBSERVED= 828.0 CM-1 CALCULATED= 817.3 CM-1 ERROR= 10.7 CM-1 OR 1.3 PERCENT									
INTERNAL COORDINATES-	26.33	C50	11.78	CCHA	9.99	CCHB	6.73	CCO9	6.04 CCO*
FORCE CONSTANTS-	43.11	CO	26.31	CC	14.79	CCO	10.58	CC	5.24 CCH
OFF DIAGONAL-	3.30	SS18	-2.88	S822	2.29	S826	-2.28	S823	-2.05 BB29 -1.81 SB25 -1.68 SB27 1.66 BB43 -1.57 SB21
NORMAL MODE 39 OBSERVED= 745.0 CM-1 CALCULATED= 801.2 CM-1 ERROR= -36.2 CM-1 OR -4.7 PERCENT									
INTERNAL COORDINATES-	9.52	4C0	9.06	C-06	8.49	C50	7.99	O9CC	0.96 C
FORCE CONSTANTS-	33.16	CO	31.98	CCO	8.06	CCO	7.37	CCH	5.91 CCC
OFF DIAGONAL-	8.23	S825	-5.46	S827	4.37	BB43	-3.65	S823	-2.42 BB41 1.90 SS18 -1.62 BB34 1.59 BB33
NORMAL MODE 40 OBSERVED= 702.0 CM-1 CALCULATED= 718.7 CM-1 ERROR= -16.7 CM-1 OR -2.4 PERCENT									
INTERNAL COORDINATES-	7.07	C9C1	6.77	C50	6.27	C2C3	6.26	O9CC	5.52 C1CC
FORCE CONSTANTS-	29.47	CCO	14.12	CC	12.71	CO	9.82	CCH	7.93 CCC
OFF DIAGONAL-	4.92	BB43	3.68	S825	-2.65	S827	2.29	S821	-1.87 SB26 -1.79 BB41 1.78 SS18 1.69 SB24
NORMAL MODE 41 OBSERVED= 660.0 CM-1 CALCULATED= 695.4 CM-1 ERROR= -35.4 CM-1 OR -5.4 PERCENT									
INTERNAL COORDINATES-	24.19	C2C3	18.64	CCO9	8.94	O8CC	5.50	C4CC	5.41 CC4H
FORCE CONSTANTS-	34.05	CCO	27.98	CC	10.57	CCO	10.14	CO	9.67 CCH
OFF DIAGONAL-	3.78	BB43	2.93	SS18	2.73	S825	-1.99	BB34	-1.71 BB41 -1.65 SB22
NORMAL MODE 42 OBSERVED= 612.0 CM-1 CALCULATED= 622.0 CM-1 ERROR= -10.0 CM-1 OR -1.6 PERCENT									
INTERNAL COORDINATES-	19.99	CCO6	13.17	CCO	13.05	CCO7	9.94	CCO*	7.04 CO* C
FORCE CONSTANTS-	21.17	CCO	14.82	CCH	13.17	O8CC	8.81	CC	6.63 CCH
OFF DIAGONAL-	-4.26	BB34	3.04	S824	-2.62	BB29	-7.56	BB42	-2.34 BB41 2.21 BB48 1.60 SB25 1.57 SS18
NORMAL MODE 43 OBSERVED= 530.0 CM-1 CALCULATED= 504.2 CM-1 ERROR= 25.8 CM-1 OR 4.9 PERCENT									
INTERNAL COORDINATES-	17.15	OC0	12.20	O*CC	12.48	O7CC	12.48	CCO8	6.70 HC2*
FORCE CONSTANTS-	55.49	CCO	17.39	CCH	17.15	OCO	8.40	CCC	5.58 CC
OFF DIAGONAL-	-9.61	BB34	4.47	BB43	3.70	S824	-3.52	BB29	-3.00 BB42 -1.88 SB26 1.58 SB25
NORMAL MODE 44 OBSERVED= 490.0 CM-1 CALCULATED= 490.8 CM-1 ERROR= -0.8 CM-1 OR -0.2 PERCENT									
INTERNAL COORDINATES-	27.10	CCO*	11.27	O*CC	11.04	HC3C	8.98	CCHB	7.75 C3CC
FORCE CONSTANTS-	59.08	CCO	23.97	CCH	9.82	CCC	5.69	CO	6.82 CCO*
OFF DIAGONAL-	-11.09	BB34	5.83	BB43	-5.18	BB29	4.00	S825	
NORMAL MODE 45 OBSERVED= 417.0 CM-1 CALCULATED= 416.1 CM-1 ERROR= 0.9 CM-1 OR 0.2 PERCENT									
INTERNAL COORDINATES-	25.82	OCO	14.85	CCO8	11.13	O7CC	8.25	O*CC	
FORCE CONSTANTS-	49.27	CCO	25.82	OCO	9.90	CCH	7.61	CC	
OFF DIAGONAL-	-6.88	BB34	6.53	S822	-3.13	BB42	2.78	BB43	-1.66 BB29
NORMAL MODE 46 OBSERVED= 407.0 CM-1 CALCULATED= 392.0 CM-1 ERROR= 15.0 CM-1 OR 3.7 PERCENT									
INTERNAL COORDINATES-	18.77	CCO7	14.88	O8CC	14.67	C2CC	13.98	C1CC	8.78 C4C5
FORCE CONSTANTS-	45.51	CCO	11.82	CC	9.42	CC	8.99	CCO*	8.01 CO* C
OFF DIAGONAL-	-4.97	BB34	-1.02	BB42	4.38	S825	-2.00	S826	1.98 SB22 -1.80 BB41 1.65 SB23
NORMAL MODE 47 OBSERVED= 358.0 CM-1 CALCULATED= 349.8 CM-1 ERROR= 8.2 CM-1 OR 2.3 PERCENT									
INTERNAL COORDINATES-	50.46	OCO	26.75	C3C4	9.36	CCO*	9.09	4C0*	
FORCE CONSTANTS-	60.46	CCO	26.75	CC	7.22	CCH	6.22	CCC	
OFF DIAGONAL-	4.89	S821	-4.63	S826	4.50	S822	3.08	S825	-2.45 BB34 -1.76 BB42 -1.59 BB36
NORMAL MODE 48 OBSERVED= 331.0 CM-1 CALCULATED= 313.9 CM-1 ERROR= 17.1 CM-1 OR 5.1 PERCENT									
INTERNAL COORDINATES-	17.21	O8CC	21.34	CCO8	11.54	CCO7	10.86	O9CC	6.42 O7CC
FORCE CONSTANTS-	85.93	CCO	11.54	T-OH	6.51	CCH			6.11 TH-3
OFF DIAGONAL-	-7.69	BB34	-4.39	BB42					
NORMAL MODE 49 OBSERVED= 299.0 CM-1 CALCULATED= 308.3 CM-1 ERROR= -9.3 CM-1 OR -3.1 PERCENT									
INTERNAL COORDINATES-	15.40	CCO9	14.80	O9CC	9.90	CCO8	8.07	TH-4	6.75 CCO*
FORCE CONSTANTS-	60.31	CCO	12.34	T-OH	9.49	CCH	6.87	CC	
OFF DIAGONAL-	6.02	S822	-4.50	BB33	-2.97	S826	2.91	S821	2.15 BB43 -1.90 BB42 -1.64 BB34
NORMAL MODE 50 OBSERVED= 268.0 CM-1 CALCULATED= 285.7 CM-1 ERROR= -17.7 CM-1 OR -6.6 PERCENT									
INTERNAL COORDINATES-	15.64	CCO	11.11	CCO6	9.46	O*CC	9.12	CCO9	8.24 C3CC
FORCE CONSTANTS-	61.72	CCO	11.54	CC	14.04	T-OH	8.89	CCH	8.00 TH-2 7.58 CCO7 7.48 C4CC
OFF DIAGONAL-	-4.32	BB33	-4.04	BB34	-3.34	BB42	-1.86	S825	
NORMAL MODE 51 OBSERVED= 254.0 CM-1 CALCULATED= 257.8 CM-1 ERROR= -3.8 CM-1 OR -1.5 PERCENT									
INTERNAL COORDINATES-	44.83	CCO	11.36	CCO9	10.07	TH-3			
FORCE CONSTANTS-	44.83	CCO	23.36	T-OH	16.13	CCH	12.41	CCC	
OFF DIAGONAL-	6.18	BB43	-3.92	BB34	-3.92	BB33	-3.88	S825	-1.77 BB29 1.76 SB22
NORMAL MODE 52 OBSERVED= 230.0 CM-1 CALCULATED= 234.2 CM-1 ERROR= -4.2 CM-1 OR -1.8 PERCENT									
INTERNAL COORDINATES-	37.88	TH-8	39.37	TH-1					
FORCE CONSTANTS-	80.21	T-OH	9.33	CCO					
OFF DIAGONAL-	NONE								
NORMAL MODE 53 OBSERVED= 0.0 CM-1 CALCULATED= 228.7 CM-1 ERROR= 0.0 CM-1 OR 0.0 PERCENT									
INTERNAL COORDINATES-	33.03	TH-3	26.03	TH-1	22.94	TH-4	5.19	TH-2	
FORCE CONSTANTS-	91.02	T-OH	5.35	CCO					
OFF DIAGONAL-	NONE								
NORMAL MODE 54 OBSERVED= 0.0 CM-1 CALCULATED= 218.1 CM-1 ERROR= 0.0 CM-1 OR 0.0 PERCENT									
INTERNAL COORDINATES-	34.56	TH-5	23.64	TH-1	10.82	TH-4	10.61	TH-3	
FORCE CONSTANTS-	81.44	T-OH	9.83	CCO					
OFF DIAGONAL-	NONE								
NORMAL MODE 55 OBSERVED= 0.0 CM-1 CALCULATED= 213.2 CM-1 ERROR= 0.0 CM-1 OR 0.0 PERCENT									
INTERNAL COORDINATES-	74.04	TH-8	14.60	CCO7					
FORCE CONSTANTS-	82.72	T-OH	14.77	CCO					
OFF DIAGONAL-	NONE								
NORMAL MODE 56 OBSERVED= 0.0 CM-1 CALCULATED= 208.3 CM-1 ERROR= 0.0 CM-1 OR 0.0 PERCENT									
INTERNAL COORDINATES-	43.71	TH-4	30.48	TH-3	8.79	CCO9	6.62	O8CC	
FORCE CONSTANTS-	74.52	T-OH	20.16	CCO					
OFF DIAGONAL-	NONE								
NORMAL MODE 57 OBSERVED= 0.0 CM-1 CALCULATED= 185.4 CM-1 ERROR= 0.0 CM-1 OR 0.0 PERCENT									
INTERNAL COORDINATES-	19.26	CCO*	11.66	CO* C	11.25	C4CC	8.69	TH-5	6.86 O9CC
FORCE CONSTANTS-	42.61	CCO	16.88	T-OH	16.33	CCC	11.66	CO C	5.12 CCH
OFF DIAGONAL-	-2.79	BB42	-2.59	BB33	-2.35	BB34	2.12	BB41	
NORMAL MODE 58 OBSERVED= 0.0 CM-1 CALCULATED= 129.4 CM-1 ERROR= 0.0 CM-1 OR 0.0 PERCENT									
INTERNAL COORDINATES-	22.81	C4CC	17.54	CC* C	8.19	TCC4			
FORCE CONSTANTS-	30.67	CCC	17.54	CO C	14.30	CCO	9.99	T-CC	8.68 T-CC
OFF DIAGONAL-	-5.01	S821	3.00	BB43	2.48	S822	2.29	BB41	-1.93 BB37 -1.57 SB25
NORMAL MODE 59 OBSERVED= 0.0 CM-1 CALCULATED= 112.0 CM-1 ERROR= 0.0 CM-1 OR 0.0 PERCENT									
INTERNAL COORDINATES-	48.11	ICC5	7.81	TCC2	6.64	C2CC	5.00	C3CC	
FORCE CONSTANTS-	64.64	T-CC	13.24	CCC	11.41	CCO	5.43	CCH	
OFF DIAGONAL-	1.65	BB43							
NORMAL MODE 60 OBSERVED= 0.0 CM-1 CALCULATED= 85.9 CM-1 ERROR= 0.0 CM-1 OR 0.0 PERCENT									
INTERNAL COORDINATES-	20.19	C2C3	14.33	TCC1	12.13	C3CC	11.45	TCC4	6.70 TCC2
FORCE CONSTANTS-	38.27	T-CC	35.42	CCC	16.13	CCO	5.91	CO C	5.91 CO* C
OFF DIAGONAL-	-3.57	S825	-3.28	BB42	2.00	BB41	-1.71	BB34	-1.68 SB21
NORMAL MODE 61 OBSERVED= 0.0 CM-1 CALCULATED= 67.6 CM-1 ERROR= 0.0 CM-1 OR 0.0 PERCENT									
INTERNAL COORDINATES-	30.04	TCC5	10.19	TCC4	7.84	C3CC	6.66	TCC3	6.38 C1CC
FORCE CONSTANTS-	53.30	T-CC	19.50	CCO	17.00	CCC			6.28 4C0* 5.96 TCC2
OFF DIAGONAL-	-1.81	BB42	-1.74	BB34					

40. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR =11.06

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR				PROBLEM 400		PAGE 1	
MOLECULE 25				-6 NG=1235 ALPHA GALACTOSE-1-D GT			
NORMAL MODE 8	OBSERVED=	1498.0 CM-1	CALCULATED=	1454.9 CM-1	ERROR=	43.1 CM-1	OR 2.9 PERCENT
INTERNAL COORDINATES-	67.85 C2OH 5.43 CC3H						
FORCE CONSTANTS-	66.33 BCOH 5.04 CCH			6.04 CCO			
OFF DIAGONAL-	4.44 BB36 3.90 SB28			1.86 BB34 -1.77 SB25			
NORMAL MODE 9	OBSERVED=	1458.0 CM-1	CALCULATED=	1449.7 CM-1	ERROR=	8.3 CM-1	OR 0.6 PERCENT
INTERNAL COORDINATES-	61.80 HCH 20.01 OCHB			18.98 OCHA			
FORCE CONSTANTS-	61.80 HCH 39.42 OCH						
OFF DIAGONAL-	-3.88 SB27						
NORMAL MODE 10	OBSERVED=	1442.0 CM-1	CALCULATED=	1429.1 CM-1	ERROR=	12.9 CM-1	OR 0.9 PERCENT
INTERNAL COORDINATES-	54.77 C3OH 9.52 C4OH			7.54 C2C3 5.10 OC3H			
FORCE CONSTANTS-	66.03 BCOH 11.48 CCH			9.35 CC 7.14 OCH			
OFF DIAGONAL-	4.66 SB28 4.24 BB36			-2.73 SB26 -2.11 SB27			
NORMAL MODE 11	OBSERVED=	1424.0 CM-1	CALCULATED=	1407.8 CM-1	ERROR=	16.2 CM-1	OR 1.1 PERCENT
INTERNAL COORDINATES-	37.34 C4OH 19.00 OC4H			10.95 C3OH 5.07 HC4C			
FORCE CONSTANTS-	50.56 BCOH 24.24 CCH			19.16 CCH 3.00 CO			
OFF DIAGONAL-	-9.35 SB27 4.82 SB28			-2.30 BB39 -1.72 BB45			
NORMAL MODE 12	OBSERVED=	1405.0 CM-1	CALCULATED=	1399.7 CM-1	ERROR=	5.3 CM-1	OR 0.4 PERCENT
INTERNAL COORDINATES-	79.52 BCOH 5.60 OCH						
FORCE CONSTANTS-	79.52 BCOH 5.60 OCH						
OFF DIAGONAL-	4.74 SB28 -1.93 SB22						
NORMAL MODE 13	OBSERVED=	1394.0 CM-1	CALCULATED=	1389.8 CM-1	ERROR=	4.2 CM-1	OR 0.3 PERCENT
INTERNAL COORDINATES-	79.84 C3OH 6.50 CCHA			5.91 OCHB 5.07 C5C4			
FORCE CONSTANTS-	80.11 BCOH 10.91 CCH			7.75 OCH 5.47 CC			
OFF DIAGONAL-	-3.94 SB26 -2.80 BB39			2.24 SB28			
NORMAL MODE 14	OBSERVED=	1380.0 CM-1	CALCULATED=	1361.3 CM-1	ERROR=	18.8 CM-1	OR 1.4 PERCENT
INTERNAL COORDINATES-	24.31 OC2H 14.50 HC2C			9.38 OC3H 6.53 C5H 6.36 CC3H 6.33 HC5C 5.16 CCH8			
FORCE CONSTANTS-	44.28 OCH 38.98 CCH			10.88 BCOH 6.46 CO			
OFF DIAGONAL-	7.25 BB29 -6.77 SB27			-3.36 BB45 -1.85 SB26 1.70 BB34 -1.63 SB25 -1.62 SB28			
NORMAL MODE 15	OBSERVED=	0.0 CM-1	CALCULATED=	1357.2 CM-1	ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	13.54 C4OH 12.90 C5H			12.14 OC2H 11.58 CCH8 10.73 HC5C 7.30 HC2C 5.89 OCH8			
FORCE CONSTANTS-	39.88 CCH 37.57 OCH			16.42 BCOH 5.78 CO			
OFF DIAGONAL-	7.76 BB29 -5.95 SB27			-3.07 BB45 -2.20 SB26 -1.74 SB25			
NORMAL MODE 16	OBSERVED=	1340.0 CM-1	CALCULATED=	1334.7 CM-1	ERROR=	5.3 CM-1	OR 0.4 PERCENT
INTERNAL COORDINATES-	19.27 C4OH 15.01 CC5H			11.29 CCH8 10.15 HC5C 5.61 C3OH 5.47 HC3C 5.46 OC3H			
FORCE CONSTANTS-	50.40 CCH 25.65 OCH			17.93 OCH 7.64 CCH			
OFF DIAGONAL-	5.11 BB29 -4.38 SB27			-3.85 SB28 -2.84 BB45 -2.81 SB26 -1.64 SB25			
NORMAL MODE 17	OBSERVED=	1322.0 CM-1	CALCULATED=	1312.5 CM-1	ERROR=	9.5 CM-1	OR 0.7 PERCENT
INTERNAL COORDINATES-	26.40 OC3H 25.05 HC3C			7.73 CCHA 6.65 OCH			
FORCE CONSTANTS-	50.63 CCH 36.91 OCH			7.06 BCOH 6.67 CO			
OFF DIAGONAL-	-3.64 BB45 -2.09 SB26			1.77 BB29			
NORMAL MODE 18	OBSERVED=	0.0 CM-1	CALCULATED=	1307.2 CM-1	ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	34.92 CCH2 13.43 C-6			10.98 OC1 10.34 OC2H 8.75 C1OH 7.58 HC2C			
FORCE CONSTANTS-	49.65 CCH 25.99 CO			21.60 OCH 11.06 BCOH 6.11 CCO			
OFF DIAGONAL-	-7.67 SB27 -4.64 SB25			-4.60 SB28 -4.11 SB26 3.62 BB34 -3.11 BB45 2.91 BB29 2.56 BB33			
NORMAL MODE 19	OBSERVED=	1290.0 CM-1	CALCULATED=	1284.9 CM-1	ERROR=	5.1 CM-1	OR 0.4 PERCENT
INTERNAL COORDINATES-	40.68 C5H 14.38 CC5H			7.23 CCHA 7.05 OCHA 5.35 OC3H			
FORCE CONSTANTS-	61.22 OCH 27.79 CCH			5.52 CO			
OFF DIAGONAL-	6.85 SB27 -3.45 BB45						
NORMAL MODE 20	OBSERVED=	1282.0 CM-1	CALCULATED=	1279.9 CM-1	ERROR=	2.1 CM-1	OR 0.2 PERCENT
INTERNAL COORDINATES-	35.46 OC4H 15.87 CCHA			12.71 CCHA 10.42 HC4C 5.41 C4OH			
FORCE CONSTANTS-	56.40 OCH 32.09 CCH			8.45 BCOH			
OFF DIAGONAL-	-3.47 BB45 -2.80 SB26			1.71 BB39			
NORMAL MODE 21	OBSERVED=	1255.0 CM-1	CALCULATED=	1254.5 CM-1	ERROR=	0.5 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	74.90 HC4C 7.00 OC4H 6.45 C3OH 5.91 OCHA 5.54 CCH8 5.01 CCHA			12.33 CCH 7.00 OC4H 6.45 C3OH 5.91 OCHA 5.54 CCH8 5.01 CCHA			
FORCE CONSTANTS-	54.00 CCH 19.67 OCH			8.70 BCOH 7.81 CO			
OFF DIAGONAL-	4.84 SB27 -3.52 BB29			3.47 BB34 -3.11 BB45 -2.70 SB25			
NORMAL MODE 22	OBSERVED=	1240.0 CM-1	CALCULATED=	1231.3 CM-1	ERROR=	8.7 CM-1	OR 0.7 PERCENT
INTERNAL COORDINATES-	16.05 C4H 13.78 OCHB			12.60 HC4C 15.43 HC5C 10.55 C5H 9.30 C4C5 6.26 OC3H			
FORCE CONSTANTS-	64.01 CCH 23.90 OCH			16.31 CC 5.85 CCO 5.51 BCOH			
OFF DIAGONAL-	-12.03 SB26 -4.85 BB29			-3.74 BB45 -3.32 SB22 3.27 BB34 -2.77 BB43 2.41 BB33			
NORMAL MODE 23	OBSERVED=	1194.0 CM-1	CALCULATED=	1212.6 CM-1	ERROR=	-18.6 CM-1	OR -1.6 PERCENT
INTERNAL COORDINATES-	20.82 CC3H 12.42 HC3C			10.39 C2OH 9.23 C4C5 9.02 C3C4 6.29 OC2H 5.10 OC1 5.06 OC3H			
FORCE CONSTANTS-	40.62 CCH 21.58 CC			18.51 CO 16.34 CCH 12.18 CCO 11.99 BCOH			
OFF DIAGONAL-	-9.53 SB26 5.35 SB27			-5.03 SB25 -4.22 SB22 3.95 BB29 3.05 BB34 -2.49 SB28 -2.38 BB45 2.20 BB33			
NORMAL MODE 24	OBSERVED=	0.0 CM-1	CALCULATED=	1169.6 CM-1	ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	29.90 OC1 18.97 C5O			10.24 C4C5 8.76 C-8 6.80 CCH2 5.69 C3C4			
FORCE CONSTANTS-	62.73 CCH 18.10 CO			18.08 CCH 16.31 CCH 12.69 OCH			
OFF DIAGONAL-	-6.73 SB25 -6.69 SB26			3.40 SS18 -2.72 SB27 -2.31 SB28 -2.12 SB21 -1.87 SB22 -1.86 BB43 -1.61 SB24			
NORMAL MODE 25	OBSERVED=	1148.0 CM-1	CALCULATED=	1161.1 CM-1	ERROR=	-13.1 CM-1	OR -1.1 PERCENT
INTERNAL COORDINATES-	39.87 OCH 22.88 C1H			18.79 CCH 13.07 CC 13.03 CCO			
FORCE CONSTANTS-	39.87 OCH 22.88 C1H			-3.74 SB22 -3.55 SB23 2.28 BB37 -1.61 SB26			
OFF DIAGONAL-	-5.38 SB27 -4.35 SB25						
NORMAL MODE 26	OBSERVED=	1132.0 CM-1	CALCULATED=	1125.2 CM-1	ERROR=	6.8 CM-1	OR 0.6 PERCENT
INTERNAL COORDINATES-	32.99 C-0 19.50 C2C3			16.54 C3C4 8.26 C-09 7.30 C1CC 6.64 C-08 5.41 CC1H			
FORCE CONSTANTS-	54.63 CO 37.47 CC			13.94 CCH 13.61 CCO 11.44 CCC 9.60 OCH			
OFF DIAGONAL-	-8.84 SB27 -8.40 SB25			-5.08 SS18 -4.91 SB21 -4.20 SB28 -3.56 SB26 -3.31 SB22			
NORMAL MODE 27	OBSERVED=	1110.0 CM-1	CALCULATED=	1108.1 CM-1	ERROR=	1.9 CM-1	OR 0.2 PERCENT
INTERNAL COORDINATES-	12.76 C2C3 9.02 C2OH			8.67 C-07 8.59 C5C4 8.26 C4C5 5.98 C1C2 5.51 C-09 5.18 C4C4			
FORCE CONSTANTS-	39.46 CC 21.24 CO			14.84 CCO 14.33 CCH 12.13 BCOH 8.28 OCH			
OFF DIAGONAL-	-8.33 SB22 6.28 SB26			-5.62 SB25 -4.50 SB28 2.39 SB27 2.11 BB43 -1.91 BB36 -1.51 SS17			
NORMAL MODE 28	OBSERVED=	1090.0 CM-1	CALCULATED=	1096.4 CM-1	ERROR=	-6.4 CM-1	OR -0.6 PERCENT
INTERNAL COORDINATES-	31.34 C-07 26.61 C-08			11.55 C3C4 9.19 C-09 8.89 OC1 6.80 C-0*			
FORCE CONSTANTS-	85.08 CO 21.45 CC			5.76 BCOH			
OFF DIAGONAL-	-8.33 SS18 -7.68 SB28			-4.35 SB27 -3.55 SB25			
NORMAL MODE 29	OBSERVED=	1080.0 CM-1	CALCULATED=	1074.7 CM-1	ERROR=	5.3 CM-1	OR 0.5 PERCENT
INTERNAL COORDINATES-	25.48 C1C2 22.46 C-0*			14.56 C-06 12.61 C5C4 10.75 C2C3 5.51 C5O*			
FORCE CONSTANTS-	25.48 C1C2 22.46 C-0*			15.58 OCH 17.55 CCH 9.87 BCOH 6.37 CCH			
OFF DIAGONAL-	-8.84 SB27 -8.60 SS18			-7.90 SB28 -6.41 SB22 -4.24 SB26 -3.65 SB21 -3.08 SB24			
NORMAL MODE 30	OBSERVED=	1064.0 CM-1	CALCULATED=	1065.8 CM-1	ERROR=	-1.8 CM-1	OR -0.2 PERCENT
INTERNAL COORDINATES-	23.30 C-0 17.26 C-08			8.80 C5C 6.60 C-09 7.55 C4CC 6.54 C3C4 5.99 C3CO 5.51 C5O*			
FORCE CONSTANTS-	56.79 CO 17.58 CC			14.97 CCC 14.84 CCO 11.21 OCH 10.06 CCH 6.58 BCOH			
OFF DIAGONAL-	-10.58 SB25 -5.94 SB21			-5.37 SB28 -5.08 SB22 -4.93 SB27 2.22 SS18 -1.61 BB43			
NORMAL MODE 31	OBSERVED=	1050.0 CM-1	CALCULATED=	1044.1 CM-1	ERROR=	5.9 CM-1	OR 0.6 PERCENT
INTERNAL COORDINATES-	32.86 C1C2 27.47 C-0*			13.73 C-09 8.22 C-06 7.96 OC1 5.03 C1H			
FORCE CONSTANTS-	59.21 CO 43.55 CC			15.31 CCH 11.82 OCH 9.43 BCOH 6.07 CCO			
OFF DIAGONAL-	-9.99 SB27 -8.65 SS18			-7.26 SB26 -7.05 SB28 -5.18 SB21 -5.11 SB22 -4.15 SB24 -1.60 BB34			
NORMAL MODE 32	OBSERVED=	995.0 CM-1	CALCULATED=	1004.0 CM-1	ERROR=	-9.0 CM-1	OR -0.9 PERCENT
INTERNAL COORDINATES-	31.88 C1H 10.78 OC1H			6.94 C4C5 6.37 C-0*			
FORCE CONSTANTS-	49.47 OCH 19.79 CC			12.15 CO 11.28 CCH 8.42 CCO			
OFF DIAGONAL-	-5.17 SB21 -2.01 SB22			-1.99 SS18			
NORMAL MODE 33	OBSERVED=	976.0 CM-1	CALCULATED=	984.6 CM-1	ERROR=	-8.6 CM-1	OR -0.9 PERCENT
INTERNAL COORDINATES-	26.80 C5C 18.71 C3C4			9.14 C-08 8.38 C4C5 7.01 CC3H 6.64 C-0* 5.87 CC5H			
FORCE CONSTANTS-	27.34 CO 20.11 CC			14.10 CCH 12.84 CCO 9.02 CC			
OFF DIAGONAL-	-10.80 SB22 -9.39 SB21			-3.77 SB25 5.82 SB26 2.34 SS18 1.90 BB43			
NORMAL MODE 34	OBSERVED=	0.0 CM-1	CALCULATED=	977.4 CM-1	ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	19.60 C-0 14.02 C-08			25.96 C4C5 14.3 C2C3 5.84 CC3H 5.31 C5C4 5.13 C-0*			
FORCE CONSTANTS-	44.96 CO 32.31 CCH			6.90 BCOH 7.58 OCH 6.26 CCO 5.80 CCC			
OFF DIAGONAL-	-6.51 SB28 -5.43 SB21			-3.73 SB24 -3.55 SB22 -3.48 SB25 -2.73 BB29 -2.71 SB27 -1.70 BB34			
NORMAL MODE 35	OBSERVED=	0.0 CM-1	CALCULATED=	958.5 CM-1	ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	50.99 OC1H 11.25 CC1H			9.49 C1C2 6.85 C-06			
FORCE CONSTANTS-	51.85 OCH 14.54 CC			12.75 CCH 10.86 CO 8.33 CCO			
OFF DIAGONAL-	8.84 SB27 -5.98 SB22			-4.30 SB26 2.03 SS18 -2.02 BB45 -2.00 SB25			

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400									
MOLECULE 75 -6 NG-1235 ALPHA GALACTOSE-1-D GT									
PAGE 2									
NORMAL MODE 36	OBSERVED=	933.0 CM-1	CALCULATED=	904.7 CM-1	ERROR=	28.3 CM-1	OR	3.0 PERCENT	
INTERNAL COORDINATES-	19.73	C-09 9.91 CCH	9.71 C4C5	8.23 C-06	5.18 CCHA	5.11 CCHB			
FORCE CONSTANTS-	41.92	CCH 34.06 CC	15.36 CC	9.06 CCO	7.54 CCH				
OFF DIAGONAL-	7.12	SB26 -4.26 SB21	-4.16 SB25	-3.60 SB27	-3.47 BB29	-2.78 SB22	2.69 SS18	-1.96 SB24	1.66 BB43
NORMAL MODE 37	OBSERVED=	864.0 CM-1	CALCULATED=	849.0 CM-1	ERROR=	15.0 CM-1	OR	1.7 PERCENT	
INTERNAL COORDINATES-	18.58	C-06 14.96 C-09	8.61 CCH2	7.90 C-02	5.42 C3C4	5.03 HC3C			
FORCE CONSTANTS-	49.72	CCO 19.66 CCH	16.60 CC	13.19 CCO	10.29 CCH				
OFF DIAGONAL-	-7.53	SB27 -6.92 SB21	-5.17 SB25	-5.10 SB26	-4.30 SB22	3.37 BB43	1.59 BB42		
NORMAL MODE 38	OBSERVED=	822.0 CM-1	CALCULATED=	807.2 CM-1	ERROR=	14.8 CM-1	OR	1.8 PERCENT	
INTERNAL COORDINATES-	13.82	4C01 9.56 C-09	8.30 CCO*	7.93 C9CC					
FORCE CONSTANTS-	33.76	CCO 23.51 CC	14.19 CCH	6.90 CC	5.94 CCH	5.08 CCC			
OFF DIAGONAL-	4.21	BB43 3.54 SB25	-2.71 SB27	-1.88 BB41	1.80 BB33	-1.76 SB21	1.54 BB34		
NORMAL MODE 39	OBSERVED=	760.0 CM-1	CALCULATED=	769.1 CM-1	ERROR=	-9.1 CM-1	OR	-1.2 PERCENT	
INTERNAL COORDINATES-	39.43	C5C6 12.96 C1H	10.05 CC1H	7.57 C-01	6.94 C0C	6.21 CCHB	6.03 CCHA		
FORCE CONSTANTS-	47.06	CCO 25.99 CCH	16.38 CCH	9.29 CCO	6.94 CCH	6.16 CC			
OFF DIAGONAL-	-6.66	SB23 -3.38 BB34	-3.35 BB37	2.72 SS18	-1.52 BB29				
NORMAL MODE 40	OBSERVED=	695.0 CM-1	CALCULATED=	707.6 CM-1	ERROR=	-12.6 CM-1	OR	-1.8 PERCENT	
INTERNAL COORDINATES-	10.58	OBCC 10.44 CC09	6.87 C5C*	6.81 C9CC	5.66 C1CC	5.62 CC1H			
FORCE CONSTANTS-	38.69	CCO 12.69 CCH	10.99 CC	9.79 CCH	8.76 CC				
OFF DIAGONAL-	4.45	BB43 3.21 SB25	-2.31 BB41	-2.28 SB26	2.11 SB22	-1.98 SB27	1.79 SS18	1.67 SB24	
NORMAL MODE 41	OBSERVED=	648.0 CM-1	CALCULATED=	686.3 CM-1	ERROR=	-38.3 CM-1	OR	-5.9 PERCENT	
INTERNAL COORDINATES-	30.68	C2C3 10.73 CC09	7.04 CC1H	14.44 CCH	7.13 CC				
FORCE CONSTANTS-	33.13	CC 22.18 CCO	14.44 CCH	2.65 SB25	2.51 SB21	2.28 SS18	-1.68 BB34		
OFF DIAGONAL-	3.77	BB43 -3.17 SB22							
NORMAL MODE 42	OBSERVED=	0.0 CM-1	CALCULATED=	612.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	22.31	CC06 12.64 CC07	11.23 CCO	0.21 CCO*	5.10 C0C*				
FORCE CONSTANTS-	49.85	CCH 15.93 CCH	11.23 CCO	11.04 CC	5.10 CCH				
OFF DIAGONAL-	-5.26	BB34 3.51 BB43	-2.42 BB29	-2.32 BB42	2.29 SB24	-2.25 BB41	1.80 SB25	1.73 SS18	
NORMAL MODE 43	OBSERVED=	0.0 CM-1	CALCULATED=	502.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	18.22	CC01 13.70 C*CC	11.72 C7CC	11.61 CCOB	7.54 C9CC	5.68 C3CC	5.68 HC2C	5.30 CC3H	
FORCE CONSTANTS-	53.27	CCO 18.22 CCO	16.00 CCH	8.93 CCH	5.80 CC				
OFF DIAGONAL-	-9.18	BB34 4.64 BB43	3.94 SB24	-3.31 BB29	-3.11 BB42	-1.63 SB26	1.55 SB25		
NORMAL MODE 44	OBSERVED=	0.0 CM-1	CALCULATED=	490.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	26.49	CC0*	13.09 C*CC	10.64 HC5C	8.62 CCHB	7.09 C3CC	6.56 CCO*		
FORCE CONSTANTS-	60.05	CCO 23.75 CCH	8.92 CCH	5.50 CC					
OFF DIAGONAL-	-11.05	BB34 5.83 BB43	-5.10 BB29	4.14 SB25					
NORMAL MODE 45	OBSERVED=	0.0 CM-1	CALCULATED=	414.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	23.70	CCO 15.75 CCOB	11.06 C7CC	7.36 C*CC	5.29 C1C2				
FORCE CONSTANTS-	49.11	CCO 23.70 CCO	10.25 CCH	8.76 CC					
OFF DIAGONAL-	-6.86	BB34 6.59 SB22	-2.96 BB42	2.64 BB43	-1.71 BB29	1.54 SB21			
NORMAL MODE 46	OBSERVED=	0.0 CM-1	CALCULATED=	389.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	28.08	CC07 14.95 OBCC	14.25 C2CC	14.05 C1CC	8.23 C0C*	7.93 C4C5			
FORCE CONSTANTS-	49.78	CCO 30.72 CCH	8.31 CC	8.93 CCH	7.67 CCH	6.93 CC			
OFF DIAGONAL-	-5.72	BB34 -4.75 BB42	4.12 SB25	-2.05 SB26	2.01 SB22	-1.92 SB21	-1.82 BB41	1.58 SB23	
NORMAL MODE 47	OBSERVED=	0.0 CM-1	CALCULATED=	349.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	21.24	C7CC 12.23 C3C4	8.44 CCO*	8.90 C4C*					
FORCE CONSTANTS-	51.54	CCO 20.71 CC	7.50 CCH	5.92 CCH					
OFF DIAGONAL-	4.77	SB21 -4.68 SB26	4.51 SB22	3.03 SB25	-2.54 BB34	-1.75 BB42	-1.61 BB36		
NORMAL MODE 48	OBSERVED=	0.0 CM-1	CALCULATED=	313.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	27.12	OBCC 21.34 CCOB	11.96 CCO7	10.54 C9CC	6.48 C7CC	6.09 TH-3			
FORCE CONSTANTS-	85.91	CCO 11.64 T-0H	6.44 CCH						
OFF DIAGONAL-	-7.69	BB34 -4.40 BB42	-1.51 BB43						
NORMAL MODE 49	OBSERVED=	0.0 CM-1	CALCULATED=	308.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	15.45	CC09 14.85 C9CC	9.83 CCOB	8.10 TH-4	6.74 CCO*				
FORCE CONSTANTS-	60.20	CCO 12.37 T-0H	9.47 CCH	6.86 CC					
OFF DIAGONAL-	6.03	SB22 -4.51 BB33	-2.96 SB26	2.91 SB21	2.16 BB43	-1.89 BB42	-1.61 BB34		
NORMAL MODE 50	OBSERVED=	0.0 CM-1	CALCULATED=	284.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	15.34	CC07 11.33 CCO6	9.62 C*CC	8.77 CCO9	8.25 C3CC	8.04 TH-2	7.43 C4CC	7.26 CCO7	5.32 TH-5
FORCE CONSTANTS-	61.38	CCO 30.72 CCH	14.05 T-0H	8.88 CCH					
OFF DIAGONAL-	-4.32	BB33 -4.06 BB34	-3.32 BB42	-1.79 SB25	1.54 BB43				
NORMAL MODE 51	OBSERVED=	0.0 CM-1	CALCULATED=	257.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	13.89	CC01 11.44 CCO9	10.03 CCH	12.52 CCH					
FORCE CONSTANTS-	44.86	CCO 22.18 T-0H	10.15 CCH	12.52 CCH					
OFF DIAGONAL-	6.18	BB43 -3.93 BB33	-3.90 BB34	-3.88 SB25	-1.77 BB29	1.70 SB22			
NORMAL MODE 52	OBSERVED=	0.0 CM-1	CALCULATED=	234.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	39.05	TH-5 34.34 TH-1							
FORCE CONSTANTS-	80.50	T-0H 9.15 CCO							
OFF DIAGONAL-	NONE								
NORMAL MODE 53	OBSERVED=	0.0 CM-1	CALCULATED=	228.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	33.20	TH-3 26.36 TH-1							
FORCE CONSTANTS-	91.13	T-0H 5.30 CCO							
OFF DIAGONAL-	NONE								
NORMAL MODE 54	OBSERVED=	0.0 CM-1	CALCULATED=	218.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	33.84	TH-5 24.50 TH-1							
FORCE CONSTANTS-	81.32	T-0H 9.86 CCO							
OFF DIAGONAL-	NONE								
NORMAL MODE 55	OBSERVED=	0.0 CM-1	CALCULATED=	213.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	74.16	TH-2 5.68 CCO7							
FORCE CONSTANTS-	82.68	T-0H 14.83 CCO							
OFF DIAGONAL-	NONE								
NORMAL MODE 56	OBSERVED=	0.0 CM-1	CALCULATED=	208.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	43.61	TH-4 30.55 TH-3							
FORCE CONSTANTS-	74.49	T-0H 20.18 CCO							
OFF DIAGONAL-	NONE								
NORMAL MODE 57	OBSERVED=	0.0 CM-1	CALCULATED=	185.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	19.63	CC0*	11.75 C0C*	11.45 C4CC	8.65 TH-5	6.82 C9CC	6.26 CCO*	6.19 C4C*	
FORCE CONSTANTS-	42.84	CCO 16.50 T-0H	16.37 CCH	11.75 CCH	5.09 CCH				
OFF DIAGONAL-	-2.81	BB42 -2.61 BB33	-2.35 BB34	2.14 BB41					
NORMAL MODE 58	OBSERVED=	0.0 CM-1	CALCULATED=	129.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	22.90	C4CC 17.66 C0C*	8.00 C7CC						
FORCE CONSTANTS-	30.83	CCO 17.66 CCH	14.23 CCH	10.01 T-CC	8.72 T-CC				
OFF DIAGONAL-	-5.14	SB21 2.99 BB43	2.48 SB22	2.30 BB41	-1.96 BB37	-1.58 SB25			
NORMAL MODE 59	OBSERVED=	0.0 CM-1	CALCULATED=	111.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	48.04	TCC5 7.72 TCC2	6.65 C2CC						
FORCE CONSTANTS-	64.49	T-CC 13.02 CCH	11.39 CCO	5.48 CCH					
OFF DIAGONAL-	1.69	BB43							
NORMAL MODE 60	OBSERVED=	0.0 CM-1	CALCULATED=	85.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	20.13	C2CC 14.28 TCC1	12.31 C1CC	11.80 TCC5	6.72 TCC2	6.09 TCC4	5.81 C0C*	5.24 CCOB	
FORCE CONSTANTS-	38.55	T-CC 35.33 CCH	16.11 CCO	5.81 CCH					
OFF DIAGONAL-	-3.56	SB25 -3.27 BB42	1.99 BB41	-1.71 BB34	-1.69 SB21				
NORMAL MODE 61	OBSERVED=	0.0 CM-1	CALCULATED=	67.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	29.64	TCC5 10.39 TCC4	7.81 C3CC	6.68 TCC3	6.52 C1CC	6.33 C4C*	5.95 TCC2	5.05 C7CC	
FORCE CONSTANTS-	53.12	T-CC 19.62 CCO	17.09 CCH						
OFF DIAGONAL-	-1.82	BB42 -1.75 BB34							

29. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 11.57

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400									
MOLECULE 26		-6 NG=1235		ALPHA		GALACTOSE		GG	
PAGE 1									
NORMAL MODE 8	OBSERVED=	1487.0	CM-1	CALCULATED=	1455.5	CM-1	ERROR=	31.5	CM-1 OR 2.1 PERCENT
INTERNAL COORDINATES-	67.27	C2OH	5.15	CC3H	6.09	CCO			
FORCE CONSTANTS-	68.00	BCOH	7.03	CCH	1.77	BB34	-1.77	SB25	
OFF DIAGONAL-	4.46	BB36	3.83	SB28					
NORMAL MODE 9	OBSERVED=	1454.0	CM-1	CALCULATED=	1450.1	CM-1	ERROR=	3.9	CM-1 OR 0.3 PERCENT
INTERNAL COORDINATES-	60.62	HCH	20.90	OCHB	19.67	OCHA			
FORCE CONSTANTS-	60.62	HCH	40.71	OCH					
OFF DIAGONAL-	-4.24	SB27							
NORMAL MODE 10	OBSERVED=	1434.0	CM-1	CALCULATED=	1430.0	CM-1	ERROR=	4.0	CM-1 OR 0.3 PERCENT
INTERNAL COORDINATES-	54.13	C3OH	8.95	C4OH	8.03	C2C3	5.18	OC3H	
FORCE CONSTANTS-	64.43	BCOH	12.52	CCH	9.65	CC	7.49	OCH	
OFF DIAGONAL-	4.63	SB28	4.19	BB36	-2.97	SB26	-2.14	SB27	-1.74
								SB21	-1.62
								BB39	-1.61
								SB22	
NORMAL MODE 11	OBSERVED=	1409.6	CM-1	CALCULATED=	1409.6	CM-1	ERROR=	0.0	CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	45.93	C1OH	23.71	CC1H	8.91	C1H			
FORCE CONSTANTS-	50.95	BCOH	37.29	OCH	8.06	CCH			
OFF DIAGONAL-	-4.93	SB27	4.47	SB28	-3.02	BB39	-1.72	BB45	
NORMAL MODE 12	OBSERVED=	1407.8	CM-1	CALCULATED=	1407.8	CM-1	ERROR=	0.0	CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	33.17	C4OH	16.93	OC4H	9.60	C3OH	6.88	C1OH	
FORCE CONSTANTS-	52.08	BCOH	23.97	OCH	18.10	CCCH	5.23	CO	
OFF DIAGONAL-	-5.38	SB27	4.83	SB28	-2.34	BB39	-1.67	BB45	
NORMAL MODE 13	OBSERVED=	1404.0	CM-1	CALCULATED=	1396.2	CM-1	ERROR=	7.8	CM-1 OR 0.5 PERCENT
INTERNAL COORDINATES-	60.20	C1OH	8.73	CCBH	7.92	OCBH	6.51	CCHA	5.25
FORCE CONSTANTS-	64.48	BCOH	20.19	CCH	10.34	OCH	5.25	HCH	
OFF DIAGONAL-	3.63	SB28	-2.69	BB39	-2.59	SB26	-2.41	SB27	
NORMAL MODE 14	OBSERVED=	1381.0	CM-1	CALCULATED=	1388.4	CM-1	ERROR=	-7.4	CM-1 OR -0.5 PERCENT
INTERNAL COORDINATES-	43.60	CC1H	25.71	C1OH	14.91	OC1H			
FORCE CONSTANTS-	60.74	OCH	27.93	BCOH	5.54	CO	5.21	CCH	
OFF DIAGONAL-	-3.96	SB27	3.13	BB37	-2.39	BB45	1.70	BB39	
NORMAL MODE 15	OBSERVED=	1375.0	CM-1	CALCULATED=	1360.8	CM-1	ERROR=	14.3	CM-1 OR 1.0 PERCENT
INTERNAL COORDINATES-	32.98	OC2H	22.87	HC2C	12.13	OC3H	9.90	CC3H	7.33
FORCE CONSTANTS-	48.86	OCH	36.87	CCH	9.61	BCOH	5.46	CO	
OFF DIAGONAL-	7.12	BB29	-6.28	SB27	-3.45	BB45	2.17	BB34	-2.11
								SB28	-1.78
								SB26	
NORMAL MODE 16	OBSERVED=	1358.0	CM-1	CALCULATED=	1347.0	CM-1	ERROR=	11.0	CM-1 OR 0.8 PERCENT
INTERNAL COORDINATES-	26.00	C4OH	24.02	C5H	11.54	C1OH	8.48	HC4C	7.87
FORCE CONSTANTS-	38.08	BCOH	30.63	OCH	29.20	CCCH	10.82	CO	
OFF DIAGONAL-	-8.39	SB27	-3.06	SB28	-2.76	SB25	2.35	BB33	-2.31
								BB45	
NORMAL MODE 17	OBSERVED=	1332.0	CM-1	CALCULATED=	1334.1	CM-1	ERROR=	-2.1	CM-1 OR -0.2 PERCENT
INTERNAL COORDINATES-	19.52	CCCH	4.58	OCHA	4.09	C1OH	11.98	HC5C	11.17
FORCE CONSTANTS-	43.60	OCH	23.04	CCBH	20.25	BCOH	6.83	CCCH	5.30
OFF DIAGONAL-	-3.12	SB27	-3.06	BB45	-2.87	SB28	-2.10	SB22	-1.85
								SB26	1.58
								BB30	1.54
								BB34	
NORMAL MODE 18	OBSERVED=	1318.4	CM-1	CALCULATED=	1318.4	CM-1	ERROR=	0.0	CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	50.30	OC3H	19.27	HC3C	14.91	CC1H	9.21	CCCH	6.83
FORCE CONSTANTS-	50.30	CCH	27.86	OCH	12.33	BCOH	8.09	CO	5.25
OFF DIAGONAL-	-3.38	BB45	-2.70	SB26	-2.10	SB28	1.75	BB34	
NORMAL MODE 19	OBSERVED=	1310.0	CM-1	CALCULATED=	1307.0	CM-1	ERROR=	3.0	CM-1 OR 0.2 PERCENT
INTERNAL COORDINATES-	20.98	OC3H	17.49	CH2	14.82	OC2H	11.44	HC3C	6.17
FORCE CONSTANTS-	48.13	OCH	39.90	CCH	8.63	CO	6.02	BCOH	
OFF DIAGONAL-	-3.63	BB45	-2.15	SB26	-2.06	SB28	-1.81	BB43	-1.70
								SB25	1.62
								BB34	
NORMAL MODE 20	OBSERVED=	1305.0	CM-1	CALCULATED=	1285.5	CM-1	ERROR=	19.5	CM-1 OR 1.5 PERCENT
INTERNAL COORDINATES-	20.34	OC4H	17.93	C5H	8.83	OC1H	7.37	CC1H	6.41
FORCE CONSTANTS-	50.69	OCH	32.41	CCH	7.69	CO			
OFF DIAGONAL-	-3.34	BB45	2.77	SB27	2.02	BB34	-1.59	SB26	-1.57
								SB25	
NORMAL MODE 21	OBSERVED=	1280.0	CM-1	CALCULATED=	1277.1	CM-1	ERROR=	2.9	CM-1 OR 0.2 PERCENT
INTERNAL COORDINATES-	21.21	OC4H	12.04	OCBH	11.25	CCBH	6.73	HC4C	
FORCE CONSTANTS-	43.21	OCH	34.63	CCH	9.49	BCOH	7.58	CO	
OFF DIAGONAL-	-3.15	BB45							
NORMAL MODE 22	OBSERVED=	1273.0	CM-1	CALCULATED=	1274.2	CM-1	ERROR=	-1.2	CM-1 OR -0.1 PERCENT
INTERNAL COORDINATES-	19.13	CCCH	32.81	C5H	11.57	OCBH	9.22	C1H	7.01
FORCE CONSTANTS-	45.28	OCH	33.66	CCH	21.80	CO	14.80	CCCH	6.80
OFF DIAGONAL-	-3.59	BB45	2.78	BB34	1.86	SB26	-1.53	SB25	6.11
								CC5H	
NORMAL MODE 23	OBSERVED=	1246.0	CM-1	CALCULATED=	1247.8	CM-1	ERROR=	-1.8	CM-1 OR -0.1 PERCENT
INTERNAL COORDINATES-	28.88	CC4H	17.35	HC4C	8.02	HC5C	6.48	C3OH	6.03
FORCE CONSTANTS-	61.23	CCH	17.35	OCH	8.55	BCOH	8.20	CO	
OFF DIAGONAL-	3.86	SB27	-3.46	BB45	-3.11	SB26	2.02	BB34	-1.65
								SB25	-1.60
								SB28	1.53
								BB33	
NORMAL MODE 24	OBSERVED=	1220.0	CM-1	CALCULATED=	1224.1	CM-1	ERROR=	5.9	CM-1 OR 0.5 PERCENT
INTERNAL COORDINATES-	11.48	CC3H	11.23	OC3H	9.27	HC5C	6.82	CC5H	5.91
FORCE CONSTANTS-	52.33	CCH	22.38	OCH	12.49	CO	10.09	BCOH	
OFF DIAGONAL-	5.94	SB27	-3.69	BB29	-3.39	SB25	-3.31	SB26	-3.18
								BB45	1.95
								BB34	
NORMAL MODE 25	OBSERVED=	1199.4	CM-1	CALCULATED=	1199.4	CM-1	ERROR=	0.0	CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	16.21	HC5C	11.65	CC5H	10.62	CC3H	9.71	HC3C	8.82
FORCE CONSTANTS-	65.68	OCH	23.72	CC	12.66	OCH	10.74	CO	9.27
OFF DIAGONAL-	-21.11	SB26	-5.37	SB22	4.13	BB33	4.05	SB27	-3.46
								BB45	-3.06
								SB25	-2.32
								BB43	-2.14
								BB30	
NORMAL MODE 26	OBSERVED=	1152.0	CM-1	CALCULATED=	1165.6	CM-1	ERROR=	-13.6	CM-1 OR -1.2 PERCENT
INTERNAL COORDINATES-	25.30	O1C1	29.39	C5O1	14.58	C4C5	6.15	OCBH	5.81
FORCE CONSTANTS-	54.48	OCH	23.71	OCH	21.80	CO	14.80	CCCH	13.00
OFF DIAGONAL-	-8.11	SB25	-5.26	SB26	-4.29	SB27	-3.18	SB22	-2.54
								SB21	-1.94
								SB24	-1.66
								SB28	-1.53
								BB43	
NORMAL MODE 27	OBSERVED=	1135.0	CM-1	CALCULATED=	1150.3	CM-1	ERROR=	-15.3	CM-1 OR -1.3 PERCENT
INTERNAL COORDINATES-	13.01	O1C1	12.90	C1O8	10.37	C1O8	9.26	C1O8	9.59
FORCE CONSTANTS-	40.15	CO	25.91	CC	17.89	OCH	15.72	CCO	10.06
OFF DIAGONAL-	-6.81	SB22	-3.82	SB25	-2.39	SB23	-2.11	SB28	-1.90
								SB21	-1.65
								SB26	-1.62
								SB27	
NORMAL MODE 28	OBSERVED=	1110.0	CM-1	CALCULATED=	1110.0	CM-1	ERROR=	-0.6	CM-1 OR -0.0 PERCENT
INTERNAL COORDINATES-	27.89	C3C4	19.12	C-O9	9.41	C-O8	9.00	C-O7	7.73
FORCE CONSTANTS-	53.20	CO	34.58	CC	16.49	OCH	13.43	CCO	12.74
OFF DIAGONAL-	-8.56	SB25	-7.74	SB21	-5.87	SB27	-5.71	SB18	-4.93
								CCC	10.95
								CCH	
								BB34	-2.67
								SB26	-2.23
								SB22	
NORMAL MODE 29	OBSERVED=	1103.0	CM-1	CALCULATED=	1106.5	CM-1	ERROR=	-3.5	CM-1 OR -0.3 PERCENT
INTERNAL COORDINATES-	19.36	C-O7	11.16	C2OH	7.77	C2C3	7.58	C1C2	7.19
FORCE CONSTANTS-	33.71	CO	25.26	CC	16.96	CCO	13.14	CCH	12.93
OFF DIAGONAL-	-9.13	SB25	-6.65	SB22	-5.58	SB28	5.55	SB27	2.47
								BB43	2.29
								SB26	-2.08
								BB36	
NORMAL MODE 30	OBSERVED=	1078.0	CM-1	CALCULATED=	1092.2	CM-1	ERROR=	-14.2	CM-1 OR -1.3 PERCENT
INTERNAL COORDINATES-	37.92	C-L7	26.28	C-O8	11.35	C2C3	7.81	O1C1	6.92
FORCE CONSTANTS-	87.94	CO	18.18	CC	5.74	OCOH			
OFF DIAGONAL-	-7.79	SB18	-7.03	SB28	-3.92	SB25	-3.36	SB27	
NORMAL MODE 31	OBSERVED=	1065.0	CM-1	CALCULATED=	1063.8	CM-1	ERROR=	1.1	CM-1 OR 0.1 PERCENT
INTERNAL COORDINATES-	12.18	O1C1	12.90	C1C2	18.21	CCH	14.68	CCC	13.00
FORCE CONSTANTS-	12.18	CO	22.73	CC	-6.47	SB18	-5.61	SB25	-5.59
OFF DIAGONAL-									

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400									
MOLECULE 26		-6 NG=1235		ALPHA		GG		PAGE 2	
GALACTOSE									
NORMAL MODE 36	OBSERVED=	955.0 CM-1	CALCULATED=	909.1 CM-1	ERROR=	45.9 CM-1	OR	4.8 PERCENT	
INTERNAL COORDINATES-	31.50	C2C3 8.23 CCHA	7.98 C2C3 7.98 CCHB	6.32 C-06					
FORCE CONSTANTS-	39.61	CC 26.76 CCH	13.91 CCO 12.74 CCO	6.98 CCH	5.82 CCC				
OFF DIAGONAL-	-8.04	SB21 -5.27 SB22	3.79 SB26 2.97 BB43	-1.92 SB24					
NORMAL MODE 37	OBSERVED=	886.0 CM-1	CALCULATED=	875.0 CM-1	ERROR=	11.0 CM-1	OR	1.3 PERCENT	
INTERNAL COORDINATES-	12.94	C2C3 9.72 C-U*	6.80 CCHB	6.30 C3C4 5.75 C50	5.04 C5C7 5.00 C0C				
FORCE CONSTANTS-	26.54	CCH 24.95 CC	19.25 CCO 16.89 CCO	7.08 CCH	5.57 CCC				
OFF DIAGONAL-	-7.77	SB21 -5.04 SB22	4.74 SB26 3.25 BB43	-2.25 SB23	1.84 SS18 -1.83 SB27				
NORMAL MODE 38	OBSERVED=	828.0 CM-1	CALCULATED=	848.9 CM-1	ERROR=	-20.9 CM-1	OR	-2.5 PERCENT	
INTERNAL COORDINATES-	23.16	C-U9 10.66 C-U6	6.74 C4C5 6.49 C-U*						
FORCE CONSTANTS-	42.09	CC 17.94 CC	11.25 CCO 10.24 CCH	6.91 CCC					
OFF DIAGONAL-	-8.86	SB21 5.36 SB26	4.84 SB25 -4.57 SB27	4.12 SS18	3.91 BB43 -1.71 SB22				
NORMAL MODE 39	OBSERVED=	765.0 CM-1	CALCULATED=	791.5 CM-1	ERROR=	-26.5 CM-1	OR	-3.5 PERCENT	
INTERNAL COORDINATES-	29.30	C50* 6.53 O9CC	5.62 C-06 5.48 CCO*	5.34 C-01					
FORCE CONSTANTS-	45.89	CC 26.13 CCO	9.10 CCH 6.72 CCH						
OFF DIAGONAL-	8.79	SB25 -6.01 SB27	-4.11 SB23 3.25 BB43	-2.03 SB24					
NORMAL MODE 40	OBSERVED=	702.0 CM-1	CALCULATED=	752.9 CM-1	ERROR=	-50.9 CM-1	OR	-7.3 PERCENT	
INTERNAL COORDINATES-	11.54	C5C3 6.64 C1CC	6.47 O8CC 5.57 CCO9	5.49 C50	5.30 C-07				
FORCE CONSTANTS-	39.15	CC 18.50 CCH	17.95 CCO 9.35 CCC	8.78 CCH					
OFF DIAGONAL-	3.87	BB43 3.34 SS18	-2.36 BB41 1.90 SB25	-1.70 SB27					
NORMAL MODE 41	OBSERVED=	660.0 CM-1	CALCULATED=	701.7 CM-1	ERROR=	-41.7 CM-1	OR	-6.3 PERCENT	
INTERNAL COORDINATES-	31.50	C2C3 7.22 CCO9	10.44 CCH 10.01 CCC	9.91 CCO					
FORCE CONSTANTS-	34.32	CC 19.85 CCO	3.21 SB21 2.86 SB25	2.80 SS18	-1.75 BB34 -1.67 SB26				
OFF DIAGONAL-	4.72	BB43 -3.22 SB22							
NORMAL MODE 42	OBSERVED=	612.0 CM-1	CALCULATED=	612.6 CM-1	ERROR=	-0.6 CM-1	OR	-0.1 PERCENT	
INTERNAL COORDINATES-	20.84	CC6C 12.90 CCO7	10.08 CCO 8.19 CCO*	7.13 C0C	6.58 CCO9				
FORCE CONSTANTS-	60.34	CC 10.08 CCO	8.64 CCH 7.58 CC	7.13 CCO	5.06 CCO				
OFF DIAGONAL-	-3.33	BB42 -2.94 BB41	2.54 SB24 -1.91 BB34	-1.56 SB23					
NORMAL MODE 43	OBSERVED=	530.0 CM-1	CALCULATED=	543.9 CM-1	ERROR=	-13.9 CM-1	OR	-2.6 PERCENT	
INTERNAL COORDINATES-	16.99	CC6C 14.21 CCO	9.52 C4C5 5.70 C4C5	5.49 CCO9					
FORCE CONSTANTS-	46.01	CC 14.21 CCO	12.88 CC 8.16 CCH	7.93 CCO					
OFF DIAGONAL-	4.77	SB24 3.76 SB21	-3.25 SB22 3.01 BB43	-2.62 BB34	-1.91 SB27 -1.69 BB42	1.69 SS18			
NORMAL MODE 44	OBSERVED=	490.0 CM-1	CALCULATED=	486.1 CM-1	ERROR=	3.9 CM-1	OR	0.8 PERCENT	
INTERNAL COORDINATES-	21.60	O*CC 15.12 O7CC	8.07 CCOB 7.61 CCO	6.03 C4C5	6.02 HC2C	5.79 CCO*	5.45 O9CC	5.36 C3C4	
FORCE CONSTANTS-	62.59	CC 16.29 CCH	11.62 CC 7.81 CCO						
OFF DIAGONAL-	-8.28	BB34 4.73 BB43	4.07 SB25 3.83 SB22	-3.32 SB26	-2.54 BB29 -2.15 BB42	-2.11 SB21			
NORMAL MODE 45	OBSERVED=	417.0 CM-1	CALCULATED=	421.9 CM-1	ERROR=	-4.9 CM-1	OR	-1.2 PERCENT	
INTERNAL COORDINATES-	24.30	OCC 22.50 CCOB	12.26 O7CC 9.07 O*CC	5.74 C3C4	5.67 C1C2				
FORCE CONSTANTS-	92.28	CC 8.64 T-0H	7.58 CCH 7.81 CCO						
OFF DIAGONAL-	-6.33	BB34 5.62 SB22	-3.23 BB42 2.42 BB43						
NORMAL MODE 46	OBSERVED=	407.0 CM-1	CALCULATED=	398.9 CM-1	ERROR=	8.26 CM-1	OR	2.0 PERCENT	
INTERNAL COORDINATES-	13.88	CC6C 14.73 C2CC	13.90 O8CC 13.79 C1CC	8.26 C0C	6.59 O9CC	6.39 CCO*			
FORCE CONSTANTS-	48.45	CC 34.06 CCH	8.26 CCO 7.04 CCH						
OFF DIAGONAL-	-5.24	BB42 -4.81 BB34	4.12 SB25 -2.25 BB41						
NORMAL MODE 47	OBSERVED=	358.0 CM-1	CALCULATED=	334.8 CM-1	ERROR=	23.2 CM-1	OR	6.5 PERCENT	
INTERNAL COORDINATES-	19.90	O9CC 16.11 O7CC	10.03 CCO9 6.63 C3C4	5.62 C4C5	5.23 CCO*	5.22 CCO6			
FORCE CONSTANTS-	64.72	CC 11.70 CCH	6.78 CCH						
OFF DIAGONAL-	8.43	SB22 -4.08 SB26	-3.93 BB33 -2.81 BB42	1.79 SB21	1.76 BB43	1.57 SB25			
NORMAL MODE 48	OBSERVED=	331.0 CM-1	CALCULATED=	318.1 CM-1	ERROR=	12.9 CM-1	OR	3.9 PERCENT	
INTERNAL COORDINATES-	29.35	CCOB 22.84 O8CC	15.44 CCO7 12.55 O7CC	9.32 O9CC					
FORCE CONSTANTS-	92.28	CC 8.64 T-0H	7.58 CCH						
OFF DIAGONAL-	-8.62	BB34 -5.05 BB42	-2.92 BB43						
NORMAL MODE 49	OBSERVED=	299.0 CM-1	CALCULATED=	299.1 CM-1	ERROR=	-0.1 CM-1	OR	-0.0 PERCENT	
INTERNAL COORDINATES-	26.87	C4C3 21.91 C4CC	8.78 CCO9 7.44 CCO*	7.13 TH-5	5.06 CCO6				
FORCE CONSTANTS-	52.60	CC 24.36 CCH	13.74 T-0H 7.63 CCH						
OFF DIAGONAL-	-4.78	BB34 -4.24 BB42	-3.15 BB33 2.50 SB21						
NORMAL MODE 50	OBSERVED=	268.0 CM-1	CALCULATED=	280.8 CM-1	ERROR=	-12.8 CM-1	OR	-4.8 PERCENT	
INTERNAL COORDINATES-	15.72	CCO 13.26 CCO9	13.10 C3CC 10.09 CCO*	6.40 CCO6	5.65 O8CC				
FORCE CONSTANTS-	57.16	CC 15.12 CCC	9.34 T-0H 8.27 CCH	5.56 CC					
OFF DIAGONAL-	7.76	SB22 -4.69 BB33	-3.29 SB21 -2.79 BB42	-2.28 SB26	2.21 BB43 -2.05 BB34				
NORMAL MODE 51	OBSERVED=	254.0 CM-1	CALCULATED=	261.2 CM-1	ERROR=	-7.2 CM-1	OR	-2.8 PERCENT	
INTERNAL COORDINATES-	20.04	CCO6 6.54 O*CC	6.20 CCH2 6.02 CCO9	6.00 TH-2	5.80 C1CC	5.48 TH-3	5.44 TH-4	5.27 CCO7	
FORCE CONSTANTS-	48.49	CC 20.82 T-0H	16.92 CCH 11.00 CCC						
OFF DIAGONAL-	6.85	BB43 -5.50 BB34	-3.86 BB33 -3.69 SB25	-1.92 BB29					
NORMAL MODE 52	OBSERVED=	230.0 CM-1	CALCULATED=	240.4 CM-1	ERROR=	-10.4 CM-1	OR	-4.5 PERCENT	
INTERNAL COORDINATES-	39.97	TH-1 7.94 TH-5	5.78 O9CC 5.72 C0C	5.08 TH-3					
FORCE CONSTANTS-	58.63	T-0H 18.75 CCO	5.72 CCO 5.42 CCH						
OFF DIAGONAL-	-2.50	BB33 2.45 SB22	2.04 BB43 -1.55 SB25						
NORMAL MODE 53	OBSERVED=	0.0 CM-1	CALCULATED=	227.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	7.25	TH-1 31.49 TH-4	18.36 TH-1 5.37 TH-2						
FORCE CONSTANTS-	NONE								
OFF DIAGONAL-	NONE								
NORMAL MODE 54	OBSERVED=	0.0 CM-1	CALCULATED=	222.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	68.95	TH-5 13.46 TH-1	5.11 CCO*						
FORCE CONSTANTS-	85.10	T-0H 8.29 CCO							
OFF DIAGONAL-	NONE								
NORMAL MODE 55	OBSERVED=	0.0 CM-1	CALCULATED=	213.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	74.95	TH-2 6.26 CCO7							
FORCE CONSTANTS-	82.72	T-0H 14.46 CCO							
OFF DIAGONAL-	NONE								
NORMAL MODE 56	OBSERVED=	0.0 CM-1	CALCULATED=	208.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	37.33	TH-3 33.65 TH-4	8.76 CCO9 7.73 O8CC						
FORCE CONSTANTS-	72.43	T-CH 20.49 CCO							
OFF DIAGONAL-	NONE								
NORMAL MODE 57	OBSERVED=	0.0 CM-1	CALCULATED=	200.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	15.26	TH-1 23.24 TH-4	10.32 O9CC 8.52 TH-5	6.46 CCO	6.23 CCO*	5.71 C4CC			
FORCE CONSTANTS-	39.22	T-CH 23.24 TH-4	7.77 CCO 6.46 CCO	6.13 CCH					
OFF DIAGONAL-	3.15	BB43 2.93 SB22	-2.49 BB33 1.64 BB41	-1.64 SB26					
NORMAL MODE 58	OBSERVED=	0.0 CM-1	CALCULATED=	131.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	23.22	C4C3 11.99 C4CC	11.31 TCC 7.40 TCO	7.26 C1CC					
FORCE CONSTANTS-	23.22	CC 19.54 CCH	14.00 CCO 11.77 T-CC	11.09 T-CC					
OFF DIAGONAL-	3.95	BB43 2.62 BB41	-2.40 BB37						
NORMAL MODE 59	OBSERVED=	0.0 CM-1	CALCULATED=	94.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	24.40	C2CC 16.27 TCC2	12.40 TCC1 6.33 C3CC	6.31 TCC5	6.16 O8CC	5.35 CCO8			
FORCE CONSTANTS-	39.01	T-CC 35.53 CCH	17.45 CCO						
OFF DIAGONAL-	-3.36	SB25 -2.49 BB42	2.13 BB41 -2.04 BB34	-1.72 SB21					
NORMAL MODE 60	OBSERVED=	0.0 CM-1	CALCULATED=	79.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	64.60	TCC5 8.24 C4CC	5.18 C3CC						
FORCE CONSTANTS-	72.78	T-CC 15.11 CCH	6.19 CCO						
OFF DIAGONAL-	NONE								
NORMAL MODE 61	OBSERVED=	0.0 CM-1	CALCULATED=	71.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	13.14	TCC4 13.09 TCC5	12.02 C1CC 10.32 C4C0*	7.03 CCO*	6.39 TCC3	5.91 TCO2	5.29 C0C		
FORCE CONSTANTS-	38.36	T-CC 28.07 CCO	19.30 CCO	6.01 T-CC					
OFF DIAGONAL-	-2.61	BB42 -1.62 BB34	-1.60 BB33						

40. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 12.85

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR GALACTOSE	PROBLEM 400	TG	PAGE 1
MOLECULE 27	-6 NG=1235		
NORMAL MODE 8 OBSERVED= 1487.0 CM-1	CALCULATED= 1455.5 CM-1	ERROR= 31.5 CM-1 OR 2.1 PERCENT	
INTERNAL COORDINATES- 67.15 C2OH 5.1 C3H			
FORCE CONSTANTS- 67.92 BCOH 7.28 CCH	6.11 CCO		
OFF DIAGONAL- 4.46 BB36 3.83 SB28	1.78 BB34 -1.78 SB25		
NORMAL MODE 9 OBSERVED= 1454.0 CM-1	CALCULATED= 1449.5 CM-1	ERROR= 4.5 CM-1 OR 0.3 PERCENT	
INTERNAL COORDINATES- 57.28 HCH 22.93 OCHA	21.46 OCHB		
FORCE CONSTANTS- 57.28 HCH 44.45 OCH			
OFF DIAGONAL- -4.77 SB27			
NORMAL MODE 10 OBSERVED= 1434.0 CM-1	CALCULATED= 1431.4 CM-1	ERROR= 2.6 CM-1 OR 0.2 PERCENT	
INTERNAL COORDINATES- 40.86 C3OH 10.06 C4OH	6.18 C2C3		
FORCE CONSTANTS- 54.72 BCOH 17.55 CCH	11.64 OCH 7.63 CC 5.33 CO		
OFF DIAGONAL- 4.49 SB28	3.49 BB36 -2.84 SB26 -1.71 BB39	1.65 BB34	
NORMAL MODE 11 OBSERVED= 0.0 CM-1	CALCULATED= 1421.3 CM-1	ERROR= 0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES- 19.62 C3OH 14.42 C'OH	10.50 CCHA 6.70 CCHB 5.36 C5O'		
FORCE CONSTANTS- 35.45 BCOH 27.69 CCH	20.45 CCO		
OFF DIAGONAL- -6.03 SB27 -5.12 SB26	3.45 BB34 3.27 SB28 2.68 BB29 -2.20 SB25 -1.76 BB45 -1.74 BB39		
NORMAL MODE 12 OBSERVED= 0.0 CM-1	CALCULATED= 1409.0 CM-1	ERROR= 0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES- 52.92 C1OH 40.79 OC1H			
FORCE CONSTANTS- 57.61 BCOH 31.38 OCH	6.68 CCH		
OFF DIAGONAL- 4.66 SB28 -4.41 SB27	-2.85 BB39		
NORMAL MODE 13 OBSERVED= 1404.0 CM-1	CALCULATED= 1401.3 CM-1	ERROR= 2.7 CM-1 OR 0.2 PERCENT	
INTERNAL COORDINATES- 41.08 C4OH 12.79 CC4H	9.36 C1OH		
FORCE CONSTANTS- 59.30 BCOH 16.39 OCH	16.34 CCH		
OFF DIAGONAL- 4.79 SB28 -3.57 SB27	-2.52 BB39		
NORMAL MODE 14 OBSERVED= 1381.0 CM-1	CALCULATED= 1385.1 CM-1	ERROR= -4.1 CM-1 OR -0.3 PERCENT	
INTERNAL COORDINATES- 41.19 C1H 20.91 C1OH	16.45 OC1H 12.34 C'OH		
FORCE CONSTANTS- 59.98 OCH 33.79 BCOH			
OFF DIAGONAL- -3.82 SB27 2.54 BB37	-2.27 BB45 -1.87 SB26 1.53 BB39		
NORMAL MODE 15 OBSERVED= 1375.0 CM-1	CALCULATED= 1363.0 CM-1	ERROR= 12.0 CM-1 OR 0.9 PERCENT	
INTERNAL COORDINATES- 31.58 C'CH 11.21 OC2H	9.22 C'CH 8.13 HC5C 6.50 HC2C		
FORCE CONSTANTS- 38.13 BCOH 29.87 OCH	26.16 CCH 5.43 CC		
OFF DIAGONAL- -5.06 SB27 4.87 BB29	2.64 BB34 -2.41 SB28 -2.25 BB45 -1.73 SB25		
NORMAL MODE 16 OBSERVED= 1358.0 CM-1	CALCULATED= 1359.2 CM-1	ERROR= -1.2 CM-1 OR -0.1 PERCENT	
INTERNAL COORDINATES- 22.11 OC2H 17.33 HC2C	11.39 C'OH 8.71 OC3H 7.78 CC3H 5.19 C3OH		
FORCE CONSTANTS- 31.92 OCH 40.77 CCH	20.47 BCOH		
OFF DIAGONAL- 6.73 BB29 -5.19 SB27	-2.99 BB45 2.32 BB34 -2.27 SB28		
NORMAL MODE 17 OBSERVED= 1332.0 CM-1	CALCULATED= 1329.7 CM-1	ERROR= 2.3 CM-1 OR 0.2 PERCENT	
INTERNAL COORDINATES- 22.68 C4OH 16.34 CC5H	12.01 HC3 11.91 OC3H 5.61 CCHA 5.24 C'CH 5.08 HC5C		
FORCE CONSTANTS- 46.12 CCH 29.67 OCH	23.89 BCOH 5.62 CO		
OFF DIAGONAL- -3.74 SB28 -3.21 BB45	-3.06 SB26 2.79 BB29 -2.69 SB27		
NORMAL MODE 18 OBSERVED= 0.0 CM-1	CALCULATED= 1315.7 CM-1	ERROR= 0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES- 12.14 CCH2 11.61 CC1H	9.17 CCHB 7.70 OC1H 7.55 C1OH		
FORCE CONSTANTS- 48.97 CCH 25.98 OCH	13.95 BCOH 7.31 CC 5.15 CO		
OFF DIAGONAL- -3.24 BB45 -2.34 SB26	1.88 BB34 -1.76 SB28 1.51 BB30		
NORMAL MODE 19 OBSERVED= 1310.0 CM-1	CALCULATED= 1309.8 CM-1	ERROR= 0.2 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES- 15.31 CCHB 11.88 CCH2	9.26 OCCH 8.54 C'OH 6.23 O'C1		
FORCE CONSTANTS- 43.60 CCH 19.34 OCH	14.49 BCOH 14.36 CO 5.94 CC		
OFF DIAGONAL- 3.18 BB34 -2.68 BB45	-2.20 SB28 -1.73 SB26 -1.62 SB22 -1.56 SB25		
NORMAL MODE 20 OBSERVED= 1305.0 CM-1	CALCULATED= 1303.4 CM-1	ERROR= 1.5 CM-1 OR 0.1 PERCENT	
INTERNAL COORDINATES- 26.76 OC3H 16.33 HC3C	13.56 C'CH 10.07 OC2H 5.87 CC5H 5.54 HC4C 5.53 OCHA 5.51 CCHA		
FORCE CONSTANTS- 31.92 OCH 40.79 CCH			
OFF DIAGONAL- -4.02 BB45 -2.86 SB27			
NORMAL MODE 21 OBSERVED= 1280.0 CM-1	CALCULATED= 1285.8 CM-1	ERROR= -5.8 CM-1 OR -0.5 PERCENT	
INTERNAL COORDINATES- 52.47 OC1H 12.09 C'CH	8.33 OC1H 8.94 CCH 6.99 HC4C 5.28 CCH2		
FORCE CONSTANTS- 52.47 OCH 30.83 CCH	6.91 CO 5.75 BCOH		
OFF DIAGONAL- -3.34 BB45 2.02 BB34	1.80 SB27		
NORMAL MODE 22 OBSERVED= 1273.0 CM-1	CALCULATED= 1273.0 CM-1	ERROR= -0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES- 20.36 CC1H 12.44 OC4H	9.75 C'CH 8.04 C'CH		
FORCE CONSTANTS- 38.99 CCH 35.42 OCH	12.52 CO		
OFF DIAGONAL- 3.49 BB34 -3.11 BB45	-2.26 SB25 2.14 SB26 1.98 SB27		
NORMAL MODE 23 OBSERVED= 1246.0 CM-1	CALCULATED= 1246.5 CM-1	ERROR= -0.5 CM-1 OR -0.0 PERCENT	
INTERNAL COORDINATES- 32.09 CCH4H 18.03 HC4C	7.57 C3OH 6.33 C'CH 5.88 OC4H 5.24 HC5C		
FORCE CONSTANTS- 63.50 CCH 18.49 OC1H	8.53 BCOH 6.34 CO		
OFF DIAGONAL- -3.70 SB26 -3.38 BB45	3.24 SB27 2.12 BB34 -1.66 SB25 1.58 BB33		
NORMAL MODE 24 OBSERVED= 1230.0 CM-1	CALCULATED= 1226.8 CM-1	ERROR= 3.2 CM-1 OR 0.3 PERCENT	
INTERNAL COORDINATES- 18.35 OCHA 12.74 HC5C	11.75 CC5H 10.09 OC3H 8.00 OCCHB 6.02 CC3H		
FORCE CONSTANTS- 4.63 CCH2H	9.77 CO		
OFF DIAGONAL- -6.03 BB29 3.75 SB27	-3.26 BB45 -2.82 SB25 2.26 BB34 -1.63 SB28		
NORMAL MODE 25 OBSERVED= 0.0 CM-1	CALCULATED= 1206.3 CM-1	ERROR= 0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES- 43.71 CC2H 21.14 HC3C	17.49 CO 12.77 CC 9.64 BB45 8.17 OCCHB 6.83 HC5C 6.36 CC5H 5.82 O'C1		
FORCE CONSTANTS- 48.68 SB26 -4.29 SB25	3.51 SB27 -3.23 BB29 -2.67 BB45 2.46 BB34 -2.26 SB22 -1.71 SB28		
NORMAL MODE 26 OBSERVED= 1152.0 CM-1	CALCULATED= 1168.1 CM-1	ERROR= -16.1 CM-1 OR -1.4 PERCENT	
INTERNAL COORDINATES- 29.93 O'C1 16.91 C5O'	11.94 C4C5 10.83 C-OB 8.54 C3C4 7.66 CCH2 5.25 HC4C 5.24 OC1H		
FORCE CONSTANTS- 61.76 CO 21.51 CCH	21.45 CC 14.59 CCO 13.65 OCH		
OFF DIAGONAL- -9.14 SB26 -6.96 SB25	-5.58 SB27 -2.74 SB22 -2.74 SS18 -2.32 BB43 -2.31 SB28 -2.14 SB21 -1.90 SB24		
NORMAL MODE 27 OBSERVED= 1132.0 CM-1	CALCULATED= 1116.0 CM-1	ERROR= 19.0 CM-1 OR 1.7 PERCENT	
INTERNAL COORDINATES- 16.94 C-OB 14.23 C-O7	13.13 C5C 10.72 C-OB 8.00 C1CC 7.47 C4C5 7.29 C2C3 5.97 C'O'C		
FORCE CONSTANTS- 50.54 CO 32.58 CCH	13.94 CCO 12.80 OCH 9.95 CCC 8.51 CCH 5.97 COC		
OFF DIAGONAL- -6.80 SB22 -6.42 SB25	-5.92 SB26 -5.30 SB27 -2.77 BB34 -2.74 SB28 -2.55 SS18 -2.02 SB21 -1.58 SB23		
NORMAL MODE 28 OBSERVED= 1110.0 CM-1	CALCULATED= 1108.7 CM-1	ERROR= 1.3 CM-1 OR 0.1 PERCENT	
INTERNAL COORDINATES- 16.80 C-O9 14.37 C-O7	9.96 C2OH 7.83 CC4H 6.16 OC3H 5.43 C1C2 5.17 C2CC 5.05 C5O'		
FORCE CONSTANTS- 43.26 CO 19.02 CCO	14.17 CCH 13.32 BCOH 12.69 CCO 12.55 OCH 8.49 BCOH		
OFF DIAGONAL- -13.26 SB25 -7.15 SB28	-5.93 SB27 -3.76 SB21 2.61 BB43 -2.20 BB36		
NORMAL MODE 29 OBSERVED= 1103.0 CM-1	CALCULATED= 1104.0 CM-1	ERROR= -1.0 CM-1 OR -0.1 PERCENT	
INTERNAL COORDINATES- 52.94 C3C4 27.97 C-O7	19.32 CCH 11.83 CCO 8.88 OCH		
FORCE CONSTANTS- 52.94 CO 27.97 CCO	-2.23 BB34 -2.20 SB21 -1.79 SS17 -1.69 SB25		
OFF DIAGONAL- -11.74 SB22 -2.35 SB28			
NORMAL MODE 30 OBSERVED= 1078.0 CM-1	CALCULATED= 1091.8 CM-1	ERROR= -13.8 CM-1 OR -1.3 PERCENT	
INTERNAL COORDINATES- 32.60 C-O7 23.44 C-OB	13.42 C2C3 12.88 C5C' 6.11 C-O8 5.09 C4C5		
FORCE CONSTANTS- 68.45 CO 31.78 CCH	6.77 BCOH 5.21 CCH		
OFF DIAGONAL- -7.36 SB28 -6.50 SS18	-4.45 SB25 -2.37 SB27		
NORMAL MODE 31 OBSERVED= 1065.0 CM-1	CALCULATED= 1064.4 CM-1	ERROR= 0.6 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES- 56.17 C-O8 9.24 C-O9	7.51 C4C5 5.13 C4CC		
FORCE CONSTANTS- 74.39 CO 14.92 CC	9.26 CCO 8.67 CCH 7.81 OCH 6.68 CCC		
OFF DIAGONAL- -7.48 SB21 -7.00 SB25	-5.55 SB28 -5.10 SS18 1.91 SB22 -1.77 SB27		
NORMAL MODE 32 OBSERVED= 1040.0 CM-1	CALCULATED= 1056.8 CM-1	ERROR= -16.8 CM-1 OR -1.6 PERCENT	
INTERNAL COORDINATES- 57.59 C1C2 16.72 C-O6	8.59 C1OH 8.50 C2C3 6.74 O'C1 6.63 C5C' 5.37 CC1H		
FORCE CONSTANTS- 74.48 CC 36.02 CO	14.55 CCH 12.13 CCO 11.01 BCOH 9.74 OCH		
OFF DIAGONAL- -12.70 SB22 -12.62 SB26	-9.29 SS18 -7.46 SB27 -6.28 SB28 -5.24 SB24 -4.39 SB21 -3.63 BB34 -1.63 BB43		
NORMAL MODE 33 OBSERVED= 0.0 CM-1	CALCULATED= 1030.3 CM-1	ERROR= 0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES- 15.51 C-O8 10.79 C5C'	10.44 C4C5 7.36 O'C1 7.15 C3CC 6.83 C-OB 6.38 C-O9 5.49 HC2C 5.26 C-O6		
FORCE CONSTANTS- 49.48 CCH 16.95 CCH	18.53 CO 11.93 CCO 11.93 CCO 11.93 CCO 11.93 CCO 11.93 CCO 11.93 CCO		
OFF DIAGONAL- -8.90 SB21 -7.75 SB27	-6.03 SB28 -5.36 SB25 -2.63 SB22 -2.43 BB29 -2.06 SS18 -2.03 SB26 -1.87 BB34		
NORMAL MODE 34 OBSERVED= 997.0 CM-1	CALCULATED= 987.7 CM-1	ERROR= 9.3 CM-1 OR 0.9 PERCENT	
INTERNAL COORDINATES- 38.19 C5C' 10.76 C3C4	11.91 C1OH 10.54 C-OB		
FORCE CONSTANTS- 70.28 CC 17.04 CO	14.61 CCO 12.85 CCH 5.94 OCH		
OFF DIAGONAL- -15.57 SB22 -4.31 SB26	-3.64 SB21 -2.34 BB34		
NORMAL MODE 35 OBSERVED= 970.0 CM-1	CALCULATED= 960.2 CM-1	ERROR= 9.8 CM-1 OR 1.0 PERCENT	
INTERNAL COORDINATES- 16.53 C-O6 13.29 C-O8	12.13 O'C1 9.00 C5O' 5.75 C-O7		
FORCE CONSTANTS- 60.38 CO 26.62 CCH	8.97 CCO 8.30 CC 6.21 OCH		
OFF DIAGONAL- -6.11 SB24 -4.59 SB25	-3.95 SB28 -2.76 SB21 -2.12 BB29 1.79 BB43 -1.74 SS18		

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400									
MOLECULE 27		-6 NG-1235		ALPHA GALACTOSE		FG		PAGE 2	
NORMAL MODE 36									
INTERNAL COORDINATES-	OBSERVED=	955.0 CM-1		CALCULATED=	937.8 CM-1	ERROR=	17.5 CM-1	OR	1.8 PERCENT
FORCE CONSTANTS-	27.92	C-09 10.22	C-06	9.63 CCHA	8.65 CCHB	7.57 CCHH			
OFF DIAGONAL-	47.92	C-04 43.23	CCH	8.50	C-25 CCH				
	-5.18	SB25 -4.73	BB29	4.21 SB26	-2.65 SB27	-2.34 SB28	-1.56 SB22		
NORMAL MODE 37									
INTERNAL COORDINATES-	OBSERVED=	886.0 CM-1		CALCULATED=	881.0 CM-1	ERROR=	5.0 CM-1	OR	0.6 PERCENT
FORCE CONSTANTS-	31.45	C2C3 10.88	C-09	9.14 CCH	7.04 CCH	5.21 C-06			
OFF DIAGONAL-	36.42	C-04 7.79	CCH	22.82 CCH	10.96 CCH	7.86 CCH	7.77 CCH		
	-9.49	SB21 -7.94	SB22	-3.85 SB27	3.11 SB26	1.73 BB43	1.69 SB25		
NORMAL MODE 38									
INTERNAL COORDINATES-	OBSERVED=	828.0 CM-1		CALCULATED=	839.1 CM-1	ERROR=	-11.1 CM-1	OR	-1.3 PERCENT
FORCE CONSTANTS-	12.87	C4C5 10.78	C-06	8.71 C-09	8.12 CCH	6.85 C-06			
OFF DIAGONAL-	30.71	C-02 22.74	CCH	20.69 CCH	13.04 CCH				
	-5.57	SB26 -5.39	SB22	-4.58 SB21	4.33 SS18	3.63 BB43	-2.13 SB27	1.95 SB25	
NORMAL MODE 39									
INTERNAL COORDINATES-	OBSERVED=	765.0 CM-1		CALCULATED=	767.9 CM-1	ERROR=	-2.9 CM-1	OR	-0.4 PERCENT
FORCE CONSTANTS-	7.94	C-06		6.81 C-06					
OFF DIAGONAL-	31.55	C-02 21.91	CCH	12.61 CCH	11.75 CCH	7.94 CCH	6.96 CCH		
	6.01	SB25 4.06	BB43	-2.83 SB27	-2.43 BB41	-2.40 SB21	2.08 SS18	-1.91 SB23	
NORMAL MODE 40									
INTERNAL COORDINATES-	OBSERVED=	702.0 CM-1		CALCULATED=	708.4 CM-1	ERROR=	-6.4 CM-1	OR	-0.9 PERCENT
FORCE CONSTANTS-	25.16	C2C3 7.63	C-06	5.80 C-06					
OFF DIAGONAL-	26.79	C-02 20.94	CCH	14.71 CCH	11.55 CCH	5.51 CCH			
	9.06	SB21 4.38	SB25	4.37 BB43	-3.60 SB22	-2.37 CCH	1.91 SS18	-1.90 SB27	1.69 BB42
NORMAL MODE 41									
INTERNAL COORDINATES-	OBSERVED=	660.0 CM-1		CALCULATED=	669.0 CM-1	ERROR=	-9.0 CM-1	OR	-1.4 PERCENT
FORCE CONSTANTS-	10.85	CCH		8.63 CCHA	7.83 CCH	7.64 CCH	7.22 C2C3	6.91 HC5C	5.26 CCHB
OFF DIAGONAL-	31.97	C-02 23.49	CCH	19.68 CCH	10.47 CCH	7.19 CCH			
	3.97	BB43 -3.91	SB21	-3.77 BB29	2.29 SB25	2.05 SS18	-1.60 BB41	-1.58 SB27	
NORMAL MODE 42									
INTERNAL COORDINATES-	OBSERVED=	612.0 CM-1		CALCULATED=	612.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
FORCE CONSTANTS-	51.34	CCH		11.97 CCH	7.48 C-06	6.60 CCH			
OFF DIAGONAL-	-3.22	BB42 3.07	SB24	-2.75 BB41	-1.57 SB23				
NORMAL MODE 43									
INTERNAL COORDINATES-	OBSERVED=	530.0 CM-1		CALCULATED=	532.2 CM-1	ERROR=	-2.2 CM-1	OR	-0.4 PERCENT
FORCE CONSTANTS-	24.87	CCH		9.48 CCH	6.18 CCH				
OFF DIAGONAL-	50.71	C-02 16.33	CCH	15.33 CCH	6.18 CCH	6.17 CCH			
	-7.42	BB34 6.49	BB43	4.65 SB25	-3.40 BB29	-1.89 SB21	-1.72 BB41	-1.60 SB27	
NORMAL MODE 44									
INTERNAL COORDINATES-	OBSERVED=	490.0 CM-1		CALCULATED=	482.3 CM-1	ERROR=	7.7 CM-1	OR	1.6 PERCENT
FORCE CONSTANTS-	21.00	CCH		16.31 CCH	14.17 CCH	7.56 CCH			
OFF DIAGONAL-	58.14	C-02 14.17	CCH	11.29 CCH	9.99 CCH				
	-8.51	BB34 4.75	SB25	-3.06 BB42	2.51 BB43	-2.34 SB27	-2.05 BB29	1.99 SB24	
NORMAL MODE 45									
INTERNAL COORDINATES-	OBSERVED=	417.0 CM-1		CALCULATED=	436.7 CM-1	ERROR=	-19.7 CM-1	OR	-4.7 PERCENT
FORCE CONSTANTS-	11.14	CCH		9.38 CCH	7.72 CCH	7.14 CCH	5.70 CCH		
OFF DIAGONAL-	22.65	C-02 18.74	CCH	18.25 CCH	10.47 CCH	6.22 CCH			
	6.85	SB21 6.40	SB22	4.98 SB25	-3.93 SB26	2.48 BB43	-1.58 BB42	1.52 SS18	
NORMAL MODE 46									
INTERNAL COORDINATES-	OBSERVED=	407.0 CM-1		CALCULATED=	403.2 CM-1	ERROR=	3.8 CM-1	OR	0.9 PERCENT
FORCE CONSTANTS-	20.36	CCH		10.00 CCH	5.76 CCH	5.29 CCH	5.20 CCH	5.12 CCH	
OFF DIAGONAL-	-10.21	BB34 4.08	SB22	3.54 BB43	-3.19 BB42	-2.06 BB29	2.03 SB26	-1.55 BB36	
NORMAL MODE 47									
INTERNAL COORDINATES-	OBSERVED=	358.0 CM-1		CALCULATED=	348.8 CM-1	ERROR=	9.2 CM-1	OR	2.6 PERCENT
FORCE CONSTANTS-	11.59	CCH		10.49 CCH	8.96 CCH	8.76 CCH	8.62 CCH	6.79 CCH	
OFF DIAGONAL-	50.45	C-02 18.75	CCH	12.91 CCH	5.74 CCH				
	4.30	SB25 -3.88	BB34	3.66 SB22	-3.57 BB42	-3.40 SB27	2.46 SB23		
NORMAL MODE 48									
INTERNAL COORDINATES-	OBSERVED=	331.0 CM-1		CALCULATED=	320.1 CM-1	ERROR=	10.9 CM-1	OR	3.3 PERCENT
FORCE CONSTANTS-	30.85	CCH		19.07 CCH	14.47 CCH	9.29 CCH	6.09 CCH		
OFF DIAGONAL-	87.70	C-02 10.15	CCH	7.34 CCH	5.87 CCH				
	-7.45	BB34 -4.41	BB42	-3.00 SB26	2.52 SB22	-2.29 BB43	-2.01 BB33		
NORMAL MODE 49									
INTERNAL COORDINATES-	OBSERVED=	299.0 CM-1		CALCULATED=	310.1 CM-1	ERROR=	-11.1 CM-1	OR	-3.7 PERCENT
FORCE CONSTANTS-	20.73	CCH		18.14 CCH	11.95 CCH	9.51 CCH	6.91 CCH	6.44 CCH	
OFF DIAGONAL-	69.68	C-02 16.52	CCH	16.93 CCH	10.76 CCH	7.97 CCH	5.74 CCH		
	-3.43	BB33 -2.84	BB34	-2.80 BB42	2.34 BB41	2.06 SB22	1.98 BB43		
NORMAL MODE 50									
INTERNAL COORDINATES-	OBSERVED=	268.0 CM-1		CALCULATED=	264.9 CM-1	ERROR=	3.1 CM-1	OR	1.1 PERCENT
FORCE CONSTANTS-	24.94	CCH		11.70 CCH	9.20 CCH	7.30 CCH			
OFF DIAGONAL-	54.71	C-02 17.56	CCH	17.56 CCH	10.90 CCH				
	5.75	BB43 -5.49	BB34	-4.35 BB33	-2.94 SB25	2.45 SB22			
NORMAL MODE 51									
INTERNAL COORDINATES-	OBSERVED=	254.0 CM-1		CALCULATED=	250.5 CM-1	ERROR=	3.5 CM-1	OR	1.4 PERCENT
FORCE CONSTANTS-	14.90	CCH		13.57 CCH	13.11 CCH	12.54 CCH	11.40 CCH		
OFF DIAGONAL-	38.07	C-02 32.09	CCH	16.09 CCH	10.59 CCH				
	4.23	SB22 -3.95	BB33	-3.44 SB25	3.09 BB43	-2.56 SB21	-2.18 SB26		
NORMAL MODE 52									
INTERNAL COORDINATES-	OBSERVED=	230.0 CM-1		CALCULATED=	236.2 CM-1	ERROR=	-6.2 CM-1	OR	-2.7 PERCENT
FORCE CONSTANTS-	42.45	CCH		11.65 CCH	9.82 CCH	8.20 CCH			
OFF DIAGONAL-	77.39	C-02 8.73	CCH	8.73 CCH					
	NONE								
NORMAL MODE 53									
INTERNAL COORDINATES-	OBSERVED=	0.0 CM-1		CALCULATED=	226.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
FORCE CONSTANTS-	49.50	CCH		20.56 CCH	20.53 CCH				
OFF DIAGONAL-	92.75	C-02 20.56	CCH						
	NONE								
NORMAL MODE 54									
INTERNAL COORDINATES-	OBSERVED=	0.0 CM-1		CALCULATED=	216.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
FORCE CONSTANTS-	37.89	CCH		15.45 CCH	13.36 CCH				
OFF DIAGONAL-	70.25	C-02 21.17	CCH	5.70 CCH					
	-2.22	BB34 -1.52	SB25						
NORMAL MODE 55									
INTERNAL COORDINATES-	OBSERVED=	0.0 CM-1		CALCULATED=	212.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
FORCE CONSTANTS-	55.01	CCH		17.93 CCH	5.94 CCH	5.52 CCH			
OFF DIAGONAL-	76.13	C-02 17.93	CCH						
	NONE								
NORMAL MODE 56									
INTERNAL COORDINATES-	OBSERVED=	0.0 CM-1		CALCULATED=	209.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
FORCE CONSTANTS-	50.91	CCH		20.56 CCH	7.82 CCH				
OFF DIAGONAL-	73.44	C-02 19.36	CCH						
	NONE								
NORMAL MODE 57									
INTERNAL COORDINATES-	OBSERVED=	0.0 CM-1		CALCULATED=	202.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
FORCE CONSTANTS-	26.82	CCH		18.55 CCH	14.55 CCH	7.88 CCH	7.32 CCH		
OFF DIAGONAL-	33.33	C-02 29.21	CCH	29.21 CCH	23.67 CCH	8.52 CCH			
	-4.57	BB34 -3.42	BB42	-2.68 SB25					
NORMAL MODE 58									
INTERNAL COORDINATES-	OBSERVED=	0.0 CM-1		CALCULATED=	146.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
FORCE CONSTANTS-	29.05	CCH		11.70 CCH	10.76 CCH	7.97 CCH	6.29 CCH		
OFF DIAGONAL-	-4.08	BB34 3.10	BB43	-2.92 BB37	1.84 BB41	-1.58 SB25			
NORMAL MODE 59									
INTERNAL COORDINATES-	OBSERVED=	0.0 CM-1		CALCULATED=	96.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
FORCE CONSTANTS-	21.33	CCH		16.21 CCH	12.30 CCH	11.91 CCH	8.40 CCH		
OFF DIAGONAL-	46.13	C-02 35.99	CCH	15.98 CCH					
	-3.94	SB25 -3.77	SB21	-2.69 BB42	2.20 BB41	-1.89 BB34			
NORMAL MODE 60									
INTERNAL COORDINATES-	OBSERVED=	0.0 CM-1		CALCULATED=	87.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
FORCE CONSTANTS-	26.60	CCH		10.09 CCH	8.72 CCH	7.27 CCH	6.22 CCH		
OFF DIAGONAL-	50.84	C-02 19.47	CCH	14.22 CCH					
	3.53	SB21 -1.63	BB34						
NORMAL MODE 61									
INTERNAL COORDINATES-	OBSERVED=	0.0 CM-1		CALCULATED=	65.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
FORCE CONSTANTS-	30.35	CCH		8.55 CCH	8.18 CCH	7.66 CCH	6.44 CCH		
OFF DIAGONAL-	44.16	C-02 18.52	CCH	16.69 CCH	8.95 CCH	6.87 CCH	5.49 CCH		
	-2.05	BB42							

40. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 7.24

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400										PAGE 1	
MOL ECULE 28		-6		NG=1235		ALPHA		TG			
NORMAL MODE 8		OBSERVED=		1498.0 CM-1		CALCULATED=		1454.9 CM-1		ERROR= 43.1 CM-1 OR 2.9 PERCENT	
INTERNAL COORDINATES-		67.51 C2CH		5.43 CC3H		6.05 CCO		1.87 BB34			
FORCE CONSTANTS-		68.30 CCOCH		7.08 CCH		1.87 BB34		-1.77 SB25			
OFF DIAGONAL-		4.44 BB36		3.91 SB28							
NORMAL MODE 9		OBSERVED=		1458.0 CM-1		CALCULATED=		1449.4 CM-1		ERROR= 8.5 CM-1 OR 0.6 PERCENT	
INTERNAL COORDINATES-		17.74 CCH		23.06 CCHA		21.61 CCHB					
FORCE CONSTANTS-		57.04 CCH		44.69 CCH							
OFF DIAGONAL-		-4.84 SB27									
NORMAL MODE 10		OBSERVED=		1442.0 CM-1		CALCULATED=		1430.1 CM-1		ERROR= 11.9 CM-1 OR 0.8 PERCENT	
INTERNAL COORDINATES-		44.88 C3OH		10.81 C4OH		6.17 C2C3		5.57 CCH			
FORCE CONSTANTS-		59.24 BCOH		15.55 CCH		9.74 CCH		7.87 CC			
OFF DIAGONAL-		4.65 SB28		3.74 BB36		-3.16 SB27		-2.73 SB28		-1.73 BB39	
NORMAL MODE 11		OBSERVED=		1424.0 CM-1		CALCULATED=		1419.6 CM-1		ERROR= 4.4 CM-1 OR 0.3 PERCENT	
INTERNAL COORDINATES-		17.11 CCH		16.52 C3OH		11.48 CCHA		7.01 CCHB		5.51 CCH	
FORCE CONSTANTS-		36.88 BCOH		30.05 CCH		17.85 CCH		7.42 CC		5.83 CCH	
OFF DIAGONAL-		-5.94 SB27		-5.64 SB26		3.48 SB28		3.38 BB34		2.97 BB29	
										-1.81 BB39 -1.73 BB45	
NORMAL MODE 12		OBSERVED=		1405.0 CM-1		CALCULATED=		1401.2 CM-1		ERROR= 3.8 CM-1 OR 0.3 PERCENT	
INTERNAL COORDINATES-		32.31 C4OH		15.17 C1UH		11.26 CCH		9.60 CCHH			
FORCE CONSTANTS-		61.29 CCH		13.59 CCH		13.59 CCH		7.72 CC		5.82 CCO	
OFF DIAGONAL-		5.06 SB28		-3.20 SB27		-2.29 BB39					
NORMAL MODE 13		OBSERVED=		1394.0 CM-1		CALCULATED=		1399.5 CM-1		ERROR= -5.5 CM-1 OR -0.4 PERCENT	
INTERNAL COORDINATES-		63.73 CCH		9.78 C4OH		6.14 CCH					
FORCE CONSTANTS-		70.29 BCOH		36 CCH		-1.58 SB22					
OFF DIAGONAL-		4.66 SB28		-1.72 SB27							
NORMAL MODE 14		OBSERVED=		1380.0 CM-1		CALCULATED=		1363.0 CM-1		ERROR= 17.0 CM-1 OR 1.2 PERCENT	
INTERNAL COORDINATES-		44.36 C3OH		10.42 C5H		9.16 HC5C		5.99 CCHA			
FORCE CONSTANTS-		50.13 BCOH		21.34 CCH		21.29 CCH		5.35 CC			
OFF DIAGONAL-		-4.18 SB27		4.06 BB29		2.75 BB34		-2.44 SB28		-1.80 SB25 -1.78 BB35 -1.70 BB45	
NORMAL MODE 15		OBSERVED=		0.0 CM-1		CALCULATED=		1359.8 CM-1		ERROR= 0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-		33.05 CCH		19.61 HC2C		12.11 OC3H		9.27 CC3H		5.52 CCH	
FORCE CONSTANTS-		46.85 CCH		32.77 CCH		16.61 BCOH		3.17 BB45		-2.56 SB28	
OFF DIAGONAL-		6.60 BB29		-6.41 SB27						2.09 BB34	
NORMAL MODE 16		OBSERVED=		1340.0 CM-1		CALCULATED=		1329.5 CM-1		ERROR= 10.5 CM-1 OR 0.8 PERCENT	
INTERNAL COORDINATES-		22.53 C4OH		16.47 C5H		11.39 HC3C		11.11 OC3H		5.84 CCHA	
FORCE CONSTANTS-		45.93 CCH		29.60 CCH		23.92 BCOH		5.98 CC		5.31 HC5C	
OFF DIAGONAL-		-3.79 SB28		-3.20 BB45		-2.96 SB26		-2.88 SB27		2.85 BB29	
NORMAL MODE 17		OBSERVED=		1322.0 CM-1		CALCULATED=		1317.7 CM-1		ERROR= 4.3 CM-1 OR 0.3 PERCENT	
INTERNAL COORDINATES-		18.40 CCHB		11.22 CCHB		10.42 CCH		9.38 HC5C		9.12 C5H	
FORCE CONSTANTS-		44.24 CCH		24.44 CCH		14.79 CCH		10.94 CCH		7.72 CC	
OFF DIAGONAL-		-3.97 SB27		3.11 BB34		-2.78 BB45		-2.29 SB22		-1.85 SB28	
</											

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400									
MOLECULE 28 -6 NG=1235 ALPHA GALACTOSE-1-D TG									
PAGE 2									
NORMAL MODE 36	OBSERVED=	933.0 CM-1	CALCULATED=	921.0 CM-1	ERROR=	12.0 CM-1	OR	1.3 PERCENT	
INTERNAL COORDINATES-	32.93	C-08 11.70 CCHA	11.13 CCHB	7.01 CCIH	6.45 CC5H				
FORCE CONSTANTS-	49.18	CCH 37.20 CO	14.47 OCH	5.54 CC					
OFF DIAGONAL-	-5.12	SB27 -4.21 BB29	-3.22 SB28	-1.62 SB25					
NORMAL MODE 37	OBSERVED=	864.0 CM-1	CALCULATED=	850.0 CM-1	ERROR=	14.0 CM-1	OR	1.6 PERCENT	
INTERNAL COORDINATES-	19.14	C-06 11.20 C2C3	9.86 CCH2	8.46 CCIH	6.83 C-09	6.66 CC08	5.65 OC1H		
FORCE CONSTANTS-	29.56	CO 24.64 CCH	16.35 CC	14.28 OCH	13.81 CCO	5.52 CCC			
OFF DIAGONAL-	-7.41	SB21 -7.39 SB27	4.83 SB25	4.48 SB26	-4.27 SB22	2.76 BB43	1.51 BB33		
NORMAL MODE 38	OBSERVED=	822.0 CM-1	CALCULATED=	828.7 CM-1	ERROR=	-6.7 CM-1	OR	-0.8 PERCENT	
INTERNAL COORDINATES-	16.43	C4C5 12.08 C5U1	8.49 OC8C	7.74 CIIH	5.42 C-09	5.05 CC0*			
FORCE CONSTANTS-	25.99	CC 23.82 CO	21.19 CCO	17.18 CCH	10.52 OCH				
OFF DIAGONAL-	-7.08	SB22 4.55 SS18	4.51 SB21	-1.51 SB21	-2.17 SB25	2.13 BB43	-1.62 SB23		
NORMAL MODE 39	OBSERVED=	760.0 CM-1	CALCULATED=	756.0 CM-1	ERROR=	4.0 CM-1	OR	0.5 PERCENT	
INTERNAL COORDINATES-	8.45	4C0*	8.14 CCIH	7.37 COC	7.12 C-07	5.02 C-09			
FORCE CONSTANTS-	26.81	CCO 25.03 CO	16.95 CCH	19.67 CC	7.64 CCC	7.37 COC			
OFF DIAGONAL-	6.22	SB25 3.60 BB43	-2.91 SB23	-2.41 BB41	-1.88 SB26	-1.88 SB27	1.86 SS18	-1.80 SB21	
NORMAL MODE 40	OBSERVED=	695.0 CM-1	CALCULATED=	691.7 CM-1	ERROR=	3.3 CM-1	OR	0.5 PERCENT	
INTERNAL COORDINATES-	20.77	C2C3 10.46 CCIH	8.27 COC	5.89 4C0*	5.58 OCO				
FORCE CONSTANTS-	23.42	CC 21.98 CCH	17.64 CCO	8.41 CO	6.56 COC	5.58 OCO			
OFF DIAGONAL-	4.18	SB21 4.15 BB43	3.53 SB25	-2.89 SB26	-2.86 SB22	1.74 BB42			
NORMAL MODE 41	OBSERVED=	648.0 CM-1	CALCULATED=	665.1 CM-1	ERROR=	-17.1 CM-1	OR	-2.6 PERCENT	
INTERNAL COORDINATES-	12.17	CC09 11.80 C2C3	9.13 C4C6	8.87 O9CC	8.07 C4C5	7.28 CCHA	7.16 OC8C	5.81 HC5C	5.34 CCHB
FORCE CONSTANTS-	33.01	CCO 23.39 CC	22.64 CCH	11.79 CCC	5.33 CO				
OFF DIAGONAL-	-4.51	SB21 3.91 BB43	-3.10 BB29	1.90 SS18	1.75 SB25	-1.69 BB41			
NORMAL MODE 42	OBSERVED=	604.8 CM-1	CALCULATED=	604.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	24.21	CC06 13.12 CCU7	10.46 OCO	6.44 COC	5.40 CCO*				
FORCE CONSTANTS-	55.93	CCO 10.46 UCO	8.51 CCH	8.38 CC	6.45 CO	6.44 COC			
OFF DIAGONAL-	-2.91	BB34 -2.79 BB42	-2.66 BB41	2.55 SB24	2.55 BB43	-1.64 SB27	1.53 SS18		
NORMAL MODE 43	OBSERVED=	526.3 CM-1	CALCULATED=	526.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	22.48	CCC*	8.91 C4CC	8.73 OCO	5.24 O7CC				
FORCE CONSTANTS-	48.97	CCO 14.78 CCH	14.26 CCH	8.73 OCO					
OFF DIAGONAL-	-7.34	BB34 6.30 BB43	4.45 SB25	-3.08 BB29	-1.70 SB27	-1.67 BB42	-1.67 SB21	-1.57 BB41	
NORMAL MODE 44	OBSERVED=	479.5 CM-1	CALCULATED=	479.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	20.70	O*CO 17.70 CCO*	13.15 OCO	7.09 O7CC	6.90 CCO8	5.53 C5U1			
FORCE CONSTANTS-	57.10	CCO 13.15 CCO	10.90 CCH	9.67 CC	8.14 CCC				
OFF DIAGONAL-	-8.29	BB34 4.75 SB25	-2.96 BB42	2.81 BB43	-2.42 SB27	-1.99 BB29	1.83 SB24		
NORMAL MODE 45	OBSERVED=	436.3 CM-1	CALCULATED=	436.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	27.91	C3CC 9.36 C*CC	7.49 OC8C	7.04 C4C5	5.61 C2CC	5.15 CCO8	5.13 OCO		
FORCE CONSTANTS-	27.91	CCO 18.57 CC	18.03 CCC	7.23 CO	6.35 CCH	5.13 OCO			
OFF DIAGONAL-	6.68	SB21 6.49 SB22	5.09 SB25	-3.98 SB26	2.50 BB43	-1.62 BB42	1.53 SS18		
NORMAL MODE 46	OBSERVED=	399.9 CM-1	CALCULATED=	399.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	21.56	O7CC 18.64 OCO	11.44 CCO8	5.81 CCO*	5.56 CCO7	5.46 O9CC	5.21 C3C4		
FORCE CONSTANTS-	60.22	CCO 18.64 OCO	13.15 CCH	8.84 CC					
OFF DIAGONAL-	-10.55	BB34 4.07 SB22	3.12 BB43	2.19 SB26	-1.99 BB29	-1.58 BB36			
NORMAL MODE 47	OBSERVED=	348.4 CM-1	CALCULATED=	348.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	11.29	CCO*	10.73 OC8C	8.93 4C0*	8.85 CCO7	8.57 C1CC	6.79 O*CI		
FORCE CONSTANTS-	50.38	CCO 18.71 CCC	12.91 CO	5.75 CC					
OFF DIAGONAL-	4.26	SB25 -3.93 BB34	3.73 SB22	-3.57 BB42	-3.38 SB27	2.48 SB23			
NORMAL MODE 48	OBSERVED=	320.0 CM-1	CALCULATED=	320.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	30.68	CCO8 19.19 O7CC	14.60 CCO7	9.14 OC8C	6.16 CCO9				
FORCE CONSTANTS-	87.74	CCO 10.24 CCH	7.27 CCH	7.27 CCH					
OFF DIAGONAL-	-7.49	BB34 -4.41 BB42	-3.02 SB26	2.50 SB22	-2.28 BB43	-2.02 BB33			
NORMAL MODE 49	OBSERVED=	310.1 CM-1	CALCULATED=	310.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	69.67	CCO 18.12 C9CC	11.50 OC8C	9.48 TH-4	7.04 CCO7	6.42 CCO6			
FORCE CONSTANTS-	69.67	CCO 16.53 T-OH	6.97 CCH						
OFF DIAGONAL-	-3.41	BB33 -2.89 BB34	-2.80 BB42	2.34 BB41	2.05 SB22	1.96 BB43			
NORMAL MODE 50	OBSERVED=	264.8 CM-1	CALCULATED=	264.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	24.63	CC06 11.69 O*CC	9.14 TH-2	7.67 CCH2	7.35 C1CC	5.06 CCO7			
FORCE CONSTANTS-	54.74	CCO 17.45 T-OH	15.01 CCH	10.96 CCC					
OFF DIAGONAL-	5.82	BB43 -5.47 BB34	-4.36 BB33	-2.94 SB25	2.44 SB22	-1.51 SB26			
NORMAL MODE 51	OBSERVED=	250.4 CM-1	CALCULATED=	250.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	14.46	CC09 13.61 TH-3	13.11 C3CC	12.51 O9CC	11.41 TH-5	7.15 TH-1			
FORCE CONSTANTS-	37.91	CCO 32.23 T-OH	16.12 CCC	10.54 CCH					
OFF DIAGONAL-	4.19	SB22 -3.93 BB33	-3.42 SB25	3.10 BB43	-2.53 SB21	-2.17 SB26			
NORMAL MODE 52	OBSERVED=	236.2 CM-1	CALCULATED=	236.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	77.68	TH-3 11.68 TH-3	9.92 CCH	8.18 TH-2	7.61 C4CC	5.30 TH-4			
FORCE CONSTANTS-	77.68	T-OH 8.77 CCO	7.89 CCC						
OFF DIAGONAL-	NONE								
NORMAL MODE 53	OBSERVED=	226.3 CM-1	CALCULATED=	226.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	95.84	TH-4 20.53 TH-4	20.51 TH-3						
FORCE CONSTANTS-	92.89	T-OH							
OFF DIAGONAL-	NONE								
NORMAL MODE 54	OBSERVED=	216.0 CM-1	CALCULATED=	216.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	37.74	TH-1 16.59 TH-2	12.84 TH-5						
FORCE CONSTANTS-	70.88	T-OH 20.58 CCO	5.55 CCH						
OFF DIAGONAL-	-2.10	BB34							
NORMAL MODE 55	OBSERVED=	212.4 CM-1	CALCULATED=	212.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	54.63	TH-2 8.68 TH-3	6.20 TH-4	5.75 TH-5					
FORCE CONSTANTS-	75.79	T-OH 18.06 CCO							
OFF DIAGONAL-	NONE								
NORMAL MODE 56	OBSERVED=	209.0 CM-1	CALCULATED=	209.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	50.46	TH-4 21.05 TH-3	7.91 CCO9						
FORCE CONSTANTS-	73.46	T-OH 19.43 CCO							
OFF DIAGONAL-	NONE								
NORMAL MODE 57	OBSERVED=	202.1 CM-1	CALCULATED=	202.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	77.77	C4CC 18.77 CCO*	14.04 TH-3	8.01 TH-4	7.35 CCO*				
FORCE CONSTANTS-	33.48	CCO 29.37 CCC	23.29 T-OH	8.64 T-CC					
OFF DIAGONAL-	-4.62	BB34 -3.45 BB42	-2.66 SB25						
NORMAL MODE 58	OBSERVED=	145.6 CM-1	CALCULATED=	145.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	29.10	CO*	11.63 TCC5	11.21 CCO*	7.29 TCC4	6.20 OCO	5.71 TCO1		
FORCE CONSTANTS-	29.10	CCO 21.38 CCO	19.69 T-CC	8.70 T-CC	6.20 OCO	5.86 CCH			
OFF DIAGONAL-	-4.19	BB34 3.10 BB43	-3.05 BB37	1.84 BB41	-1.61 SB25				
NORMAL MODE 59	OBSERVED=	96.2 CM-1	CALCULATED=	96.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	21.49	C2CC 15.73 TCC5	12.32 TCC1	12.17 TCC2	8.27 C1CC	6.63 OC8C	5.06 C3CC		
FORCE CONSTANTS-	45.86	T-CC 36.15 CCC	16.04 CCO						
OFF DIAGONAL-	-3.94	SB25 -3.78 SB21	-2.69 BB42	2.21 BB41	-1.91 BB34				
NORMAL MODE 60	OBSERVED=	87.2 CM-1	CALCULATED=	87.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	27.13	TCC5 10.31 TCC4	8.43 TCC2	7.34 O*CC	6.01 C3CC	5.13 TCC3			
FORCE CONSTANTS-	51.14	T-CC 19.18 CCO	14.05 CCC						
OFF DIAGONAL-	3.50	SB21 -1.60 BB34							
NORMAL MODE 61	OBSERVED=	65.5 CM-1	CALCULATED=	65.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	46.65	TCC5 8.48 CO*	16.83 CCO	7.48 CCO	6.98 TCC4	6.44 TCO2	5.47 C4CC		
FORCE CONSTANTS-	46.65	T-CC 18.60 CCC	16.83 CCO	7.48 CCO	6.98 TCC4	6.44 TCO2	5.47 C4CC		
OFF DIAGONAL-	-2.66	BB42							

29. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 8.97

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400									
MOLECULE 29 -6 NG=1236 BETA GALACTOSE GT									
PAGE 1									
NORMAL MODE 8	OBSERVED=	1466.0 CM-1	CALCULATED=	1449.7 CM-1	ERROR=	16.3 CM-1	OR	1.1 PERCENT	
INTERNAL COORDINATES-	62.19 HCH	19.88 CCHB	18.68 OCHA						
FORCE CONSTANTS-	56.13 OCH	23.91 BCOH	13.20 CCH	7.93 CO	2.65 CCO				
OFF DIAGONAL-	-3.80 SB27								
NORMAL MODE 9	OBSERVED=	1420.0 CM-1	CALCULATED=	1421.6 CM-1	ERROR=	-1.6 CM-1	OR	-0.1 PERCENT	
INTERNAL COORDINATES-	32.67 CCH	17.74 OC1H	14.31 C1OH	9.04 C2OH	8.02 C1H	5.15 OC2H			
FORCE CONSTANTS-	56.13 OCH	23.91 BCOH	13.20 CCH	7.93 CO	2.65 CCO				
OFF DIAGONAL-	-9.61 SB27	2.76 BB29	-2.61 SB25	-2.54 BB45	2.30 BB34	-2.11 BB43	-2.02 BB39		
NORMAL MODE 10	OBSERVED=	0.0 CM-1	CALCULATED=	1414.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	37.77 C4OH	13.82 OC4H	8.84 C3OH	6.31 HC4C	5.47 OC3H	5.34 HC3C			
FORCE CONSTANTS-	47.44 BCOH	28.01 OCH	18.02 CCH	6.31 CO	2.14 BB36	-1.74 BB45	-1.56 SB25		
OFF DIAGONAL-	5.88 SB28	-5.62 SB27	-2.57 BB39						
NORMAL MODE 11	OBSERVED=	1405.0 CM-1	CALCULATED=	1407.3 CM-1	ERROR=	-2.3 CM-1	OR	-0.2 PERCENT	
INTERNAL COORDINATES-	28.59 CCH	19.78 C1OH	14.26 C2OH	13.41 OC1H	6.63 OC2H				
FORCE CONSTANTS-	50.56 OCH	36.45 BCOH	6.13 CCH						
OFF DIAGONAL-	2.35 SB28	-2.17 SB26	-2.11 BB45						
NORMAL MODE 12	OBSERVED=	0.0 CM-1	CALCULATED=	1396.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	64.23 CCH	6.94 OCHA	6.20 C3OH	5.55 CCHB					
FORCE CONSTANTS-	71.94 BCOH	13.53 CCH	10.57 OCH						
OFF DIAGONAL-	-4.56 SB26	3.27 SB28	-2.24 BB39	-1.66 SB27					
NORMAL MODE 13	OBSERVED=	0.0 CM-1	CALCULATED=	1391.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	52.02 C3OH	10.40 OC3H	9.19 C4OH	8.14 C1OH					
FORCE CONSTANTS-	72.19 CCH	18.75 OCH	6.78 CCH						
OFF DIAGONAL-	-4.01 SB28	-2.90 SB27	-2.89 BB39	-1.84 SB26					
NORMAL MODE 14	OBSERVED=	0.0 CM-1	CALCULATED=	1389.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	49.39 C1OH	32.99 C2OH	10.22 HC3C						
FORCE CONSTANTS-	79.65 BCOH	32.18 CCH	6.65 OCH	5.27 CC					
OFF DIAGONAL-	3.58 SB28	-2.48 SB26	-1.69 BB39						
NORMAL MODE 15	OBSERVED=	1380.0 CM-1	CALCULATED=	1361.0 CM-1	ERROR=	18.9 CM-1	OR	1.4 PERCENT	
INTERNAL COORDINATES-	28.66 C2OH	11.54 OC2H	11.55 CC3H	10.34 C3OH	9.03 HC2C				
FORCE CONSTANTS-	37.06 BCOH	31.30 CCH	23.02 OCH						
OFF DIAGONAL-	6.79 BB29	-3.82 SB27	-2.90 SB28	2.55 BB34	-2.12 BB45	1.99 BB39	-1.94 BB36		
NORMAL MODE 16	OBSERVED=	0.0 CM-1	CALCULATED=	1356.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	15.81 C5H	15.13 C4OH	11.39 HC5C	11.09 CCHB	6.73 CCHB	6.04 C5O	5.31 CCHA		
FORCE CONSTANTS-	38.71 CCH	32.65 OCH	21.13 BCOH	6.99 CO					
OFF DIAGONAL-	6.58 BB29	-5.70 SB27	-2.86 BB45	-1.95 SB25					
NORMAL MODE 17	OBSERVED=	1341.0 CM-1	CALCULATED=	1331.0 CM-1	ERROR=	10.0 CM-1	OR	0.8 PERCENT	
INTERNAL COORDINATES-	17.05 C4OH	13.90 CC5H	13.82 CCHB	10.90 OCMB	8.00 C1OH	6.81 HC5C	5.21 OC4H		
FORCE CONSTANTS-	47.86 CCH	26.34 BCOH	21.35 OCH	6.18 CO					
OFF DIAGONAL-	-4.57 SB27	4.57 BB29	-3.58 SB28	-3.10 SB26	-2.88 BB45	1.93 BB39			
NORMAL MODE 18	OBSERVED=	1320.0 CM-1	CALCULATED=	1310.7 CM-1	ERROR=	9.3 CM-1	OR	0.7 PERCENT	
INTERNAL COORDINATES-	14.63 C4OH	11.53 HC3C	11.41 CCH2	6.63 CC3H	5.44 OC4H	5.19 CCHA	5.11 CC1H		
FORCE CONSTANTS-	69.19 CCH	11.71 OCH	7.71 BCOH	5.39 CC					
OFF DIAGONAL-	-6.45 SB26	6.34 BB29	-3.58 BB45	1.58 BB34					
NORMAL MODE 19	OBSERVED=	1306.0 CM-1	CALCULATED=	1305.2 CM-1	ERROR=	0.8 CM-1	OR	0.1 PERCENT	
INTERNAL COORDINATES-	19.39 C2OH	14.77 CCH2	8.33 CC1H	5.65 OC1H	5.09 CCHA				
FORCE CONSTANTS-	50.20 CCH	31.90 OCH	11.18 BCOH						
OFF DIAGONAL-	6.18 BB29	-3.44 BB45	-1.79 SB26	-1.52 SB28					
NORMAL MODE 20	OBSERVED=	0.0 CM-1	CALCULATED=	1284.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	24.20 OC4H	12.75 C5H	7.57 OC2H	7.14 CC5H	6.95 HC2C	5.61 CC4H			
FORCE CONSTANTS-	51.05 OCH	27.88 CCH	7.86 CO						
OFF DIAGONAL-	7.72 SB27	-3.16 BB45							
NORMAL MODE 21	OBSERVED=	0.0 CM-1	CALCULATED=	1276.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	21.27 C5H	17.13 CCHA	12.26 OC3H	11.90 OCHA	10.72 CC3H				
FORCE CONSTANTS-	51.21 OCH	35.64 CCH	5.39 CO						
OFF DIAGONAL-	-3.42 BB45	3.08 SB27							
NORMAL MODE 22	OBSERVED=	1273.0 CM-1	CALCULATED=	1269.6 CM-1	ERROR=	3.4 CM-1	OR	0.3 PERCENT	
INTERNAL COORDINATES-	18.85 HC4C	10.29 CCHA	8.04 CC4H	7.61 OC2H	7.38 CCHA	7.34 HC5C	6.41 C5H		
FORCE CONSTANTS-	57.82 CCH	13.13 OCH	3.43 BB34	2.50 SB27					
OFF DIAGONAL-	-3.95 BB29	28.66 BB45							
NORMAL MODE 23	OBSERVED=	1246.0 CM-1	CALCULATED=	1256.6 CM-1	ERROR=	-10.6 CM-1	OR	-0.8 PERCENT	
INTERNAL COORDINATES-	43.34 C5H	9.60 CCH	9.76 OC1H	7.76 CCH	7.56 CC2H	6.99 CC3H	5.35 CC4H		
FORCE CONSTANTS-	35.95 CCH	29.11 OCH	26.42 CO	7.05 CCO					
OFF DIAGONAL-	6.99 SB27	-5.39 SB25	-2.67 BB45	2.18 BB34	-1.86 SB28	-1.85 BB29	-1.62 SB26	1.53 BB43	
NORMAL MODE 24	OBSERVED=	1218.0 CM-1	CALCULATED=	1229.3 CM-1	ERROR=	-11.3 CM-1	OR	-0.9 PERCENT	
INTERNAL COORDINATES-	16.06 HC5C	11.89 CC5H	11.76 OCMB	10.31 OC1H	6.50 C4C5	5.81 OC3H	5.73 C-06	5.13 CC4H	5.05 OCHA
FORCE CONSTANTS-	53.09 CCH	24.78 OCH	18.44 CO	9.45 CC	9.25 CCO	5.91 BCOH			
OFF DIAGONAL-	-8.83 SB26	-4.59 BB29	4.33 BB34	-3.29 BB45	-2.79 SB25	-2.53 BB43	-2.31 SB22	2.01 BB33	
NORMAL MODE 25	OBSERVED=	0.0 CM-1	CALCULATED=	1211.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	15.68 C-06	13.88 C4C5	12.87 OC1H	8.61 CC3H	8.39 HC3C	8.03 C3C4	7.90 CC4H	7.42 HC4C	
FORCE CONSTANTS-	42.70 CCH	37.36 CO	24.29 CC	14.51 CCO	8.02 BCOH	7.88 OCH			
OFF DIAGONAL-	-13.73 SB26	-6.13 SB25	-4.16 SB22	-4.13 SB28	3.50 BB34	-2.83 BB29	2.74 BB33	-2.33 BB43	-2.21 BB45
NORMAL MODE 26	OBSERVED=	1166.0 CM-1	CALCULATED=	1170.6 CM-1	ERROR=	-4.6 CM-1	OR	-0.4 PERCENT	
INTERNAL COORDINATES-	18.64 CC1H	14.62 OC1H	11.04 OC1H	8.98 OC2H	8.48 C-06	7.80 C-08	7.00 CCH2		
FORCE CONSTANTS-	32.78 CCH	32.70 CO	27.44 CCH	2.75 CCH					
OFF DIAGONAL-	-6.05 BB29	-5.34 SB25	-3.23 SB28	2.40 BB34	-2.23 BB45	-1.79 SB22			
NORMAL MODE 27	OBSERVED=	1138.0 CM-1	CALCULATED=	1150.5 CM-1	ERROR=	-12.5 CM-1	OR	-1.1 PERCENT	
INTERNAL COORDINATES-	37.79 C4H	17.44 OC4H	17.73 CCO	12.31 OCHA	10.33 CCO	8.99 C5O	5.34 OC9C		
FORCE CONSTANTS-	39.78 CC	30.77 OCH	17.13 CCO	12.13 CO	7.50 CCH				
OFF DIAGONAL-	-9.45 SB22	-3.39 SB25	-2.77 SB23						
NORMAL MODE 28	OBSERVED=	1111.0 CM-1	CALCULATED=	1119.5 CM-1	ERROR=	-8.5 CM-1	OR	-0.8 PERCENT	
INTERNAL COORDINATES-	23.14 C-08	18.88 C5C	17.78 C5O	13.08 C3OH	5.91 CCO	5.81 C-08	5.73 C-09		
FORCE CONSTANTS-	58.92 CO	25.13 CC	10.94 CCO	9.44 BCOH	9.24 OCH	8.88 CCC	8.61 CCH		
OFF DIAGONAL-	-7.93 SB25	-6.77 SB28	-6.17 SS18	-3.48 SB27	-3.39 SB26				
NORMAL MODE 29	OBSERVED=	1096.0 CM-1	CALCULATED=	1101.7 CM-1	ERROR=	-5.7 CM-1	OR	-0.5 PERCENT	
INTERNAL COORDINATES-	19.26 C-07	17.68 C1C2	8.02 C2C3	7.75 C3C4	6.31 CCH2	5.20 OC1H			
FORCE CONSTANTS-	39.50 CC	33.67 CO	15.72 CCH	10.28 CCO	9.65 OCH				
OFF DIAGONAL-	-5.88 SB22	4.35 SB27	-4.30 SB25	-3.29 SS18	-2.99 BB29	1.63 BB34	-1.60 SB24		
NORMAL MODE 30	OBSERVED=	1086.0 CM-1	CALCULATED=	1094.3 CM-1	ERROR=	-8.3 CM-1	OR	-0.8 PERCENT	
INTERNAL COORDINATES-	25.41 C3C4	17.49 C-U*	15.73 C2C3	14.97 C-09	13.64 C-07	7.12 C5O	6.67 C4CC	5.16 C2OH	
FORCE CONSTANTS-	54.56 CO	42.26 CC	14.44 OCH	13.87 CCO	12.15 CCC	9.73 BCOH			
OFF DIAGONAL-	-9.44 SB21	-7.95 SB25	-7.38 SB27	-7.14 SB28	-5.20 SS18	-4.40 SB22	-3.81 SB26	-1.84 BB43	-1.73 BB34
NORMAL MODE 31	OBSERVED=	1068.0 CM-1	CALCULATED=	1065.2 CM-1	ERROR=	2.8 CM-1	OR	0.3 PERCENT	
INTERNAL COORDINATES-	41.92 C-07	13.99 C2C3	11.51 C-09	8.68 C2OH	6.76 C-08				
FORCE CONSTANTS-	69.78 CO	33.72 CC	13.00 CCO	12.86 BCOH	10.56 CCH	10.44 OCH	9.60 CCC		
OFF DIAGONAL-	-10.88 SB27	-10.74 SB28	-8.64 SB21	-6.77 SB25	-5.89 SS18	-1.81 SB22			
NORMAL MODE 32	OBSERVED=	1056.0 CM-1	CALCULATED=	1054.6 CM-1	ERROR=	1.4 CM-1	OR	0.1 PERCENT	
INTERNAL COORDINATES-	43.34 C-08	30.44 C-08	10.42 CCH	8.36 OCH	6.09 BCOH				
FORCE CONSTANTS-	90.20 CO	17.40 CC	-7.21 SS18	-3.84 SB25	-2.28 SB26	-2.27 SB21	-1.76 BB29		
OFF DIAGONAL-	-12.03 SB27	-8.86 SB28							
NORMAL MODE 33	OBSERVED=	1035.0 CM-1	CALCULATED=	1039.9 CM-1	ERROR=	-4.9 CM-1	OR	-0.5 PERCENT	
INTERNAL COORDINATES-	50.81 C1C2	13.18 C-0*	6.27 C-09	6.18 CC1H	5.77 CC3H	5.76 C1OH	5.68 C-06	5.53 OC1H	5.06 OC1H
FORCE CONSTANTS-	57.34 CC	35.08 CO	20.95 CCH	12.85 OCH	12.65 CCO	8.24 BCOH			
OFF DIAGONAL-	-12.39 SB22	-8.38 SB27	-6.75 SS18	-5.44 SB26	-4.77 SB28	-4.76 SB21	-3.61 SB24	-2.47 BB29	-2.25 BB34
NORMAL MODE 34	OBSERVED=	0.0 CM-1	CALCULATED=	987.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	27.57 C5C	19.03 C3C4	15.47 C-08	14.74 C1C2	12.13 C-0*	5.04 C-09			
FORCE CONSTANTS-	56.96 CC	42.31 CO	14.73 CCH	12.99 CCH					
OFF DIAGONAL-	-13.68 SB22	-7.51 SB26	-3.61 SB21	-3.54 SB25	-3.52 SB27	-2.95 SB28	-2.91 BB34	1.57 SS18	
NORMAL MODE 35	OBSERVED=	0.0 CM-1	CALCULATED=	967.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	31.35 C2C	23.37 C4C5	12.49 C-06	6.11 OC1H					
FORCE CONSTANTS-	39.48 CC	22.44 CO	12.12 CCH	10.56 CCH	5.30 OCH				
OFF DIAGONAL-	6.33 SB26	-6.31 SB21	-5.99 SB22	-4.93 SB24	1.90 SS18	-1.54 SB23			

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400									
MOLECULE 29		-6 NG=1236		BETA GALACTOSE		GT		PAGE 2	
NORMAL MODE 36	OBSERVED=	949.0 CM-1		CALCULATED=	948.7 CM-1	ERROR=	0.3 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	19.48	C-06	19.18	C5C	8.93 O'C1	7.29 C1C2	6.37	C-08	
FORCE CONSTANTS-	37.17	CO	24.20	CC	11.62 CCH	19.31 OCH	11.79	CCO	8.98 CCC
OFF DIAGONAL-	-9.33	SB21	-6.37	SB22	-5.15 SB24	3.92 SB27	2.98	BB43	2.88 SB26 2.14 SS18 -1.87 SB25 -1.57 SB28
NORMAL MODE 37	OBSERVED=	906.0 CM-1		CALCULATED=	879.8 CM-1	ERROR=	26.2 CM-1	OR	2.9 PERCENT
INTERNAL COORDINATES-	24.26	C-03	11.19	C3C4	7.02 O'CC	6.24 HC3C		C2C3	5.58 CCHB
FORCE CONSTANTS-	34.92	CO	27.53	CCH	21.75 CC	13.15 CCO	6.14		5.32 CCHA
OFF DIAGONAL-	6.54	SB26	-6.00	SB21	-5.39 SB22	3.63 SS18	-2.48	BB29	-2.21 SB25 2.08 BB43 -1.80 SB27
NORMAL MODE 38	OBSERVED=	889.0 CM-1		CALCULATED=	871.8 CM-1	ERROR=	17.2 CM-1	OR	1.9 PERCENT
INTERNAL COORDINATES-	25.65	C5C	8.84	CCHA	8.71 OCO	8.24 C5C	6.90	CCHB	6.16 C4C5
FORCE CONSTANTS-	31.75	CO	20.30	CCH	16.04 CC	8.71 OCO	7.82	OGH	7.80 CCO
OFF DIAGONAL-	-4.23	SB23	4.09	SS18	-3.85 SB27	-3.80 SB21	3.55	SB26	-2.73 SB22 2.57 BB43
NORMAL MODE 39	OBSERVED=	784.0 CM-1		CALCULATED=	792.7 CM-1	ERROR=	-8.7 CM-1	OR	-1.1 PERCENT
INTERNAL COORDINATES-	17.61	4CO*	11.95	C9CC	9.92 C-09	6.27 CCO*			
FORCE CONSTANTS-	39.79	CCO	21.01	CCO	9.31 CCH	6.34 CCC	5.79	OGH	
OFF DIAGONAL-	7.54	SB25	4.70	BB43	-4.68 SB27	2.42 BB33	-2.27	BB41	2.09 BB34
NORMAL MODE 40	OBSERVED=	703.0 CM-1		CALCULATED=	604.8 CM-1	ERROR=	-1.7 CM-1	OR	-0.3 PERCENT
INTERNAL COORDINATES-	15.51	CCO*	10.25	CLHB	7.43 OCO	6.33 CCO7	5.91	O*CC	5.52 HC5C
FORCE CONSTANTS-	44.36	CCO	14.61	CC	12.11 CCH	10.98 CCC	9.04	CO	5.34 CO*CC
OFF DIAGONAL-	4.48	BB43	3.66	SB25	-2.12 BB41	-2.11 BB34	2.04	SS18	
NORMAL MODE 41	OBSERVED=	623.0 CM-1		CALCULATED=	704.7 CM-1	ERROR=	18.2 CM-1	OR	2.9 PERCENT
INTERNAL COORDINATES-	21.79	CCO	13.07	CCH	10.58 C2C3	5.83 C4C5			
FORCE CONSTANTS-	37.68	CCO	23.41	CCH	11.62 CCH	10.98 CCC	6.28	CCO	6.69 CC
OFF DIAGONAL-	-6.54	BB34	5.14	BB43	4.44 SB22	-4.41 BB29	3.50	SB27	2.86 SB24 2.75 SB25 -2.42 SB23 -2.25 BB33
NORMAL MODE 42	OBSERVED=	560.0 CM-1		CALCULATED=	560.1 CM-1	ERROR=	-0.1 CM-1	OR	-0.0 PERCENT
INTERNAL COORDINATES-	24.48	CCO	20.15	CCO6	10.95 CH2	9.86 HC2C	8.19	CC1H	7.44 O'CC
FORCE CONSTANTS-	71.12	CCO	38.57	CCH	5.72 CC				5.71 O*CC 5.05 CC3H
OFF DIAGONAL-	-22.21	BB34	9.85	BB43	-8.50 BB29	-2.37 SB22			
NORMAL MODE 43	OBSERVED=	536.0 CM-1		CALCULATED=	513.2 CM-1	ERROR=	22.8 CM-1	OR	4.3 PERCENT
INTERNAL COORDINATES-	12.55	OGC	11.48	C-06	7.97 CO*CC	7.59 C5O*	7.50	O*CC	5.88 O9CC
FORCE CONSTANTS-	26.54	CCO	20.85	CCO	12.55 OCO	10.22 CC	7.97	CCO	7.15 CCC
OFF DIAGONAL-	8.45	SB24	4.42	SB21	4.13 SB22	-2.97 SB27	-2.97	SB22	2.21 SS18 1.74 BB43 -1.68 BB42 -1.56 BB34
NORMAL MODE 44	OBSERVED=	478.0 CM-1		CALCULATED=	491.5 CM-1	ERROR=	-13.5 CM-1	OR	-2.8 PERCENT
INTERNAL COORDINATES-	21.65	CCO*	10.33	C3CC	9.88 O'CC	8.40 HC5C	6.40	CCHB	
FORCE CONSTANTS-	53.57	CCO	17.38	CCH	12.91 CCC	5.71 CC			
OFF DIAGONAL-	-7.64	BB34	4.92	BB43	3.92 SB25	-3.64 BB29	1.76	SB22	-1.65 BB41
NORMAL MODE 45	OBSERVED=	435.0 CM-1		CALCULATED=	423.9 CM-1	ERROR=	11.1 CM-1	OR	2.6 PERCENT
INTERNAL COORDINATES-	12.90	C1CC	9.07	C2CC	8.00 CCO*	7.19 C4C5	5.52	OCO	
FORCE CONSTANTS-	29.17	CCO	23.41	CCH	12.91 CCC	5.71 CC			
OFF DIAGONAL-	4.81	SB22	3.70	BB43	3.25 SB25	-2.86 SB26	-1.69	BB42	5.52 CCO
NORMAL MODE 46	OBSERVED=	400.0 CM-1		CALCULATED=	387.2 CM-1	ERROR=	12.8 CM-1	OR	3.1 PERCENT
INTERNAL COORDINATES-	27.25	O'CC	9.95	O8CC	7.99 CCH2	7.76 CC1H	7.54	CCO7	6.70 CCO9
FORCE CONSTANTS-	64.75	CCO	26.16	CCH	8.92 CCH	6.09 CC			
OFF DIAGONAL-	-13.21	BB34	-5.51	BB29	4.62 BB43	-2.18 BB36	-2.04	SB26	1.95 SB22 1.70 SB21
NORMAL MODE 47	OBSERVED=	363.0 CM-1		CALCULATED=	346.1 CM-1	ERROR=	16.9 CM-1	OR	4.6 PERCENT
INTERNAL COORDINATES-	8.65	CCO*	7.98	O9CC	7.54 O'CC	6.51 CCO8	5.74	CO*CC	5.37 C1CC
FORCE CONSTANTS-	43.57	CCO	14.12	CC	11.59 CCC	8.39 CCH	5.74	CCO	
OFF DIAGONAL-	5.15	SB21	3.78	SB22	-3.77 BB34	-3.36 SB26	3.14	BB43	2.00 SB25
NORMAL MODE 48	OBSERVED=	329.0 CM-1		CALCULATED=	320.9 CM-1	ERROR=	8.1 CM-1	OR	2.5 PERCENT
INTERNAL COORDINATES-	35.94	CCO7	15.24	O7CC	12.05 CCO6	10.94 OCO	7.38	CCO8	7.16 TH-2
FORCE CONSTANTS-	78.07	CCO	12.38	T-OH	10.94 OCO				
OFF DIAGONAL-	-6.60	BB34	-5.31	BB42	-3.00 BB43	-1.95 SB24			
NORMAL MODE 49	OBSERVED=	311.0 CM-1		CALCULATED=	320.3 CM-1	ERROR=	-9.3 CM-1	OR	-3.0 PERCENT
INTERNAL COORDINATES-	20.19	O8CC	13.58	O9CC	10.70 CCO8	7.22 CCO6	6.45	4CO*	5.86 TH-3
FORCE CONSTANTS-	65.50	CCO	13.36	CC	9.88 T-OH				
OFF DIAGONAL-	4.38	SB21	-3.56	BB42	3.04 SB22	-2.54 BB34			
NORMAL MODE 50	OBSERVED=	292.0 CM-1		CALCULATED=	293.0 CM-1	ERROR=	-1.0 CM-1	OR	-0.3 PERCENT
INTERNAL COORDINATES-	15.93	O9CC	10.46	CCO6	8.25 CCO	7.98 CCO8	6.19	TH-4	5.15 C1CC
FORCE CONSTANTS-	51.27	CCO	14.77	CCH	11.25 T-OH	7.21 CCC	6.33	CC	
OFF DIAGONAL-	6.96	SB22	5.96	BB43	-5.83 BB34	-3.30 BB33	-2.45	SB21	-2.18 BB29 -1.91 SB26
NORMAL MODE 51	OBSERVED=	256.0 CM-1		CALCULATED=	262.7 CM-1	ERROR=	-6.7 CM-1	OR	-2.6 PERCENT
INTERNAL COORDINATES-	26.39	CCO9	11.28	C3CC	8.47 TH-4	5.71 O7CC	5.46	O8CC	5.36 C4CC
FORCE CONSTANTS-	51.13	CCO	21.97	CCC	12.44 CCH	12.07 T-OH	5.01	T-CC	5.24 CCO*
OFF DIAGONAL-	3.87	BB43	-3.85	BB33	-2.94 SB25	-2.45 BB34	-2.38	SB21	-1.97 BB36
NORMAL MODE 52	OBSERVED=	240.0 CM-1		CALCULATED=	230.7 CM-1	ERROR=	9.3 CM-1	OR	3.9 PERCENT
INTERNAL COORDINATES-	35.43	TH-1	26.34	TH-2	16.88 TH-3	5.33 TH-5			
FORCE CONSTANTS-	87.90	T-OH	6.86	CCO					
OFF DIAGONAL-	NONE								
NORMAL MODE 53	OBSERVED=	200.0 CM-1		CALCULATED=	226.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	82.62	TH-1	6.35	CCO					
FORCE CONSTANTS-	84.54	T-OH							
OFF DIAGONAL-	NONE								
NORMAL MODE 54	OBSERVED=	200.0 CM-1		CALCULATED=	216.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	42.45	TH-1	21.59	TH-3	18.88 TH-4				
FORCE CONSTANTS-	87.46	T-OH	7.53	CCO					
OFF DIAGONAL-	NONE								
NORMAL MODE 55	OBSERVED=	200.0 CM-1		CALCULATED=	214.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	59.17	TH-2	11.86	TH-3	6.44 TH-4	5.77 CCO7			
FORCE CONSTANTS-	81.15	T-OH	16.68	CCO					
OFF DIAGONAL-	-1.53	BB34							
NORMAL MODE 56	OBSERVED=	200.0 CM-1		CALCULATED=	212.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	46.07	TH-4	34.00	TH-3	7.42 O8CC	6.06 CCO9			
FORCE CONSTANTS-	80.46	T-OH	17.49	CCO					
OFF DIAGONAL-	NONE								
NORMAL MODE 57	OBSERVED=	200.0 CM-1		CALCULATED=	195.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	26.89	CCO	15.68	CO*CC	8.03 C4CC	7.39 TH-1	5.53	OCO	
FORCE CONSTANTS-	49.56	CCO	19.80	T-OH	15.68 CCH	9.57 CCH	6.08	CCH	5.53 OCO
OFF DIAGONAL-	-2.97	BB34	-2.43	BB42	-2.28 BB33	-1.95 SB23			5.18 T-CC
NORMAL MODE 58	OBSERVED=	200.0 CM-1		CALCULATED=	141.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	34.37	CCC	23.88	CCO	10.85 COC	7.38 T-CCO	6.51	T-CC	5.69 CCH
FORCE CONSTANTS-	44.88	SB21	3.14	SB22	2.89 BB43	-2.54 SB25	-1.96	BB42	1.68 BB41
OFF DIAGONAL-									
NORMAL MODE 59	OBSERVED=	200.0 CM-1		CALCULATED=	107.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	44.81	TCC5	9.55	C2CC	8.63 TCC2	5.06 C3CC			
FORCE CONSTANTS-	61.76	T-CC	16.73	CCC	12.03 CCO	5.23 CCH			
OFF DIAGONAL-	-1.64	SB25							
NORMAL MODE 60	OBSERVED=	200.0 CM-1		CALCULATED=	86.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	18.23	C2CC	14.56	TCC5	13.31 TCC1	13.07 C1CC	9.09	TCC4	
FORCE CONSTANTS-	41.62	T-CC	34.14	CCC	17.30 CCO				
OFF DIAGONAL-	-3.55	SB25	-3.37	BB42	1.80 BB41	-1.68 BB34	-1.56	SB21	
NORMAL MODE 61	OBSERVED=	200.0 CM-1		CALCULATED=	67.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	29.05	TCC5	10.73	TCC4	8.35 C3CC	7.13 TCC2	6.84	TCC3	6.28 4CO*
FORCE CONSTANTS-	59.91	T-CC	19.95	CCO	16.58 CCC				5.15 O*CC
OFF DIAGONAL-	-1.88	BB42	-1.58	BB34					

35. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 9.05

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400 GG									
MOLECULE 30 -6 NG=1236 BETA GALACTOSE									
PAGE 1									
NORMAL MODE 8	OBSERVED=	1466.0 CM-1	CALCULATED=	1450.1 CM-1	ERROR=	15.9 CM-1	OR	1.1 PERCENT	
INTERNAL COORDINATES-	61.38 HCH 20.29 OCHB		19.63 OCHA						
FORCE CONSTANTS-	41.38 HCH 40.05 OCH								
OFF DIAGONAL-	-4.13 SB27								
NORMAL MODE 9	OBSERVED=	1420.0 CM-1	CALCULATED=	1421.7 CM-1	ERROR=	-1.7 CM-1	OR	-0.1 PERCENT	
INTERNAL COORDINATES-	32.99 C1H 17.91 OC1H		14.18 C1OH 8.94 C2OH		8.04 CC1H 5.10 OC2H				
FORCE CONSTANTS-	56.59 OCH 23.61 BC0H		13.27 CCH 7.82 CO		5.62 CCO				
OFF DIAGONAL-	-9.58 SB27 3.72 SB28		-2.76 SB27 -2.59 SB25		-2.56 BB45 2.30 BB34		-2.11 BB43 -2.02 BB39		
NORMAL MODE 10	OBSERVED=	0.0 CM-1	CALCULATED=	1414.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	37.57 C4OH 13.84 OC4H		9.09 C3OH 6.72 HC4C		5.46 UC3H 5.38 HC3C				
FORCE CONSTANTS-	47.71 HC0H 26.30 OCH		17.86 CCH 6.37 CO		-1.76 BB45 -1.56 SB25				
OFF DIAGONAL-	5.89 SB28 -5.61 SB27		-2.60 BB39 2.14 BB36						
NORMAL MODE 11	OBSERVED=	1405.0 CM-1	CALCULATED=	1407.3 CM-1	ERROR=	-2.3 CM-1	OR	-0.2 PERCENT	
INTERNAL COORDINATES-	27.68 C1H 19.45 C1OH		14.36 C2OH 13.09 OC1H		6.88 OC2H				
FORCE CONSTANTS-	49.93 OCH 36.63 CCH		6.44 CCH						
OFF DIAGONAL-	-2.46 SB28 -2.21 SB26		-2.11 BB45						
NORMAL MODE 12	OBSERVED=	0.0 CM-1	CALCULATED=	1393.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	53.23 C1OH 25.16 C3OH		6.92 OCHA						
FORCE CONSTANTS-	70.59 BC0H 13.88 OCH		11.97 CCH						
OFF DIAGONAL-	3.74 SB28 -2.47 SB27		-2.34 BB39						
NORMAL MODE 13	OBSERVED=	0.0 CM-1	CALCULATED=	1391.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	40.62 C3OH 20.77 C1OH		10.74 C4OH 8.81 OC3H						
FORCE CONSTANTS-	73.96 BC0H 17.16 OCH		6.63 CCH						
OFF DIAGONAL-	4.11 SB28 -2.65 BB39		-2.51 SB27 -2.25 SB26						
NORMAL MODE 14	OBSERVED=	0.0 CM-1	CALCULATED=	1389.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	43.67 C1OH 35.47 C2OH								
FORCE CONSTANTS-	80.64 HC0H 7.66 CCH		5.92 OCH 5.28 CC						
OFF DIAGONAL-	3.48 SB28 -2.22 SB26		-1.67 BB39						
NORMAL MODE 15	OBSERVED=	1380.0 CM-1	CALCULATED=	1361.0 CM-1	ERROR=	19.0 CM-1	OR	1.4 PERCENT	
INTERNAL COORDINATES-	24.62 C2OH 12.59 CC3H		12.44 OC2H 10.84 C3OH		9.64 HC2C				
FORCE CONSTANTS-	38.76 BC0H 30.76 CCH		13.22 OCH						
OFF DIAGONAL-	6.51 BB29 -3.68 SB27		-3.22 SB28 2.74 BB34		2.24 BB39 -2.17 BB36		-2.02 BB45		
NORMAL MODE 16	OBSERVED=	0.0 CM-1	CALCULATED=	1352.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	18.93 C1SH 16.36 CCHB		16.09 C4OH 8.52 OC4H		8.99 HC9C 7.51 C1OH		6.88 C5O1 5.49 HC4C		
FORCE CONSTANTS-	16.96 CCH 2.92 OCH		25.66 CCH 9.60 CO						
OFF DIAGONAL-	-6.23 SB27 -2.74 BB45		-2.29 SB28 -2.05 SB25		1.62 BB33				
NORMAL MODE 17	OBSERVED=	1341.0 CM-1	CALCULATED=	1338.1 CM-1	ERROR=	2.9 CM-1	OR	0.2 PERCENT	
INTERNAL COORDINATES-	22.57 CCH4 17.67 CC5H		13.86 C4OH 8.15 OCHA		7.04 C4C3 6.84 HC5C		6.38 C1OH		
FORCE CONSTANTS-	53.59 CCH 20.96 BC0H		16.13 OCH 7.49 CC		5.30 CO				
OFF DIAGONAL-	-4.22 SB27 -3.01 SB28		-2.88 BB45 2.69 BB34		-2.46 SB26 -1.75 SB22		1.61 BB30		
NORMAL MODE 18	OBSERVED=	1320.0 CM-1	CALCULATED=	1309.9 CM-1	ERROR=	10.1 CM-1	OR	0.8 PERCENT	
INTERNAL COORDINATES-	15.47 CC4H 12.46 HC3C		11.83 CCH2 7.68 OC4H		6.94 CC3H				
FORCE CONSTANTS-	61.53 CCH 19.92 OCH		7.36 BC0H 6.95 CC		5.54 CO				
OFF DIAGONAL-	5.97 BB29 -5.74 SB26		-3.61 BB45 2.21 BB34						
NORMAL MODE 19	OBSERVED=	1306.0 CM-1	CALCULATED=	1305.6 CM-1	ERROR=	0.4 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	19.59 OC3H 14.33 CCH2		11.52 HC3C 8.91 CC1H		5.31 OC1H 5.04 C3OH				
FORCE CONSTANTS-	48.78 CCH 31.03 OCH		11.57 BC0H						
OFF DIAGONAL-	6.18 BB29 -3.37 BB45		1.61 BB34 -1.58 SB28						
NORMAL MODE 20	OBSERVED=	0.0 CM-1	CALCULATED=	1286.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	33.57 C1SH 14.89 CC4H		7.79 CC5H						
FORCE CONSTANTS-	59.08 CCH 2.22 CCH		6.38 CO						
OFF DIAGONAL-	8.19 SB27 -3.26 BB45								
NORMAL MODE 21	OBSERVED=	0.0 CM-1	CALCULATED=	1283.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	53.16 OCHB 12.01 OC3H		11.87 CCHB		9.85 OC4H 7.87 OC2H		6.17 C1SH 5.94 HC2C		5.38 HC3C
FORCE CONSTANTS-	53.81 OCH 30.63 CCH		5.52 CO						
OFF DIAGONAL-	-3.32 BB45 2.18 SB27		-2.02 SB26						
NORMAL MODE 22	OBSERVED=	1273.0 CM-1	CALCULATED=	1267.4 CM-1	ERROR=	5.6 CM-1	OR	0.4 PERCENT	
INTERNAL COORDINATES-	20.65 HC4C 12.54 OC2H		7.35 CC4H 6.76 CC3H		5.63 OC4H				
FORCE CONSTANTS-	45.67 CCH 36.82 OCH		6.98 CC 6.93 CO						
OFF DIAGONAL-	-3.82 SB26 3.77 SB27		-3.44 BB45 2.69 BB34		-2.38 BB29 -1.71 SB25				
NORMAL MODE 23	OBSERVED=	1246.0 CM-1	CALCULATED=	1256.3 CM-1	ERROR=	-10.3 CM-1	OR	-0.8 PERCENT	
INTERNAL COORDINATES-	11.78 CC4H 11.34 O1C1		9.75 OC4H 8.94 C-06		7.81 CCH2				
FORCE CONSTANTS-	42.15 CCH 28.16 CO		20.52 OCH 7.10 CCO						
OFF DIAGONAL-	4.96 SB27 -4.75 SB25		-2.69 BB45 1.99 BB34		-1.94 SB28 -1.71 SB26				
NORMAL MODE 24	OBSERVED=	1218.0 CM-1	CALCULATED=	1220.8 CM-1	ERROR=	-2.8 CM-1	OR	-0.2 PERCENT	
INTERNAL COORDINATES-	14.67 HC5C 13.02 O1C1		15.17 C-06 10.71 CC5H		7.33 OC3H 7.25 HC2C		6.13 CCH2		
FORCE CONSTANTS-	47.01 C-09 9.89 CO		15.17 C-06 10.71 CC5H						
OFF DIAGONAL-	-6.22 SB25 -3.25 SB26		-2.66 BB45 -2.63 SB28		-2.53 BB29 2.11 BB34		1.74 SB27		
NORMAL MODE 25	OBSERVED=	0.0 CM-1	CALCULATED=	1206.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	10.14 HC5C 14.06 CC5H		9.84 C-08 8.03 HC3C		7.89 CC4H 7.45 C4C5		6.41 C5C1		6.39 CC3H
FORCE CONSTANTS-	61.61 CCH 24.01 CO		19.99 CC 12.22 OCH		9.06 CCO				
OFF DIAGONAL-	-19.66 SB26 -3.97 SB25		-3.97 SB22 3.54 BB33		-3.25 BB45 -2.20 BB43		-2.17 SB28 -2.08 BB30		1.62 BB34
NORMAL MODE 26	OBSERVED=	1166.0 CM-1	CALCULATED=	1168.8 CM-1	ERROR=	-2.8 CM-1	OR	-0.2 PERCENT	
INTERNAL COORDINATES-	17.97 CC1H 14.06 OC1H		9.81 O1C1 8.41 C-08		8.09 OC2H 7.52 C-06		6.90 CCH2		
FORCE CONSTANTS-	36.35 CCH 31.28 CO		26.31 OCH 9.88 CCO		8.26 CC				
OFF DIAGONAL-	-6.11 BB29 -5.28 SB25		-3.03 BB28 2.44 BB34		-2.38 BB45 -2.17 SB22		-1.55 SB26		
NORMAL MODE 27	OBSERVED=	1138.0 CM-1	CALCULATED=	1141.8 CM-1	ERROR=	-3.8 CM-1	OR	-0.3 PERCENT	
INTERNAL COORDINATES-	19.88 C4C5 14.68 OCHA		13.32 C5C1 13.07 C-07		9.79 CCO1 9.30 C1OH		8.76 OCHB 8.40 C5O1		5.02 O9CC
FORCE CONSTANTS-	38.45 CC 25.08 OCH		24.20 CO 16.96 CCO		9.66 BC0H 5.24 CCH				
OFF DIAGONAL-	-8.59 SB22 -4.06 SB25		-4.05 SB28 -2.64 SB23		-2.61 SB26 -1.78 SS18				
NORMAL MODE 28	OBSERVED=	1111.0 CM-1	CALCULATED=	1124.8 CM-1	ERROR=	-13.8 CM-1	OR	-1.2 PERCENT	
INTERNAL COORDINATES-	25.18 C5O1 20.91 C5C1		19.50 C-08 6.43 C3OH		6.28 C2C3 6.04 CCO1		5.45 OC4H		
FORCE CONSTANTS-	53.49 CO 27.57 CC		12.56 CO 11.16 CCH		10.97 CCH 10.28 CC		7.9 BC0H		
OFF DIAGONAL-	-8.56 SB25 -5.53 SS18		-4.46 SB28 -4.06 SB27		-4.04 SB26 -3.80 SB21		-2.29 SB22		
NORMAL MODE 29	OBSERVED=	1096.0 CM-1	CALCULATED=	1100.6 CM-1	ERROR=	-4.6 CM-1	OR	-0.4 PERCENT	
INTERNAL COORDINATES-	32.21 C-07 14.89 C1C2		8.19 C-08 5.92 C-07		5.70 C1C1 5.34 CCH2		5.06 O7CC		
FORCE CONSTANTS-	52.21 CO 23.21 CC		13.61 CCH 11.94 OCH		11.61 CCO				
OFF DIAGONAL-	-8.25 SB25 -4.84 SS18		-4.37 SB28 -3.23 SB21		2.80 SB27 -2.56 BB29				
NORMAL MODE 30	OBSERVED=	1086.0 CM-1	CALCULATED=	1092.8 CM-1	ERROR=	-6.8 CM-1	OR	-0.6 PERCENT	
INTERNAL COORDINATES-	38.21 C3C4 18.28 C-09		15.12 C2C3 9.90 C-08						
FORCE CONSTANTS-	58.15 CC 38.86 CO		14.07 OCH 10.12 CCH		10.08 CCO 9.30 BC0H		9.00 CCC		
OFF DIAGONAL-	-8.66 SB27 -7.48 SB21		-6.97 SB22 -6.70 SB26		-6.22 SS18 -5.45 SB28		-2.90 SB25 -1.76 BB43		-1.71 BB34
NORMAL MODE 31	OBSERVED=	1068.0 CM-1	CALCULATED=	1069.0 CM-1	ERROR=	-1.0 CM-1	OR	-0.1 PERCENT	
INTERNAL COORDINATES-	40.56 C-07 18.84 C2C3		12.23 C-07 8.85 C2OH		8.37 C-09 5.40 C4C5				
FORCE CONSTANTS-	70.08 CO 27.86 CC		12.21 BC0H 11.24 CCH		10.32 CCO 9.66 OCH		5.66 CCC		
OFF DIAGONAL-	-10.46 SB28 -10.15 SB27		-7.91 SS18 -7.21 SB21		-5.47 SB25				
NORMAL MODE 32	OBSERVED=	1056.0 CM-1	CALCULATED=	1043.9 CM-1	ERROR=	12.1 CM-1	OR	1.1 PERCENT	
INTERNAL COORDINATES-	42.49 C1C2 19.32 C-08		7.98 CC3H 6.72 OC1H		6.22 CC1H 6.13 C-06		5.21 C1OH 5.10 C-07		
FORCE CONSTANTS-	14.89 C-07 34.95 CO		27.36 CCH 15.65 OCH		13.67 CCO 9.37 CCH		6.01 CCC		
OFF DIAGONAL-	-10.45 SB22 -8.71 SB27		-6.06 SB28 -5.68 SS18		-5.20 SB21 -4.21 BB29		-3.82 SB26 -3.79 SB25		-2.75 BB34
NORMAL MODE 33	OBSERVED=	1035.0 CM-1	CALCULATED=	1016.6 CM-1	ERROR=	18.4 CM-1	OR	1.8 PERCENT	
INTERNAL COORDINATES-	25.10 C-07 18.50 C3C4		15.71 C5C1 11.72 C1C2		8.52 C-08 8.05 O1C1		5.88 C-06 5.86 C-09		5.69 C-07
FORCE CONSTANTS-	42.00 CO 43.52 CC		13.38 CCH 7.64 CCO		9.01 BC0H				
OFF DIAGONAL-	-9.27 SB26 -6.94 SB27		-6.51 SB22 -5.58 SB28		-4.48 SB24 -3.84 SS18				
NORMAL MODE 34	OBSERVED=	0.0 CM-1	CALCULATED=	979.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	18.00 C-07 12.28 C2C3		10.20 C1C2 7.95 C5C1		7.30 C-08 6.23 CC5H		5.71 CCO1 5.51 HC4C		
FORCE CONSTANTS-	35.07 CO 33.62 CC		19.28 CCH 15.39 CCO		7.35 OCH				
OFF DIAGONAL-	-10.42 SB22 -5.78 SB21		5.52 SB26 -4.99 SB25		-3.12 SB27 -2.37 SB28				
NORMAL MODE 35	OBSERVED=	0.0 CM-1	CALCULATED=	966.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	26.17 C-06 12.44 C-08		8.88 O1C1 8.33 C1C2		7.05 C2C3 5.87 C4C5				
FORCE CONSTANTS-	49.14 CO 24.59 CC		10.47 CCH 7.71 CCH						
OFF DIAGONAL-	-6.06 SB24 -4.87 SB22		4.84 SS18 2.98 SB27						

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400									
-6 NG=1236 BETA GALACTOSE GG									
PAGE 2									
MOLECULE 30									
NORMAL MODE 36	OBSERVED=	949.0 CM-1	CALCULATED=	918.7 CM-1	ERROR=	30.3 CM-1	OR	3.2 PERCENT	
INTERNAL COORDINATES-	23.53	C-U9 10.45 CCHA	8.47 CCHB	6.96 C4C5					
FORCE CONSTANTS-	33.79	CC 30.58 CCH	16.12 CC	13.62 OCH	7.44 CCO				
OFF DIAGONAL-	-3.37	SB22 -3.08 SB21	-2.69 SB27	-2.34 SB24	-2.06 SB28				
NORMAL MODE 37	OBSERVED=	906.0 CM-1	CALCULATED=	900.7 CM-1	ERROR=	5.3 CM-1	OR	0.6 PERCENT	
INTERNAL COORDINATES-	12.70	CCHB 11.79 C5C*	10.90 C5C*	9.52 C-U9	6.82 CCHA	6.68 C3C4	5.40 CCO*		
FORCE CONSTANTS-	28.30	CC 23.65 CCO	23.13 CC	10.36 CCO	6.46 OCH	5.40 CCO			
OFF DIAGONAL-	6.16	SB26 -4.96 SB21	-4.08 SB22	3.97 SS18	-3.45 SB25	-3.04 SB23	-2.42 SB27	1.54 BB43	
NORMAL MODE 38	OBSERVED=	889.0 CM-1	CALCULATED=	863.9 CM-1	ERROR=	25.1 CM-1	OR	2.8 PERCENT	
INTERNAL COORDINATES-	20.32	C4C5 8.69 C5C*	17.91 CCO	9.80 CCH	6.73 CCO	5.56 C3CC			
FORCE CONSTANTS-	34.60	CC 23.06 CCO	-5.18 SB22	5.04 SS18	4.06 BB43	-1.73 SB27			
OFF DIAGONAL-	-10.74	SB21 7.37 SB26							
NORMAL MODE 39	OBSERVED=	784.0 CM-1	CALCULATED=	734.3 CM-1	ERROR=	42.8 CM-1	OR	-5.5 PERCENT	
INTERNAL COORDINATES-	12.76	CCO 12.16 C2C3	8.89 C-U9	7.47 CCO*	6.71 CCH	6.05 OCH			
FORCE CONSTANTS-	30.59	CC 28.86 CCO	7.62 OCH	7.41 CCO	5.91 CCO				
OFF DIAGONAL-	11.42	SB25 -6.40 SB27	5.73 BB43	-2.99 SB21	2.72 BB33	-1.71 BB41	-1.56 SB24		
NORMAL MODE 40	OBSERVED=	703.0 CM-1	CALCULATED=	826.8 CM-1	ERROR=	-31.3 CM-1	OR	-4.4 PERCENT	
INTERNAL COORDINATES-	10.94	C-U9 10.54 CCO*	9.55 C-U9	9.36 OCH	8.28 CCO*	6.72 C4CC	5.91 CCO		
FORCE CONSTANTS-	35.46	CCO 17.22 CC	13.13 CCO	12.12 CCO	11.82 CCH				
OFF DIAGONAL-	5.11	SB25 4.14 BB43	-2.38 BB41	2.29 SB21	-2.04 BB34	1.92 SS18	-1.62 SB27		
NORMAL MODE 41	OBSERVED=	623.0 CM-1	CALCULATED=	610.5 CM-1	ERROR=	12.4 CM-1	OR	2.0 PERCENT	
INTERNAL COORDINATES-	12.16	CCO*	8.87 CCO9	8.24 CCO*	5.29 OCH	5.11 CCHA			
FORCE CONSTANTS-	51.71	CCO 18.86 CCH	8.20 OCH	6.46 CCO	5.97 CCO				
OFF DIAGONAL-	-4.90	BB34 4.02 BB43	3.73 SB25	-2.57 SB27	-2.56 BB29	2.12 SB22	-1.77 BB41	-1.63 SB23	
NORMAL MODE 42	OBSERVED=	560.0 CM-1	CALCULATED=	555.3 CM-1	ERROR=	4.7 CM-1	OR	0.8 PERCENT	
INTERNAL COORDINATES-	24.20	CCO8 23.13 CCO6	10.67 CCH2	8.76 CCO7	7.23 HC2C	6.97 OCH	6.70 CCO1H		
FORCE CONSTANTS-	29.50	CCO 32.06 CCH	6.64 CCO	3.94 CCO					
OFF DIAGONAL-	-19.89	BB34 -8.20 BB43	-19.49 BB29	-2.76 SB22	-2.72 BB42	-1.62 SB21	-1.51 BB41		
NORMAL MODE 43	OBSERVED=	536.0 CM-1	CALCULATED=	540.8 CM-1	ERROR=	-4.8 CM-1	OR	-0.9 PERCENT	
INTERNAL COORDINATES-	11.81	CCO*	7.19 CCO	6.40 C4C5	6.00 C2C3	5.79 C3C4	5.67 CCO	5.29 C5O*	
FORCE CONSTANTS-	25.25	CCO 23.18 C-U9	19.67 CCO	7.67 CCO					
OFF DIAGONAL-	5.60	SB24 4.44 SS18	-4.36 SB27	3.63 SB21	2.95 BB43	2.54 SB23	-1.97 SB22		
NORMAL MODE 44	OBSERVED=	478.0 CM-1	CALCULATED=	489.9 CM-1	ERROR=	-11.9 CM-1	OR	-2.5 PERCENT	
INTERNAL COORDINATES-	14.28	OCH 12.82 CCO	7.77 CCO*	6.08 CCO*	5.22 C4C5				
FORCE CONSTANTS-	41.83	CCO 12.82 CCO	9.47 CC	9.21 CCO	8.77 CCH	7.77 CCO	5.20 CCO		
OFF DIAGONAL-	-3.79	SB26 3.65 SB22	3.61 SB25	2.48 BB43	2.47 SB24	-1.87 BB42			
NORMAL MODE 45	OBSERVED=	445.0 CM-1	CALCULATED=	425.9 CM-1	ERROR=	9.1 CM-1	OR	2.1 PERCENT	
INTERNAL COORDINATES-	15.74	C1CC 11.71 C2CC	7.46 CCO*	7.42 OCH	5.14 OCH				
FORCE CONSTANTS-	39.37	CCO 30.49 CCO	7.03 CC	5.91 CCO	5.57 CCH				
OFF DIAGONAL-	4.29	SB25 -3.59 BB42	3.12 SB21	-2.32 BB41	1.76 SB22	-1.58 SB26			
NORMAL MODE 46	OBSERVED=	400.0 CM-1	CALCULATED=	389.4 CM-1	ERROR=	10.6 CM-1	OR	2.7 PERCENT	
INTERNAL COORDINATES-	24.98	OCH 10.29 CCH2	9.08 OCH	8.96 CCO9	8.70 CCO1H	8.14 OCH	6.76 CCO7	5.56 C3CC	
FORCE CONSTANTS-	61.49	CCO 29.62 CCH	8.04 CCO	6.49 BB43	2.11 SB22	-2.05 BB36	1.83 SB21	-1.59 SB26	
OFF DIAGONAL-	-13.37	BB34 -6.50 BB29	6.49 BB43						
NORMAL MODE 47	OBSERVED=	363.0 CM-1	CALCULATED=	329.3 CM-1	ERROR=	33.7 CM-1	OR	9.3 PERCENT	
INTERNAL COORDINATES-	19.71	CCO8 14.05 OCH	11.32 CCO7	6.88 OCH	5.36 TH-3	5.31 CCO*	5.23 CCO*		
FORCE CONSTANTS-	66.37	CCO 8.62 CCH	8.37 T-OH	8.29 CCO	6.89 CCO	5.31 CCO			
OFF DIAGONAL-	-7.55	BB34 -2.87 BB42	2.65 SB22	2.08 BB43	-1.76 SB26	-1.65 SB21			
NORMAL MODE 48	OBSERVED=	329.0 CM-1	CALCULATED=	323.9 CM-1	ERROR=	5.1 CM-1	OR	1.6 PERCENT	
INTERNAL COORDINATES-	28.39	OCH 7.51 CCO*	7.29 OCH	6.71 CCO*	5.36 C3CC				
FORCE CONSTANTS-	63.25	CCO 11.34 CCO	7.27 CC	6.74 T-OH					
OFF DIAGONAL-	5.49	SB22 -3.73 BB42	3.21 SB21	-2.50 BB33	1.63 SB25				
NORMAL MODE 49	OBSERVED=	311.0 CM-1	CALCULATED=	320.4 CM-1	ERROR=	-9.4 CM-1	OR	-3.0 PERCENT	
INTERNAL COORDINATES-	24.67	CCO7 20.46 CCO6	13.75 CCO	12.55 OCH	5.39 TH-2				
FORCE CONSTANTS-	67.09	CCO 13.75 CCO	10.88 T-OH	6.25 CC					
OFF DIAGONAL-	-4.93	BB42 4.78 SB22	-4.22 BB34	-2.49 SB24	-2.14 SB21	-1.84 BB43			
NORMAL MODE 50	OBSERVED=	292.0 CM-1	CALCULATED=	285.5 CM-1	ERROR=	6.5 CM-1	OR	2.2 PERCENT	
INTERNAL COORDINATES-	32.88	CCO 18.74 TH-5	14.94 C4CC	8.56 CCO	5.46 CCO				
FORCE CONSTANTS-	41.62	CCO 23.44 T-OH	12.33 CCO	6.69 CCH	1.88 SB22	1.82 SB25			
OFF DIAGONAL-	-3.83	BB34 -3.18 BB42	-2.83 BB33	2.35 SB24					
NORMAL MODE 51	OBSERVED=	256.0 CM-1	CALCULATED=	266.4 CM-1	ERROR=	-10.4 CM-1	OR	-4.1 PERCENT	
INTERNAL COORDINATES-	19.71	CCO 19.19 TH-4	10.39 T-OH	15.47 CCH	5.70 CCO*	5.50 CCO8	5.22 OCH		
FORCE CONSTANTS-	44.71	CCO 19.19 CCO	-2.71 BB33	-2.65 SB25	-2.32 BB29				
OFF DIAGONAL-	6.48	BB43 -4.96 BB34							
NORMAL MODE 52	OBSERVED=	240.0 CM-1	CALCULATED=	249.1 CM-1	ERROR=	-9.1 CM-1	OR	-3.8 PERCENT	
INTERNAL COORDINATES-	12.15	CCO 10.94 CCO9	10.91 OCH	9.26 CCO*	8.10 C3CC	8.10 TH-3			
FORCE CONSTANTS-	40.32	CCO 13.27 CCO	12.15 CCO	9.50 CCH	8.89 T-OH	7.54 T-CC			
OFF DIAGONAL-	5.50	SB22 -4.03 BB33	3.52 BB43	-2.97 SB25	-2.77 SB26	-1.68 SB21			
NORMAL MODE 53	OBSERVED=	0.0 CM-1	CALCULATED=	226.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	38.97	TH-1 37.72 TH-2	10.51 TH-5	7.86 TH-3					
FORCE CONSTANTS-	95.86	T-OH							
OFF DIAGONAL-	NONE								
NORMAL MODE 54	OBSERVED=	0.0 CM-1	CALCULATED=	216.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	34.09	TH-1 18.22 TH-2	15.69 TH-3	14.19 TH-4					
FORCE CONSTANTS-	86.17	T-OH 8.35 CCO							
OFF DIAGONAL-	NONE								
NORMAL MODE 55	OBSERVED=	0.0 CM-1	CALCULATED=	212.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	54.40	TH-3 7.80 TH-4	8.55 CCO*	5.46 TH-1					
FORCE CONSTANTS-	71.14	T-OH 14.17 CCO	9.91 CCO						
OFF DIAGONAL-	1.79	SB22							
NORMAL MODE 56	OBSERVED=	0.0 CM-1	CALCULATED=	212.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	54.47	TH-3 25.57 TH-2	6.00 CCO8						
FORCE CONSTANTS-	82.21	T-OH 16.11 CCO							
OFF DIAGONAL-	-1.96	BB34							
NORMAL MODE 57	OBSERVED=	0.0 CM-1	CALCULATED=	211.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	54.42	TH-4 9.25 TH-1	6.54 TH-2	6.32 TH-5	5.95 CCO9				
FORCE CONSTANTS-	78.81	T-OH 14.85 CCO							
OFF DIAGONAL-	NONE								
NORMAL MODE 58	OBSERVED=	0.0 CM-1	CALCULATED=	137.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	16.33	CO-C 12.42 C4CC	8.31 TCC4	6.10 CCO*	5.57 TCO1	5.33 CCO			
FORCE CONSTANTS-	24.76	CCO 18.16 CCO	18.33 CCO	9.09 T-CC	8.91 T-CC	7.29 CCH	5.33 CCO		
OFF DIAGONAL-	4.14	BB43 -2.37 BB33	2.24 BB41	-2.15 SB25					
NORMAL MODE 59	OBSERVED=	0.0 CM-1	CALCULATED=	95.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	25.43	C2CC 14.90 TCC2	13.05 TCC	7.26 TCC5	5.92 OCH	5.73 C1CC	5.36 CCO8	5.30 C3CC	
FORCE CONSTANTS-	39.76	T-CC 16.96 CCO	17.52 CCO						
OFF DIAGONAL-	-3.71	SB25 -2.65 BB42	2.14 BB41	-2.00 BB34	-1.80 SB21				
NORMAL MODE 60	OBSERVED=	0.0 CM-1	CALCULATED=	76.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	68.16	TCC5 5.67 C4CC	5.87 CCO						
FORCE CONSTANTS-	75.73	T-CC 11.96 CCO							
OFF DIAGONAL-	NONE								
NORMAL MODE 61	OBSERVED=	0.0 CM-1	CALCULATED=	72.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	14.96	TCC4 11.80 C1CC	11.35 CCO*	8.25 TCC5	7.40 TCC3	7.05 CCO*	5.60 TCO2		
FORCE CONSTANTS-	36.54	T-CC 30.33 CCO	20.07 CCO	5.82 T-CC					
OFF DIAGONAL-	-2.70	BB42 -1.72 BB33	-1.67 BB34	1.53 BB41					

35. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR =11.35

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400									
MOLECULE 31 -6 NG=1236 BETA GALACTOSE TG PAGE 1									
NORMAL MODE 8	OBSERVED=	1466.0 CM-1	CALCULATED=	1449.3 CM-1	ERROR=	16.7 CM-1	OR	1.1 PERCENT	
INTERNAL COORDINATES-	59.15 HCH	22.33 OCHA	20.37 OCHB						
FORCE CONSTANTS-	59.15 HCH	42.72 OCH							
OFF DIAGONAL-	-4.41 SB2								
NORMAL MODE 9	OBSERVED=	1420.0 CM-1	CALCULATED=	1421.9 CM-1	ERROR=	-1.9 CM-1	OR	-0.1 PERCENT	
INTERNAL COORDINATES-	30.26 C1H	16.53 OC1H	13.66 C1OH	8.11 C2OH	7.32 C1CH				
FORCE CONSTANTS-	53.39 OCH	24.65 SB2H	14.49 CCH	8.48 CO	5.61 CCO				
OFF DIAGONAL-	-9.48 SB27	3.83 SB2H	-2.76 SB25	2.58 BB29	-2.50 BB45	2.45 BB34	-2.08 BB39	-1.99 BB43	
NORMAL MODE 10	OBSERVED=	0.0 CM-1	CALCULATED=	1418.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	25.81 C4OH	19.34 OC4H	7.85 HC4C	7.21 C5H	5.17 CCHA				
FORCE CONSTANTS-	22.51 BCOH	32.22 UCH	26.16 CCH	8.24 CO					
OFF DIAGONAL-	-7.72 SB27	4.78 SB28	-2.47 SB25	-2.29 BB39	-2.28 BB45	1.86 BB34	-1.81 SB26	1.54 BB29	
NORMAL MODE 11	OBSERVED=	1405.0 CM-1	CALCULATED=	1407.6 CM-1	ERROR=	-2.6 CM-1	OR	-0.2 PERCENT	
INTERNAL COORDINATES-	27.30 C1H	20.12 C1OH	15.49 C2OH	12.63 OC1H	6.45 OC2H				
FORCE CONSTANTS-	47.83 OCH	37.40 BCOH	6.59 CCH						
OFF DIAGONAL-	2.44 SB28	-2.03 BB45	-1.98 SB26						
NORMAL MODE 12	OBSERVED=	0.0 CM-1	CALCULATED=	1402.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	20.75 C1OH	18.57 C3UH	9.76 CCHA	8.77 C4OH	7.93 CCHA	6.28 OC3H	5.11 CCHB		
FORCE CONSTANTS-	48.53 BCOH	20.10 CCH	18.57 OCH	5.91 CO					
OFF DIAGONAL-	-4.88 SB27	4.61 SB28	-3.81 SB26	2.65 BB34	-2.41 BB39	2.33 BB29	-1.58 SB21		
NORMAL MODE 13	OBSERVED=	0.0 CM-1	CALCULATED=	1390.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	39.06 C3OH	14.71 C4OH	12.79 C1OH	9.26 OC3H	5.97 C1OH	5.15 OC4H			
FORCE CONSTANTS-	72.25 CCH	19.33 CCH	14.85 CCH						
OFF DIAGONAL-	4.28 SB28	-2.72 BB39	-2.67 SB27	-2.54 SB26					
NORMAL MODE 14	OBSERVED=	0.0 CM-1	CALCULATED=	1389.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	38.09 C1OH	35.09 C2UH	5.90 OCH						
FORCE CONSTANTS-	82.06 BCOH	36.69 CCH	-1.71 BB39						
OFF DIAGONAL-	3.33 SB28	-1.91 SB26							
NORMAL MODE 15	OBSERVED=	1380.0 CM-1	CALCULATED=	1376.9 CM-1	ERROR=	3.1 CM-1	OR	0.2 PERCENT	
INTERNAL COORDINATES-	44.29 C1OH	11.83 C4OH	7.86 HC5C	7.00 C5H	6.68 CCHA	5.73 OCHB			
FORCE CONSTANTS-	59.95 BCOH	18.52 CCH	13.58 OCH						
OFF DIAGONAL-	3.41 BB29	-3.38 SB27	2.69 BB34	-2.48 SB28					
NORMAL MODE 16	OBSERVED=	0.0 CM-1	CALCULATED=	1360.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	26.57 C2OH	14.12 CC3H	13.78 OC2H	10.68 HC2C	10.31 C3OH	5.55 OC3H			
FORCE CONSTANTS-	37.69 BCOH	30.97 CCH	22.23 OCH						
OFF DIAGONAL-	7.13 BB29	-3.57 SB27	-3.25 SB28	3.00 BB34	-2.35 BB36	2.28 BB39	-2.05 BB45		
NORMAL MODE 17	OBSERVED=	1341.0 CM-1	CALCULATED=	1328.4 CM-1	ERROR=	12.5 CM-1	OR	0.9 PERCENT	
INTERNAL COORDINATES-	17.23 CC5H	13.53 C4UH	13.12 HC5C	9.00 OCHB	8.92 CCHB	7.46 HC3C	6.06 CCHA		
FORCE CONSTANTS-	58.35 CCH	21.26 LCH	15.77 BCOH	5.15 CC					
OFF DIAGONAL-	4.41 BB29	-4.18 SB26	-3.48 BB45	-2.65 SB28					
NORMAL MODE 18	OBSERVED=	1320.0 CM-1	CALCULATED=	1320.2 CM-1	ERROR=	-0.2 CM-1	OR	-0.0 PERCENT	
INTERNAL COORDINATES-	19.51 CCHB	16.62 C5H	16.44 OCHB	13.12 C4OH	6.65 HC5C				
FORCE CONSTANTS-	14.28 CCH	11.26 CCH	14.99 BCOH						
OFF DIAGONAL-	-4.63 SB27	-3.11 BB45	2.49 BB34	-1.71 SB28					
NORMAL MODE 19	OBSERVED=	1306.0 CM-1	CALCULATED=	1308.4 CM-1	ERROR=	-2.4 CM-1	OR	-0.2 PERCENT	
INTERNAL COORDINATES-	33.49 CCHH	11.72 CC1H	8.09 OC1H	7.90 HC2C	6.96 CC3H	6.58 C1OH	6.18 CC4H	5.08 OC4H	
FORCE CONSTANTS-	60.46 CCH	20.55 OCH	8.06 BCOH	6.44 CO					
OFF DIAGONAL-	11.57 BB29	-7.37 SB26	-3.56 BB45	1.55 BB34					
NORMAL MODE 20	OBSERVED=	0.0 CM-1	CALCULATED=	1297.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	22.17 UC3H	19.36 HC3C	10.99 HC4C	9.61 CC4H	5.99 C5H				
FORCE CONSTANTS-	52.86 CCH	35.51 OCH	5.69 BCOH						
OFF DIAGONAL-	-3.75 BB45	-2.19 SB27							
NORMAL MODE 21	OBSERVED=	0.0 CM-1	CALCULATED=	1284.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	23.62 OC4H	19.86 C5H	6.82 OC2H	6.38 HC2C	5.81 CC5H				
FORCE CONSTANTS-	52.86 CCH	35.51 OCH	8.09 CO						
OFF DIAGONAL-	8.07 SB27	-3.12 BB45							
NORMAL MODE 22	OBSERVED=	1273.0 CM-1	CALCULATED=	1268.7 CM-1	ERROR=	4.3 CM-1	OR	0.3 PERCENT	
INTERNAL COORDINATES-	18.18 HC4C	15.18 OC2H	8.07 C5H	7.60 OC3H	7.18 CC3H	6.59 CC4H			
FORCE CONSTANTS-	41.83 CCH	4.43 CCH	8.07 CO						
OFF DIAGONAL-	6.10 SB27	-3.38 BB45	-2.96 BB29	2.58 BB34	-2.29 SB25	-2.28 SB26			
NORMAL MODE 23	OBSERVED=	1246.0 CM-1	CALCULATED=	1254.0 CM-1	ERROR=	-8.0 CM-1	OR	-0.6 PERCENT	
INTERNAL COORDINATES-	0.11 C1H	11.02 CC4H	10.93 C1OH	9.26 OC4H	5.93 HC3C				
FORCE CONSTANTS-	39.22 CCH	31.12 CO	21.23 OCH	7.74 CCO					
OFF DIAGONAL-	-5.49 SB25	4.99 SB27	-2.55 BB45	-2.52 SB26	-1.88 SB28	1.68 BB34			
NORMAL MODE 24	OBSERVED=	1218.0 CM-1	CALCULATED=	1219.4 CM-1	ERROR=	-1.4 CM-1	OR	-0.1 PERCENT	
INTERNAL COORDINATES-	3.64 OC1H	11.12 C-U6	8.90 HC5C	8.16 OCHA	6.64 HC2C	6.24 OC3H	6.10 C-O9	5.91 CC5H	
FORCE CONSTANTS-	37.73 CCH	35.95 CO	22.23 OCH	10.25 CCO	8.61 BCOH				
OFF DIAGONAL-	-6.28 SB25	-5.02 BB29	3.15 BB34	-3.14 SB28	-2.40 BB45				
NORMAL MODE 25	OBSERVED=	0.0 CM-1	CALCULATED=	1203.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	15.86 OCHA	11.17 HC5C	10.86 CC5H	10.30 OCHB	8.18 C-O6	7.46 C4C5	6.13 HC3C	5.92 CC4H	5.88 C3C4
FORCE CONSTANTS-	47.77 CCH	31.00 OCH	18.74 CCH	17.67 CO	6.19 CCO				
OFF DIAGONAL-	-13.41 SB26	-3.35 BB29	-3.03 BB45	-2.89 SB22	-2.41 SB25	2.14 BB33	-2.11 BB43		
NORMAL MODE 26	OBSERVED=	1166.0 CM-1	CALCULATED=	1170.1 CM-1	ERROR=	-4.1 CM-1	OR	-0.3 PERCENT	
INTERNAL COORDINATES-	18.37 CC1H	23.49 OC1H	8.40 OC1H	8.15 OC2H	7.81 C-O8	7.57 CCH2	5.86 C-O6		
FORCE CONSTANTS-	33.29 CCH	33.99 CCH	27.52 CCH	9.45 CCH					
OFF DIAGONAL-	-6.64 BB29	-5.18 SB25	3.19 BB34	-2.55 SB28	-2.37 BB45	2.09 SB27			
NORMAL MODE 27	OBSERVED=	1138.0 CM-1	CALCULATED=	1124.9 CM-1	ERROR=	13.1 CM-1	OR	1.1 PERCENT	
INTERNAL COORDINATES-	43.77 C-O8	26.06 C4C5	8.53 C-O9	8.11 C-O9	7.33 OC1H	6.13 CCHH	5.15 CCO*		
FORCE CONSTANTS-	46.25 CO	35.43 CCH	21.42 CCO	13.90 CCH	9.89 OCH	5.27 BCOH			
OFF DIAGONAL-	-10.02 SB25	-8.97 SB26	-6.36 SB22	-3.08 SS18	-2.82 SB21	-2.62 SB28	-1.96 BB34	-1.60 SB23	
NORMAL MODE 28	OBSERVED=	1111.0 CM-1	CALCULATED=	1117.7 CM-1	ERROR=	-6.7 CM-1	OR	-0.6 PERCENT	
INTERNAL COORDINATES-	25.36 C5C	14.48 C-U8	12.09 C4C5	10.47 C2C3	6.48 CCO				
FORCE CONSTANTS-	50.54 CCH	26.52 CO	14.34 CCO	12.61 CCH	7.00 OCH	6.29 CCC			
OFF DIAGONAL-	-9.91 SB22	-3.47 SB25	-3.34 SB28	-2.58 SB27	-2.03 SS18				
NORMAL MODE 29	OBSERVED=	1096.0 CM-1	CALCULATED=	1097.9 CM-1	ERROR=	-1.9 CM-1	OR	-0.2 PERCENT	
INTERNAL COORDINATES-	27.40 C-O7	13.99 C1C2	9.53 C-O8	5.94 OC1H	5.23 C-O7				
FORCE CONSTANTS-	54.81 CO	19.21 CC	12.38 CCH	12.12 OCH	10.54 CCO				
OFF DIAGONAL-	-7.44 SB25	5.48 SB27	-4.37 SS18	-4.29 SB28	-2.27 BB29	-2.23 SB24			
NORMAL MODE 30	OBSERVED=	1086.0 CM-1	CALCULATED=	1084.2 CM-1	ERROR=	1.8 CM-1	OR	0.2 PERCENT	
INTERNAL COORDINATES-	31.23 C3C4	22.01 C2C3	13.91 C-O9	7.94 C5OH	7.37 C-O7				
FORCE CONSTANTS-	61.83 CCH	33.99 CCH	27.52 CCH	12.81 CCH	11.26 CCH	9.42 BCOH	8.32 CCC		
OFF DIAGONAL-	-8.93 SB22	-8.73 SB27	-7.92 SB21	-7.30 SB26	-5.55 SS18	-5.44 SB28	-3.59 BB34	-2.66 SB25	-1.69 BB43
NORMAL MODE 31	OBSERVED=	1068.0 CM-1	CALCULATED=	1068.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	14.28 C-O8	14.77 C-U7	8.53 C-O9	8.11 C-O9	7.33 OC1H	6.13 CCHH	5.15 CCO*		
FORCE CONSTANTS-	86.99 CO	9.75 CCO	8.49 CCH	8.47 BCOH	7.12 OCH	6.91 CCH			
OFF DIAGONAL-	-9.33 SB28	-8.03 SB27	-5.54 SB25	-3.15 SS18	-2.76 SB21				
NORMAL MODE 32	OBSERVED=	1056.0 CM-1	CALCULATED=	1054.3 CM-1	ERROR=	1.8 CM-1	OR	0.2 PERCENT	
INTERNAL COORDINATES-	42.26 C-O8	11.66 C5C	11.77 C-O7	11.04 C2C3	10.34 C-O9	5.96 C1OH			
FORCE CONSTANTS-	67.55 CO	27.49 CC	11.14 BCOH	9.11 OCH	9.00 CCM	6.41 CCC	6.03 CCO		
OFF DIAGONAL-	-10.06 SB28	-8.06 SB21	-7.69 SB27	-6.54 SS18	-4.12 SB25				
NORMAL MODE 33	OBSERVED=	1035.0 CM-1	CALCULATED=	1043.8 CM-1	ERROR=	-8.8 CM-1	OR	-0.8 PERCENT	
INTERNAL COORDINATES-	43.63 C1C2	18.27 C-O8	7.79 CC3H	7.33 C-O6	7.02 OC1H	6.61 CC1H	5.58 C1OH		
FORCE CONSTANTS-	46.81 CC	35.89 CO	27.41 CCH	15.94 OCH	13.30 CCO	9.51 BCOH	5.60 CCC		
OFF DIAGONAL-	-10.48 SB22	-8.91 SB27	-6.11 SB28	-5.98 SS18	-5.17 SB21	-4.20 BB29	-3.67 SB26	-3.15 SB25	-2.69 BB34
NORMAL MODE 34	OBSERVED=	0.0 CM-1	CALCULATED=	991.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	25.63 C5C	24.28 C1C2	23.06 C-O8	11.98 C3C4	8.89 C5O				
FORCE CONSTANTS-	62.37 CCH	38.56 CCH	12.27 CO	12.27 CO	9.44 CCHA				
OFF DIAGONAL-	-14.69 SB22	-7.85 SB26	-3.56 SB27	-2.01 SB28	-2.00 BB34				
NORMAL MODE 35	OBSERVED=	0.0 CM-1	CALCULATED=	962.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	33.18 C2C3	10.25 CC5H	18.08 CO	11.22 CCO	8.97 OCH	5.74 CCH			
FORCE CONSTANTS-	33.18 CCH	25.89 CC	4.85 SB26	-2.77 SB24	-2.31 SB23	-1.74 SB25	1.64 SS18	-1.63 BB29	
OFF DIAGONAL-	-7.96 SB22								

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400									
MOLECULE 31 -6 NG=1236 BETA GALACTOSE TG									
PAGE 2									
NORMAL MODE 36	OBSERVED=	949.0 CM-1	CALCULATED=	944.6 CM-1	ERROR=	4.4 CM-1	OR	0.5 PERCENT	
INTERNAL COORDINATES-	24.72	C-06 15.52 O-C1	11.01 C5C*	7.50 OCO	5.15	C-08			
FORCE CONSTANTS-	50.17	CO-16.29 CC	21.36 CC	8.24 CCH	7.94	CCO	7.50 OCO	5.94 CCC	
OFF DIAGONAL-	-10.34	SB24 4.27 SB27	-4.18 SB21	-3.28 SB22	-2.64	SB23	2.46 BB43	2.15 SS18	-1.73 SB28
NORMAL MODE 37	OBSERVED=	906.0 CM-1	CALCULATED=	908.8 CM-1	ERROR=	-2.8 CM-1	OR	-0.3 PERCENT	
INTERNAL COORDINATES-	29.30	C-09 10.81 C2C3	9.48 CCHA	9.21 CCHB	5.97	HC3C			
FORCE CONSTANTS-	35.04	CCH 33.32 CO	21.36 CC	8.94 CCO	8.71	OCB			
OFF DIAGONAL-	-5.12	SB22 -4.48 SB27	-3.15 SB21	-2.90 BB29	-2.09	SB28	1.54 SB26		
NORMAL MODE 38	OBSERVED=	889.0 CM-1	CALCULATED=	863.6 CM-1	ERROR=	25.4 CM-1	OR	2.9 PERCENT	
INTERNAL COORDINATES-	19.28	C4C5 8.94 OC8C	6.62 C-09	6.31 C5O*	5.90	C3C4	5.54 O9CC	5.42 C5C*	
FORCE CONSTANTS-	32.13	CC 23.07 CCO	18.95 CO	12.63 CCH	5.08	CC			
OFF DIAGONAL-	-8.32	SB21 6.76 SB26	-6.33 SB22	4.39 BB43	4.17	SS18			
NORMAL MODE 39	OBSERVED=	784.0 CM-1	CALCULATED=	759.3 CM-1	ERROR=	24.7 CM-1	OR	3.1 PERCENT	
INTERNAL COORDINATES-	14.36	C4C5 19.79 C-09	7.07 C1C2	5.47 CC4*	5.26	C-07			
FORCE CONSTANTS-	30.17	CCO 19.79 CO	14.38 CCH	12.19 CC	5.58	CCC			
OFF DIAGONAL-	8.07	SB25 3.92 BB43	-3.52 SB27	-1.91 SB22	-1.83	BB41	1.62 SB21		
NORMAL MODE 40	OBSERVED=	703.0 CM-1	CALCULATED=	674.2 CM-1	ERROR=	28.8 CM-1	OR	4.1 PERCENT	
INTERNAL COORDINATES-	13.70	C4C5 17.98 C4C5	6.83 O9CC	6.69 CCHA	5.64	OC8C	5.51 C4CC	5.48 C2C3	
FORCE CONSTANTS-	34.60	CCO 22.54 CCH	17.28 CC	8.96 CCC	7.09	CO			
OFF DIAGONAL-	4.50	BB43 -3.55 BB29	-2.55 SB21	1.98 SB25	1.96	SS18	-1.55 BB41		
NORMAL MODE 41	OBSERVED=	623.0 CM-1	CALCULATED=	617.0 CM-1	ERROR=	6.0 CM-1	OR	1.0 PERCENT	
INTERNAL COORDINATES-	13.48	UCO 11.62 CCO*	5.71 O-C1	5.55 CCO*	5.09	CCO7			
FORCE CONSTANTS-	38.29	CCO 19.80 CO	13.48 OCO	8.96 OCH	7.23	CCH	5.69 CC		
OFF DIAGONAL-	5.92	SB24 -5.84 SB27	3.44 SB25	3.36 SB22	2.65	BB43	1.66 SS18	-1.58 BB34	-1.54 BB42
NORMAL MODE 42	OBSERVED=	560.0 CM-1	CALCULATED=	578.7 CM-1	ERROR=	-18.7 CM-1	OR	-3.3 PERCENT	
INTERNAL COORDINATES-	14.70	CCO* 12.57 O-C1	8.34 C-C*	7.16 CCO8	6.55	C4CC	6.45 HC2C	5.38 HC5C	5.31 O9CC
FORCE CONSTANTS-	51.65	CLO 28.72 CCH	8.89 CC	8.28 CCO					
OFF DIAGONAL-	-11.83	BB34 7.94 BB43	-6.26 BB29	2.51 SB25	-2.14	BB41			
NORMAL MODE 43	OBSERVED=	536.0 CM-1	CALCULATED=	547.2 CM-1	ERROR=	-11.2 CM-1	OR	-2.1 PERCENT	
INTERNAL COORDINATES-	22.53	CCO6 17.71 CCOB	13.04 C-C*	9.01 CCO7	7.19	CH2	5.81 C2C3	5.66 CC1H	5.55 CCO*
FORCE CONSTANTS-	23.17	CCO 23.54 CCH	13.04 C-C*	10.61 CC					
OFF DIAGONAL-	-14.72	BB34 6.95 BB43	-4.85 BB29	-3.21 SB22	2.64	SB25			
NORMAL MODE 44	OBSERVED=	478.0 CM-1	CALCULATED=	458.5 CM-1	ERROR=	19.5 CM-1	OR	4.1 PERCENT	
INTERNAL COORDINATES-	11.41	C1C2 17.42 C2CC	9.53 C1C2	6.04 C-08	5.39	CCO8			
FORCE CONSTANTS-	23.02	CCC 20.34 CCO	19.30 CC	14.55 CO					
OFF DIAGONAL-	6.20	SB25 5.33 SB21	4.60 SB22	3.00 SS18	-2.77	SB26	2.39 BB43	-1.60 SB27	-1.51 BB42
NORMAL MODE 45	OBSERVED=	435.0 CM-1	CALCULATED=	438.6 CM-1	ERROR=	-3.6 CM-1	OR	-0.8 PERCENT	
INTERNAL COORDINATES-	17.76	O-C1 14.28 CCO*	14.23 OCO	6.79 C3CC	5.90	C5O*			
FORCE CONSTANTS-	42.77	CCO 14.73 UCO	13.42 CCC	10.28 CO	10.09	CCH	7.92 CC		
OFF DIAGONAL-	-5.62	BB34 5.49 SB21	4.21 BB43	-2.41 BB42	1.90	SB24	-1.74 BB29	-1.69 SB26	
NORMAL MODE 46	OBSERVED=	400.0 CM-1	CALCULATED=	388.1 CM-1	ERROR=	11.9 CM-1	OR	3.0 PERCENT	
INTERNAL COORDINATES-	27.89	UCC 9.69 CH2	9.05 CCO9	8.77 CC1H	6.97	OC8C	6.36 O-C1	6.11 CCO7	
FORCE CONSTANTS-	61.54	CCO 29.31 CCH	5.91 CCC	5.82 CC					
OFF DIAGONAL-	-13.06	BB34 6.43 BB29	6.31 BB43	2.63 SB22	-2.08	BB36	-1.80 SB26		
NORMAL MODE 47	OBSERVED=	363.0 CM-1	CALCULATED=	347.3 CM-1	ERROR=	15.8 CM-1	OR	4.3 PERCENT	
INTERNAL COORDINATES-	11.21	OC8C 8.73 CCO*	7.94 O9CC	7.08 C1CC	6.45	CCO*	5.45 O-C1	5.29 CO-C	5.07 C2CC
FORCE CONSTANTS-	44.44	CCO 19.97 CCH	13.87 CCO	8.28 C-C*					
OFF DIAGONAL-	4.19	SB25 3.33 SB22	-3.08 SB27	-2.83 BB34	2.80	SB23	-2.33 BB42		
NORMAL MODE 48	OBSERVED=	329.0 CM-1	CALCULATED=	324.6 CM-1	ERROR=	4.4 CM-1	OR	1.3 PERCENT	
INTERNAL COORDINATES-	33.55	CCC 22.00 CCO8	12.44 O7CC	8.03 OC8C	6.65	TH-2			
FORCE CONSTANTS-	87.50	CCO 12.14 T-OH	6.19 CCH						
OFF DIAGONAL-	-8.25	BB34 -4.73 BB42	-1.89 BB43						
NORMAL MODE 49	OBSERVED=	311.0 CM-1	CALCULATED=	317.4 CM-1	ERROR=	-6.4 CM-1	OR	-2.1 PERCENT	
INTERNAL COORDINATES-	22.56	CCO6 15.51 CCO	6.88 OC8C	6.24 O9CC	5.64	CCO7	5.19 O7CC		
FORCE CONSTANTS-	58.10	CCO 15.51 CCO	10.26 T-OH	9.55 CC					
OFF DIAGONAL-	5.99	SB22 -4.24 BB42	-2.21 BB34						
NORMAL MODE 50	OBSERVED=	292.0 CM-1	CALCULATED=	288.4 CM-1	ERROR=	3.6 CM-1	OR	1.2 PERCENT	
INTERNAL COORDINATES-	16.77	O9CC 11.34 TH-4	9.24 CCO9	6.64 C1CC	6.38	CCO6	5.81 CCO8		
FORCE CONSTANTS-	48.82	CCO 11.34 CCH	12.74 CCC	13.81 T-OH					
OFF DIAGONAL-	7.98	BB43 -5.97 BB34	4.29 SB22	-3.06 BB33	-2.83	BB29	-1.78 SB25		
NORMAL MODE 51	OBSERVED=	256.0 CM-1	CALCULATED=	253.9 CM-1	ERROR=	2.1 CM-1	OR	0.8 PERCENT	
INTERNAL COORDINATES-	20.09	CCO9 18.23 CCO*	12.44 C3CC	10.79 O9CC	5.75	CO-C			
FORCE CONSTANTS-	57.09	CCO 18.23 CCO*	11.64 CCO	5.75 CCO	5.66	T-OH	5.12 T-CC		
OFF DIAGONAL-	-4.57	BB33 -3.96 SB25	-3.30 SB21	2.91 SB22	2.86	BB43	-1.99 BB34	-1.80 BB42	-1.69 BB36
NORMAL MODE 52	OBSERVED=	240.0 CM-1	CALCULATED=	244.6 CM-1	ERROR=	-4.6 CM-1	OR	-1.9 PERCENT	
INTERNAL COORDINATES-	25.93	TH-0 9.41 C4CC	18.18 CCO	5.12 TH-1					
FORCE CONSTANTS-	65.00	T-OH 15.63 CCO	13.14 CCC						
OFF DIAGONAL-	-2.03	BB34 1.56 SB22							
NORMAL MODE 53	OBSERVED=	0.0 CM-1	CALCULATED=	226.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	30.71	TH-2 29.59 TH-1	17.01 TH-3	13.99 TH-5	5.28	TH-4			
FORCE CONSTANTS-	96.58	I-CH							
OFF DIAGONAL-	NONE								
NORMAL MODE 54	OBSERVED=	0.0 CM-1	CALCULATED=	216.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	41.18	TH-1 22.40 TH-3	22.37 TH-4						
FORCE CONSTANTS-	86.73	T-OH 7.91 CCO							
OFF DIAGONAL-	NONE								
NORMAL MODE 55	OBSERVED=	0.0 CM-1	CALCULATED=	214.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	35.25	TH-2 14.57 TH-3	11.82 TH-1	6.29 CCO7					
FORCE CONSTANTS-	89.34	T-OH 14.13 CCO							
OFF DIAGONAL-	-1.78	BB34							
NORMAL MODE 56	OBSERVED=	0.0 CM-1	CALCULATED=	211.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	81.39	TH-0 29.49 TH-3	6.92 OC8C	5.59 CCO9					
FORCE CONSTANTS-	NONE	T-OH 16.52 CCO							
OFF DIAGONAL-	NONE								
NORMAL MODE 57	OBSERVED=	0.0 CM-1	CALCULATED=	191.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	25.48	C4CC 24.78 TH-5	12.56 TCC5						
FORCE CONSTANTS-	30.24	CCC 27.62 T-OH	15.63 CCO	14.03 T-CC					
OFF DIAGONAL-	-2.31	BB42 -1.66 SB21							
NORMAL MODE 58	OBSERVED=	0.0 CM-1	CALCULATED=	153.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	27.08	CCO* 22.46 CO-C	9.81 CCO*	5.93 OCO	5.19	TCC4			
FORCE CONSTANTS-	44.87	CCO 22.46 CO-C	8.91 CCH	8.48 T-CC	6.13	T-CC	5.93 OCO	5.34 CCC	
OFF DIAGONAL-	-8.00	BB34 -3.32 SB25	2.31 BB43						
NORMAL MODE 59	OBSERVED=	0.0 CM-1	CALCULATED=	97.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	21.06	C2CC 18.34 TCC5	12.49 TCC1	10.22 TCC2	9.02	C1CC	5.99 OC8C	5.01 TCC4	
FORCE CONSTANTS-	47.52	T-CC 18.34 TCC5	16.00 CCO						
OFF DIAGONAL-	-4.05	SB25 -3.75 SB21	-2.80 BB42	2.16 BB41	-1.65	BB34			
NORMAL MODE 60	OBSERVED=	0.0 CM-1	CALCULATED=	86.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	50.99	T-CC 19.39 TCC2	6.76 O-C1	6.37					
FORCE CONSTANTS-	3.35	SB21	14.34 CCC						
OFF DIAGONAL-									
NORMAL MODE 61	OBSERVED=	0.0 CM-1	CALCULATED=	67.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	32.63	TCC5 8.59 TCC4	8.34 C1CC	7.97 C4C*	5.63	TCC2	5.55 CO-C	5.19 C4CC	
FORCE CONSTANTS-	50.08	T-CC 18.26 TCC4	17.54 CCO	5.65 T-CC	5.55	CCO			
OFF DIAGONAL-	-2.01	BB42							

35. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 8.15

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400	GT	PAGE 1
MOLECULE 32	-6 NG=1237 ALPHA MANNDSE	
NORMAL MODE 8 OBSERVED= 1460.0 CM-1	CALCULATED= 1449.6 CM-1	ERROR= 10.4 CM-1 OR 0.7 PERCENT
INTERNAL COORDINATES- 62.00 HCH 19.99 CCHB 19.17 OCHA		
FORCE CONSTANTS- 62.00 HCH 39.46 OCH		
OFF DIAGONAL- -3.85 SB27		
NORMAL MODE 9 OBSERVED= 1420.0 CM-1	CALCULATED= 1415.3 CM-1	ERROR= -4.7 CM-1 OR -0.4 PERCENT
INTERNAL COORDINATES- 13.85 C3OH 11.19 C2OH 9.17 OC1H 7.75 OC4H 7.46 C1OH		
FORCE CONSTANTS- 59.69 BCOH 16.82 CCH 11.51 OCH 8.33 CC 5.51 CCO		
OFF DIAGONAL- -3.72 SB26 3.48 SB28 -3.44 SB27 3.38 BB36 2.35 BB29 2.19 BB34 -2.11 SB25 -1.86 BB43		
NORMAL MODE 10 OBSERVED= 1407.9 CM-1	CALCULATED= 1407.9 CM-1	ERROR= 0.0 CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES- 31.87 C1OH 16.02 C3OH 11.13 OC1H 8.81 C2OH		
FORCE CONSTANTS- 36.55 BCOH 34.80 OCH 17.33 CCH 8.18 CO		
OFF DIAGONAL- -7.18 SB27 5.00 SB28 -2.82 SB26 -2.65 SB25 -2.57 BB39 2.50 BB29 2.21 BB34 -1.99 BB45		
NORMAL MODE 11 OBSERVED= 1400.0 CM-1	CALCULATED= 1426.3 CM-1	ERROR= -7.9 CM-1 OR -0.6 PERCENT
INTERNAL COORDINATES- 40.08 C3OH 14.82 C4OH 11.29 CCH		
FORCE CONSTANTS- 58.67 BCOH 22.76 OCH -2.80 BB39 -2.67 SB26		
OFF DIAGONAL- 4.93 SB28 -4.66 SB27		
NORMAL MODE 12 OBSERVED= 1395.0 CM-1	CALCULATED= 1394.7 CM-1	ERROR= 0.3 CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES- 41.27 C1OH 17.87 C2OH 12.69 C1H 6.85 OC2H 5.31 CH2		
FORCE CONSTANTS- 69.18 BCOH 22.84 OCH 8.07 CCH		
OFF DIAGONAL- -3.85 SB27 1.51 BB34		
NORMAL MODE 13 OBSERVED= 1392.0 CM-1	CALCULATED= 1390.8 CM-1	ERROR= 1.2 CM-1 OR 0.1 PERCENT
INTERNAL COORDINATES- 42.51 C1OH 17.13 C2OH 10.72 C1H 8.26 OC1H		
FORCE CONSTANTS- 62.54 BCOH 25.61 OCH 7.80 CCH		
OFF DIAGONAL- -3.01 SB26 2.70 SB28 -2.28 BB39 -1.92 SB27		
NORMAL MODE 14 OBSERVED= 1382.0 CM-1	CALCULATED= 1386.8 CM-1	ERROR= -4.8 CM-1 OR -0.3 PERCENT
INTERNAL COORDINATES- 35.51 C1OH 21.90 C1H 13.61 OC1H 12.83 C2OH		
FORCE CONSTANTS- 51.23 BCOH 40.31 OCH 6.54 CCH		
OFF DIAGONAL- -3.14 SB27 -1.72 BB45 1.68 SB28 -1.66 SB26		
NORMAL MODE 15 OBSERVED= 1371.0 CM-1	CALCULATED= 1372.4 CM-1	ERROR= -1.4 CM-1 OR -0.1 PERCENT
INTERNAL COORDINATES- 56.48 C4OH 10.88 C5H 6.83 CC5H 5.73 HC4C		
FORCE CONSTANTS- 61.17 BCOH 19.33 CCH 16.67 OC4H		
OFF DIAGONAL- 3.18 BB29 -2.73 BB36 -2.33 SB27		
NORMAL MODE 16 OBSERVED= 1356.0 CM-1	CALCULATED= 1359.4 CM-1	ERROR= -3.4 CM-1 OR -0.3 PERCENT
INTERNAL COORDINATES- 14.51 HC3C 10.08 HC5C 8.79 C5H 9.30 CC4H 8.10 CCHB 5.82 C4OH		
FORCE CONSTANTS- 51.91 CCH 32.86 OCH 7.95 BCOH 5.19 CO		
OFF DIAGONAL- 10.44 BB29 -5.68 SB27 -4.10 SB26 -3.54 BB45 2.42 BB34		
NORMAL MODE 17 OBSERVED= 1333.0 CM-1	CALCULATED= 1336.3 CM-1	ERROR= -3.3 CM-1 OR -0.3 PERCENT
INTERNAL COORDINATES- 17.61 HC5C 16.78 CCHB 9.49 CC5H 6.30 CCHB 6.04 HC3C 5.66 OC3H 5.50 HC4C		
FORCE CONSTANTS- 67.49 CCH 14.04 OCH 6.29 BCOH 6.21 CO		
OFF DIAGONAL- 13.84 BB29 -8.27 SB26 -3.51 BB45 -3.01 SB27		
NORMAL MODE 18 OBSERVED= 1327.0 CM-1	CALCULATED= 1319.1 CM-1	ERROR= 7.9 CM-1 OR 0.6 PERCENT
INTERNAL COORDINATES- 23.00 C1H 18.62 HC2C 12.58 OC1H 9.45 CCH2 6.59 OC3H		
FORCE CONSTANTS- 57.69 CCH 23.16 OCH 7.23 BCOH 6.54 CC		
OFF DIAGONAL- -3.56 BB45 3.15 BB34 1.61 BB30		
NORMAL MODE 19 OBSERVED= 1312.0 CM-1	CALCULATED= 1315.7 CM-1	ERROR= -3.7 CM-1 OR -0.3 PERCENT
INTERNAL COORDINATES- 22.35 OC2H 20.32 CH2 15.73 C2OH 12.10 OC1		
FORCE CONSTANTS- 31.91 CCH 26.78 OCH 22.08 CCH 16.28 BCOH		
OFF DIAGONAL- -4.05 SB25 -2.41 BB45 2.25 BB34 1.95 BB33 -1.84 SB28 1.72 BB39 1.53 BB29		
NORMAL MODE 20 OBSERVED= 1293.0 CM-1	CALCULATED= 1296.9 CM-1	ERROR= -3.9 CM-1 OR -0.3 PERCENT
INTERNAL COORDINATES- 25.90 OC4H 22.15 CCH 16.73 OC4H 12.10 OC1		
FORCE CONSTANTS- 55.86 OCH 17.03 CCH 6.55 BCOH		
OFF DIAGONAL- -3.66 BB45 -2.78 SB27 -1.98 BB29		
NORMAL MODE 21 OBSERVED= 1281.0 CM-1	CALCULATED= 1281.0 CM-1	ERROR= -0.0 CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES- 21.19 C5H 7.89 CC5H 7.74 OC1H 7.63 HC2C 6.61 OCHA 5.65 CCHA		
FORCE CONSTANTS- 51.91 OCH 34.27 CCH 5.82 CO		
OFF DIAGONAL- -3.46 BB45 2.74 SB27 -1.74 BB29		
NORMAL MODE 22 OBSERVED= 1274.0 CM-1	CALCULATED= 1269.5 CM-1	ERROR= 4.5 CM-1 OR 0.3 PERCENT
INTERNAL COORDINATES- 22.23 OC3H 17.74 C4H 12.91 CC3H 11.70 OC4H 5.76 OCHA		
FORCE CONSTANTS- 45.54 OCH 43.52 CCH		
OFF DIAGONAL- -3.64 BB45 3.44 SB27 1.52 BB34		
NORMAL MODE 23 OBSERVED= 1255.0 CM-1	CALCULATED= 1260.3 CM-1	ERROR= -5.3 CM-1 OR -0.4 PERCENT
INTERNAL COORDINATES- 13.82 OC2H 11.22 CC1H 10.49 C5H 9.81 HC2C 5.30 OCHA		
FORCE CONSTANTS- 19.25 CCH 37.4 CCH 11.09 CO		
OFF DIAGONAL- -3.25 BB45 2.71 BB34 2.47 SB27 -1.98 SB25		
NORMAL MODE 24 OBSERVED= 1239.0 CM-1	CALCULATED= 1234.4 CM-1	ERROR= 4.6 CM-1 OR 0.4 PERCENT
INTERNAL COORDINATES- 16.78 HC5C 16.77 OC6H 9.63 OCHB 7.47 C5H 6.58 HC3C 6.18 CCHB		
FORCE CONSTANTS- 46.89 CCH 36.23 OCH 3.75 BB34 -3.35 BB45 -3.07 SB26 -2.03 SB25		
OFF DIAGONAL- -5.91 BB29 5.77 SB27		
NORMAL MODE 25 OBSERVED= 1210.0 CM-1	CALCULATED= 1197.0 CM-1	ERROR= 13.0 CM-1 OR 1.1 PERCENT
INTERNAL COORDINATES- 10.93 C5H 10.28 CC4H 9.83 HC4C 9.10 HC5C 8.95 OCHB 8.78 CC3H 6.03 HC3C 5.72 C3OH 5.15 C-O7		
FORCE CONSTANTS- 58.40 CCH 17.40 OCH 12.86 CO 10.41 CCO 7.92 BCOH		
OFF DIAGONAL- -10.35 BB29 5.29 BB34 -5.02 SB25 4.41 SB27 -2.88 SB28 -2.84 BB45 -1.92 BB36		
NORMAL MODE 26 OBSERVED= 1169.0 CM-1	CALCULATED= 1152.5 CM-1	ERROR= 16.5 CM-1 OR 1.4 PERCENT
INTERNAL COORDINATES- 22.20 C5O 11.25 C-O7 7.99 OCHB 7.30 OCHA 6.66 C-O8 5.17 OC1		
FORCE CONSTANTS- 48.13 CO 27.18 OCH 16.83 CCO 10.61 CCH 8.24 CC 7.30 BCOH		
OFF DIAGONAL- -12.74 SB25 -4.09 SB28 -2.54 SB26 -1.66 SB21 1.58 SB27		
NORMAL MODE 27 OBSERVED= 1140.0 CM-1	CALCULATED= 1146.7 CM-1	ERROR= -6.7 CM-1 OR -0.6 PERCENT
INTERNAL COORDINATES- 19.01 C-O6 16.60 OC1 10.70 C3C4 7.70 OC2H 6.85 CCH2 6.45 C4C5 6.13 OCHB 5.22 HC2C		
FORCE CONSTANTS- 40.30 CO 23.50 CC 19.14 OCH 16.16 CCH 13.85 CCO		
OFF DIAGONAL- -9.72 SB25 -5.31 SB22 -2.81 SB21 -2.34 SB23 -2.19 SB26 -1.76 SB27 -1.62 SB28		
NORMAL MODE 28 OBSERVED= 1115.0 CM-1	CALCULATED= 1112.8 CM-1	ERROR= 2.2 CM-1 OR 0.2 PERCENT
INTERNAL COORDINATES- 13.37 C5O 11.69 C-O8 11.42 C4C5 10.84 C-O9 6.22 C1C2 5.83 C2C3 5.38 CCO 5.22 CCO		
FORCE CONSTANTS- 49.73 CCH 30.29 CO 22.88 CCO 12.22 OCH		
OFF DIAGONAL- -11.48 SB22 -5.24 SB25 -3.36 SB28 1.75 SB21		
NORMAL MODE 29 OBSERVED= 1104.0 CM-1	CALCULATED= 1097.5 CM-1	ERROR= 6.5 CM-1 OR 0.6 PERCENT
INTERNAL COORDINATES- 11.92 C-O9 19.80 C4C5 11.71 C5C 11.40 C-O8 10.65 C-O6 6.31 C2C3 5.32 C1C2		
FORCE CONSTANTS- 51.22 CO 46.40 CCH 11.51 CCO 7.08 CCH		
OFF DIAGONAL- -7.32 SB22 -4.29 SB26 -3.37 SB25 -3.32 SB28 -3.14 SS18		
NORMAL MODE 30 OBSERVED= 1085.0 CM-1	CALCULATED= 1084.9 CM-1	ERROR= 0.1 CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES- 29.54 C-O8 21.37 C4C5 14.83 C3C4 9.65 C5O 7.63 C-O7 6.07 CCH2 5.11 C1C2		
FORCE CONSTANTS- 53.70 CO 42.84 CCH 12.30 CCH 9.26 CCO 7.33 OCH 6.33 CCH 5.42 BCOH		
OFF DIAGONAL- -6.37 SS18 -5.79 SB27 -5.77 SB21 -5.17 SB28 -4.45 SB22 -4.23 SB25 -1.98 SB26		
NORMAL MODE 31 OBSERVED= 1064.0 CM-1	CALCULATED= 1066.7 CM-1	ERROR= -2.7 CM-1 OR -0.3 PERCENT
INTERNAL COORDINATES- 25.25 C2C3 13.47 C-O7 12.14 C-O8 9.19 C-O9 8.85 C1C2		
FORCE CONSTANTS- 41.76 CO 38.79 CCH 18.87 CCO 17.98 OCH 8.76 CCH		
OFF DIAGONAL- -8.56 SB22 -6.79 SB25 -6.49 SB26 -5.27 SB21 -5.21 SB28 -3.60 SB27 -2.02 SS18 -1.51 BB34		
NORMAL MODE 32 OBSERVED= 1053.0 CM-1	CALCULATED= 1059.6 CM-1	ERROR= -6.6 CM-1 OR -0.6 PERCENT
INTERNAL COORDINATES- 28.63 C-O8 12.36 C-O8 11.74 C5C 9.60 C-O8 5.18 C4C5		
FORCE CONSTANTS- 82.15 CO 16.18 CC 10.31 CCH 9.69 BCOH 7.04 CCH 6.52 CCO		
OFF DIAGONAL- -9.58 SB28 -7.90 SB27 -5.42 SB25 -4.07 SB26 -3.13 SB22 2.22 SB21 -1.87 BB34 -1.71 SB24		
NORMAL MODE 33 OBSERVED= 1043.0 CM-1	CALCULATED= 1041.0 CM-1	ERROR= 2.0 CM-1 OR 0.2 PERCENT
INTERNAL COORDINATES- 29.74 C-O8 20.29 C1C2 10.67 OC1 8.94 C-O8 7.45 C1OH 6.58 OCO 5.79 OCH 5.52 CCC 5.10 CCO		
FORCE CONSTANTS- 69.93 CO 25.50 CC 10.81 CCH 8.91 BCOH 6.58 CCO		
OFF DIAGONAL- -10.91 SB24 -8.16 SB28 -6.98 SS18 -5.47 SB21 -2.69 SB27 -2.27 SB26		
NORMAL MODE 34 OBSERVED= 1018.0 CM-1	CALCULATED= 1035.9 CM-1	ERROR= -17.9 CM-1 OR -1.8 PERCENT
INTERNAL COORDINATES- 21.99 C-O7 21.40 C-O9 16.69 C5C 12.42 C4C5 7.96 C1C2 6.84 C5O 5.88 C3C4 5.67 C4CC 5.47 HC3C		
FORCE CONSTANTS- 56.73 CO 41.43 CCH 16.52 CCH 12.88 CCC 9.39 OCH 8.43 BCOH 7.57 CCO		
OFF DIAGONAL- -15.98 SB21 -11.07 SB27 -7.45 SB28 -2.50 SB25 -2.00 BB34 -1.75 BB29		
NORMAL MODE 35 OBSERVED= 964.0 CM-1	CALCULATED= 978.4 CM-1	ERROR= -14.4 CM-1 OR -1.5 PERCENT
INTERNAL COORDINATES- 24.07 C5C 21.78 C-O8 9.34 C-O7 8.16 CC4H 6.76 HC3C 6.33 C1C2 5.97 C-O8 5.50 OC1		
FORCE CONSTANTS- 47.16 CO 33.94 CCH 33.93 CCH 10.33 CCO		
OFF DIAGONAL- -8.02 SB22 -5.70 SB25 -5.50 BB29 -4.93 SB26 -4.41 SB21 -3.05 SB27 -2.80 SB28 -1.84 SB24 -1.64 BB34		

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400				PAGE 2	
MOLECULE	32	6	NG-1237 ALPHA MANNOSE 400 GT		
NORMAL MODE 36	OBSERVED=	958.0 CM-1	CALCULATED=	957.6 CM-1	ERROR= 0.4 CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	24.97	C3C4 13.42 C1C2	10.80	O*CI 8.99 CC*H	7.33 C-O* 5.08 CCH2
FORCE CONSTANTS-	45.03	CCO 21.93 CCO	21.47	CCO 14.37 CCO	6.47 CCH 6.28 CCC
OFF DIAGONAL-	-10.43	SB21 -9.79 SB22	-4.14	SB27 -1.88 SB28	1.78 SB25
NORMAL MODE 37	OBSERVED=	883.0 CM-1	CALCULATED=	889.2 CM-1	ERROR= -6.2 CM-1 OR -0.7 PERCENT
INTERNAL COORDINATES-	48.30	CCO 21.93 CCO	13.89	C3C4 7.94 CCH	6.80 CC3H 5.86 CC08
FORCE CONSTANTS-	48.30	CCO 21.93 CCO	13.94	CCO 11.77 CCH	5.11 C1C2
OFF DIAGONAL-	-11.92	SB22 -8.71 SB21	7.08	SB26 3.84 SS18	3.02 HB43
NORMAL MODE 38	OBSERVED=	842.0 CM-1	CALCULATED=	825.1 CM-1	ERROR= 16.9 CM-1 OR 2.0 PERCENT
INTERNAL COORDINATES-	24.96	C3C4 14.62 CCHA	13.21	CCHB 9.50 O*CI	6.51 C3C1
FORCE CONSTANTS-	36.37	CCO 35.85 CCH	12.93	CCO 9.52 CCO	6.53 CCH
OFF DIAGONAL-	-3.75	SB25 -3.51 HB29	2.37	SS18 -2.08 SB22	1.84 HB43 -1.80 SB24 1.73 SB26
NORMAL MODE 39	OBSERVED=	814.0 CM-1	CALCULATED=	788.0 CM-1	ERROR= 26.0 CM-1 OR 3.2 PERCENT
INTERNAL COORDINATES-	12.84	O*CC 10.19 C0*C	8.86	O*CI 6.48 C3C4	5.65 C1CC 5.09 C-O9
FORCE CONSTANTS-	21.34	CCH 19.30 CCO	18.70	CCO 16.08	CCO 10.19 CCH 8.99 CCC
OFF DIAGONAL-	4.68	HB43 4.33 SB25	-4.32	SB26 -3.90 SB23	-2.54 BB34 -2.35 BB41 1.92 SS18 -1.84 SB27 -1.81 HB29
NORMAL MODE 40	OBSERVED=	685.0 CM-1	CALCULATED=	685.4 CM-1	ERROR= -0.4 CM-1 OR -0.1 PERCENT
INTERNAL COORDINATES-	16.14	O*CC 6.74 C-U7	5.55	C3C4 5.20 CCO*	5.11 CC08
FORCE CONSTANTS-	33.26	CCO 18.75 CCO	16.16	CCH 8.72 CC	6.75 CO
OFF DIAGONAL-	7.44	SB25 5.75 HB43	-3.10	SB27 -2.88 BB34	-2.73 HB29 1.82 SB21
NORMAL MODE 41	OBSERVED=	606.0 CM-1	CALCULATED=	602.5 CM-1	ERROR= 3.5 CM-1 OR 0.6 PERCENT
INTERNAL COORDINATES-	15.13	UBCC 11.11 CCO*	9.74	OCO 8.19 CC5H	7.81 HC4C
FORCE CONSTANTS-	15.13	UBCC 11.11 CCO*	10.44	CCO 9.14 CCO	6.89 CCH
OFF DIAGONAL-	-7.62	BB34 6.61 BB43	-4.31	HB29 4.08 SB24	3.11 SB25 -2.08 SB27
NORMAL MODE 42	OBSERVED=	576.0 CM-1	CALCULATED=	573.7 CM-1	ERROR= 2.3 CM-1 OR 0.4 PERCENT
INTERNAL COORDINATES-	17.60	OCO 11.58 CCO*	7.75	CC08 7.41 CCO7	7.20 O7CC 7.03 CCO*
FORCE CONSTANTS-	57.95	CCO 17.80 CCO	17.46	CCH 5.69 CO	6.67 CCHB 6.60 HC5C
OFF DIAGONAL-	-7.85	HB34 3.89 BB43	-3.58	HB29 -2.99 BB42	2.10 SB25 1.89 SB24
NORMAL MODE 43	OBSERVED=	530.0 CM-1	CALCULATED=	532.8 CM-1	ERROR= -2.8 CM-1 OR -0.5 PERCENT
INTERNAL COORDINATES-	11.24	4CO* 6.01 C2C3	6.36	CC09 6.23 C1C2	5.83 CC4H
FORCE CONSTANTS-	32.92	CCO 22.58 CCH	16.27	CCH 13.60 CCO	4.06 SS18 -3.17 BB29 -2.77 SB27 -2.65 SB26
OFF DIAGONAL-	6.01	SB22 5.53 SB25	-5.14	BB34 4.67 BB43	
NORMAL MODE 44	OBSERVED=	475.0 CM-1	CALCULATED=	468.0 CM-1	ERROR= 7.0 CM-1 OR 1.5 PERCENT
INTERNAL COORDINATES-	10.39	CO*CC 10.17 CC06	9.43	O9CC 8.46 C1CC	7.84 4CO* 7.67 C4CC 6.99 O8CC
FORCE CONSTANTS-	50.50	CCO 20.35 CCH	10.39	CCO 8.86 CCH	8.04 CC 7.19 CO
OFF DIAGONAL-	-7.08	BB34 5.19 SB22	3.58	BB43 -2.94 SB21	-2.88 BB42 -2.80 BB41 -1.93 BB37 -1.66 SB27
NORMAL MODE 45	OBSERVED=	450.0 CM-1	CALCULATED=	437.6 CM-1	ERROR= 12.3 CM-1 OR 2.7 PERCENT
INTERNAL COORDINATES-	24.99	CC06 13.36 CCO	11.29	C3CC 10.94 CCO7	8.06 C2CC
FORCE CONSTANTS-	52.14	CCO 19.25 CCO	12.12	CCO 12.12 CCO	6.75 CO
OFF DIAGONAL-	-7.66	BB34 -4.23 BB42	3.62	SB25 -2.32 BB41	-2.11 SB24
NORMAL MODE 46	OBSERVED=	398.0 CM-1	CALCULATED=	389.9 CM-1	ERROR= 8.0 CM-1 OR 2.0 PERCENT
INTERNAL COORDINATES-	14.07	O9CC 13.11 CCO	9.56	O*CC 9.11 CC08	8.53 C2CC
FORCE CONSTANTS-	49.31	CCO 16.79 CCH	13.11	OCO 7.54 CC	5.97 CCH
OFF DIAGONAL-	-4.19	BB42 -4.06 BB34	3.55	SB22 3.09 SB25	2.82 SB21
NORMAL MODE 47	OBSERVED=	373.0 CM-1	CALCULATED=	372.3 CM-1	ERROR= 0.7 CM-1 OR 0.2 PERCENT
INTERNAL COORDINATES-	24.51	CC09 11.71 CCO*	11.07	O7CC 6.84 HC4C	6.44 4CO* 5.54 C2C3
FORCE CONSTANTS-	63.52	CCO 25.63 CCH	6.77	CC	
OFF DIAGONAL-	-10.75	BB34 5.82 BB43	-5.27	BB29 3.38 SB22 -2.01	BB33 -1.63 SB26
NORMAL MODE 48	OBSERVED=	359.0 CM-1	CALCULATED=	349.3 CM-1	ERROR= 9.7 CM-1 OR 2.7 PERCENT
INTERNAL COORDINATES-	17.59	CC0* 10.85 CCO7	9.78	C4C5 7.05 4CO*	5.40 CC09
FORCE CONSTANTS-	56.10	CCO 7.09 CCO	7.21	CCH	
OFF DIAGONAL-	5.22	SB21 -9.09 BB34	3.58	SB22 -2.61 SB26 2.57	BB43 -1.70 BB42
NORMAL MODE 49	OBSERVED=	308.0 CM-1	CALCULATED=	309.0 CM-1	ERROR= -1.0 CM-1 OR -0.3 PERCENT
INTERNAL COORDINATES-	23.62	UBCC 20.96 CC08	19.34	O9CC 10.99 CC09	5.66 TH-3
FORCE CONSTANTS-	83.16	CCO 11.58 T-UH	7.40	CCH	
OFF DIAGONAL-	-9.12	BB34 -4.09 BB42	-1.52	SB21	
NORMAL MODE 50	OBSERVED=	274.0 CM-1	CALCULATED=	292.4 CM-1	ERROR= -18.4 CM-1 OR -6.7 PERCENT
INTERNAL COORDINATES-	15.20	CC07 12.82 CC08	12.47	O7CC 9.52 TH-2	
FORCE CONSTANTS-	59.54	CCO 12.92 T-UH	10.76	CCH 6.88 CCC	6.03 CC
OFF DIAGONAL-	-4.98	BB34 3.76 SB21	2.18	SB22 -1.84	SB25 -1.66 BB42 -1.53 BB33
NORMAL MODE 51	OBSERVED=	249.0 CM-1	CALCULATED=	242.5 CM-1	ERROR= 6.4 CM-1 OR 2.6 PERCENT
INTERNAL COORDINATES-	23.42	TH-5 10.83 TH-3	8.69	TH-4 7.63 CO*CC	5.73 C4CC 5.35 TH-1 5.08 O7CC
FORCE CONSTANTS-	51.83	T-OH 23.32 CCO	10.93	CCC 7.63 CCO	5.17 CCH
OFF DIAGONAL-	-2.40	BB34 -1.90 SB25	1.68	BB43	
NORMAL MODE 52	OBSERVED=	236.0 CM-1	CALCULATED=	231.7 CM-1	ERROR= 4.3 CM-1 OR 1.8 PERCENT
INTERNAL COORDINATES-	36.48	TH-1 22.30 TH-3	18.87	TH-5 5.36 TH-2	
FORCE CONSTANTS-	86.63	T-OH 9.32 CCO			
OFF DIAGONAL-	NONE				
NORMAL MODE 53	OBSERVED=	0.0 CM-1	CALCULATED=	226.4 CM-1	ERROR= 0.0 CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	38.62	TH-1 16.63 TH-5			
FORCE CONSTANTS-	76.41	T-OH 19.10 CCO			
OFF DIAGONAL-	-1.68	HB34			
NORMAL MODE 54	OBSERVED=	222.0 CM-1	CALCULATED=	220.8 CM-1	ERROR= 1.2 CM-1 OR 0.5 PERCENT
INTERNAL COORDINATES-	53.40	TH-4 17.22 TH-3	9.48	CC07 5.44 CC06	
FORCE CONSTANTS-	67.65	T-OH 24.60 CCO	6.60	CCC	
OFF DIAGONAL-	-2.62	BB34 -1.71 SB25			
NORMAL MODE 55	OBSERVED=	0.0 CM-1	CALCULATED=	217.9 CM-1	ERROR= 0.0 CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	35.95	TH-3 34.94 TH-2	15.77	TH-4	
FORCE CONSTANTS-	88.44	T-OH 11.45 CCO			
OFF DIAGONAL-	NONE				
NORMAL MODE 56	OBSERVED=	208.0 CM-1	CALCULATED=	210.8 CM-1	ERROR= -2.8 CM-1 OR -1.4 PERCENT
INTERNAL COORDINATES-	39.25	TH-2 15.21 TH-3	13.06	O7CC 8.55 TH-1	7.32 TH-4
FORCE CONSTANTS-	70.38	T-OH 20.85 CCO	6.09	CCH	
OFF DIAGONAL-	-1.74	BB33 -1.71 BB34			
NORMAL MODE 57	OBSERVED=	196.0 CM-1	CALCULATED=	189.4 CM-1	ERROR= 6.6 CM-1 OR 3.3 PERCENT
INTERNAL COORDINATES-	28.21	CC0* 13.24 TH-5	12.65	C4CC 6.88 CCO	6.30 TCC5 6.29 CCO*
FORCE CONSTANTS-	51.73	CCO 16.75 CCO	11.97	T-OH 8.57 T-OH	6.68 CCO 6.56 CCH
OFF DIAGONAL-	-4.75	BB34 -3.50 BB42	-2.74	BB33 -2.22 SB25 -1.67	SB21 1.53 BB41
NORMAL MODE 58	OBSERVED=	0.0 CM-1	CALCULATED=	132.8 CM-1	ERROR= 0.0 CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	19.49	CO*CC 11.98 C4CC	13.42	CCO 10.02 T-CC	9.19 T-CO
FORCE CONSTANTS-	27.24	CCC 19.09 CCO	2.19	SB22 -2.07 BB37	2.02 BB41
OFF DIAGONAL-	-3.98	SB21 3.42 BB43			
NORMAL MODE 59	OBSERVED=	0.0 CM-1	CALCULATED=	102.5 CM-1	ERROR= 0.0 CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	58.83	ICC5 7.28 C3CC	6.02	O9CC	
FORCE CONSTANTS-	68.19	T-CC 16.22 CCO	13.50	CCC	
OFF DIAGONAL-	-2.81	BB34 -2.60 SB25	-1.67	BB42	
NORMAL MODE 60	OBSERVED=	0.0 CM-1	CALCULATED=	82.6 CM-1	ERROR= 0.0 CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	26.34	C2CC 10.24 C1CC	8.83	CO*CC 8.18	5.95 TCC4 5.56 O8CC 5.55 CC08 5.00 C3CC
FORCE CONSTANTS-	42.83	CCC 23.48 T-CC	15.81	CCO 8.83 CCO	6.10 T-CO
OFF DIAGONAL-	-3.62	SB25 3.27 BB42	-2.36	SB41 -2.13 SB21	
NORMAL MODE 61	OBSERVED=	0.0 CM-1	CALCULATED=	64.3 CM-1	ERROR= 0.0 CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	27.03	TCC5 21.35 C3CC	8.17	TCC4 7.46 TCC2	7.20 TCC3 6.16 4CO* 5.51 O*CC
FORCE CONSTANTS-	50.67	T-OH 21.65 CCO	19.89	CCC	
OFF DIAGONAL-	-2.36	BB42 -1.60 BB34			

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400									
MOLECULE 33 -6 NG-1237 ALPHA MANNOSE-1-D GT									
PAGE 1									
NORMAL MODE 8	OBSERVED=	1456.0	CM-1	CALCULATED=	1449.6	CM-1	ERROR=	6.4	CM-1 OR 0.4 PERCENT
INTERNAL COORDINATES-	62.00	HCH	19.99	OC4H	19.18	OC4A			
FORCE CONSTANTS-	62.00	HCH	39.45	UCH					
OFF DIAGONAL-	-3.85	SB27							
NORMAL MODE 9	OBSERVED=	1435.0	CM-1	CALCULATED=	1426.1	CM-1	ERROR=	8.9	CM-1 OR 0.6 PERCENT
INTERNAL COORDINATES-	42.19	C3OH	14.51	C4OH	6.78	OC4H			
FORCE CONSTANTS-	57.77	BCOH	15.94	CCH	10.69	OCB	8.44	CC	5.36
OFF DIAGONAL-	-3.63	SB26	3.60	SB28	3.51	BB36	-3.25	SB27	2.14
								2.01	BB34 -1.94
								SB25	-1.90
								BB43	
NORMAL MODE 10	OBSERVED=	1422.0	CM-1	CALCULATED=	1412.5	CM-1	ERROR=	9.5	CM-1 OR 0.7 PERCENT
INTERNAL COORDINATES-	20.43	C3OH	13.31	OC4H	8.31	OC3H	7.60	C4OH	6.41
FORCE CONSTANTS-	36.24	BCOH	27.44	UCH	22.42	CCH	7.30	CO	
OFF DIAGONAL-	-6.62	SB27	4.93	SB28	4.12	BB29	2.36	BB34	-2.69
								SB26	-2.49
								SB25	-2.35
								BB39	-1.95
								BB45	
NORMAL MODE 11	OBSERVED=	0.0	CM-1	CALCULATED=	1401.4	CM-1	ERROR=	0.0	CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	34.44	C2OH	30.73	C1OH	9.24	C3OH	5.55	C1C2	5.23
FORCE CONSTANTS-	74.74	BCOH	8.55	UCH	7.49	CC	5.58	CCH	
OFF DIAGONAL-	5.64	SB28	-2.63	SB27	-2.37	SB26	-1.91	BB39	
NORMAL MODE 12	OBSERVED=	1395.0	CM-1	CALCULATED=	1391.6	CM-1	ERROR=	3.4	CM-1 OR 0.2 PERCENT
INTERNAL COORDINATES-	55.56	C1CH	25.38	C2OH	7.17	OC2H			
FORCE CONSTANTS-	81.87	BCOH	8.62	UCH					
OFF DIAGONAL-	-1.66	BB39	-1.58	SB27					
NORMAL MODE 13	OBSERVED=	0.0	CM-1	CALCULATED=	1389.2	CM-1	ERROR=	0.0	CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	79.95	C*OH	6.86	GCHB	5.16	C5C*	5.16	CCHB	
FORCE CONSTANTS-	80.30	BCOH	10.37	CCH	7.99	OCB	5.43	CC	
OFF DIAGONAL-	-3.99	SB26	-2.77	BB39	2.29	SB28			
NORMAL MODE 14	OBSERVED=	1380.0	CM-1	CALCULATED=	1373.1	CM-1	ERROR=	6.9	CM-1 OR 0.5 PERCENT
INTERNAL COORDINATES-	60.23	C4CH	9.75	C5H	6.96	CC5H	6.32	HC4C	
FORCE CONSTANTS-	63.40	BCOH	20.62	CCH	12.43	GCH			
OFF DIAGONAL-	-3.32	BB29	-2.82	BB36	-2.22	SB27	-1.70	SB26	
NORMAL MODE 15	OBSERVED=	1358.0	CM-1	CALCULATED=	1359.4	CM-1	ERROR=	-1.4	CM-1 OR -0.1 PERCENT
INTERNAL COORDINATES-	19.02	HC3C	14.95	OC3H	9.75	HC5C	4.62	CC4H	8.90
FORCE CONSTANTS-	51.86	CCH	32.68	UCH	7.81	BCOH	5.41	CO	
OFF DIAGONAL-	10.56	BB29	-5.70	SB27	-4.01	SB26	-3.53	BB45	2.45
								BB34	
NORMAL MODE 16	OBSERVED=	1330.0	CM-1	CALCULATED=	1336.2	CM-1	ERROR=	-6.2	CM-1 OR -0.5 PERCENT
INTERNAL COORDINATES-	17.52	HC5C	16.72	CCHB	9.52	CC5H	6.29	OC3H	6.26
FORCE CONSTANTS-	66.42	CCH	14.69	UCH	6.67	BCOH	6.46	CO	
OFF DIAGONAL-	13.91	BB29	-8.08	SB26	-3.49	BB45	-1.18	SB27	
NORMAL MODE 17	OBSERVED=	1318.0	CM-1	CALCULATED=	1323.4	CM-1	ERROR=	-5.4	CM-1 OR -0.4 PERCENT
INTERNAL COORDINATES-	27.37	CC2H	17.56	C2OH	13.08	OC2H	16.02	O*Cl	6.89
FORCE CONSTANTS-	37.16	CCH	24.93	UCH	23.29	OCB	17.77	BCOH	7.30
OFF DIAGONAL-	-7.70	SB27	-4.83	SB25	3.07	BB34	-2.53	BB45	2.34
								BB33	-1.63
								SB28	1.61
								BB29	-1.56
								SB26	1.54
								BB39	
NORMAL MODE 18	OBSERVED=	1305.0	CM-1	CALCULATED=	1298.2	CM-1	ERROR=	6.8	CM-1 OR 0.5 PERCENT
INTERNAL COORDINATES-	21.85	OC4A	21.61	GCHB	13.57	OC4H	12.47	HC2C	5.50
FORCE CONSTANTS-	50.17	CCH	41.84	UCH	6.02	BCOH			
OFF DIAGONAL-	-3.72	BB45	-3.68	SB27	-1.53	SB26			
NORMAL MODE 19	OBSERVED=	1288.0	CM-1	CALCULATED=	1295.4	CM-1	ERROR=	-7.4	CM-1 OR -0.6 PERCENT
INTERNAL COORDINATES-	21.09	HC2C	20.59	OC3H	11.64	CC3H	9.81	OC2H	
FORCE CONSTANTS-	45.93	CCH	38.93	UCH	8.66	BCOH			
OFF DIAGONAL-	-3.51	BB45	1.60	BB39					
NORMAL MODE 20	OBSERVED=	0.0	CM-1	CALCULATED=	1280.3	CM-1	ERROR=	0.0	CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	35.75	C5OH	10.51	OC4A	9.61	CC5H			
FORCE CONSTANTS-	63.45	UCH	27.17	CCH	9.19	OC4H	9.04	CC4A	6.56
OFF DIAGONAL-	6.17	SB27	-3.51	BB45	-3.33	BB29			
NORMAL MODE 21	OBSERVED=	1255.0	CM-1	CALCULATED=	1268.3	CM-1	ERROR=	-13.3	CM-1 OR -1.1 PERCENT
INTERNAL COORDINATES-	18.88	CC4H	16.15	OC3H	11.43	OC2H	10.80	CC3H	6.79
FORCE CONSTANTS-	45.96	CCH	41.04	UCH					
OFF DIAGONAL-	4.79	SB27	-3.59	BB45	2.27	BB34			
NORMAL MODE 22	OBSERVED=	1226.0	CM-1	CALCULATED=	1240.8	CM-1	ERROR=	-14.8	CM-1 OR -1.2 PERCENT
INTERNAL COORDINATES-	16.58	OC4H	13.62	CC3H	8.59	HC3C	7.31	HC5C	6.95
FORCE CONSTANTS-	45.37	CCH	31.19	UCH	11.55	CO	5.22	CCO	
OFF DIAGONAL-	7.58	SB27	-5.18	BB29	3.68	BB34	-3.54	SB25	-3.08
								BB45	-2.39
								SB26	
NORMAL MODE 23	OBSERVED=	1212.0	CM-1	CALCULATED=	1199.2	CM-1	ERROR=	12.8	CM-1 OR 1.1 PERCENT
INTERNAL COORDINATES-	12.46	OCBH	11.79	HC5C	11.12	CC5H	8.44	CC4H	8.02
FORCE CONSTANTS-	54.02	CCH	22.31	UCH	15.32	CCO	9.43	CCO	5.22
OFF DIAGONAL-	-9.64	BB29	-5.18	SB25	4.96	SB27	4.69	BB34	-2.72
								BB45	-2.04
								SB28	
NORMAL MODE 24	OBSERVED=	1170.0	CM-1	CALCULATED=	1166.3	CM-1	ERROR=	3.7	CM-1 OR 0.3 PERCENT
INTERNAL COORDINATES-	34.36	C5OH	11.50	OC4A	10.98	OCBH	5.67	C*OH	
FORCE CONSTANTS-	48.72	CO	31.62	UCH	13.27	CCH	12.41	CCO	5.54
OFF DIAGONAL-	-10.31	SB25	-2.53	SB28					
NORMAL MODE 25	OBSERVED=	1155.0	CM-1	CALCULATED=	1159.3	CM-1	ERROR=	-4.3	CM-1 OR -0.4 PERCENT
INTERNAL COORDINATES-	22.25	C*OH	20.43	O*Cl	11.27	CC2H	8.06	OC2H	6.64
FORCE CONSTANTS-	48.14	CO	23.81	UCH	23.77	CCH	17.02	CC	16.50
OFF DIAGONAL-	-10.94	SB27	-6.75	SB25	-5.05	SB26	-4.31	SB22	-3.36
								SB28	-2.86
								SB21	-2.10
								BB43	-1.95
								SB23	-1.54
								BB45	
NORMAL MODE 26	OBSERVED=	1130.0	CM-1	CALCULATED=	1121.5	CM-1	ERROR=	8.5	CM-1 OR 0.8 PERCENT
INTERNAL COORDINATES-	27.94	C4C5	13.40	C2C3	12.86	C*OH	9.69	C5C*	7.28
FORCE CONSTANTS-	56.73	CO	26.74	CO	22.00	CCO	11.40	UCH	8.01
OFF DIAGONAL-	-10.62	SB22	-6.08	SB26	-5.88	SB25	-5.04	SB28	-1.96
								SB21	-1.95
								SS17	-1.87
								SS18	-1.76
								SB27	
NORMAL MODE 27	OBSERVED=	1110.0	CM-1	CALCULATED=	1114.0	CM-1	ERROR=	-4.0	CM-1 OR -0.4 PERCENT
INTERNAL COORDINATES-	25.33	C2C3	21.77	C*OH	10.85	C3C4	10.00	C1C2	6.03
FORCE CONSTANTS-	47.89	CCH	27.77	UCH	17.07	CCO	7.88	UCH	6.05
OFF DIAGONAL-	-12.35	SB22	-3.88	SB25	1.93	SS18	-1.87	SS17	
NORMAL MODE 28	OBSERVED=	1090.0	CM-1	CALCULATED=	1099.3	CM-1	ERROR=	-9.3	CM-1 OR -0.8 PERCENT
INTERNAL COORDINATES-	24.11	C5C*	19.70	C*OH	12.01	C*OH	7.29	C3C4	6.61
FORCE CONSTANTS-	50.06	CO	43.42	UCH	9.15	UCH	9.58	CO	6.43
OFF DIAGONAL-	-5.77	SB22	-5.67	SS18	-4.92	SB28	-4.23	SB27	-2.45
								SB26	-1.68
								SB25	
NORMAL MODE 29	OBSERVED=	1080.0	CM-1	CALCULATED=	1080.9	CM-1	ERROR=	-0.9	CM-1 OR -0.1 PERCENT
INTERNAL COORDINATES-	25.85	CO	38.35	C*OH	22.94	C4C5	10.92	C2C3	8.51
FORCE CONSTANTS-	62.13	CO	38.32	CC	11.86	CCO	10.96	BCOH	9.91
OFF DIAGONAL-	-10.02	SB27	-9.80	SB21	-8.77	SB28	-7.54	SS18	-6.06
								SB25	-2.54
								SB22	-2.05
								BB36	
NORMAL MODE 30	OBSERVED=	1065.0	CM-1	CALCULATED=	1060.1	CM-1	ERROR=	4.9	CM-1 OR 0.5 PERCENT
INTERNAL COORDINATES-	64.49	C*OH	9.76	C*OH	7.46	C4C5			
FORCE CONSTANTS-	77.80	CO	9.80	CCO	9.00	CC	6.91	CCH	5.91
OFF DIAGONAL-	-6.89	SB28	-6.58	SB25	-5.22	SB27	-3.77	SB22	2.78
								SB21	-1.64
								SB26	
NORMAL MODE 31	OBSERVED=	1045.0	CM-1	CALCULATED=	1041.6	CM-1	ERROR=	3.4	CM-1 OR 0.3 PERCENT
INTERNAL COORDINATES-	38.88	C*OH	28.39	C1C2	9.95	O*Cl	8.88	C1OH	6.80
FORCE CONSTANTS-	68.22	CO	34.36	CC	15.13	CCH	11.26	UCH	9.98
OFF DIAGONAL-	-9.42	SB24	-8.34	SB27	-7.89	SS18	-7.84	SB28	-6.30
								SB21	-4.59
								SB26	-3.70
								SB22	2.08
								SB25	-1.85
								BB43	

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400									
MOLECULE 33 -6 NG=1237 ALPHA MANNOS-1-D GT									
PAGE 2									
NORMAL MODE 36	OBSERVED=	930.0 CM-1	CALCULATED=	930.6 CM-1	ERROR=	-0.6 CM-1	OR	-0.1 PERCENT	
INTERNAL COORDINATES-	20.72	C-07	19.70	C3C4	16.11	CC1H	10.28	OC1H	7.02
FORCE CONSTANTS-	36.00	CCH	29.98	CC	21.05	CC	20.09	OCH	8.69
OFF DIAGONAL-	-6.08	SB27	-5.25	SB21	-5.21	SB22	-2.54	BB34	-2.02
NORMAL MODE 37	OBSERVED=	864.0 CM-1	CALCULATED=	863.7 CM-1	ERROR=	-0.3 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	21.55	C2C3	9.74	CC1H	9.26	CC08	8.97	CC09	8.24
FORCE CONSTANTS-	33.91	CC	23.50	CCO	20.42	CCH	11.01	OCH	9.59
OFF DIAGONAL-	-7.96	SB22	-7.01	SB21	6.95	SB26	3.11	BB43	-2.86
NORMAL MODE 38	OBSERVED=	818.0 CM-1	CALCULATED=	809.4 CM-1	ERROR=	-8.6 CM-1	OR	1.0 PERCENT	
INTERNAL COORDINATES-	23.41	C5O1	12.12	CCHA	10.82	CC0H	7.13	CC1H	7.09
FORCE CONSTANTS-	33.25	CC	28.74	CCCH	13.23	CC	11.10	OCH	10.70
OFF DIAGONAL-	-4.18	SB29	-2.76	BB29	2.28	SS18	2.28	BB43	-1.54
NORMAL MODE 39	OBSERVED=	790.0 CM-1	CALCULATED=	771.6 CM-1	ERROR=	-18.4 CM-1	OR	2.3 PERCENT	
INTERNAL COORDINATES-	12.83	CC1H	9.33	C*CC	8.25	CC0C	6.91	O*CC	6.88
FORCE CONSTANTS-	32.37	CCH	17.73	CC	17.40	CCO	15.03	CC	8.95
OFF DIAGONAL-	-5.52	SB26	-3.85	SB23	3.80	BB43	-3.29	BB34	-2.76
NORMAL MODE 40	OBSERVED=	670.0 CM-1	CALCULATED=	677.3 CM-1	ERROR=	-7.3 CM-1	OR	-1.1 PERCENT	
INTERNAL COORDINATES-	13.04	O7CC	6.52	C-07	11.23	CC0H	5.73	CC1H	5.72
FORCE CONSTANTS-	31.37	CCO	19.85	CCH	15.64	CC	7.78	CC	5.72
OFF DIAGONAL-	7.74	SB25	5.74	BB43	-3.25	BB34	-3.00	BB29	-2.88
NORMAL MODE 41	OBSERVED=	0.0 CM-1	CALCULATED=	601.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	14.45	O8CC	11.09	CCU	10.10	CCO*	7.84	CC5H	7.53
FORCE CONSTANTS-	43.18	CCO	19.69	CCH	11.09	OC01	10.50	CCO	6.59
OFF DIAGONAL-	-6.92	BB34	6.46	BB43	4.35	SB24	-4.08	BB29	3.06
NORMAL MODE 42	OBSERVED=	0.0 CM-1	CALCULATED=	563.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	15.62	UCO	12.76	CCO*	7.63	O7CC	7.54	HC5C	6.97
FORCE CONSTANTS-	55.45	CCO	20.74	CCH	15.62	CCO	6.05	CC	6.05
OFF DIAGONAL-	-8.72	BB34	5.11	BB43	-4.11	BB29	3.53	SB25	-2.18
NORMAL MODE 43	OBSERVED=	0.0 CM-1	CALCULATED=	526.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	9.84	CCO*	9.53	C2C3	6.90	C1C2	6.33	CC09	5.14
FORCE CONSTANTS-	32.77	CCO	24.52	CC	18.27	CC	12.65	CC	8.95
OFF DIAGONAL-	-5.19	SB22	-5.04	BB34	4.54	BB43	4.20	SB25	3.94
NORMAL MODE 44	OBSERVED=	0.0 CM-1	CALCULATED=	466.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	50.41	CCO	20.05	CCC	10.30	CDC	8.93	CCH	8.08
FORCE CONSTANTS-	50.41	CCO	20.05	CCC	10.30	CDC	8.93	CCH	8.08
OFF DIAGONAL-	-7.16	BB34	5.14	SB22	3.43	BB43	-2.98	SB21	-2.87
NORMAL MODE 45	OBSERVED=	0.0 CM-1	CALCULATED=	436.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	23.09	CC06	13.06	CCU	11.23	CCO7	11.02	C3CC	7.79
FORCE CONSTANTS-	52.60	CCO	24.42	CCC	13.06	CCO	12.37	CCH	6.80
OFF DIAGONAL-	-7.75	BB34	-4.20	BB42	3.74	SB25	-2.30	BB41	-2.18
NORMAL MODE 46	OBSERVED=	0.0 CM-1	CALCULATED=	382.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	14.38	U9CC	12.57	CCU	9.59	O1CC	9.37	CC08	8.68
FORCE CONSTANTS-	49.61	CCO	17.17	CCG	12.57	OC01	7.47	CC	6.06
OFF DIAGONAL-	-4.22	BB34	-4.18	BB42	3.44	SB27	3.12	SB25	2.88
NORMAL MODE 47	OBSERVED=	0.0 CM-1	CALCULATED=	371.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	24.09	CC09	11.64	CCO*	11.13	O7CC	6.84	HC4C	6.60
FORCE CONSTANTS-	51.31	CCO	25.41	CCH	6.64	CC	6.42	CCO*	5.42
OFF DIAGONAL-	-10.66	BB34	5.80	BB43	-5.22	BB29	3.39	SB22	-1.99
NORMAL MODE 48	OBSERVED=	0.0 CM-1	CALCULATED=	347.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	55.88	CCO	17.13	CC	9.78	C4C5	7.03	4C0*	5.78
FORCE CONSTANTS-	55.88	CCO	17.13	CC	9.78	C4C5	7.03	4C0*	5.78
OFF DIAGONAL-	-5.38	BB34	5.19	SB21	3.44	SB22	-2.57	SB26	2.53
NORMAL MODE 49	OBSERVED=	0.0 CM-1	CALCULATED=	309.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	24.64	O8CC	20.92	CC08	19.64	O9CC	11.05	CC09	5.66
FORCE CONSTANTS-	83.24	CCO	11.60	T-OH	7.37	CCH	7.37	CCH	7.37
OFF DIAGONAL-	-9.11	BB34	-4.10	BB42	-1.51	SB21			
NORMAL MODE 50	OBSERVED=	0.0 CM-1	CALCULATED=	292.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	15.39	CCO7	12.79	CC08	12.67	O7CC	9.69	TH-2	7.47
FORCE CONSTANTS-	59.62	CCO	13.04	T-UH	10.98	CCH	6.84	CCG	5.84
OFF DIAGONAL-	-5.09	BB34	3.68	SB21	2.96	BB43	2.14	SB22	-1.84
NORMAL MODE 51	OBSERVED=	0.0 CM-1	CALCULATED=	242.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	24.91	TH-5	11.08	TH-3	8.68	TH-4	7.48	COYC	5.66
FORCE CONSTANTS-	52.24	CCO	22.54	CCO	10.67	CCO	7.48	COC	5.02
OFF DIAGONAL-	-2.35	BB34	-1.83	SB25	1.65	BB43			
NORMAL MODE 52	OBSERVED=	0.0 CM-1	CALCULATED=	231.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	36.42	TH-1	22.97	TH-3	18.68	TH-5			
FORCE CONSTANTS-	86.96	T-UH	9.10	CCO					
OFF DIAGONAL-	NONE								
NORMAL MODE 53	OBSERVED=	0.0 CM-1	CALCULATED=	226.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	39.27	TH-1	35.50	TH-5					
FORCE CONSTANTS-	76.08	T-OH	15.31	CCO					
OFF DIAGONAL-	-1.72	BB34							
NORMAL MODE 54	OBSERVED=	0.0 CM-1	CALCULATED=	220.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	54.17	TH-4	6.44	CCO7	6.14	TH-3	5.58	CC06	
FORCE CONSTANTS-	66.90	T-OH	25.25	CCO	6.80	CCC			
OFF DIAGONAL-	-2.12	BB34	-1.76	SB25					
NORMAL MODE 55	OBSERVED=	0.0 CM-1	CALCULATED=	217.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	35.98	TH-3	35.67	TH-2	14.64	TH-4			
FORCE CONSTANTS-	88.12	T-OH	11.69	CCO					
OFF DIAGONAL-	-1.53	BB34							
NORMAL MODE 56	OBSERVED=	0.0 CM-1	CALCULATED=	210.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	39.18	TH-2	15.23	TH-3	13.23	O7CC	8.22	TH-1	7.47
FORCE CONSTANTS-	70.13	T-OH	11.77	CCO	6.14	CCC			
OFF DIAGONAL-	-1.77	BB33	-1.73	BB34	-1.53	SB25			
NORMAL MODE 57	OBSERVED=	0.0 CM-1	CALCULATED=	189.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	28.50	CCO*	13.09	TH-5	12.83	C4C5	6.75	O1CC	6.42
FORCE CONSTANTS-	51.62	CCO	16.83	CCC	15.77	T-UH	8.72	T-CC	6.75
OFF DIAGONAL-	-4.75	BB34	-3.50	BB42	-2.74	BB33	-2.16	SB25	-1.65
NORMAL MODE 58	OBSERVED=	0.0 CM-1	CALCULATED=	132.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	19.28	COYC	18.96	C4CC	8.76	TCC4	6.14	C1CC	5.69
FORCE CONSTANTS-	27.27	CCC	19.28	COC	13.36	CCO	9.96	T-CC	9.27
OFF DIAGONAL-	-4.05	SB21	3.41	BB43	2.18	SB22	-2.12	BB37	2.04
NORMAL MODE 59	OBSERVED=	0.0 CM-1	CALCULATED=	102.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	58.93	TCC5	7.19	C3CC	5.99	O9CC			
FORCE CONSTANTS-	68.27	T-CC	16.21	CCO	13.34	CCC			
OFF DIAGONAL-	-2.82	BB34	-2.58	SB25	-1.65	BB42			
NORMAL MODE 60	OBSERVED=	0.0 CM-1	CALCULATED=	82.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	26.34	C2CC	10.27	C1CC	8.80	TCC1	8.78	COYC	8.20
FORCE CONSTANTS-	42.93	CCC	23.55	T-CC	19.81	CCO	8.78	COC	6.07
OFF DIAGONAL-	-3.62	SB25	-3.27	BB42	2.36	BB41	-2.14	SB21	
NORMAL MODE 61	OBSERVED=	0.0 CM-1	CALCULATED=	64.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	26.80	TCC5	13.33	C3CC	8.80	TCC4	7.44	TCC2	7.22
FORCE CONSTANTS-	50.58	T-CC	21.70	CCO	19.95	CCC			
OFF DIAGONAL-	-2.37	BB42	-1.61	BB34					

30. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 7.13

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400										PAGE 1	
MOLCULE 34											
NORMAL MODE 8											
INTERNAL COORDINATES-											
FORCE CONSTANTS-											
OFF DIAGONAL-											
OBSERVED= 1460.0 CM-1										CALCULATED= 1450.2 CM-1	
60.53 HCH 20.63 OCH										ERROR= 9.8 CM-1 OR 0.7 PERCENT	
-4.23 SB27											
NORMAL MODE 9											
INTERNAL COORDINATES-											
FORCE CONSTANTS-											
OFF DIAGONAL-											
OBSERVED= 1422.0 CM-1										CALCULATED= 1426.1 CM-1	
60.53 HCH 20.63 OCH										ERROR= -4.1 CM-1 OR -0.3 PERCENT	
-3.71 SB27											
NORMAL MODE 10											
INTERNAL COORDINATES-											
FORCE CONSTANTS-											
OFF DIAGONAL-											
OBSERVED= 1400.0 CM-1										CALCULATED= 1415.1 CM-1	
60.53 HCH 20.63 OCH										ERROR= 0.0 CM-1 OR 0.0 PERCENT	
-3.71 SB27											
NORMAL MODE 11											
INTERNAL COORDINATES-											
FORCE CONSTANTS-											
OFF DIAGONAL-											
OBSERVED= 1400.0 CM-1										CALCULATED= 1407.9 CM-1	
60.53 HCH 20.63 OCH										ERROR= -7.9 CM-1 OR -0.6 PERCENT	
-3.71 SB27											
NORMAL MODE 12											
INTERNAL COORDINATES-											
FORCE CONSTANTS-											
OFF DIAGONAL-											
OBSERVED= 1395.0 CM-1										CALCULATED= 1396.7 CM-1	
60.53 HCH 20.63 OCH										ERROR= -1.7 CM-1 OR -0.1 PERCENT	
-3.71 SB27											
NORMAL MODE 13											
INTERNAL COORDINATES-											
FORCE CONSTANTS-											
OFF DIAGONAL-											
OBSERVED= 1391.0 CM-1										CALCULATED= 1394.2 CM-1	
60.53 HCH 20.63 OCH										ERROR= -3.2 CM-1 OR -0.2 PERCENT	
-3.71 SB27											
NORMAL MODE 14											
INTERNAL COORDINATES-											
FORCE CONSTANTS-											
OFF DIAGONAL-											
OBSERVED= 1380.0 CM-1										CALCULATED= 1389.0 CM-1	
60.53 HCH 20.63 OCH										ERROR= -9.0 CM-1 OR -0.6 PERCENT	
-3.71 SB27											
NORMAL MODE 15											
INTERNAL COORDINATES-											
FORCE CONSTANTS-											
OFF DIAGONAL-											
OBSERVED= 1372.0 CM-1										CALCULATED= 1371.1 CM-1	
60.53 HCH 20.63 OCH										ERROR= 0.9 CM-1 OR 0.1 PERCENT	
-3.71 SB27											
NORMAL MODE 16											
INTERNAL COORDINATES-											
FORCE CONSTANTS-											
OFF DIAGONAL-											
OBSERVED= 1359.0 CM-1										CALCULATED= 1353.0 CM-1	
60.53 HCH 20.63 OCH										ERROR= 6.0 CM-1 OR 0.4 PERCENT	
-3.71 SB27											
NORMAL MODE 17											
INTERNAL COORDINATES-											
FORCE CONSTANTS-											
OFF DIAGONAL-											
OBSERVED= 1333.0 CM-1										CALCULATED= 1330.7 CM-1	
60.53 HCH 20.63 OCH										ERROR= 2.3 CM-1 OR 0.2 PERCENT	
-4.00 SB27											
NORMAL MODE 18											
INTERNAL COORDINATES-											
FORCE CONSTANTS-											
OFF DIAGONAL-											
OBSERVED= 1327.0 CM-1										CALCULATED= 1319.1 CM-1	
60.53 HCH 20.63 OCH										ERROR= 7.9 CM-1 OR 0.6 PERCENT	
-3.58 SB45											
NORMAL MODE 19											
INTERNAL COORDINATES-											
FORCE CONSTANTS-											
OFF DIAGONAL-											
OBSERVED= 1313.0 CM-1										CALCULATED= 1315.8 CM-1	
60.53 HCH 20.63 OCH										ERROR= -2.8 CM-1 OR -0.2 PERCENT	
-4.45 SB25											
NORMAL MODE 20											
INTERNAL COORDINATES-											
FORCE CONSTANTS-											
OFF DIAGONAL-											
OBSERVED= 1293.0 CM-1										CALCULATED= 1294.9 CM-1	
60.53 HCH 20.63 OCH										ERROR= -1.9 CM-1 OR -0.1 PERCENT	
-3.90 SB45											
NORMAL MODE 21											
INTERNAL COORDINATES-											
FORCE CONSTANTS-											
OFF DIAGONAL-											
OBSERVED= 1280.0 CM-1										CALCULATED= 1282.8 CM-1	
60.53 HCH 20.63 OCH										ERROR= -2.8 CM-1 OR -0.2 PERCENT	
-3.26 SB45											
NORMAL MODE 22											
INTERNAL COORDINATES-											
FORCE CONSTANTS-											
OFF DIAGONAL-											
OBSERVED= 1274.0 CM-1										CALCULATED= 1266.8 CM-1	
60.53 HCH 20.63 OCH										ERROR= 7.2 CM-1 OR 0.6 PERCENT	
-3.71 SB45											
NORMAL MODE 23											
INTERNAL COORDINATES-											
FORCE CONSTANTS-											
OFF DIAGONAL-											
OBSERVED= 1255.0 CM-1										CALCULATED= 1260.1 CM-1	
60.53 HCH 20.63 OCH										ERROR= -5.1 CM-1 OR -0.4 PERCENT	
-3.17 SB45											
NORMAL MODE 24											
INTERNAL COORDINATES-											
FORCE CONSTANTS-											
OFF DIAGONAL-											
OBSERVED= 1240.0 CM-1										CALCULATED= 1234.0 CM-1	
60.53 HCH 20.63 OCH										ERROR= 6.0 CM-1 OR 0.5 PERCENT	
-6.82 SB27											
NORMAL MODE 25											
INTERNAL COORDINATES-											
FORCE CONSTANTS-											
OFF DIAGONAL-											
OBSERVED= 1210.0 CM-1										CALCULATED= 1154.1 CM-1	
60.53 HCH 20.63 OCH										ERROR= 19.0 CM-1 OR 1.6 PERCENT	
-8.66 SB29											
NORMAL MODE 26											
INTERNAL COORDINATES-											
FORCE CONSTANTS-											
OFF DIAGONAL-											
OBSERVED= 1169.0 CM-1										CALCULATED= 1191.0 CM-1	
60.53 HCH 20.63 OCH										ERROR= 14.9 CM-1 OR 1.3 PERCENT	
-7.66 SB22											
NORMAL MODE 27											
INTERNAL COORDINATES-											
FORCE CONSTANTS-											
OFF DIAGONAL-											
OBSERVED= 1140.0 CM-1										CALCULATED= 1146.3 CM-1	
60.53 HCH 20.63 OCH										ERROR= -6.3 CM-1 OR -0.5 PERCENT	
-11.98 SB25											
NORMAL MODE 28											
INTERNAL COORDINATES-											
FORCE CONSTANTS-											
OFF DIAGONAL-											
OBSERVED= 1115.0 CM-1										CALCULATED= 1120.6 CM-1	
60.53 HCH 20.63 OCH										ERROR= -5.6 CM-1 OR -0.5 PERCENT	
-14.26 SB22											
NORMAL MODE 29											
INTERNAL COORDINATES-											
FORCE CONSTANTS-											
OFF DIAGONAL-											
OBSERVED= 1103.0 CM-1										CALCULATED= 1103.2 CM-1	
60.53 HCH 20.63 OCH										ERROR= -0.2 CM-1 OR -0.0 PERCENT	
-6.16 SB22											
NORMAL MODE 30											
INTERNAL COORDINATES-											
FORCE CONSTANTS-											
OFF DIAGONAL-											
OBSERVED= 1083.0 CM-1										CALCULATED= 1086.5 CM-1	
60.53 HCH 20.63 OCH										ERROR= -3.5 CM-1 OR -0.3 PERCENT	
-5.13 SB18											
NORMAL MODE 31											
INTERNAL COORDINATES-											
FORCE CONSTANTS-											
OFF DIAGONAL-											
OBSERVED= 1064.0 CM-1										CALCULATED= 1064.7 CM-1	
60.53 HCH 20.63 OCH										ERROR= -0.7 CM-1 OR -0.1 PERCENT	
-8.09 SB22											
NORMAL MODE 32											
INTERNAL COORDINATES-											
FORCE CONSTANTS-											
OFF DIAGONAL-											
OBSERVED= 1052.0 CM-1										CALCULATED= 1050.0 CM-1	
60.53 HCH 20.63 OCH										ERROR= 2.0 CM-1 OR 0.2 PERCENT	
-13.20 SB21											
NORMAL MODE 33											
INTERNAL COORDINATES-											
FORCE CONSTANTS-											
OFF DIAGONAL-											
OBSERVED= 1043.0 CM-1										CALCULATED= 1043.8 CM-1	
60.53 HCH 20.63 OCH										ERROR= -0.8 CM-1 OR -0.1 PERCENT	
-10.42 SB24											
NORMAL MODE 34											
INTERNAL COORDINATES-											
FORCE CONSTANTS-											
OFF DIAGONAL-											
OBSERVED= 1018.0 CM-1										CALCULATED= 1007.1 CM-1	
60.53 HCH 20.63 OCH										ERROR= 10.9 CM-1 OR 1.1 PERCENT	
-63.19 SB22											
NORMAL MODE 35											
INTERNAL COORDINATES-											
FORCE CONSTANTS-											
OFF DIAGONAL-											
OBSERVED= 958.0 CM-1										CALCULATED= 983.5 CM-1	
60.53 HCH 20.63 OCH										ERROR= -25.5 CM-1 OR -2.7 PERCENT	
-6.65 SB22											

TABLE XXXIV (Continued)

COUNDED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400											PAGE 2
MOLULE 34 -6 NG=1237 ALPHA MANNOSE GG											
NORMAL MODE 36	OBSERVED=	915.0 CM-1	CALCULATED=	913.1 CM-1	ERROR=	0.9 CM-1	OR	0.1 PERCENT			
INTERNAL COORDINATES=	30.91	C20 18.23 C5C	16.00 CCM	6.93 CCH	6.38 CCO						
FORCE CONSTANTS=	43.32	C20 18.23 C5C	16.00 CCM	6.93 CCH	6.38 CCO						
OFF DIAGONAL=	-10.21	S821 -6.22 SB27	5.69 SB26	-5.69 SB22	2.21 SS18	1.76 BB43					
NORMAL MODE 37	OBSERVED=	883.0 CM-1	CALCULATED=	891.5 CM-1	ERROR=	-8.5 CM-1	OR	-1.0 PERCENT			
INTERNAL COORDINATES=	25.59	C20 10.58 CC09	10.58 C1C2	7.09 CC08	6.88 C-07	6.13 CC3H	5.74 C3C4				
FORCE CONSTANTS=	49.15	CC 24.15 CCO	10.69 CCH	10.45 CC							
OFF DIAGONAL=	-12.46	SB22 7.63 SB26	-7.31 SB21	3.66 BB43	3.60 SS18						
NORMAL MODE 38	OBSERVED=	944.0 CM-1	CALCULATED=	835.1 CM-1	ERROR=	8.9 CM-1	OR	1.0 PERCENT			
INTERNAL COORDINATES=	22.93	CC01 16.85 CCH	16.52 CCHB	16.49 O*CI	5.30 C4C5	5.11 CCH					
FORCE CONSTANTS=	41.85	CC 38.64 CCH	12.98 CC	8.02 CCO	7.09 OCH	5.11 CCH					
OFF DIAGONAL=	-5.87	SB23 -2.89 BB34	-2.62 SB25	-2.04 SB22	-1.98 SB21	-1.87 BB33	-1.68 SB24				
NORMAL MODE 39	OBSERVED=	780.0 CM-1	CALCULATED=	805.4 CM-1	ERROR=	-25.4 CM-1	OR	-3.3 PERCENT			
INTERNAL COORDINATES=	12.28	CC01 7.26 C5C	6.66 CCH	5.81 C1C2	5.72 HC2C	5.66 C2C3	5.58 C-09	5.29 C3C4			
FORCE CONSTANTS=	21.13	CC 19.53 CCH	14.10 CCH	11.54 CC	10.63 CCH	6.66 CCH					
OFF DIAGONAL=	5.75	BB43 3.24 SB25	-3.03 SB26	-2.56 BB41	-1.99 SB27	1.72 SS18	1.69 BB42				
NORMAL MODE 40	OBSERVED=	720.0 CM-1	CALCULATED=	686.6 CM-1	ERROR=	33.4 CM-1	UR	4.6 PERCENT			
INTERNAL COORDINATES=	12.57	CC01 9.32 C7CC	5.72 CC3H	5.44 C4CC							
FORCE CONSTANTS=	42.37	CC 21.83 CCH	12.97 CCH	8.99 CCH							
OFF DIAGONAL=	8.37	SB25 2.47 BB43	-4.57 BB34	-4.18 BB29	-3.20 SB27	-1.96 BB41	1.53 BB42				
NORMAL MODE 41	OBSERVED=	684.0 CM-1	CALCULATED=	660.0 CM-1	ERROR=	24.0 CM-1	OR	3.5 PERCENT			
INTERNAL COORDINATES=	13.92	CC01 10.14 CC09	10.00 CCH	9.91 CCH	5.07 CCO						
FORCE CONSTANTS=	38.05	CC 19.77 CC	14.00 CC	9.31 CCH	5.07 CCO						
OFF DIAGONAL=	5.41	SB25 -4.23 SB22	3.25 BB43	2.40 SS18	-2.17 SB27	1.97 SB21	1.63 SB23				
NORMAL MODE 42	OBSERVED=	575.0 CM-1	CALCULATED=	565.2 CM-1	ERROR=	9.8 CM-1	OR	1.7 PERCENT			
INTERNAL COORDINATES=	23.18	CC01 10.50 CC07	9.07 C1C2	8.36 C-06	6.79 O*CC						
FORCE CONSTANTS=	31.47	CC 23.18 CCO	16.60 CC	13.46 CC							
OFF DIAGONAL=	8.32	SB24 3.08 SS18	-2.61 BB42	-2.59 SB27	2.21 BB43	-1.63 SB26					
NORMAL MODE 43	OBSERVED=	531.0 CM-1	CALCULATED=	512.6 CM-1	ERROR=	18.4 CM-1	OR	3.5 PERCENT			
INTERNAL COORDINATES=	21.18	OC0C 10.23 C4C5	7.89 C4CC	6.27 C5C0	5.34 O8CC						
FORCE CONSTANTS=	38.43	CC 13.48 CCH	11.68 CC	9.78 CCH	7.96 CCH						
OFF DIAGONAL=	9.79	SB22 7.42 SB25	-5.37 SB21	3.04 BB43	2.86 SS18	-2.13 SB27	-1.61 SB26	-1.59 BB42			
NORMAL MODE 44	OBSERVED=	475.0 CM-1	CALCULATED=	494.8 CM-1	ERROR=	-19.8 CM-1	OR	-4.2 PERCENT			
INTERNAL COORDINATES=	25.56	CC01 15.66 C8CC	10.71 CC09	9.09 CCO0	7.58 CC06	6.15 CCO0					
FORCE CONSTANTS=	79.55	CC 19.57 CCH	8.04 CCH								
OFF DIAGONAL=	-13.99	BB34 5.35 BB43	-2.71 BB42	-2.60 BB29	-1.90 BB41	-1.61 SB22					
NORMAL MODE 45	OBSERVED=	449.0 CM-1	CALCULATED=	445.5 CM-1	ERROR=	3.4 CM-1	OR	0.8 PERCENT			
INTERNAL COORDINATES=	32.41	CC06 14.29 CCO	11.87 CCH	8.21 C0CC	7.33 C1CC	6.71 CC09	5.30 C2CC				
FORCE CONSTANTS=	59.97	CC 19.97 CCH	12.97 CCH	8.99 CCH	7.21 CCH						
OFF DIAGONAL=	-6.94	BB34 5.34 SB25	-5.23 BB42	-2.95 SB24	-2.88 BB41	-2.08 BB43	2.03 SB22				
NORMAL MODE 46	OBSERVED=	197.0 CM-1	CALCULATED=	411.4 CM-1	ERROR=	-14.4 CM-1	OR	-3.6 PERCENT			
INTERNAL COORDINATES=	3.33	C3C 9.08 CLO9	10.00 CCH	6.56 CCH	6.11 U7CC	5.82 HC4C	5.13 C2CC				
FORCE CONSTANTS=	39.73	CC 28.48 CCH	16.17 CCH	8.67 CCH							
OFF DIAGONAL=	-6.34	BB34 6.20 BB43	3.24 SB22	-2.84 BB29	-2.14 B041	1.58 SB21					
NORMAL MODE 47	OBSERVED=	373.0 CM-1	CALCULATED=	390.0 CM-1	ERROR=	-17.0 CM-1	OR	-4.5 PERCENT			
INTERNAL COORDINATES=	12.50	OC0C 11.73 CCO	8.99 OBCC	8.25 O*CC	8.02 CC08	7.74 CC09	5.89 C2CC	5.11 C1C2			
FORCE CONSTANTS=	55.64	CC 11.73 CCO	11.51 CCH	10.51 CCH	6.45 CC						
OFF DIAGONAL=	-7.27	BB34 3.81 SB22	-2.73 BB42	2.57 SB21	-2.48 BB29	2.12 BB43					
NORMAL MODE 48	OBSERVED=	358.0 CM-1	CALCULATED=	317.6 CM-1	ERROR=	40.4 CM-1	OR	11.3 PERCENT			
INTERNAL COORDINATES=	24.61	UBCC 17.57 CC09	13.47 OC0C	11.36 CC08	5.63 TH-3						
FORCE CONSTANTS=	77.47	CC 10.63 T-0H	7.40 CC	2.95 SB22	-2.01 SB26	-1.51 BB36					
OFF DIAGONAL=	-9.37	BB34 -4.00 BB42									
NORMAL MODE 49	OBSERVED=	306.0 CM-1	CALCULATED=	300.4 CM-1	ERROR=	5.6 CM-1	OR	1.8 PERCENT			
INTERNAL COORDINATES=	23.54	CC08 10.50 T-0H	11.78 CCH	9.27 TH-2	6.68 CC06						
FORCE CONSTANTS=	72.54	CC 10.50 T-0H	11.97 CCH								
OFF DIAGONAL=	-4.82	BB34 -2.73 BB42	2.39 SB22	2.16 SB21	1.75 BB43	1.71 BB41					
NORMAL MODE 50	OBSERVED=	260.0 CM-1	CALCULATED=	277.1 CM-1	ERROR=	-9.1 CM-1	OR	-3.4 PERCENT			
INTERNAL COORDINATES=	34.54	CC08 15.09 C4CC	11.99 OC0C	11.29 T-0H	5.48 TH-4						
FORCE CONSTANTS=	56.08	CC 19.17 T-0H	18.93 CCH	9.63 CCH							
OFF DIAGONAL=	-6.90	BB34 -3.79 BB42	-2.84 BB33	-2.20 SB25							
NORMAL MODE 51	OBSERVED=	254.0 CM-1	CALCULATED=	252.3 CM-1	ERROR=	1.7 CM-1	OR	0.7 PERCENT			
INTERNAL COORDINATES=	19.17	TH-1 14.40 TH-5	12.92 CC00	5.26 CCO	5.05 C0*CC						
FORCE CONSTANTS=	33.88	TH-2 29.10 CCO	10.00 CCH	6.87 CCC	5.26 CCO	5.05 CCO					
OFF DIAGONAL=	4.60	BB43 2.91 SB22	-2.80 BB34	-2.30 BB33	-2.00 SB25	-1.99 SB26					
NORMAL MODE 52	OBSERVED=	230.0 CM-1	CALCULATED=	233.7 CM-1	ERROR=	-3.7 CM-1	OR	-1.6 PERCENT			
INTERNAL COORDINATES=	19.61	TH-1 11.93 C7CC	10.43 CC07	9.41 CC06	8.49 C1CC	8.48 O*CC	7.72 TH-3	5.75 TH-5			
FORCE CONSTANTS=	44.32	CC 37.14 T-0H	11.13 CCH	6.83 CCH							
OFF DIAGONAL=	-3.88	BB34 -3.20 SB25	-2.20 BB33	-2.13 BB42							
NORMAL MODE 53	OBSERVED=	0.0 CM-1	CALCULATED=	226.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES=	48.73	TH-3 21.79 TH-4	13.11 TH-1								
FORCE CONSTANTS=	87.83	TH-3 7.47 CCO									
OFF DIAGONAL=	NONE										
NORMAL MODE 54	OBSERVED=	0.0 CM-1	CALCULATED=	223.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES=	26.79	TH-4 0.83 TH-1	20.59 TH-5	6.90 TH-2							
FORCE CONSTANTS=	76.97	TH-4 17.34 CCO									
OFF DIAGONAL=	-1.59	BB34									
NORMAL MODE 55	OBSERVED=	0.0 CM-1	CALCULATED=	217.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES=	53.54	TH-2 22.07 TH-3	9.72 TH-4								
FORCE CONSTANTS=	87.57	TH-0 11.67 CCO									
OFF DIAGONAL=	NONE										
NORMAL MODE 56	OBSERVED=	0.0 CM-1	CALCULATED=	212.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES=	34.15	TH-3 27.52 TH-4	6.86 C4CC	5.53 CCO0							
FORCE CONSTANTS=	68.81	T-0H 19.67 CCO	7.56 CCC	5.13 CCH							
OFF DIAGONAL=	-2.39	BB34									
NORMAL MODE 57	OBSERVED=	0.0 CM-1	CALCULATED=	206.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES=	50.25	TH-2 16.51 TH-2	8.50 O7CC	8.36 TH-5	8.17 TH-3						
FORCE CONSTANTS=	50.85	T-0H 20.19 CCH	1.53 CCH								
OFF DIAGONAL=	2.40	BB43 -2.23 BB34	-1.53 BB33								
NORMAL MODE 58	OBSERVED=	0.0 CM-1	CALCULATED=	134.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES=	21.40	CC01 11.13 TC44	16.39 CCO	10.16 CCH	6.58 TC01	6.47 T-0C	5.71 CCH	5.15 OCH			
FORCE CONSTANTS=	21.40	CCC 21.04 CCO	16.39 CCO	12.50 T-CC	9.47 T-CC						
OFF DIAGONAL=	3.79	BB43 2.42 BB41	-2.27 BB37	-2.13 SB21	-1.73 SB25						
NORMAL MODE 59	OBSERVED=	0.0 CM-1	CALCULATED=	87.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES=	32.75	TCC5 17.84 C2CC	7.90 TCC2	5.83 C3CC							
FORCE CONSTANTS=	47.49	T-CC 30.34 CCC	13.09 CCH								
OFF DIAGONAL=	-3.06	SB25 -2.46 BB42	-1.65 BB34	-1.63 SB21	1.54 BB41						
NORMAL MODE 60	OBSERVED=	0.0 CM-1	CALCULATED=	75.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES=	47.50	TCC5 10.78 C3CC	8.83 C2CC	7.92 TCC2							
FORCE CONSTANTS=	58.64	T-CC 23.20 CCC	10.82 CCO								
OFF DIAGONAL=	-2.17	SB25 -2.13 BB42	-1.96 SB21								
NORMAL MODE 61	OBSERVED=	0.0 CM-1	CALCULATED=	69.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES=	13.46	TCC4 11.63 C4CC	9.41 C1CC	8.39 T3CC	8.30 TCC3	6.02 CCO0	5.97 TCC2	5.53 O*CC			
FORCE CONSTANTS=	33.50	CC 10.20 CCH	10.20 CCH	6.28 T-CC							
OFF DIAGONAL=	-3.79	BB42 -2.09 BB34	2.59 BB41								

44. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 9.38

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400										PAGE 1			
MOLECULE 35 -6 NG=1237 ALPHA MANNOSE-1-D GG													
NORMAL MODE 8	OBSERVED=	1456.0 CM-1	CALCULATED=	1450.2 CM-1	ERROR=	5.8 CM-1	OR	0.4 PERCENT					
INTERNAL COORDINATES-	60.54	HCH 20.65	OCBH	19.72	OCBH								
FORCE CONSTANTS-	60.54	HCH 40.54	OCBH										
OFF DIAGONAL-	-4.23	SB27											
NORMAL MODE 9	OBSERVED=	1439.0 CM-1	CALCULATED=	1425.9 CM-1	ERROR=	9.1 CM-1	OR	0.6 PERCENT					
INTERNAL COORDINATES-	43.44	C3OH 14.13	C4OH	6.38	OC4H								
FORCE CONSTANTS-	58.76	BCOH 15.37	CCH	10.45	CC	8.50	5.30	CCO	1.87	BB34	-1.87		
OFF DIAGONAL-	3.63	SB28	-3.60	SB26		-3.16	SB27	2.00	BB29	5.89	BB43		
NORMAL MODE 10	OBSERVED=	1422.0 CM-1	CALCULATED=	1412.1 CM-1	ERROR=	9.9 CM-1	OR	0.7 PERCENT					
INTERNAL COORDINATES-	18.98	C3OH 13.64	OC4H	8.29	OC3H	8.08	C4OH	6.56	CC5H	6.26	CC2H		
FORCE CONSTANTS-	36.03	BCOH 27.80	OCM	22.59	CCH	1.37	CO	2.84	BB34	-2.49	BB25		
OFF DIAGONAL-	-6.70	SB27	4.99	SB28		-2.94	SB26		BB39	-1.98	BB45		
NORMAL MODE 11	OBSERVED=	0.0 CM-1	CALCULATED=	1401.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT					
INTERNAL COORDINATES-	37.03	C2OH 28.04	C1OH	8.8	C3OH	5.24	OC2H	5.24	C1C2				
FORCE CONSTANTS-	73.66	BCOH 9.05	OCM	7.28	CC	6.23	CCH						
OFF DIAGONAL-	5.60	SB28	-2.75	SB27		-2.37	SB26		-1.95	BB39			
NORMAL MODE 12	OBSERVED=	1395.0 CM-1	CALCULATED=	1396.0 CM-1	ERROR=	-1.0 CM-1	OR	-0.1 PERCENT					
INTERNAL COORDINATES-	55.14	C1OH 8.24	C1OH	7.49	CCBH	6.98	OCBH	6.78	CCHA				
FORCE CONSTANTS-	64.74	BCOH 19.70	CCH	10.20	OCM								
OFF DIAGONAL-	3.38	SB28	-2.63	SB26		-2.56	BB39		-2.43	SB27			
NORMAL MODE 13	OBSERVED=	1380.0 CM-1	CALCULATED=	1391.4 CM-1	ERROR=	-11.4 CM-1	OR	-0.8 PERCENT					
INTERNAL COORDINATES-	49.86	C1OH 25.77	C2OH	7.17	OC2H								
FORCE CONSTANTS-	81.63	BCOH 8.70	OCM										
OFF DIAGONAL-	-1.77	BB39	1.68	SB28		-1.55	SB27						
NORMAL MODE 14	OBSERVED=	0.0 CM-1	CALCULATED=	1371.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT					
INTERNAL COORDINATES-	64.11	C4OH 9.57	CC5H	5.83	HC4C								
FORCE CONSTANTS-	64.11	CCH 11.60	OCM	6.17	OCM								
OFF DIAGONAL-	-3.21	BB36	3.17	BB29		-2.22	SB28		-1.79	SB26	-1.52		
NORMAL MODE 15	OBSERVED=	1358.0 CM-1	CALCULATED=	1352.8 CM-1	ERROR=	5.2 CM-1	OR	0.4 PERCENT					
INTERNAL COORDINATES-	52.20	CCM 16.50	OC3H	13.29	CC4H	12.67	CC5H	6.65	C1OH	6.28	HC4C		
FORCE CONSTANTS-	52.20	CCH 32.64	OCM	8.89	BCOH	8.10	CO	1.93	BB34	-1.66	SB25		
OFF DIAGONAL-	9.91	BB29	-7.09	SB27		-6.35	SB26		-3.59	BB45			
NORMAL MODE 16	OBSERVED=	1330.0 CM-1	CALCULATED=	1334.5 CM-1	ERROR=	-4.5 CM-1	OR	-0.3 PERCENT					
INTERNAL COORDINATES-	15.66	CC4H 15.60	C1OH	14.2	HC5C	11.79	OC4H	6.86	CC5H				
FORCE CONSTANTS-	45.78	CCH 24.94	OCM	18.36	BCOH	6.48	CC	5.97	CO				
OFF DIAGONAL-	-4.13	SB27	-2.93	BB45		2.45	BB29		-2.28	SB26	-2.09		
NORMAL MODE 17	OBSERVED=	1318.0 CM-1	CALCULATED=	1321.5 CM-1	ERROR=	-3.5 CM-1	OR	-0.3 PERCENT					
INTERNAL COORDINATES-	28.27	CC2H 16.67	C2OH	15.34	C1C1	13.19	OC2H	6.50	C-06				
FORCE CONSTANTS-	37.35	CCH 24.00	CO	21.64	OCM	19.60	BCOH	6.53	CCO				
OFF DIAGONAL-	-6.56	SB27	-4.62	SB25		3.09	BB34		2.61	BB33	-2.44		
NORMAL MODE 18	OBSERVED=	1305.0 CM-1	CALCULATED=	1298.4 CM-1	ERROR=	6.6 CM-1	OR	0.5 PERCENT					
INTERNAL COORDINATES-	23.69	HC2C 12.29	OC2H	11.79	OC4H								
FORCE CONSTANTS-	23.69	CCH 4.53	OCM	2.49	BB34								
OFF DIAGONAL-	-3.19	BB45	2.53	SB27									
NORMAL MODE 19	OBSERVED=	1288.0 CM-1	CALCULATED=	1293.6 CM-1	ERROR=	-5.6 CM-1	OR	-0.4 PERCENT					
INTERNAL COORDINATES-	47.45	OCM 10.18	HC2C	10.09	OC4H	8.40	CC5H	8.06	OC4H	5.84	CC4H		
FORCE CONSTANTS-	47.45	OCM 39.20	CCM	9.73	BCOH	5.35	CO						
OFF DIAGONAL-	-3.58	BB45											
NORMAL MODE 20	OBSERVED=	0.0 CM-1	CALCULATED=	1281.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT					
INTERNAL COORDINATES-	30.22	C5H 16.88	CCBH	15.02	OCBH	8.12	OC4H	7.82	CC5H	5.71	C1OH		
FORCE CONSTANTS-	58.49	OCM 29.39	CCH	6.72	BCOH								
OFF DIAGONAL-	5.24	SB27	-3.26	BB45		-2.29	BB29						
NORMAL MODE 21	OBSERVED=	1255.0 CM-1	CALCULATED=	1265.5 CM-1	ERROR=	-10.5 CM-1	OR	-0.8 PERCENT					
INTERNAL COORDINATES-	18.45	CC4H 14.93	OC3H	12.02	CC3H	11.03	OC2H	7.49	HC2C	6.05	HC4C		
FORCE CONSTANTS-	50.13	CCH 38.46	OCM	10.78	OCM	10.51	CCO	6.04					
OFF DIAGONAL-	4.36	SB27	-3.71	BB45		2.04	BB34		1.98	BB29			
NORMAL MODE 22	OBSERVED=	1226.0 CM-1	CALCULATED=	1238.5 CM-1	ERROR=	-12.5 CM-1	OR	-1.0 PERCENT					
INTERNAL COORDINATES-	16.98	OC4H 12.32	CC3H	9.70	HC5C	8.86	HC3C	7.61	OC2H	5.48	OC4H		
FORCE CONSTANTS-	44.39	CCH 33.11	OCM	13.12	OCM	10.91	CCO	6.04					
OFF DIAGONAL-	8.70	SB27	-3.58	BB25		-3.12	BB45		-2.84	BB29	-1.93		
NORMAL MODE 23	OBSERVED=	1200.0 CM-1	CALCULATED=	1192.3 CM-1	ERROR=	7.7 CM-1	OR	0.6 PERCENT					
INTERNAL COORDINATES-	15.27	HC3C 18.84	CC5H	8.94	HC4C	8.76	CC4H	7.36	CCO	6.16	CC3H		
FORCE CONSTANTS-	15.27	CCH 18.78	OCM	10.78	OCM	10.51	CCO	6.04					
OFF DIAGONAL-	-8.00	BB29	6.65	SB27		-6.35	SB25		3.80	BB34	-3.10		
NORMAL MODE 24	OBSERVED=	1170.0 CM-1	CALCULATED=	1167.4 CM-1	ERROR=	-2.6 CM-1	OR	0.2 PERCENT					
INTERNAL COORDINATES-	12.97	C5H 13.96	OCBH	11.08	OCBH	8.77	CC	7.71	CCH	5.76	COC		
FORCE CONSTANTS-	37.59	OCM 36.50	CO	12.84	CCO	8.37	CC	7.71	CCH	5.19	COC		
OFF DIAGONAL-	-8.53	SB25	-3.51	SB23		2.32	BB37		1.80	SB26			
NORMAL MODE 25	OBSERVED=	1155.0 CM-1	CALCULATED=	1161.5 CM-1	ERROR=	-6.5 CM-1	OR	-0.6 PERCENT					
INTERNAL COORDINATES-	23.90	C1C1 14.37	C-06	14.08	C5H	11.07	CC2H	7.86	OC2H	6.99	C-08		
FORCE CONSTANTS-	61.55	CO 24.77	CCH	17.64	CC	14.84	CCO	13.01	OCM	6.56	BCOH		
OFF DIAGONAL-	-7.86	SB27	-7.80	SB26		-7.06	SB25		-3.66	SB22	-3.61		
NORMAL MODE 26	OBSERVED=	1130.0 CM-1	CALCULATED=	1128.2 CM-1	ERROR=	1.8 CM-1	OR	0.2 PERCENT					
INTERNAL COORDINATES-	25.94	C5H 25.72	C4C5	10.91	C2C3	8.46	C-07	7.82	4CO	7.05	OC4H		
FORCE CONSTANTS-	64.72	CC 24.77	CCO	17.23	CO	16.86	CCH	12.38	OCM	5.38	BCOH		
OFF DIAGONAL-	-16.64	SB22	-15.53	SB26		-4.39	SB25		-3.01	SB28	-1.97		
NORMAL MODE 27	OBSERVED=	1110.0 CM-1	CALCULATED=	1115.0 CM-1	ERROR=	-5.0 CM-1	OR	-0.4 PERCENT					
INTERNAL COORDINATES-	30.59	C-08 12.89	C2C3	17.80	C1C1	6.59	CC	5.61	OTCC				
FORCE CONSTANTS-	54.61	CO 32.98	CC	17.74	CCO	11.37	OCM	1.17	CCH				
OFF DIAGONAL-	-7.17	SB22	-6.32	SB25		-3.48	SB28		1.85	BB43	1.65		
NORMAL MODE 28	OBSERVED=	1090.0 CM-1	CALCULATED=	1104.8 CM-1	ERROR=	-14.8 CM-1	OR	-1.4 PERCENT					
INTERNAL COORDINATES-	56.00	C-08 15.74	C3C4	13.83	C5C	12.14	C-08	6.20	C5O	5.92	C-08		
FORCE CONSTANTS-	56.00	CC 38.46	CCO	10.68	OCM	9.23	CCO	6.23	BCOH	5.77	CCH		
OFF DIAGONAL-	-8.88	SB22	-5.80	SB27		-4.22	SS18		-3.81	SB26	-3.40		
NORMAL MODE 29	OBSERVED=	1080.0 CM-1	CALCULATED=	1081.2 CM-1	ERROR=	-1.2 CM-1	OR	-0.1 PERCENT					
INTERNAL COORDINATES-	31.03	C-08 22.68	C-07	17.13	C4C5	8.75	C3OH	8.32	C2C3	5.05	C2CC		
FORCE CONSTANTS-	68.55	CO 30.78	CC	11.21	BCOH	10.55	CCO	10.53	OCM	10.31	CCC		
OFF DIAGONAL-	-10.39	SB27	-9.54	SB28		-9.15	SB21		-7.27	SS18	-7.18		
NORMAL MODE 30	OBSERVED=	1065.0 CM-1	CALCULATED=	1050.4 CM-1	ERROR=	14.6 CM-1	OR	1.4 PERCENT					
INTERNAL COORDINATES-	33.28	C-09 24.70	C-08	9.81	C4C5	8.74	C3C4	7.56	C5C	7.09	C-07		
FORCE CONSTANTS-	76.32	CO 27.11	CC	11.39	CCO	9.88	CCH	9.20	OCM	8.18	BCOH		
OFF DIAGONAL-	-13.04	SB21	-11.08	SB27		-9.02	SB28		-8.98	SS18	-3.80		
NORMAL MODE 31	OBSERVED=	1045.0 CM-1	CALCULATED=	1042.8 CM-1	ERROR=	2.2 CM-1	OR	0.2 PERCENT					
INTERNAL COORDINATES-	30.04	C1C1 28.12	C-06	11.76	C1C1	7.99	CC1H	7.12	C1OH	5.46	OCO		
FORCE CONSTANTS-	54.61	CO 32.98	CC	24.67	CCH	11.48	BCOH	7.91	CCO	8.71	OCM		
OFF DIAGONAL-	-8.64	SB24	-7.91	SB28		-7.46	SS18		-7.32	SB27	-6.36		
NORMAL MODE 32	OBSERVED=	1025.0 CM-1	CALCULATED=	1007.7 CM-1	ERROR=	17.3 CM-1	OR	1.7 PERCENT					
INTERNAL COORDINATES-	49.51	CO 27.47	CCH	20.93	OCM	9.09	CC	5.03	BCOH				
FORCE CONSTANTS-	53.39	SB28	-3.30	SB25		-3.23	BB29		-2.38	SB26	-2.04		
OFF DIAGONAL-													
NORMAL MODE 33	OBSERVED=	1000.0 CM-1	CALCULATED=	1006.5 CM-1	ERROR=	-6.5 CM-1	OR	-0.6 PERCENT					
INTERNAL COORDINATES-	20.19	C1C1 16.36	C3C4	13.03	C1H	8.28	C-06	7.63	C-08	6.19	CCBH		
FORCE CONSTANTS-	38.47	CC 22.70	CCO	20.70	OCM	19.71	CCH	11.03	CCO				
OFF DIAGONAL-	-10.02	SB22	-4.91	SB26		-2.97	SB28		-2.58	SB21			
NORMAL MODE 34	OBSERVED=	973.0 CM-1	CALCULATED=	968.5 CM-1	ERROR=	4.5 CM-1	OR	0.5 PERCENT					
INTERNAL COORDINATES-	43.45	OC1H 11.16	C-06	8.76	C1H	6.38	C1C2	6.29	C3C4				
FORCE CONSTANTS-	52.86	OCM 20.81	CO	14.32	CC	5.45	CCH	5.42	CCO				
OFF DIAGONAL-	7.14	SB27	-4.29	SB22		-2.92	SB24		-1.80	BB45	-1.60		
NORMAL MODE 35	OBSERVED=	966.0 CM-1	CALCULATED=	941.8 CM-1	ERROR=	24.2 CM-1	OR	2.5 PERCENT					
INTERNAL COORDINATES-	14.50	CC1H 12.90	CC1H	10.65	C-08	10.36	C-07	9.12	C3C4	7.03	C1H		
FORCE CONSTANTS-	27.54	CO 24.77	CC	23.61	CCO	20.74	OCM	6.78	CCO				
OFF DIAGONAL-	-4.36	SB22	-3.64	SB27		2.21	SS18		1.90	BB37	-1.83		

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400									
MOLECULE 35 -6 NG=1237 ALPHA MANNOSE-1-0 GG									
PAGE 2									
NORMAL MODE 36	OBSERVED=	930.0 CM-1	CALCULATED=	908.8 CM-1	ERROR=	21.2 CM-1	OR	2.3 PERCENT	
INTERNAL COORDINATES-	22.50	C-O	10.57	C-O	6.78	C-O	5.97	CC3H	
FORCE CONSTANTS-	39.53	CO	26.31	CC	6.64	CC	8.07	CCO	
OFF DIAGONAL-	-10.44	SB21	-6.38	SB22	-5.89	SB27	4.54	SB26	2.27 BB43
NORMAL MODE 37	OBSERVED=	864.0 CM-1	CALCULATED=	870.6 CM-1	ERROR=	-6.6 CM-1	OR	-0.8 PERCENT	
INTERNAL COORDINATES-	11.13	C2C	11.94	O-C1	8.88	CCO	7.99	C1C2	7.77 C1H
FORCE CONSTANTS-	35.49	CC	24.39	CCO	18.56	CC	12.03	CO	7.90 CCH
OFF DIAGONAL-	-4.93	SB22	-3.65	SB23	-5.50	SB21	-3.39	SB27	2.86 BB43
NORMAL MODE 38	OBSERVED=	818.0 CM-1	CALCULATED=	813.7 CM-1	ERROR=	4.3 CM-1	OR	0.5 PERCENT	
INTERNAL COORDINATES-	24.34	C5O	14.24	CCHB	13.99	CC	11.91	C1H	8.75 O-C1
FORCE CONSTANTS-	35.51	CO	35.08	CC	16.48	CC	13.68	CC	8.02 CCO
OFF DIAGONAL-	-4.93	SB25	-3.65	SB23	-5.50	SB21	-3.39	SB27	2.86 BB43
NORMAL MODE 39	OBSERVED=	790.0 CM-1	CALCULATED=	792.2 CM-1	ERROR=	-2.2 CM-1	OR	-0.3 PERCENT	
INTERNAL COORDINATES-	11.45	C1H	9.64	O-C1	7.48	C2C3	7.03	HC2C	6.26 CO-C
FORCE CONSTANTS-	23.08	CC	21.69	CCO	17.65	CC	10.44	CC	9.26 CO
OFF DIAGONAL-	5.69	BB43	-4.21	SB26	3.31	SB25	-2.46	BB41	-1.90 BB34
NORMAL MODE 40	OBSERVED=	705.0 CM-1	CALCULATED=	677.3 CM-1	ERROR=	27.7 CM-1	OR	3.9 PERCENT	
INTERNAL COORDINATES-	16.70	CCO	7.30	C8CC	6.59	CC5H	6.08	C4CC	
FORCE CONSTANTS-	40.56	CCO	24.95	CC	12.78	CO	7.95	CC	
OFF DIAGONAL-	7.67	SB25	-5.55	BB43	-5.52	BB34	-4.21	BB29	-2.22 SB27
NORMAL MODE 41	OBSERVED=	0.0 CM-1	CALCULATED=	655.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	19.13	OCC	9.79	C3C4	6.43	CO	6.85	CC	5.40 C-O
FORCE CONSTANTS-	30.10	CCO	17.86	CC	2.90	BB43	-2.39	SB27	2.07 SS18
OFF DIAGONAL-	5.93	SB25	-3.24	SB22	-2.90	BB43	-2.39	SB27	2.07 SS18
NORMAL MODE 42	OBSERVED=	0.0 CM-1	CALCULATED=	557.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	22.65	CCO	8.37	CCO7	7.97	C1C2	7.12	O-C1	6.72 C-O
FORCE CONSTANTS-	31.05	CCO	22.65	CCO	16.95	CC	12.19	CO	
OFF DIAGONAL-	7.75	SB24	-3.20	SB27	3.12	BB43	2.87	SS18	-2.49 BB42
NORMAL MODE 43	OBSERVED=	0.0 CM-1	CALCULATED=	508.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	19.57	OCC	8.81	C4C5	6.88	C4CC	6.76	CCO	6.61 C5O
FORCE CONSTANTS-	37.37	CCO	12.25	CC	12.24	CO	8.95	CC	7.49 CCH
OFF DIAGONAL-	9.54	SB22	7.78	SB25	-4.69	SB21	2.97	BB43	2.78 SS18
NORMAL MODE 44	OBSERVED=	0.0 CM-1	CALCULATED=	490.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	22.05	CCO	16.18	C8CC	10.41	CCO6	9.80	CCO9	9.43 CCO
FORCE CONSTANTS-	78.73	CCO	19.86	CC	9.14	CC			
OFF DIAGONAL-	-14.25	BB34	5.50	BB43	-2.97	BB42	-2.46	BB29	-1.84 BB41
NORMAL MODE 45	OBSERVED=	0.0 CM-1	CALCULATED=	443.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	30.21	CCO6	12.73	CCO	12.02	CCO7	8.29	CO	8.22 CCO9
FORCE CONSTANTS-	77.55	CCO	10.72	T-OH	5.04	BB42	-2.83	BB41	-2.75 SB24
OFF DIAGONAL-	-7.39	BB34	5.17	SB25	-5.04	BB42	-2.83	BB41	-2.75 SB24
NORMAL MODE 46	OBSERVED=	0.0 CM-1	CALCULATED=	410.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	40.11	CCO	29.01	CC	16.27	CC	7.96	CC	
FORCE CONSTANTS-	60.11	CCO	6.21	BB43	2.97	SB22	-2.80	BB29	-2.19 BB41
OFF DIAGONAL-	-6.51	BB34	6.21	BB43	2.97	SB22	-2.80	BB29	-2.19 BB41
NORMAL MODE 47	OBSERVED=	0.0 CM-1	CALCULATED=	389.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	12.76	OCC	11.64	CCO	8.75	OBCC	8.21	CCO8	8.19 O-C1
FORCE CONSTANTS-	55.53	CC	11.64	CCO	11.33	CC	10.63	CC	8.44 CC
OFF DIAGONAL-	-7.20	BB34	3.86	SB22	-2.76	BB42	2.55	SB21	-2.44 BB29
NORMAL MODE 48	OBSERVED=	0.0 CM-1	CALCULATED=	317.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	24.55	OBCC	17.68	CCO9	13.79	OCC	11.23	CCO8	5.62 TH-3
FORCE CONSTANTS-	72.61	CCO	10.72	T-OH	7.36	CC	7.06	CC	
OFF DIAGONAL-	-5.97	BB34	-4.01	BB42	2.95	SB22	-2.00	SB26	-1.51 BB36
NORMAL MODE 49	OBSERVED=	0.0 CM-1	CALCULATED=	300.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	23.17	CCO	10.62	T-OH	12.11	OCC	9.43	TH-2	6.58 CCO6
FORCE CONSTANTS-	72.61	CCO	10.62	T-OH	8.19	CC			
OFF DIAGONAL-	-4.95	BB34	-2.73	BB42	2.36	SB22	2.10	SB21	1.76 BB43
NORMAL MODE 50	OBSERVED=	0.0 CM-1	CALCULATED=	276.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	34.61	CCO	15.46	C4CC	11.66	TH-5	11.56	OCC	5.40 TH-4
FORCE CONSTANTS-	55.39	CCO	19.54	T-OH	19.16	CC	9.50	CC	
OFF DIAGONAL-	-6.84	BB34	-3.80	BB42	-2.81	BB33	-2.06	SB25	
NORMAL MODE 51	OBSERVED=	0.0 CM-1	CALCULATED=	252.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	19.69	TH-1	14.13	TH-5	12.96	CCO*	5.26	CCO	5.06 CO-C
FORCE CONSTANTS-	34.19	T-OH	28.88	CCO	10.14	CC	6.59	CC	5.26 CCO
OFF DIAGONAL-	4.60	BB43	2.96	SB22	-2.85	BB34	-2.29	BB33	-1.99 SB26
NORMAL MODE 52	OBSERVED=	0.0 CM-1	CALCULATED=	233.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	18.53	TH-1	11.81	O7CC	10.68	CCO7	9.53	CCO6	8.64 C1CC
FORCE CONSTANTS-	44.47	CCO	37.14	T-OH	11.20	CC	7.03	CC	
OFF DIAGONAL-	-4.02	BB34	-3.27	SB25	-2.18	BB33	-2.15	BB42	
NORMAL MODE 53	OBSERVED=	0.0 CM-1	CALCULATED=	226.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	17.56	TH-3	22.91	TH-4	12.67	TH-1			
FORCE CONSTANTS-	87.28	T-OH	7.97	CCO					
OFF DIAGONAL-	NONE								
NORMAL MODE 54	OBSERVED=	0.0 CM-1	CALCULATED=	223.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	75.96	TH-2	21.83	TH-1	20.04	TH-5	6.41	TH-2	
FORCE CONSTANTS-	76.92	T-OH	17.34	CCO					
OFF DIAGONAL-	-1.62	BB34							
NORMAL MODE 55	OBSERVED=	0.0 CM-1	CALCULATED=	217.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	54.26	TH-2	21.51	TH-3	9.28	TH-4			
FORCE CONSTANTS-	87.45	T-OH	11.78	CCO					
OFF DIAGONAL-	NONE								
NORMAL MODE 56	OBSERVED=	0.0 CM-1	CALCULATED=	212.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	34.13	TH-5	27.53	TH-4	6.86	C4CC	5.54	CCO*	
FORCE CONSTANTS-	68.76	T-OH	19.73	CCO	7.56	CC	5.14	CC	
OFF DIAGONAL-	-2.39	BB34							
NORMAL MODE 57	OBSERVED=	0.0 CM-1	CALCULATED=	206.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	20.06	TH-1	16.63	TH-2	8.51	O7CC	8.40	TH-5	8.20 TH-3
FORCE CONSTANTS-	59.86	T-OH	20.29	CCO	7.18	CC			
OFF DIAGONAL-	2.39	BB43	-2.23	BB34	-1.53	BB33			
NORMAL MODE 58	OBSERVED=	0.0 CM-1	CALCULATED=	133.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	21.37	CCO	11.12	TCC4	10.10	C4CC	10.07	C1C2	6.58 CCO1
FORCE CONSTANTS-	3.81	BB43	2.43	BB41	-2.37	BB37	-2.17	SB21	-1.74 SB25
OFF DIAGONAL-									
NORMAL MODE 59	OBSERVED=	0.0 CM-1	CALCULATED=	87.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	32.30	TCC5	18.00	C2CC	8.01	TCC2	5.94	C3CC	
FORCE CONSTANTS-	47.22	T-CC	30.59	CC	13.21	CCO			
OFF DIAGONAL-	-3.69	SB25	-2.48	BB42	-1.67	SB21	-1.66	BB34	1.56 BB41
NORMAL MODE 60	OBSERVED=	0.0 CM-1	CALCULATED=	75.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	48.30	TCC5	10.38	C3CC	8.75	C2CC	7.66	TCC2	
FORCE CONSTANTS-	59.07	T-CC	22.62	CC	10.66	CCO			
OFF DIAGONAL-	-2.11	SB25	-2.07	BB42	-1.89	SB21			
NORMAL MODE 61	OBSERVED=	0.0 CM-1	CALCULATED=	69.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	13.59	TCC4	11.67	CCO*	9.44	C1CC	8.64	C3CC	8.40 TCC3
FORCE CONSTANTS-	30.29	T-CC	30.29	CCO	22.82	CC	8.26	T-CC	5.92 TCC2
OFF DIAGONAL-	-2.81	BB42	-2.08	BB34	1.60	BB41			5.90 CCO*

30. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 8.56

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR	400	PAGE	1
MOLECULE 36	-6 NG=1237 ALPHA	PROBLEM	TG
NORMAL MODE 8 INTERNAL COORDINATES- FORCE CONSTANTS- OFF DIAGONAL-	OBSERVED= 1460.0 CM-1 58.27 HCH 22.23 OCHA 58.27 HCH 43.13 OCH -4.48 SB27	CALCULATED= 1449.5 CM-1 20.76 OCHB	ERROR= 10.5 CM-1 OR 0.7 PERCENT
NORMAL MODE 9 INTERNAL COORDINATES- FORCE CONSTANTS- OFF DIAGONAL-	OBSERVED= 1420.0 CM-1 8.55 CCHA 8.46 C3OH 39.53 CCH 29.00 OCH -7.89 SB27 6.27 BB34	CALCULATED= 1433.2 CM-1 8.18 C4OH 7.31 HC4C 23.97 BCOM 10.90 C4OH 6.95 CCO -5.67 SB26 4.94 BB29 -4.20 SB25	ERROR= -13.2 CM-1 OR -0.9 PERCENT 7.27 C4OH 6.55 C5OH 6.07 C5H 2.91 SB28 -2.19 BB45
NORMAL MODE 10 INTERNAL COORDINATES- FORCE CONSTANTS- OFF DIAGONAL-	OBSERVED= 1400.0 CM-1 49.18 C3OH 5.49 CCH3 60.62 BCOM 14.16 OCH 4.05 SB28 -3.37 SB27	CALCULATED= 1421.2 CM-1 12.26 CCH 6.27 CC 3.33 BB36 -2.36 SB26 -2.02 BB39	ERROR= 0.0 CM-1 OR 0.0 PERCENT
NORMAL MODE 11 INTERNAL COORDINATES- FORCE CONSTANTS- OFF DIAGONAL-	OBSERVED= 1400.0 CM-1 36.77 C1OH 17.16 C2OH 63.16 BCOM 23.10 OCH 5.39 SB28 -4.55 SB27	CALCULATED= 1409.4 CM-1 15.72 OC1H 6.90 C3OH 7.79 CCH 6.81 CC -3.22 SB26 -2.93 BB39	ERROR= -9.4 CM-1 OR -0.7 PERCENT
NORMAL MODE 12 INTERNAL COORDINATES- FORCE CONSTANTS- OFF DIAGONAL-	OBSERVED= 1395.0 CM-1 21.84 C4OH 16.64 C4OH 46.01 BCOM 24.20 OCH 5.17 SB28 -5.12 SB27	CALCULATED= 1400.2 CM-1 12.28 OC4H 5.54 C3OH 5.36 OC3H 19.53 CCH 5.33 CC4H -4.49 SB26 3.61 BB29 -2.75 BB39	ERROR= -5.2 CM-1 OR -0.4 PERCENT 5.33 CC4H 5.33 CC4H -1.69 BB45
NORMAL MODE 13 INTERNAL COORDINATES- FORCE CONSTANTS- OFF DIAGONAL-	OBSERVED= 1392.0 CM-1 42.88 C1OH 22.87 C2OH 19.11 CCH 19.11 OCH -3.50 SB27 1.59 BB34	CALCULATED= 1394.7 CM-1 9.56 C1H 7.60 OC2H 5.64 C2OH 8.23 CCH	ERROR= -2.7 CM-1 OR -0.2 PERCENT CC2H
NORMAL MODE 14 INTERNAL COORDINATES- FORCE CONSTANTS- OFF DIAGONAL-	OBSERVED= 1382.0 CM-1 34.50 C1H 23.61 C2OH 58.89 OCH 35.27 BCOM -3.49 SB27 -2.22 BB45	CALCULATED= 1386.4 CM-1 21.87 OC1H 10.20 C4OH 1.82 SB28 1.66 BB37	ERROR= -4.4 CM-1 OR -0.3 PERCENT
NORMAL MODE 15 INTERNAL COORDINATES- FORCE CONSTANTS- OFF DIAGONAL-	OBSERVED= 1371.0 CM-1 51.46 C4OH 14.14 C4OH 68.74 BCOM 16.78 CCH 2.72 SB29 -2.63 BB36	CALCULATED= 1369.7 CM-1 6.69 CC5H 6.12 C5H 5.14 HC3C 11.66 OCH -2.20 SB28 -1.71 SB27	ERROR= 1.3 CM-1 OR 0.1 PERCENT HC3C
NORMAL MODE 16 INTERNAL COORDINATES- FORCE CONSTANTS- OFF DIAGONAL-	OBSERVED= 1356.0 CM-1 11.04 CC5H 10.48 HC4C 36.90 CCH 29.74 BCOM 7.57 BB29 -4.76 SB27	CALCULATED= 1335.6 CM-1 10.31 CCHA 8.74 HC3C 8.61 HC5C 26.93 OCH 3.09 BB34 -2.65 BB45	ERROR= -4.8 CM-1 OR -0.3 PERCENT 7.38 OC3H 6.95 OCHA 6.26 HC2C -2.24 SB28 -1.69 SB26
NORMAL MODE 17 INTERNAL COORDINATES- FORCE CONSTANTS- OFF DIAGONAL-	OBSERVED= 1333.0 CM-1 25.08 C1CH 12.70 HC3C 64.60 CCH 20.28 OCH 12.89 BB29 -7.46 SB26	CALCULATED= 1360.8 CM-1 9.68 OC3H 9.10 HC5C 8.87 CCO -3.72 BB45 -2.68 SB27	ERROR= -2.6 CM-1 OR -0.2 PERCENT C5H 6.40 CC4H 5.61 CCHA
NORMAL MODE 18 INTERNAL COORDINATES- FORCE CONSTANTS- OFF DIAGONAL-	OBSERVED= 1327.0 CM-1 18.95 C1H 13.23 HC2C 58.72 CCH 24.06 OCH -3.55 BB45 2.33 BB34	CALCULATED= 1319.7 CM-1 12.95 OC1H 11.25 CCH2 6.79 OC3H 6.63 BCOM 1.51 CCH -1.91 SB26 1.65 BB29	ERROR= 7.3 CM-1 OR 0.5 PERCENT OC3H 1.63 BB30
NORMAL MODE 19 INTERNAL COORDINATES- FORCE CONSTANTS- OFF DIAGONAL-	OBSERVED= 1312.0 CM-1 33.31 OC2H 18.62 C2OH 28.21 OCH 26.06 CCH -4.42 SB25 2.98 BB34	CALCULATED= 1315.5 CM-1 17.17 CCH2 13.40 C1C 23.15 CO 19.26 BCOM 6.36 CCO -2.59 SB28 -2.18 BB45 1.94 BB39	ERROR= -3.5 CM-1 OR -0.3 PERCENT 1.88 BB33
NORMAL MODE 20 INTERNAL COORDINATES- FORCE CONSTANTS- OFF DIAGONAL-	OBSERVED= 1293.0 CM-1 26.92 CCHB 17.17 OCHB 44.02 CCH 31.99 OCH -3.12 BB45 2.97 BB34	CALCULATED= 1304.8 CM-1 11.62 C4OH 9.21 C5H 6.67 HC5C 12.76 BCOM 5.59 CC 1.87 SB26 -1.66 SB22 -1.61 SB27	ERROR= -11.8 CM-1 OR -0.9 PERCENT CC5H
NORMAL MODE 21 INTERNAL COORDINATES- FORCE CONSTANTS- OFF DIAGONAL-	OBSERVED= 1281.0 CM-1 27.68 C5H 24.67 OC4H 69.47 OCH 31.40 CCH -5.28 BB29 -3.95 BB45	CALCULATED= 1289.3 CM-1 7.67 HC4C 7.51 OCHA 7.04 CC5H	ERROR= -8.3 CM-1 OR -0.6 PERCENT CC5H
NORMAL MODE 22 INTERNAL COORDINATES- FORCE CONSTANTS- OFF DIAGONAL-	OBSERVED= 1274.0 CM-1 24.00 OC3H 12.94 CCH 42.63 OCH 0.01 CCH -3.19 BB45 2.00 SB27	CALCULATED= 1271.2 CM-1 12.22 CC1H 5.25 BCOM 13.14 CO	ERROR= -2.8 CM-1 OR -0.2 PERCENT CC4H 6.80 OC4H 5.35 OC1C
NORMAL MODE 23 INTERNAL COORDINATES- FORCE CONSTANTS- OFF DIAGONAL-	OBSERVED= 1255.0 CM-1 18.75 OC2H 12.91 HC2C 47.85 CCH 34.16 OCH -3.45 BB45 3.07 SB27	CALCULATED= 1263.6 CM-1 11.54 CC4H 1.46 HC4C 5.58 CC3H 7.30 CO 2.13 SB26	ERROR= -8.6 CM-1 OR -0.7 PERCENT 5.28 CC1H
NORMAL MODE 24 INTERNAL COORDINATES- FORCE CONSTANTS- OFF DIAGONAL-	OBSERVED= 1239.0 CM-1 14.42 OC4H 12.32 CC3H 45.34 CCH 41.56 OCH 5.22 SB27 -5.16 BB29	CALCULATED= 1234.6 CM-1 12.11 OCHA 11.38 HC5C 7.67 HC3C 7.67 CO -3.32 BB45	ERROR= -4.4 CM-1 OR -0.3 PERCENT 6.43 OCHB 6.04 CC5H
NORMAL MODE 25 INTERNAL COORDINATES- FORCE CONSTANTS- OFF DIAGONAL-	OBSERVED= 1210.0 CM-1 12.45 CC5H 11.60 OCHA 56.66 CCH 24.73 OCH -9.69 BB29 -4.60 SB25	CALCULATED= 1193.7 CM-1 9.36 HC5C 9.18 HC4C 8.87 CC4H 11.47 CO 9.19 CCO 7.61 BCOM 4.52 BB34 3.86 SB27 -3.21 SB28	ERROR= -16.3 CM-1 OR -1.3 PERCENT 8.76 CC3H 5.70 C3OH 5.50 HC3C -2.82 BB45 -1.92 BB36
NORMAL MODE 26 INTERNAL COORDINATES- FORCE CONSTANTS- OFF DIAGONAL-	OBSERVED= 1169.0 CM-1 22.23 C5OH 13.27 OC1C 17.77 CO 14.37 CCH -11.10 SB25 -4.36 SB28	CALCULATED= 1153.2 CM-1 11.21 C-O7 8.25 C-O8 6.07 OC2H 17.29 CO 13.17 CCH 7.37 CCH -3.08 SB26 -2.65 SB27 -2.37 SB21	ERROR= -15.8 CM-1 OR -1.3 PERCENT 6.07 C2OH 5.11 C3C4 7.62 BCOM
NORMAL MODE 27 INTERNAL COORDINATES- FORCE CONSTANTS- OFF DIAGONAL-	OBSERVED= 1140.0 CM-1 45.33 C-O7 10.25 C-O9 CO 19.28 CCO -11.50 SB25 5.14 SB27	CALCULATED= 1137.5 CM-1 17.47 OCH 15.56 CCH 9.13 CC -3.50 SB22 -3.00 SB28 -2.58 SB21	ERROR= 2.5 CM-1 OR 0.2 PERCENT 2.32 BB43 -1.86 SB23 -1.68 BB34
NORMAL MODE 28 INTERNAL COORDINATES- FORCE CONSTANTS- OFF DIAGONAL-	OBSERVED= 1115.0 CM-1 33.11 C2C 12.37 C1C2 CO 25.49 CO -15.39 SB22 -6.73 SB26	CALCULATED= 1103.0 CM-1 12.06 C5C 8.88 C-O9 7.40 C-O6 20.06 CCO 13.55 OCH 6.81 CCO 2.37 SS18 -2.12 SB25 -1.83 BB34	ERROR= -12.0 CM-1 OR -1.1 PERCENT 6.81 C1C 6.97 C4C5 6.11 OC1H
NORMAL MODE 29 INTERNAL COORDINATES- FORCE CONSTANTS- OFF DIAGONAL-	OBSERVED= 1104.0 CM-1 32.47 C4C5 22.93 C5C 61.25 CCO 41.92 CO -7.94 SB22 -4.94 SB26	CALCULATED= 1097.6 CM-1 17.57 C-O9 7.77 C-O8 7.45 C-O8 9.82 CCO 7.63 CCH -4.45 SS18 -3.24 SB28 -2.68 SB27	ERROR= 6.4 CM-1 OR 0.6 PERCENT -1.83 SS17 -1.60 SB25
NORMAL MODE 30 INTERNAL COORDINATES- FORCE CONSTANTS- OFF DIAGONAL-	OBSERVED= 1085.0 CM-1 41.10 C-O8 15.34 C3C4 67.78 CCH 35.25 CC -7.10 SB28 -6.91 SS18	CALCULATED= 1086.5 CM-1 9.77 C5OH 9.43 C-O7 9.06 C4C5 10.48 CCH 9.55 CCH -6.40 SB27 -4.82 SB25 -4.27 SB21	ERROR= -1.5 CM-1 OR -0.1 PERCENT 5.80 C3OH 6.94 BCOM
NORMAL MODE 31 INTERNAL COORDINATES- FORCE CONSTANTS- OFF DIAGONAL-	OBSERVED= 1064.0 CM-1 65.95 CCO 16.19 C4C5 -8.45 SB25 -5.29 SB21	CALCULATED= 1065.3 CM-1 13.64 CCO 9.32 CCH 7.74 OCH -3.83 SB28 -2.63 BB34 2.59 SB27	ERROR= -1.3 CM-1 OR -0.1 PERCENT -2.00 SS18
NORMAL MODE 32 INTERNAL COORDINATES- FORCE CONSTANTS- OFF DIAGONAL-	OBSERVED= 1053.0 CM-1 1.19 C1C2 20.79 C2C3 61.03 CO 45.32 CC -9.55 SB27 -9.49 SB28	CALCULATED= 1058.9 CM-1 20.25 C-O6 15.66 C-O9 8.25 C-O8 13.43 BCOM 12.73 CCH 10.60 OCH -8.38 SB27 -7.32 SB22 -5.63 SS18	ERROR= -5.9 CM-1 OR -0.6 PERCENT 7.51 CC1H 7.01 C-O7 6.03 C5OH 8.10 CCO 5.69 CCC -3.95 SB24 -3.62 SB21
NORMAL MODE 33 INTERNAL COORDINATES- FORCE CONSTANTS- OFF DIAGONAL-	OBSERVED= 1043.0 CM-1 30.17 C-O9 14.71 C-O7 61.91 CO 27.39 CC -12.21 SB21 -8.58 SB27	CALCULATED= 1038.3 CM-1 13.10 C3C4 11.47 C5C 10.40 C-O6 15.64 CCH 14.53 CCC 10.32 CCO -8.51 SB28 -4.71 SS18 -3.92 SB25	ERROR= -4.7 CM-1 OR -0.4 PERCENT 7.63 C3C4 6.83 C4OH 6.58 C4CC 9.38 BCOM 9.17 OCH -3.05 BB34 -2.79 SB22
NORMAL MODE 34 INTERNAL COORDINATES- FORCE CONSTANTS- OFF DIAGONAL-	OBSERVED= 1018.0 CM-1 22.56 C1C2 16.07 C-O7 34.15 CCO 23.93 CC -8.62 SB21 -8.15 SS18	CALCULATED= 1019.2 CM-1 15.88 C-O6 9.10 C-O8 8.73 C5OH 15.33 CCH 9.35 OCH 8.39 CCO -6.50 SB28 -5.04 SB24 -4.82 SB27	ERROR= -1.2 CM-1 OR -0.1 PERCENT 7.49 C3C4 6.31 OC1C 5.62 C1CC 8.04 BCOM 9.44 CCC -2.66 SB26 -2.25 SB22
NORMAL MODE 35 INTERNAL COORDINATES- FORCE CONSTANTS- OFF DIAGONAL-	OBSERVED= 964.0 CM-1 50.68 C5C 34.93 C-O8 CO 34.48 CC -12.35 SB22 -8.13 SB26	CALCULATED= 980.6 CM-1 9.44 C1C2 12.82 C4H 28.18 CCH 12.87 CCO -4.59 BB29 -3.04 SB25	ERROR= -16.6 CM-1 OR -1.7 PERCENT SB21 -2.50 SB28 -2.14 SB27 -1.53 BB34

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400										PAGE 2
MOLECULE 36		-6 NG=1237 ALPHA		MANNNOSE		TG				
NORMAL MODE 36		OBSERVED= 958.0 CM-1		CALCULATED= 944.3 CM-1		ERROR= 13.7 CM-1		OR 1.4 PERCENT		
INTERNAL COORDINATES-	22.41	O'C1	11.05	C3C4	9.51	C-O7	5.39	C-O6	5.17	
FORCE CONSTANTS-	46.69	CC	25.68	CC	22.12	CCH	15.00	CCO	5.55	
OFF DIAGONAL-	-7.42	SB22	-4.11	SB24	-2.79	SB21	-2.48	BB34	-2.38	
NORMAL MODE 37		OBSERVED= 883.0 CM-1		CALCULATED= 886.3 CM-1		ERROR= -3.3 CM-1		OR -0.4 PERCENT		
INTERNAL COORDINATES-	28.19	C2C3	9.86	C1C2	8.78	O'C1	8.29	CCO8	8.10	
FORCE CONSTANTS-	46.09	CC	22.97	CCO	15.13	CO	10.75	CCH	5.51	
OFF DIAGONAL-	-11.08	SB22	6.70	SB26	-5.54	SB21	3.61	SS18	3.48	
NORMAL MODE 38		OBSERVED= 832.0 CM-1		CALCULATED= 851.1 CM-1		ERROR= -19.1 CM-1		OR -2.3 PERCENT		
INTERNAL COORDINATES-	19.20	CCBH	17.49	CCHA	11.80	C4C5	7.12	CC5H	6.52	
FORCE CONSTANTS-	58.62	CCH	18.94	CC	9.82	OCH	8.19	CCO	7.94	
OFF DIAGONAL-	-8.09	BB29	-4.67	SB21	-3.32	SB22	2.34	SB25	1.89	
NORMAL MODE 39		OBSERVED= 814.0 CM-1		CALCULATED= 788.3 CM-1		ERROR= 25.7 CM-1		OR 3.2 PERCENT		
INTERNAL COORDINATES-	13.43	O'CC	8.97	CUC'	7.33	C3C4	5.97	C1CC	5.26	
FORCE CONSTANTS-	23.08	CCH	20.53	CCO	19.38	CC	14.34	CO	9.51	
OFF DIAGONAL-	4.94	BB43	-4.87	SB26	3.43	SB25	-2.79	BB34	-2.41	
NORMAL MODE 40		OBSERVED= 685.0 CM-1		CALCULATED= 676.7 CM-1		ERROR= 8.3 CM-1		OR 1.2 PERCENT		
INTERNAL COORDINATES-	18.86	O7CC	8.47	C3C4	7.59	C-O7	7.42	CCO8	7.21	
FORCE CONSTANTS-	34.35	CCO	14.74	CC	12.53	CCO	12.53	CCH	7.21	
OFF DIAGONAL-	7.85	SB25	4.52	BB43	-3.38	SB27	-1.51	BB41		
NORMAL MODE 41		OBSERVED= 606.0 CM-1		CALCULATED= 586.6 CM-1		ERROR= 19.3 CM-1		OR 3.2 PERCENT		
INTERNAL COORDINATES-	25.61	OCO	8.61	O'CC	7.65	CCO7	6.70	4CO*	6.23	
FORCE CONSTANTS-	33.90	CCO	25.65	CCO	12.89	CCH	10.87	CO		
OFF DIAGONAL-	5.63	SB24	3.84	BB43	-3.09	BB34	3.00	SB25	-2.79	
NORMAL MODE 42		OBSERVED= 576.0 CM-1		CALCULATED= 541.9 CM-1		ERROR= 34.1 CM-1		OR 5.9 PERCENT		
INTERNAL COORDINATES-	12.19	C5O*	10.75	4CO*	7.91	CCO*	5.67	C2C3		
FORCE CONSTANTS-	33.28	CCO	22.38	CCO	16.64	CC				
OFF DIAGONAL-	7.66	SB25	5.06	SB22	3.83	SS18	-3.82	SB27	3.52	
NORMAL MODE 43		OBSERVED= 530.0 CM-1		CALCULATED= 524.2 CM-1		ERROR= 5.8 CM-1		OR 1.1 PERCENT		
INTERNAL COORDINATES-	17.33	CCO*	15.21	C4CC	11.55	O8CC	8.09	HC5C	7.38	
FORCE CONSTANTS-	41.33	CCC	23.69	CCH	20.33	CCC	9.89	CC	6.07	
OFF DIAGONAL-	-10.54	BB34	8.34	BB43	-5.18	BB29	-1.82	SB21	-1.56	
NORMAL MODE 44		OBSERVED= 475.0 CM-1		CALCULATED= 496.7 CM-1		ERROR= -21.7 CM-1		OR -4.6 PERCENT		
INTERNAL COORDINATES-	14.11	O9CC	13.46	O8CC	10.13	C4C5	9.42	CCO*	9.00	
FORCE CONSTANTS-	61.53	CCO	15.05	CCH	14.27	CC				
OFF DIAGONAL-	-9.41	BB34	5.81	BB43	-2.58	BB29	2.39	SB22	-1.90	
NORMAL MODE 45		OBSERVED= 450.0 CM-1		CALCULATED= 442.0 CM-1		ERROR= 7.9 CM-1		OR 1.8 PERCENT		
INTERNAL COORDINATES-	29.79	CCO8	13.03	CCO7	10.36	OCO	7.78	C2CC	5.63	
FORCE CONSTANTS-	58.82	CCO	18.20	CCC	10.36	OCO	8.99	CCH	7.93	
OFF DIAGONAL-	-6.87	BB34	-4.76	BB42	4.63	SB25	-3.18	SB24	-2.90	
NORMAL MODE 46		OBSERVED= 398.0 CM-1		CALCULATED= 389.6 CM-1		ERROR= 8.4 CM-1		OR 2.1 PERCENT		
INTERNAL COORDINATES-	15.91	OCO	9.72	4CO*	8.94	O'CC	7.01	CCO*	6.72	
FORCE CONSTANTS-	49.12	CCO	15.91	OCO	8.31	CO	6.27	CCC	6.00	
OFF DIAGONAL-	6.01	SB22	-3.62	BB34	-3.06	BB42	-2.21	SB27	2.03	
NORMAL MODE 47		OBSERVED= 373.0 CM-1		CALCULATED= 388.1 CM-1		ERROR= -15.1 CM-1		OR -4.0 PERCENT		
INTERNAL COORDINATES-	13.76	O9CC	13.54	C3CC	8.33	CCO*	8.32	CCO*	6.69	
FORCE CONSTANTS-	53.30	CCO	21.57	CCC	7.57	CO	7.29	CC	6.41	
OFF DIAGONAL-	6.11	SB25	-5.52	BB34	3.57	SB21	3.40	SB22	-3.13	
NORMAL MODE 48		OBSERVED= 359.0 CM-1		CALCULATED= 357.8 CM-1		ERROR= 1.2 CM-1		OR 0.3 PERCENT		
INTERNAL COORDINATES-	33.74	CCO9	10.52	O7CC	6.42	C2C3	5.96	CCO*		
FORCE CONSTANTS-	65.35	CCO	19.66	CCH	6.90	CC	5.31	CCC		
OFF DIAGONAL-	-8.68	BB34	5.63	BB43	4.34	SB22	-4.00	BB29	-1.89	
NORMAL MODE 49		OBSERVED= 308.0 CM-1		CALCULATED= 308.4 CM-1		ERROR= -0.4 CM-1		OR -0.1 PERCENT		
INTERNAL COORDINATES-	25.81	O8CC	20.91	CCO8	18.47	O'CC	8.42	CCO9	5.96	
FORCE CONSTANTS-	78.70	CCO	11.79	T-OH	7.85	CCH	5.98	CC		
OFF DIAGONAL-	-8.99	BB34	-3.74	BB42	1.73	SB22				
NORMAL MODE 50		OBSERVED= 274.0 CM-1		CALCULATED= 294.1 CM-1		ERROR= -20.1 CM-1		OR -7.3 PERCENT		
INTERNAL COORDINATES-	19.42	CCO7	11.52	CCO8	10.53	O7CC	9.63	TH-2	5.55	
FORCE CONSTANTS-	58.68	CCO	14.67	CCH	12.29	T-OH	7.82	CCC		
OFF DIAGONAL-	-6.35	BB34	4.90	BB43	-2.37	SB25	-2.21	BB29	1.86	
NORMAL MODE 51		OBSERVED= 249.0 CM-1		CALCULATED= 237.6 CM-1		ERROR= 11.4 CM-1		OR 4.6 PERCENT		
INTERNAL COORDINATES-	39.32	TH-1	16.86	TH-5	6.72	TH-3	5.96	TH-4	5.92	
FORCE CONSTANTS-	68.86	T-OH	14.20	CCO	8.01	CCC				
OFF DIAGONAL-	-11.53	BB34								
NORMAL MODE 52		OBSERVED= 236.0 CM-1		CALCULATED= 231.7 CM-1		ERROR= 4.3 CM-1		OR 1.8 PERCENT		
INTERNAL COORDINATES-	40.86	TH-3	13.16	TH-4	6.18	TH-5	5.92	C1CC	5.91	
FORCE CONSTANTS-	66.12	T-OH	21.33	CCO	7.24	CCC				
OFF DIAGONAL-	-2.38	BB34	-1.90	SB25						
NORMAL MODE 53		OBSERVED= 0.0 CM-1		CALCULATED= 225.1 CM-1		ERROR= 0.0 CM-1		OR 0.0 PERCENT		
INTERNAL COORDINATES-	36.00	TH-3	36.99	TH-1	7.00	TH-2				
FORCE CONSTANTS-	81.36	T-OH	15.06	CCO						
OFF DIAGONAL-	NONE									
NORMAL MODE 54		OBSERVED= 222.0 CM-1		CALCULATED= 222.8 CM-1		ERROR= -0.8 CM-1		OR -0.4 PERCENT		
INTERNAL COORDINATES-	66.40	TH-5	5.00	TH-1						
FORCE CONSTANTS-	75.18	T-OH	16.86	CCO	5.11	CCC				
OFF DIAGONAL-	-1.79	BB34								
NORMAL MODE 55		OBSERVED= 0.0 CM-1		CALCULATED= 217.7 CM-1		ERROR= 0.0 CM-1		OR 0.0 PERCENT		
INTERNAL COORDINATES-	43.38	TH-2	23.62	TH-3	18.88	TH-4				
FORCE CONSTANTS-	87.65	T-OH	12.14	CCO						
OFF DIAGONAL-	NONE									
NORMAL MODE 56		OBSERVED= 208.0 CM-1		CALCULATED= 209.9 CM-1		ERROR= -1.9 CM-1		OR -0.9 PERCENT		
INTERNAL COORDINATES-	30.79	TH-2	14.40	O7CC	13.00	TH-4	12.88	TH-3	8.87	
FORCE CONSTANTS-	65.55	T-OH	26.69	CCO	6.83	CCH				
OFF DIAGONAL-	-2.25	BB34	-2.00	BB33	-1.96	SB25				
NORMAL MODE 57		OBSERVED= 196.0 CM-1		CALCULATED= 194.9 CM-1		ERROR= 1.1 CM-1		OR 0.5 PERCENT		
INTERNAL COORDINATES-	27.85	C4CC	19.44	CCO*	10.96	TCC5	7.73	CCO*	6.03	
FORCE CONSTANTS-	40.59	CCO	31.33	CCC	14.15	T-OH	11.36	T-CC	5.45	
OFF DIAGONAL-	-6.29	BB34	-4.20	SB25	-3.85	BB42	1.88	SB21		
NORMAL MODE 58		OBSERVED= 0.0 CM-1		CALCULATED= 141.6 CM-1		ERROR= 0.0 CM-1		OR 0.0 PERCENT		
INTERNAL COORDINATES-	27.43	CO*	14.87	CCO*	8.42	TCC4	6.06	TCC5	5.44	
FORCE CONSTANTS-	27.95	CCO	27.43	CUC	15.81	T-CC	7.40	T-CC	7.13	
OFF DIAGONAL-	-5.23	BB34	-2.79	BB37	2.78	BB43	-2.45	SB25	1.96	
NORMAL MODE 59		OBSERVED= 0.0 CM-1		CALCULATED= 92.8 CM-1		ERROR= 0.0 CM-1		OR 0.0 PERCENT		
INTERNAL COORDINATES-	41.21	TCC5	10.62	C1CC	10.39	TCC4				
FORCE CONSTANTS-	57.43	T-CC	20.25	CCC	14.95	CCO				
OFF DIAGONAL-	-1.92	SB25	-1.62	BB42						
NORMAL MODE 60		OBSERVED= 0.0 CM-1		CALCULATED= 80.9 CM-1		ERROR= 0.0 CM-1		OR 0.0 PERCENT		
INTERNAL COORDINATES-	19.46	C3CC	18.30	C2CC	16.95	TCC2	6.56	CCO9	5.61	
FORCE CONSTANTS-	38.01	CCC	30.41	T-CC	23.05	CCO	5.22	T-CC	1.96	
OFF DIAGONAL-	-4.04	SB25	-3.75	BB42	-2.22	BB34	2.18	BB41	-1.55	
NORMAL MODE 61		OBSERVED= 0.0 CM-1		CALCULATED= 63.9 CM-1		ERROR= 0.0 CM-1		OR 0.0 PERCENT		
INTERNAL COORDINATES-	28.96	TCC5	9.10	4CO*	6.92	CO*	6.37	C1CC	6.08	
FORCE CONSTANTS-	45.98	T-CC	18.49	CCO	18.20	CCC	6.92	CO	6.10	
OFF DIAGONAL-	-2.10	BB34	-2.02	BB42						

47. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 8.69

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400										PAGE 1
MOLECULE 37 -6 NG-1238 BETA MANNOSE GT										
NORMAL MODE 8										
INTERNAL COORDINATES-	OBSERVED=	1478.0	CM-1	CALCULATED=	1449.6	CM-1	ERROR=	28.3	CM-1 OR 1.9 PERCENT	
FORCE CONSTANTS-	62.30	HCH	39.90	OCHB	18.69	OCHA				
OFF DIAGONAL-	-3.77	SB27								
NORMAL MODE 9										
INTERNAL COORDINATES-	OBSERVED=	1428.0	CM-1	CALCULATED=	1421.1	CM-1	ERROR=	6.9	CM-1 OR 0.5 PERCENT	
FORCE CONSTANTS-	34.84	OCH	31.97	BCOH	23.18	CCH	6.48	CO	5.33	
OFF DIAGONAL-	-6.29	SB27	-5.38	SB26	4.13	BB29	4.04	SB28	-2.31	
								BB45	2.25	
								BB34	-2.16	
								SB25	2.13	
								BB36	-1.83	
								BB43		
NORMAL MODE 10										
INTERNAL COORDINATES-	OBSERVED=	1419.0	CM-1	CALCULATED=	1418.6	CM-1	ERROR=	0.4	CM-1 OR 0.0 PERCENT	
FORCE CONSTANTS-	34.95	C1H	16.72	OC1H	9.40	C4OH	8.29	C2OH	7.18	
OFF DIAGONAL-	-10.22	OCH	22.89	BCOH	17.55	CCH	8.19	CO	5.33	
		SB27	-2.94	BB45	1.84	SB28	-2.05	BB43	-1.63	
								SB25		
NORMAL MODE 11										
INTERNAL COORDINATES-	OBSERVED=	1406.0	CM-1	CALCULATED=	1404.8	CM-1	ERROR=	1.3	CM-1 OR 0.1 PERCENT	
FORCE CONSTANTS-	29.53	C3OH	13.07	OC3H	10.29	C1OH	7.53	HC3C	5.60	
OFF DIAGONAL-	-47.50	BCOH	25.14	OCH	17.23	CCH	8.61	CO		
		SB27	4.15	SB28	2.70	BB29	-2.67	SB26	-1.98	
								BB39	-1.80	
								SB25	-1.62	
								BB45		
NORMAL MODE 12										
INTERNAL COORDINATES-	OBSERVED=	1402.0	CM-1	CALCULATED=	1402.4	CM-1	ERROR=	0.0	CM-1 OR 0.0 PERCENT	
FORCE CONSTANTS-	47.85	C1OH	8.93	C1H	7.92	C2OH	7.09	C1C2		
OFF DIAGONAL-	-4.75	BCOH	16.16	OCH	7.78	CC	6.06	CCH		
		SB28	-3.15	SB26	-1.95	SB22				
NORMAL MODE 13										
INTERNAL COORDINATES-	OBSERVED=	1395.0	CM-1	CALCULATED=	1395.2	CM-1	ERROR=	0.0	CM-1 OR 0.0 PERCENT	
FORCE CONSTANTS-	70.96	C*OH	7.25	OC*H	6.34	CCHB				
OFF DIAGONAL-	-3.43	SB26	2.84	SB28	2.37	BB29	-2.03	BB39		
NORMAL MODE 14										
INTERNAL COORDINATES-	OBSERVED=	1387.0	CM-1	CALCULATED=	1387.8	CM-1	ERROR=	0.0	CM-1 OR 0.0 PERCENT	
FORCE CONSTANTS-	56.46	C2OH	12.46	C1OH	7.03	OC1H	6.50	OC2H		
OFF DIAGONAL-	-3.97	BCOH	18.63	OCH	5.29	CCH				
		SB28	-3.49	SB27	-2.55	BB39				
NORMAL MODE 15										
INTERNAL COORDINATES-	OBSERVED=	1368.0	CM-1	CALCULATED=	1375.2	CM-1	ERROR=	-7.2	CM-1 OR -0.5 PERCENT	
FORCE CONSTANTS-	33.73	C4OH	24.02	C3OH	11.68	C5H	7.29	CC5H		
OFF DIAGONAL-	-3.06	BCOH	16.45	OCH	16.18	OCH				
		SB27	2.47	BB29	2.31	BB34	-1.70	BB36		
NORMAL MODE 16										
INTERNAL COORDINATES-	OBSERVED=	1363.0	CM-1	CALCULATED=	1354.2	CM-1	ERROR=	8.8	CM-1 OR 0.6 PERCENT	
FORCE CONSTANTS-	14.54	C3OH	13.06	CC4H	12.94	HC3C	9.08	HC5C	8.26	
OFF DIAGONAL-	-47.43	CCH	25.63	OCH	18.56	BCOH	8.08	CC5H	5.42	
		BB29	-4.25	SB27	-3.06	BB45	-2.49	SB26	2.26	
								BB34	-2.11	
								SB28		
NORMAL MODE 17										
INTERNAL COORDINATES-	OBSERVED=	1350.0	CM-1	CALCULATED=	1344.9	CM-1	ERROR=	5.0	CM-1 OR 0.4 PERCENT	
FORCE CONSTANTS-	27.60	CC2H	15.20	O*Cl	11.57	C1OH	8.92	C-06	8.29	
OFF DIAGONAL-	-27.70	CCH	25.01	CO	20.60	OCH	18.57	BCOH	6.08	
		SB27	-4.47	SB28	-4.29	SB25	3.88	BB34	-1.99	
								BB45	1.74	
								BB33		
NORMAL MODE 18										
INTERNAL COORDINATES-	OBSERVED=	1330.0	CM-1	CALCULATED=	1328.8	CM-1	ERROR=	1.2	CM-1 OR 0.1 PERCENT	
FORCE CONSTANTS-	14.83	CCBH	11.26	OCBH	11.01	HC5C	10.65	CC5H	7.88	
OFF DIAGONAL-	-63.07	CCH	19.02	OCH	9.73	BCOH	6.59	HC4C	6.52	
		BB29	-7.36	SB26	-3.57	BB45	-2.51	SB27	-1.61	
								SB28		
NORMAL MODE 19										
INTERNAL COORDINATES-	OBSERVED=	1311.0	CM-1	CALCULATED=	1311.5	CM-1	ERROR=	-0.5	CM-1 OR -0.0 PERCENT	
FORCE CONSTANTS-	26.20	HC2C	21.44	CC3H	18.89	OC3H	9.19	OC2H	7.83	
OFF DIAGONAL-	-3.64	BB45	2.66	BB34	-2.04	SB28	-2.01	SB27	1.55	
								BB30		
NORMAL MODE 20										
INTERNAL COORDINATES-	OBSERVED=	1292.0	CM-1	CALCULATED=	1295.0	CM-1	ERROR=	-3.0	CM-1 OR -0.2 PERCENT	
FORCE CONSTANTS-	27.18	CC4H	15.48	OCHA	10.58	OC4H	8.27	HC4C	6.52	
OFF DIAGONAL-	-49.65	CCH	42.50	OCH	6.06	BCOH	5.10	HCH		
		BB45	-2.80	SB27	-1.81	BB29	1.55	BB39		
								CC5H	5.10	
								HCH		
NORMAL MODE 21										
INTERNAL COORDINATES-	OBSERVED=	1278.0	CM-1	CALCULATED=	1272.6	CM-1	ERROR=	5.4	CM-1 OR 0.4 PERCENT	
FORCE CONSTANTS-	23.42	C5H	15.40	OC4H	14.76	CC4H	11.23	OCHA	9.66	
OFF DIAGONAL-	-56.31	OCH	32.60	CCH	-2.75	BB29				
		SB27	-3.50	BB45						
NORMAL MODE 22										
INTERNAL COORDINATES-	OBSERVED=	1261.0	CM-1	CALCULATED=	1263.8	CM-1	ERROR=	-2.8	CM-1 OR -0.2 PERCENT	
FORCE CONSTANTS-	15.94	OC2H	11.11	C5H	9.55	CC4H	7.74	CC3H	7.39	
OFF DIAGONAL-	-42.40	OCH	38.15	CCH	6.92	CO	5.23	BCOH		
		SB27	-3.26	BB45	1.95	BB34	-1.64	SB25		
NORMAL MODE 23										
INTERNAL COORDINATES-	OBSERVED=	1238.0	CM-1	CALCULATED=	1250.0	CM-1	ERROR=	-12.4	CM-1 OR -1.0 PERCENT	
FORCE CONSTANTS-	12.26	OC4H	11.45	OC2H	8.45	HC3C	7.36	CC3H	6.68	
OFF DIAGONAL-	-35.43	CCH	38.64	OCH	11.08	CO	8.67	CO	5.33	
		SB27	-4.95	BB29	-3.75	SB25	3.53	BB34	-3.11	
								BB45	-1.61	
								SB28		
NORMAL MODE 24										
INTERNAL COORDINATES-	OBSERVED=	1212.0	CM-1	CALCULATED=	1210.8	CM-1	ERROR=	1.2	CM-1 OR 0.1 PERCENT	
FORCE CONSTANTS-	18.39	C1H	11.81	OC1H	10.74	OC3H	8.67	HC4C	6.67	
OFF DIAGONAL-	-52.54	CCH	33.15	OCH	9.39	CO	6.93	BCOH	6.37	
		BB29	-3.41	BB45	-2.95	SB25	2.93	BB34	-1.60	
								SB28		
NORMAL MODE 25										
INTERNAL COORDINATES-	OBSERVED=	1183.0	CM-1	CALCULATED=	1183.4	CM-1	ERROR=	0.0	CM-1 OR 0.0 PERCENT	
FORCE CONSTANTS-	15.04	CC1H	11.19	OC1H	8.16	OCBH	7.62	C2C3	7.38	
OFF DIAGONAL-	-46.97	CCH	29.35	OCH	19.06	CCO	10.93	CC	9.06	
		SB26	-4.53	BB29	-4.13	SB25	-3.46	SB28	-3.20	
								SB27	-2.84	
								BB45	2.57	
								BB34	-2.43	
								SB22	-2.32	
								BB43		
NORMAL MODE 26										
INTERNAL COORDINATES-	OBSERVED=	1167.0	CM-1	CALCULATED=	1157.5	CM-1	ERROR=	9.4	CM-1 OR 0.8 PERCENT	
FORCE CONSTANTS-	17.87	CC2H	17.44	O*Cl	12.73	C-08	10.80	C-06	9.41	
OFF DIAGONAL-	-48.73	CO	42.22	CCH	15.33	CC	14.50	OCH	9.61	
		SB26	-6.53	SB25	-6.11	SB27	-4.57	SB28	-2.89	
								BB43	-2.81	
								SB21	-2.41	
								BB45	-2.28	
								SS18		
NORMAL MODE 27										
INTERNAL COORDINATES-	OBSERVED=	1124.0	CM-1	CALCULATED=	1142.2	CM-1	ERROR=	-18.2	CM-1 OR -1.6 PERCENT	
FORCE CONSTANTS-	13.86	C5H	11.73	OCBH	10.39	OCHA	8.19	C2C3	6.10	
OFF DIAGONAL-	-8.69	CCO	27.21	CO	18.91	OCH	15.36	CCO	6.44	
		SB25	-3.76	SB22	3.06	SB27	-2.39	BB43		
NORMAL MODE 28										
INTERNAL COORDINATES-	OBSERVED=	1118.0	CM-1	CALCULATED=	1128.3	CM-1	ERROR=	-10.3	CM-1 OR -0.9 PERCENT	
FORCE CONSTANTS-	40.19	C3C	17.25	C4C5	8.67	CCO	7.65	C-04	7.34	
OFF DIAGONAL-	-14.56	SB22	-7.95	SB26	-4.23	SS18	-3.01	SB28	-2.29	
								SB24	2.13	
								SB21	-2.01	
								BB34	-1.91	
								SB27	-1.51	
								SS17		
NORMAL MODE 29										
INTERNAL COORDINATES-	OBSERVED=	1113.0	CM-1	CALCULATED=	1106.8	CM-1	ERROR=	6.2	CM-1 OR 0.6 PERCENT	
FORCE CONSTANTS-	26.29	C3C4	21.10	C2C3	10.61	C-09	9.36	C4C5	8.80	
OFF DIAGONAL-	-65.62	CC	27.42	CO	13.21	CCO	12.89	CCH		
		SB22	-3.12	SB26	-3.01	SS18	-2.78	SB25	-2.63	
								SS17		
NORMAL MODE 30										
INTERNAL COORDINATES-	OBSERVED=	1086.0	CM-1	CALCULATED=	1097.7	CM-1	ERROR=	-11.7	CM-1 OR -1.1 PERCENT	
FORCE CONSTANTS-	26.15	C5O	21.27	C-09	6.05	C-08	7.15	C2C3	5.50	
OFF DIAGONAL-	-63.50	CO	16.78	CC	12.54	CCO	9.92	CCH	9.71	
		SB25	-3.08	SB28	-3.03	SB22	-1.99	SB21	-1.85	
								BB2		
NORMAL MODE 31										
INTERNAL COORDINATES-	OBSERVED=	1070.0	CM-1	CALCULATED=	1066.5	CM-1	ERROR=	3.5	CM-1 OR 0.3 PERCENT	
FORCE CONSTANTS-	80.47	CO	25.94	C1C2	8.43	BCOH	6.69	CO	6.13	
OFF DIAGONAL-	-8.75	SB28	-7.29	SB27	-5.96	SS18	-3.90	SB25	-3.20	
								SB24	-3.14	
								SB22	-1.96	
								SB26	-1.62	
								SB21		
NORMAL MODE 32										
INTERNAL COORDINATES-	OBSERVED=	1057.0	CM-1	CALCULATED=	1048.4	CM-1	ERROR=	8.6	CM-1 OR 0.8 PERCENT	
FORCE CONSTANTS-	19.40	C-08	17.69	C4C5	15.62	C-07	12.25	C-04	11.14	
OFF DIAGONAL-	-58.95	CO	32.11	CC	14.26	OC3H	13.46	CCH	11.58	
		SB27	-8.71	SB28	-7.87	SB21	-7.08	SB25	-5.97	
								SS18	-3.04	
								BB34	-2.51	
								BB36	-2.20	
								SB22		
								1.53	SB26	
NORMAL MODE 33										
INTERNAL COORDINATES-	OBSERVED=	1041.0	CM-1	CALCULATED=	1039.5	CM-1	ERROR=	1.4	CM-1 OR 0.1 PERCENT	
FORCE CONSTANTS-	28.59	C-09	25.11	C-07	17.33	C1C2	11.29	C2C3	6.31	
OFF DIAGONAL-	-59.49	CO	37.70	CC	14.23	CC3H	13.86	OCH	12.86	
		SB27	-11.10	SB21	-9.52	SB28	-8.08	SS18	-5.29	
								SB26	-5.19	
								SB22	-3.68	
								SB25	-2.42	
								BB43	-2.07	
								BB34		
NORMAL MODE 34										
INTERNAL COORDINATES-	OBSERVED=	1032.0	CM-1	CALCULATED=	1023.0	CM-1	ERROR=	9.0	CM-1 OR 0.9 PERCENT	
FORCE CONSTANTS-	27.42	C4C5	20.86	C-06	20.23	C-08	7.90	C-04	6.96	
OFF DIAGONAL-	-9.32	SB21	-9.18	SB22	-9.93	SB27	-4.78	SB28	-4.12	
								SS18	-2.44	
								SB24	1.89	
								SB25		
NORMAL MODE 35										
INTERNAL COORDINATES-	OBSERVED=	1007.0	CM-1	CALCULATED=	978.9	CM-1	ERROR=	28.1	CM-1 OR 2.8 PERCENT	
FORCE CONSTANTS-										

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400									
MOLECULE 37 -6 NG-1238 BETA MANNOSIDE GT PAGE 2									
NORMAL MODE 36	OBSERVED=	933.0 CM-1		CALCULATED=	931.9 CM-1	ERROR=	1.1 CM-1	OR	0.1 PERCENT
INTERNAL COORDINATES-	17.35	C3C4 11.11	O1C1	9.08	C-06	7.92	C2C3	6.88	C-07
FORCE CONSTANTS-	36.15	CC 31.45	CC 31.45	14.77	CC 11.08	11.08	CC 11.08	6.74	CC 3H
OFF DIAGONAL-	-10.78	SB21 -6.21	SB22	4.77	SB26	2.74	SB24	2.15	SS18
NORMAL MODE 37	OBSERVED=	896.0 CM-1		CALCULATED=	894.6 CM-1	ERROR=	1.4 CM-1	OR	0.2 PERCENT
INTERNAL COORDINATES-	16.00	C5C6 11.16	C5O*	9.30	C3C4	8.47	C3C4	7.68	C-07
FORCE CONSTANTS-	31.64	CC 22.18	CC 22.18	21.32	CC 13.32	CC 13.32	CC 13.32	6.66	CC 13.32
OFF DIAGONAL-	-6.32	SB22 4.24	SS18	3.68	SB26	-2.38	SB21	-2.19	SB25
NORMAL MODE 38	OBSERVED=	855.0 CM-1		CALCULATED=	825.9 CM-1	ERROR=	29.1 CM-1	OR	3.4 PERCENT
INTERNAL COORDINATES-	43.95	O1C1 12.27	C-07	12.23	C1C2	9.82	CC 8.32	CC 8.32	C5O*
FORCE CONSTANTS-	37.43	CC 28.87	CC 28.87	13.61	CC 7.42	CC 7.42	CC 7.42	6.66	CC 5.07
OFF DIAGONAL-	-5.14	SB23 -4.88	SB24	4.32	SS18	4.20	SB26	-3.36	BB29
NORMAL MODE 39	OBSERVED=	769.0 CM-1		CALCULATED=	767.8 CM-1	ERROR=	1.2 CM-1	OR	0.1 PERCENT
INTERNAL COORDINATES-	18.83	O1C1 10.63	CC07	10.09	C-07	8.89	UCH	7.73	CC 5.14
FORCE CONSTANTS-	33.26	CC 20.83	CC 20.83	9.77	CC 8.89	CC 8.89	CC 8.89	1.84	BB33
OFF DIAGONAL-	-8.65	SB25 5.04	BB43	-3.80	SB27	-1.97	BB41	1.84	BB33
NORMAL MODE 40	OBSERVED=	730.0 CM-1		CALCULATED=	728.2 CM-1	ERROR=	1.8 CM-1	OR	0.3 PERCENT
INTERNAL COORDINATES-	14.04	CC06 13.31	O7CC	9.87	CC08	8.97	CC07	7.45	C3C4
FORCE CONSTANTS-	51.01	CC 13.20	CC 13.20	10.07	CC 7.79	CC 7.79	CC 7.79	7.11	CC 5.34
OFF DIAGONAL-	-6.47	BB43 5.11	SB25	-4.13	BB34	-2.96	SB27	-1.74	BB41
NORMAL MODE 41	OBSERVED=	618.0 CM-1		CALCULATED=	617.1 CM-1	ERROR=	0.9 CM-1	OR	0.1 PERCENT
INTERNAL COORDINATES-	20.30	CC08 18.93	OBCC	8.65	O9CC	8.34	CC3H	6.86	HC4C
FORCE CONSTANTS-	69.84	CC 28.66	CC 28.66	7.76	CC 5.08	CC 5.08	CC 5.08	6.30	CC 5.08
OFF DIAGONAL-	-14.91	BB34 7.21	BB43	-6.04	BB29	3.90	SB25	-2.69	BB42
NORMAL MODE 42	OBSERVED=	599.0 CM-1		CALCULATED=	603.6 CM-1	ERROR=	-4.6 CM-1	OR	-0.8 PERCENT
INTERNAL COORDINATES-	15.01	CC 13.32	CC0*	15.01	CC 13.32	CC 13.32	CC 13.32	6.66	CC 13.32
FORCE CONSTANTS-	36.15	CC 22.18	CC 22.18	21.32	CC 13.32	CC 13.32	CC 13.32	6.66	CC 13.32
OFF DIAGONAL-	-5.99	SB24 -3.59	BB29	3.49	SB22	-3.37	BB34	3.14	BB43
NORMAL MODE 43	OBSERVED=	492.0 CM-1		CALCULATED=	500.5 CM-1	ERROR=	-8.5 CM-1	OR	-1.7 PERCENT
INTERNAL COORDINATES-	9.94	CC0*	8.04	OBCC	7.73	CC09	7.09	HC5C	6.95
FORCE CONSTANTS-	31.15	CC 22.57	CC 22.57	13.64	CC 12.99	CC 12.99	CC 12.99	11.78	CC 11.78
OFF DIAGONAL-	-10.06	BB34 7.80	BB43	-4.92	BB29	2.69	SB24	2.14	SB21
NORMAL MODE 44	OBSERVED=	444.0 CM-1		CALCULATED=	468.7 CM-1	ERROR=	-24.7 CM-1	OR	-5.6 PERCENT
INTERNAL COORDINATES-	10.53	CC0*	8.87	C1CC	8.15	CC0*	7.41	CC0*	6.75
FORCE CONSTANTS-	30.97	CC 14.83	CC 14.83	13.91	CC 11.04	CC 11.04	CC 11.04	8.15	CC 7.96
OFF DIAGONAL-	-6.12	SB22 3.61	BB43	-3.35	SB26	-2.68	BB34	2.68	SB25
NORMAL MODE 45	OBSERVED=	423.0 CM-1		CALCULATED=	416.4 CM-1	ERROR=	6.6 CM-1	OR	1.6 PERCENT
INTERNAL COORDINATES-	18.88	CC06 9.38	O7CC	8.97	CC0*	6.65	CC0*	6.55	C3CC
FORCE CONSTANTS-	48.81	CC 12.39	CC 12.39	12.10	CC 8.97	CC 8.97	CC 8.97	8.34	CC 8.34
OFF DIAGONAL-	-4.54	BB34 2.87	SB25	1.93	BB43	-1.81	BB33	1.74	SB22
NORMAL MODE 46	OBSERVED=	394.0 CM-1		CALCULATED=	387.3 CM-1	ERROR=	6.7 CM-1	OR	1.7 PERCENT
INTERNAL COORDINATES-	15.29	CC09 13.61	CC08	12.02	O9CC	9.49	CC 7.31	C3CC	6.18
FORCE CONSTANTS-	34.55	CC 20.77	CC 20.77	14.90	CC 6.18	CC 6.18	CC 6.18	5.32	CC 5.32
OFF DIAGONAL-	-8.61	BB34 -3.03	BB42	2.91	SB21	-2.63	BB29	2.49	SB25
NORMAL MODE 47	OBSERVED=	370.0 CM-1		CALCULATED=	365.7 CM-1	ERROR=	4.3 CM-1	OR	1.2 PERCENT
INTERNAL COORDINATES-	12.89	CC0*	12.46	CC0*	12.12	CC07	8.69	CC0*	5.23
FORCE CONSTANTS-	49.61	CC 11.49	CC 11.49	11.27	CC 8.69	CC 8.69	CC 8.69	6.16	CC 6.16
OFF DIAGONAL-	-5.79	BB34 3.72	BB43	2.90	SB25	2.67	SB21	2.36	SB22
NORMAL MODE 48	OBSERVED=	326.0 CM-1		CALCULATED=	327.9 CM-1	ERROR=	-1.9 CM-1	OR	-0.6 PERCENT
INTERNAL COORDINATES-	22.74	O9CC 17.18	OBCC	14.25	CC08	13.76	CC09	12.50	CC07
FORCE CONSTANTS-	87.24	CC 10.95	T-OH	5.93	CC 5.93	CC 5.93	CC 5.93	6.66	CC 6.66
OFF DIAGONAL-	-7.03	BB34 -4.53	BB42	1.91	BB41				
NORMAL MODE 49	OBSERVED=	0.0 CM-1		CALCULATED=	309.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	14.32	CC06 8.67	CC08	8.46	OBCC	6.94	C4C5	6.90	CC03
FORCE CONSTANTS-	46.18	CC 20.21	CC 20.21	12.27	T-OH	10.61	T-OH	7.64	OBCC
OFF DIAGONAL-	-6.48	SB22 4.38	SB21	-2.91	BB42	-2.18	BB34	-1.69	SB26
NORMAL MODE 50	OBSERVED=	288.0 CM-1		CALCULATED=	292.3 CM-1	ERROR=	-4.3 CM-1	OR	-1.5 PERCENT
INTERNAL COORDINATES-	14.67	CC07 11.80	O7CC	10.08	TH-2	8.46	O9CC	7.64	OBCC
FORCE CONSTANTS-	62.65	CC 14.22	T-OH	14.13	CC 6.44	CC 6.44	CC 6.44	6.66	CC 6.66
OFF DIAGONAL-	-5.99	BB34 4.84	BB43	2.94	SB22	-2.74	BB33	-2.30	SB25
NORMAL MODE 51	OBSERVED=	258.0 CM-1		CALCULATED=	259.2 CM-1	ERROR=	-1.2 CM-1	OR	-0.5 PERCENT
INTERNAL COORDINATES-	22.00	U7CC 14.74	C1CC	9.92	CC07	6.64	O1CC	5.46	CC0*
FORCE CONSTANTS-	49.05	CC 18.60	CC 18.60	15.53	T-OH	11.21	CC 5.46	CC 5.46	CC 5.46
OFF DIAGONAL-	-4.29	BB33 4.15	SB22	3.52	BB43	-3.29	SB25	-2.73	SB21
NORMAL MODE 52	OBSERVED=	239.0 CM-1		CALCULATED=	232.7 CM-1	ERROR=	6.3 CM-1	OR	2.6 PERCENT
INTERNAL COORDINATES-	35.29	TH-1 26.18	TH-4	13.77	TH-3	6.82	CC0*	6.24	TH-2
FORCE CONSTANTS-	82.27	T-CH 10.30	CC 10.30						
OFF DIAGONAL-	NONE								
NORMAL MODE 53	OBSERVED=	0.0 CM-1		CALCULATED=	224.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	81.01	TH-5							
FORCE CONSTANTS-	85.11	T-CH 7.30	CC 7.30						
OFF DIAGONAL-	NONE								
NORMAL MODE 54	OBSERVED=	0.0 CM-1		CALCULATED=	218.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	43.91	TH-1 19.36	TH-3	11.71	TH-2	10.11	TH-4		
FORCE CONSTANTS-	86.52	T-CH 9.33	CC 9.33						
OFF DIAGONAL-	NONE								
NORMAL MODE 55	OBSERVED=	0.0 CM-1		CALCULATED=	213.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	41.99	TH-2 34.40	TH-4						
FORCE CONSTANTS-	83.78	T-CH 13.24	CC 13.24						
OFF DIAGONAL-	NONE								
NORMAL MODE 56	OBSERVED=	0.0 CM-1		CALCULATED=	209.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	47.16	TH-3 24.07	TH-2	8.23	CC08	7.67	TH-4		
FORCE CONSTANTS-	79.39	T-OH 18.89	CC 18.89						
OFF DIAGONAL-	-1.71	BB34							
NORMAL MODE 57	OBSERVED=	0.0 CM-1		CALCULATED=	193.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	31.26	CC0*	12.46	C4CC	10.03	CC0*	7.27	TH-4	7.25
FORCE CONSTANTS-	43.93	CC 15.97	T-OH	13.98	CC 10.03	CC 10.03	CC 10.03	8.10	T-CC
OFF DIAGONAL-	-3.60	BB34 -3.13	BB42	-2.73	BB33				
NORMAL MODE 58	OBSERVED=	0.0 CM-1		CALCULATED=	150.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	22.12	C4CC 16.21	CC0*	6.33	TCC4	6.27	CC06	6.16	TCC1
FORCE CONSTANTS-	44.17	CC 20.69	CC 20.69	16.21	CC 10.61	CC 10.61	CC 10.61	7.24	T-CC
OFF DIAGONAL-	-4.16	SB21 3.50	BB43	-2.40	BB34	-1.98	SB25	1.86	SB22
NORMAL MODE 59	OBSERVED=	0.0 CM-1		CALCULATED=	98.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	57.43	TCC5 8.33	C3CC	9.95	O9CC				
FORCE CONSTANTS-	66.44	T-CC 16.96	CC 16.96	15.15	CC 15.15	CC 15.15	CC 15.15	6.66	CC 6.66
OFF DIAGONAL-	-2.79	BB34 -2.75	SB25	-1.98	BB42				
NORMAL MODE 60	OBSERVED=	0.0 CM-1		CALCULATED=	86.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	25.55	C2CC 11.96	C1CC	11.22	TCC4	9.42	TCC1	6.14	TCC2
FORCE CONSTANTS-	41.99	CC 28.28	T-CC	16.39	CC 5.03	CC 5.03	CC 5.03	6.66	CC 6.66
OFF DIAGONAL-	-3.24	SB25 -2.96	BB42	2.08	BB41	-1.56	SB21		
NORMAL MODE 61	OBSERVED=	0.0 CM-1		CALCULATED=	65.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	26.96	TCC5 14.46	C3CC	8.72	TCC2	8.02	TCC4	7.09	TCC3
FORCE CONSTANTS-	21.21	T-CC 22.18	CC 22.18	20.19	CC 20.19	CC 20.19	CC 20.19	6.66	CC 6.66
OFF DIAGONAL-	-2.52	BB42 -1.85	BB34						

40. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 7.39

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400										PAGE 1
MOLECULE 38 -6 NG=1238 BETA MANNOSE-1-0 GT										
NORMAL MODE 8 OBSERVED= 1480.0 CM-1 CALCULATED= 1449.6 CM-1 ERROR= 30.3 CM-1 OR 2.0 PERCENT										
INTERNAL COORDINATES- 62.31 HCH 19.91 OCHB 18.70 OCHA										
FORCE CONSTANTS- 62.31 HCH 38.94 OCH										
OFF DIAGONAL- -3.77 SB27										
NORMAL MODE 9 OBSERVED= 1420.0 CM-1 CALCULATED= 1420.5 CM-1 ERROR= -0.5 CM-1 OR -0.0 PERCENT										
INTERNAL COORDINATES- 38.51 C4OH 18.09 OC4H 13.27 HC4C 5.45 C4C5 5.27 CC5H										
FORCE CONSTANTS- 43.88 BCOH 22.23 OCH 21.42 CCH 6.93 CO 6.07 CC										
OFF DIAGONAL- -5.93 SB26 -5.66 SB27 5.09 SB28 4.06 BB29 2.82 BB36 -2.38 BB39 -2.33 SB25 2.25 BB34 -1.94 BB43										
NORMAL MODE 10 OBSERVED= 1405.0 CM-1 CALCULATED= 1398.9 CM-1 ERROR= -1.2 CM-1 OR -0.1 PERCENT										
INTERNAL COORDINATES- 39.72 C1OH 15.42 C2OH 10.89 C1OH 5.31 C1C2										
FORCE CONSTANTS- 46.32 BCOH 24.28 OCH 20.46 CCH 5.32 CO										
OFF DIAGONAL- -5.31 SB27 3.81 SB28 3.34 BB29 -3.33 SB26 -1.96 BB39 -1.76 BB45 1.58 BB34 -1.57 SB25										
NORMAL MODE 11 OBSERVED= 1400.0 CM-1 CALCULATED= 1406.2 CM-1 ERROR= 0.0 CM-1 OR 0.0 PERCENT										
INTERNAL COORDINATES- 34.17 C3OH 17.70 OC3H 8.56 HC3C 6.61 C2OH										
FORCE CONSTANTS- 68.94 BCOH 7.73 OCH 7.71 CCH 7.41 CO 5.84 CC										
OFF DIAGONAL- 6.32 SB28 -2.68 SB26 -2.49 SB27 -1.80 BB39										
NORMAL MODE 12 OBSERVED= 1395.0 CM-1 CALCULATED= 1395.0 CM-1 ERROR= 0.0 CM-1 OR 0.0 PERCENT										
INTERNAL COORDINATES- 62.58 C1OH 6.55 C1OH 6.14 OCHA 5.77 CCHB										
FORCE CONSTANTS- 74.41 BCOH 11.57 CCH 8.93 OCH										
OFF DIAGONAL- 3.16 SB28 -3.12 SB26 2.17 BB29 -2.01 BB39 -1.61 SB27										
NORMAL MODE 13 OBSERVED= 1387.1 CM-1 CALCULATED= 1387.1 CM-1 ERROR= 0.0 CM-1 OR 0.0 PERCENT										
INTERNAL COORDINATES- 49.45 C2OH 27.19 C1OH 6.85 OC2H										
FORCE CONSTANTS- 81.38 BCOH 8.36 OCH										
OFF DIAGONAL- 4.27 SB28 -2.06 BB39 -1.59 SB27										
NORMAL MODE 14 OBSERVED= 1373.0 CM-1 CALCULATED= 1375.1 CM-1 ERROR= -2.1 CM-1 OR -0.2 PERCENT										
INTERNAL COORDINATES- 34.64 C4OH 24.07 C3OH 12.05 C5H 7.51 CC5H										
FORCE CONSTANTS- 61.22 BCOH 16.53 OCH 16.26 CCH										
OFF DIAGONAL- -2.96 SB27 2.54 BB29 2.29 BB34 -1.70 BB36										
NORMAL MODE 15 OBSERVED= 1348.0 CM-1 CALCULATED= 1354.2 CM-1 ERROR= -6.2 CM-1 OR -0.5 PERCENT										
INTERNAL COORDINATES- 13.84 C3OH 12.53 CC4H 12.74 HC3C 9.34 HC5C 8.52 CCHB										
FORCE CONSTANTS- 10.19 BB29 -4.18 SB27 -3.11 BB45 -2.55 SB26 2.23 BB34 -2.07 SB28										
OFF DIAGONAL- 10.19 BB29 -4.18 SB27 -3.11 BB45 -2.55 SB26 2.23 BB34 -2.07 SB28										
NORMAL MODE 16 OBSERVED= 1339.0 CM-1 CALCULATED= 1350.4 CM-1 ERROR= -11.4 CM-1 OR -0.9 PERCENT										
INTERNAL COORDINATES- 30.10 CCH2 21.75 C1C1 12.96 C1OH 11.34 C06 8.60 OC2H 5.73 CC06										
FORCE CONSTANTS- 35.93 CCH 34.06 CO 18.86 BCOH 14.67 OCH 8.28 CCO										
OFF DIAGONAL- -7.02 SB27 -5.67 SB25 5.59 BB34 -4.99 SB28 -2.16 BB45 2.01 BB33										
NORMAL MODE 17 OBSERVED= 1328.8 CM-1 CALCULATED= 1328.8 CM-1 ERROR= 0.0 CM-1 OR 0.0 PERCENT										
INTERNAL COORDINATES- 15.87 CCHB 12.06 OCHB 11.39 HC5C 11.10 CC5H 7.58 HC3C 6.69 CC4H 6.33 HC4C 5.88 C1OH										
FORCE CONSTANTS- 63.27 CCH 19.31 CCH 9.64 BCOH										
OFF DIAGONAL- 13.69 BB29 -7.39 SB26 -3.58 BB45 -2.84 SB27 -1.56 SB28										
NORMAL MODE 18 OBSERVED= 1318.0 CM-1 CALCULATED= 1310.6 CM-1 ERROR= 7.4 CM-1 OR 0.6 PERCENT										
INTERNAL COORDINATES- 26.77 HC2C 21.38 CC3H 17.92 OC3H 14.54 OC2H 7.29 C2OH										
FORCE CONSTANTS- 52.33 HC45 34.61 OCH 7.81 BCOH										
OFF DIAGONAL- -3.70 BB45 2.52 BB34 -2.24 SB27 1.68 BB30 -1.56 SB28										
NORMAL MODE 19 OBSERVED= 1300.0 CM-1 CALCULATED= 1295.1 CM-1 ERROR= 4.9 CM-1 OR 0.4 PERCENT										
INTERNAL COORDINATES- 26.37 CCHA 14.99 OCHA 10.72 OC4H 8.48 HC4C 7.36 OC3H 6.50 CCHB 6.10 C5H										
FORCE CONSTANTS- 49.12 CCH 13.13 OCH 11.38 CCH 9.61 CO 6.72 BCOH										
OFF DIAGONAL- -3.71 BB45 -2.82 SB27 -1.81 BB29 1.55 BB39										
NORMAL MODE 20 OBSERVED= 1278.0 CM-1 CALCULATED= 1272.9 CM-1 ERROR= 5.1 CM-1 OR 0.4 PERCENT										
INTERNAL COORDINATES- 23.96 C5H 15.48 CCHA 15.01 OC4H 11.76 OCHA 9.69 CC5H										
FORCE CONSTANTS- 56.32 OCH 32.77 CCH										
OFF DIAGONAL- 4.83 SB27 -3.51 BB45 -2.82 BB29										
NORMAL MODE 21 OBSERVED= 1261.6 CM-1 CALCULATED= 1261.6 CM-1 ERROR= 0.0 CM-1 OR 0.0 PERCENT										
INTERNAL COORDINATES- 13.37 CC4H 13.13 C5H 10.44 OC3H 8.35 OC2H 7.77 OC4H 6.79 HC5C 6.07 CC3H 5.57 HC2C										
FORCE CONSTANTS- 44.31 OCH 38.88 CCH 5.53 CO										
OFF DIAGONAL- 6.75 SB27 -3.36 BB45 2.63 BB34 -2.17 BB29										
NORMAL MODE 22 OBSERVED= 1242.0 CM-1 CALCULATED= 1243.9 CM-1 ERROR= -1.9 CM-1 OR -0.2 PERCENT										
INTERNAL COORDINATES- 17.99 CC3H 15.38 OC2H 9.99 HC3C 9.81 OC4H 6.22 C07 5.46 HC5C 5.11 HC2C										
FORCE CONSTANTS- 45.02 CCH 33.32 OCH 12.11 CO 5.58 CCO										
OFF DIAGONAL- 7.61 SB27 -3.97 SB26 -3.65 SB25 -3.45 BB29 -3.17 BB45 3.08 BB34 -1.62 SB28 1.55 BB33										
NORMAL MODE 23 OBSERVED= 1216.0 CM-1 CALCULATED= 1197.2 CM-1 ERROR= 18.8 CM-1 OR 1.5 PERCENT										
INTERNAL COORDINATES- 12.16 HC4C 12.06 CC5H 11.49 HC5C 10.81 OCHB 9.89 CC4H 5.68 C08										
FORCE CONSTANTS- 64.93 CCH 22.30 OCH 11.38 CO 9.61 CO 6.72 BCOH										
OFF DIAGONAL- -10.55 BB29 6.07 BB34 -4.31 SB25 4.30 SB27 -2.89 BB45 -1.84 SB28										
NORMAL MODE 24 OBSERVED= 1161.8 CM-1 CALCULATED= 1161.8 CM-1 ERROR= 0.0 CM-1 OR 0.0 PERCENT										
INTERNAL COORDINATES- 37.54 C1O1 17.82 C1O1 10.87 C08 7.69 C5C										
FORCE CONSTANTS- 60.81 CO 24.75 CCH 18.92 OCH 11.47 BCOH 10.37 CCO										
OFF DIAGONAL- -9.40 SB25 -7.30 SB27 -6.33 SB28 -3.57 SB26 -2.33 BB43 -1.77 SB21 -1.56 BB45										
NORMAL MODE 25 OBSERVED= 1130.0 CM-1 CALCULATED= 1143.4 CM-1 ERROR= -13.4 CM-1 OR -1.2 PERCENT										
INTERNAL COORDINATES- 12.55 OCHB 9.71 OCHA 9.70 C5O 6.38 C09 5.23 C3C4 5.04 CCO										
FORCE CONSTANTS- 32.61 OCH 26.51 CO 13.99 CCO 10.75 CC 10.08 CCH										
OFF DIAGONAL- -8.90 SB25 4.09 SB27 2.90 BB43 -2.71 SB22 2.34 SB26 -1.69 SB23										
NORMAL MODE 26 OBSERVED= 1125.0 CM-1 CALCULATED= 1132.4 CM-1 ERROR= -7.4 CM-1 OR -0.7 PERCENT										
INTERNAL COORDINATES- 31.64 C5C 17.57 C1C2 10.22 C4C5 9.47 C06 6.87 CO1C 6.68 CCO 6.24 C2C3 6.06 C0*										
FORCE CONSTANTS- 65.70 CC 27.24 CO 20.28 CCH 6.87 CUC 6.11 CCH 5.67 BCOH										
OFF DIAGONAL- -14.82 SB22 -9.76 SB26 -4.94 SS18 -3.88 SB24 -3.13 SB28 -2.10 SB27 1.58 BB33										
NORMAL MODE 27 OBSERVED= 1120.0 CM-1 CALCULATED= 1120.4 CM-1 ERROR= -0.4 CM-1 OR -0.0 PERCENT										
INTERNAL COORDINATES- 38.78 C2C3 16.38 C3C4 14.41 C1O1 13.54 C4C5 8.86 C1C2 6.85 CCO7 5.94 C09 5.39 HC2C										
FORCE CONSTANTS- 64.10 CO 23.70 CCH 13.94 CCH 12.76 CCH										
OFF DIAGONAL- -15.08 SB26 -13.08 SB22 -4.59 SB25 -3.36 SS17 -3.05 SB27 -2.97 SS18 -2.72 SB28 -2.69 SB21 -2.05 BB34										
NORMAL MODE 28 OBSERVED= 1106.0 CM-1 CALCULATED= 1100.7 CM-1 ERROR= 5.3 CM-1 OR 0.5 PERCENT										
INTERNAL COORDINATES- 30.46 C5O 24.19 C09 10.87 C08 7.69 C5C										
FORCE CONSTANTS- 68.61 CO 24.55 CCH 18.92 OCH 11.47 BCOH 10.37 CCO										
OFF DIAGONAL- -6.24 SB25 -3.77 SB28 -3.01 SB27 -2.78 SS18 -2.42 SB21 -1.88 SB22										
NORMAL MODE 29 OBSERVED= 1080.0 CM-1 CALCULATED= 1076.9 CM-1 ERROR= 3.1 CM-1 OR 0.3 PERCENT										
INTERNAL COORDINATES- 30.53 C0* 20.47 C3C4 13.50 C07 8.96 C08 7.26 C3C4 5.04 CCO										
FORCE CONSTANTS- 62.41 CO 26.17 CCH 11.34 CCH 10.34 CCO 6.94 OCH 5.77 BCOH										
OFF DIAGONAL- -5.79 SB25 -5.79 SB28 -4.22 SB22 -4.04 SB27 -3.08 SS18 -1.63 SB21										
NORMAL MODE 30 OBSERVED= 1066.0 CM-1 CALCULATED= 1067.6 CM-1 ERROR= -1.6 CM-1 OR -0.1 PERCENT										
INTERNAL COORDINATES- 29.00 C06 19.86 C08 17.36 C07 16.98 C1C2 6.02 C1C1 6.01 C4C5										
FORCE CONSTANTS- 77.30 CO 30.22 CCH 11.42 BCOH 9.16 CCH 9.15 OCH 5.89 CCC										
OFF DIAGONAL- -10.37 SB27 -9.97 SB28 -8.42 SS18 -4.91 SB25 -4.49 SB21 -3.01 SB22 -2.88 SB26 -2.03 SB24 -1.79 BB36										
NORMAL MODE 31 OBSERVED= 1055.0 CM-1 CALCULATED= 1043.4 CM-1 ERROR= 11.6 CM-1 OR 1.1 PERCENT										
INTERNAL COORDINATES- 42.07 C09 11.62 C07 9.56 C1C2 7.62 C4C5 6.27 C4OH 6.17 C3CC 5.32 HC3C 5.17 C2C3 5.11 OC4H										
FORCE CONSTANTS- 62.10 CO 26.54 CCH 15.24 CCH 14.10 CCH 13.27 CCH 11.81 BCOH 9.88 CCO										
OFF DIAGONAL- -10.28 SB21 -10.03 SB28 -9.51 SB27 -5.55 SS18 -5.66 SB25 -2.60 BB34 -2.20 SB22 -2.03 BB43 -1.56 BB29										
NORMAL MODE 32 OBSERVED= 1033.0 CM-1 CALCULATED= 1025.5 CM-1 ERROR= 7.5 CM-1 OR 0.7 PERCENT										
INTERNAL COORDINATES- 30.11 C5C 17.62 C0* 10.85 C08 7.33 C2C3 8.16 C06										
FORCE CONSTANTS- 60.11 CO 24.55 CCH 10.99 CCH 7.33 CCH 5.23 BCOH										
OFF DIAGONAL- -9.24 SB21 -6.84 SB22 -5.50 SB27 -3.95 SB28 -3.68 SS18 3.17 SB25 -1.74 SB24										
NORMAL MODE 33 OBSERVED= 985.0 CM-1 CALCULATED= 1007.4 CM-1 ERROR= -22.4 CM-1 OR -2.3 PERCENT										
INTERNAL COORDINATES- 37.18 C1H 23.49 OC1H 14.67 C08										
FORCE CONSTANTS- 62.20 OCH 25.80 CCH										
OFF DIAGONAL- -3.99 SB27 -3.59 BB29 -3.44 BB37 -3.07 BB45 -2.79 SB28 -2.38 SB25										
NORMAL MODE 34 OBSERVED= 969.0 CM-1 CALCULATED= 982.8 CM-1 ERROR= -13.8 CM-1 OR -1.4 PERCENT										
INTERNAL COORDINATES- 20.43 C5C 16.32 OC1H 11.33 C08 9.08 C1H 8.15 C1C2 7.71 C0*										
FORCE CONSTANTS- 34.30 CCH 27.83 CCH 27.80 CCH 20.87 CCH 8.82 CCO										
OFF DIAGONAL- -7.67 SB22 -4.04 SB21 -3.68 BB29 -3.49 SB25 -3.28 SB26 -2.22 SB27 -1.80 SB28 -1.79 SB24 -1.64 BB45										
NORMAL MODE 35 OBSERVED= 930.0 CM-1 CALCULATED= 930.5 CM-1 ERROR= -0.5 CM-1 OR -0.1 PERCENT										
INTERNAL COORDINATES- 29.40 C3C4 10.75 C2C3 8.52 CCH 7.99 OC1H 7.01 C06 6.77 C07 5.62 C06										
FORCE CONSTANTS- 22.10 CCH 12.34 C										

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400									
MOLECULE 38		-6 NG=1238		BETA MANNOSYL-1-D		GT		PAGE 2	
NORMAL MODE 36	OBSERVED=	911.0 CM-1		CALCULATED=	908.1 CM-1		ERROR=	4.9 CM-1	OR 0.5 PERCENT
INTERNAL COORDINATES-	18.38	CC1 8.38	CC1H	8.38	CC1H	8.38	CC1H	5.37	CC1H
FORCE CONSTANTS-	34.99	CC 19.03	CO	17.65	CC 12.18	CC 11.75	CCO	5.28	CC1H
OFF DIAGONAL-	-6.27	SB22 4.06	SS18	-3.69	SB21 3.00	SB27			
NORMAL MODE 37	OBSERVED=	828.0 CM-1		CALCULATED=	843.7 CM-1		ERROR=	-15.7 CM-1	OR -1.9 PERCENT
INTERNAL COORDINATES-	19.84	CC1H 14.08	CC1H	10.25	CC1H	9.36	CC1H	9.05	CC1H
FORCE CONSTANTS-	36.44	CC 34.81	CC 20.53	CC 20.53	CC 5.30	CC 8.03	CCO	2.49	CC1H
OFF DIAGONAL-	5.52	SB27 -3.95	SB23	-3.69	SB24 -2.63	SB25	-2.61	BB37 -2.59	BB29 2.49 BB43 -2.03 SB26
NORMAL MODE 38	OBSERVED=	790.0 CM-1		CALCULATED=	805.4 CM-1		ERROR=	-15.4 CM-1	OR -1.9 PERCENT
INTERNAL COORDINATES-	20.49	CC1H 13.52	C-O7	9.55	CC1H	7.50	CC1H	6.60	CC1H
FORCE CONSTANTS-	36.57	CC 28.94	CC 12.57	CC 12.57	CC 12.29	CC 8.03	CCO	2.49	CC1H
OFF DIAGONAL-	6.47	SB26 -4.57	SB27	-2.82	SB23 2.67	SS18	-2.59	SB24 -1.87	SB21 -1.86 BB29 -1.72 BB33
NORMAL MODE 39	OBSERVED=	758.0 CM-1		CALCULATED=	759.6 CM-1		ERROR=	-1.6 CM-1	OR -0.2 PERCENT
INTERNAL COORDINATES-	14.59	CC1H 13.87	C-O7	7.46	CC1H	5.33	CC1H	5.00	CC1H
FORCE CONSTANTS-	27.76	CC 23.20	CC 11.34	CC 11.34	CC 11.17	CC 6.45	CCO	2.49	CC1H
OFF DIAGONAL-	8.77	SB25 4.87	BB43	-3.30	SB27 2.46	SS18	-1.66	BB41	
NORMAL MODE 40	OBSERVED=	725.0 CM-1		CALCULATED=	716.2 CM-1		ERROR=	8.8 CM-1	OR 1.2 PERCENT
INTERNAL COORDINATES-	15.01	CC1H 12.29	CCO7	9.59	CC1H	7.04	CC1H	6.12	CC1H
FORCE CONSTANTS-	49.95	CC 12.01	CC 12.01	CC 12.01	CC 6.03	CC 5.66	CCO	2.49	CC1H
OFF DIAGONAL-	7.26	BB43 4.21	SB25	-3.41	BB34 3.05	BB33	-2.11	SB27 -1.55	BB41
NORMAL MODE 41	OBSERVED=	0.0 CM-1		CALCULATED=	616.8 CM-1		ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	20.38	CCO7 19.38	BBCC	8.54	CCO7	7.07	CCO7	5.66	CCO7
FORCE CONSTANTS-	69.77	CC 28.57	CC 7.91	CC 7.91	CC 5.52	CC 5.52	CCO	2.49	CCO7
OFF DIAGONAL-	-14.86	BB34 7.41	BB43	-6.03	BB29 3.97	SB25	-2.61	BB42 -1.86	BB41 -1.60 SB24
NORMAL MODE 42	OBSERVED=	0.0 CM-1		CALCULATED=	600.5 CM-1		ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	15.33	CCO 13.18	CCO7	8.03	CCO7	10.58	CCO	5.36	CCO7
FORCE CONSTANTS-	36.27	CC 19.61	CC 15.33	CC 15.33	CC 10.58	CC 5.36	CCO	2.49	CCO7
OFF DIAGONAL-	5.72	SB24 3.62	SB22	3.61	BB43 -3.57	BB29 -3.32	BB34	-2.69	SB27
NORMAL MODE 43	OBSERVED=	0.0 CM-1		CALCULATED=	500.0 CM-1		ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	11.18	CCO7 8.04	CCO7	7.75	CCO7	7.08	CCO7	6.61	CCO7
FORCE CONSTANTS-	31.49	CC 22.50	CC 13.39	CC 13.39	CC 11.53	CC 11.53	CCO	2.49	CCO7
OFF DIAGONAL-	-10.11	BB34 7.85	BB43	-4.92	BB29 2.69	SB24 2.06	SS18	2.02	SB21 -1.78 SB27 1.75 SB23
NORMAL MODE 44	OBSERVED=	0.0 CM-1		CALCULATED=	467.4 CM-1		ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	10.50	CCO7 8.82	CCO7	7.59	CCO7	7.28	CCO7	6.73	CCO7
FORCE CONSTANTS-	30.40	CC 14.62	CC 10.41	CC 10.41	CC 8.01	CC 7.59	CCO	2.49	CCO7
OFF DIAGONAL-	6.06	SB22 3.75	BB43	-3.19	SB26 2.68	CCO7 -2.64	BB34 -1.83	BB41 1.68	SB21
NORMAL MODE 45	OBSERVED=	0.0 CM-1		CALCULATED=	414.2 CM-1		ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	10.50	CCO7 8.82	CCO7	7.59	CCO7	7.28	CCO7	6.73	CCO7
FORCE CONSTANTS-	48.63	CC 12.35	CC 11.86	CC 11.86	CC 8.91	CC 8.51	CCO	2.49	CCO7
OFF DIAGONAL-	-4.49	BB34 2.87	SB25	2.06	BB43 -1.82	BB33 -1.72	SB24 1.71	SB22 1.65	SB23 -1.63 BB42 -1.58 BB29
NORMAL MODE 46	OBSERVED=	0.0 CM-1		CALCULATED=	387.1 CM-1		ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	15.33	CCO7 13.54	CCO7	12.45	CCO7	10.41	CCO7	9.22	CCO7
FORCE CONSTANTS-	54.66	CC 20.50	CC 14.62	CC 14.62	CC 10.41	CC 8.01	CCO	2.49	CCO7
OFF DIAGONAL-	-8.86	BB34 -2.99	BB42	2.92	SB21 2.67	BB29 2.44	SB25 -1.77	SB26 1.57	BB43
NORMAL MODE 47	OBSERVED=	0.0 CM-1		CALCULATED=	365.6 CM-1		ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	12.87	CCO7 12.45	CCO7	11.93	CCO7	8.76	CCO7	5.24	CCO7
FORCE CONSTANTS-	49.43	CC 11.48	CC 11.29	CC 11.29	CC 8.76	CC 6.24	CCO	2.49	CCO7
OFF DIAGONAL-	-5.77	BB34 3.69	BB43	2.93	SB25 2.66	SB21 2.33	SB22 -1.63	BB33	
NORMAL MODE 48	OBSERVED=	0.0 CM-1		CALCULATED=	327.0 CM-1		ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	22.76	CCO7 16.91	CCO7	14.72	CCO7	14.10	CCO7	11.96	CCO7
FORCE CONSTANTS-	87.34	CC 11.14	CC 11.14	CC 11.14	CC 8.23	CC 8.23	CCO	2.49	CCO7
OFF DIAGONAL-	-7.13	BB34 -4.55	BB42	1.91	BB41				
NORMAL MODE 49	OBSERVED=	0.0 CM-1		CALCULATED=	309.3 CM-1		ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	14.88	CCO7 12.15	CCO7	10.20	CCO7	8.34	CCO7	7.49	CCO7
FORCE CONSTANTS-	61.80	CC 14.47	CC 14.30	CC 14.30	CC 10.41	CC 8.01	CCO	2.49	CCO7
OFF DIAGONAL-	-5.98	BB34 4.93	BB43	2.85	SB22 -2.83	BB33 -2.34	SB25 -2.22	BB29	
NORMAL MODE 50	OBSERVED=	0.0 CM-1		CALCULATED=	292.0 CM-1		ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	14.88	CCO7 12.15	CCO7	10.20	CCO7	8.34	CCO7	7.49	CCO7
FORCE CONSTANTS-	61.80	CC 14.47	CC 14.30	CC 14.30	CC 10.41	CC 8.01	CCO	2.49	CCO7
OFF DIAGONAL-	-5.98	BB34 4.93	BB43	2.85	SB22 -2.83	BB33 -2.34	SB25 -2.22	BB29	
NORMAL MODE 51	OBSERVED=	0.0 CM-1		CALCULATED=	257.6 CM-1		ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	21.92	CCO7 14.71	CCO7	10.52	CCO7	6.91	CCO7	5.66	CCO7
FORCE CONSTANTS-	48.75	CC 18.59	CC 15.74	CC 15.74	CC 11.58	CC 8.01	CCO	2.49	CCO7
OFF DIAGONAL-	-4.48	BB33 4.07	SB22	3.52	BB43 -3.41	SB25 -2.62	SB21 -1.95	SB26 -1.77	BB36
NORMAL MODE 52	OBSERVED=	0.0 CM-1		CALCULATED=	232.7 CM-1		ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	35.47	TH-1 26.33	TH-4	14.00	TH-3	6.78	CCO7	6.26	TH-2
FORCE CONSTANTS-	80.00	CC 10.16	CCO						
OFF DIAGONAL-	NONE								
NORMAL MODE 53	OBSERVED=	0.0 CM-1		CALCULATED=	224.6 CM-1		ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	43.78	TH-1 19.49	TH-3	11.74	TH-2	9.63	TH-4		
FORCE CONSTANTS-	86.43	CC 9.37	CCO						
OFF DIAGONAL-	NONE								
NORMAL MODE 54	OBSERVED=	0.0 CM-1		CALCULATED=	218.4 CM-1		ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	43.78	TH-1 19.49	TH-3	11.74	TH-2	9.63	TH-4		
FORCE CONSTANTS-	86.43	CC 9.37	CCO						
OFF DIAGONAL-	NONE								
NORMAL MODE 55	OBSERVED=	0.0 CM-1		CALCULATED=	213.8 CM-1		ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	41.28	TH-2 34.46	TH-4						
FORCE CONSTANTS-	83.69	CC 13.30	CCO						
OFF DIAGONAL-	NONE								
NORMAL MODE 56	OBSERVED=	0.0 CM-1		CALCULATED=	209.4 CM-1		ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	47.05	TH-3 24.06	TH-2	8.23	CCO8	7.74	TH-4		
FORCE CONSTANTS-	79.34	CC 18.91	CCO						
OFF DIAGONAL-	-1.71	BB34							
NORMAL MODE 57	OBSERVED=	0.0 CM-1		CALCULATED=	192.9 CM-1		ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	41.28	CCO7 16.72	C4CC	9.77	CCO7	7.24	CCO7	7.12	TH-1
FORCE CONSTANTS-	31.22	CC 16.72	T-OH	14.27	CCO	9.77	CCO	8.11	T-CC
OFF DIAGONAL-	-3.59	BB34 -3.14	BB42	-2.75	BB33				
NORMAL MODE 58	OBSERVED=	0.0 CM-1		CALCULATED=	148.8 CM-1		ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	21.88	C4CC 16.57	C0'C	6.50	TCC4	6.25	TCC1	6.20	CCO8
FORCE CONSTANTS-	28.64	CC 20.46	CCO	16.57	CCO	10.74	T-CC	7.41	T-CC
OFF DIAGONAL-	-4.22	SB21 3.33	BB43	-2.35	BB34 -1.99	SB25 1.87	SB22		
NORMAL MODE 59	OBSERVED=	0.0 CM-1		CALCULATED=	98.4 CM-1		ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	57.57	TCC5 8.29	C3CC	5.96	O9CC				
FORCE CONSTANTS-	66.51	T-CC 16.93	CCO	15.08	CCO				
OFF DIAGONAL-	-2.79	BB34 -2.75	SB25	-1.97	BB42				
NORMAL MODE 60	OBSERVED=	0.0 CM-1		CALCULATED=	86.5 CM-1		ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	25.52	C2CC 11.95	C1CC	11.06	TCC4	9.39	TCC1	6.19	TCC2
FORCE CONSTANTS-	42.02	CC 28.27	T-CC	16.28	CCO	5.11	CCO	5.45	BBCC
OFF DIAGONAL-	-3.24	SB25 -2.97	BB42	2.08	BB41 -1.56	SB21			
NORMAL MODE 61	OBSERVED=	0.0 CM-1		CALCULATED=	65.1 CM-1		ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	26.68	TCC5 25.44	C3CC	8.66	TCC2	8.18	TCC4	7.12	TCC3
FORCE CONSTANTS-	51.09	T-CC 22.00	CCO	20.23	CCO				
OFF DIAGONAL-	-2.53	BB42 -1.86	BB34						

27. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 8.28

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400										PAGE 1	
MOLECULE 39		-6 NG-1238		BETA MANNOSE		GG					
NORMAL MODE 8		OBSERVED=	1478.0 CM-1	CALCULATED=		1450.1 CM-1	ERROR=		27.9 CM-1	OR	1.9 PERCENT
INTERNAL COORDINATES-		61.32 HCH	20.21 CCHB	19.67 OCHA							
FORCE CONSTANTS-		61.32 HCH	40.04 OCH								
OFF DIAGONAL-		-4.14 SB27									
NORMAL MODE 9		OBSERVED=	1428.0 CM-1	CALCULATED=		1421.2 CM-1	ERROR=		6.8 CM-1	OR	0.5 PERCENT
INTERNAL COORDINATES-		29.27 C4OH	15.90 OC4H	11.55 HC5C		6.74 C1H	5.97 CC3H		5.09 C4C5		
FORCE CONSTANTS-		34.19 OCH	32.69 BC0H	23.05 CCH		6.48 CO	5.83 CC				
OFF DIAGONAL-		-6.26 SB27	-5.63 SB26	4.14 BB29		4.08 SB28	-2.26 BB45		2.16 BB36	-2.14 SB25	2.13 BB34 -1.83 BB43
NORMAL MODE 10		OBSERVED=	1419.0 CM-1	CALCULATED=		1418.6 CM-1	ERROR=		0.4 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-		34.58 C1H	16.54 OC1H	9.75 C4OH		8.20 C2OH	7.11 CC1H		6.92 CCH2	5.16 C3OH	
FORCE CONSTANTS-		59.20 OCH	23.26 BC0H	17.55 CCH		8.22 CO	-1.64 SB25				
OFF DIAGONAL-		-10.20 SB27	-2.92 BB45								
NORMAL MODE 11		OBSERVED=	1406.0 CM-1	CALCULATED=		1404.5 CM-1	ERROR=		1.5 CM-1	OR	0.1 PERCENT
INTERNAL COORDINATES-		31.16 C3OH	14.04 OC3H	8.58 C1OH		8.09 HC3C	5.01 C4OH				
FORCE CONSTANTS-		45.70 BC0H	26.84 OCH	17.68 CCH		8.47 CO	-2.02 BB39		-1.89 SB25	-1.69 BB45	
OFF DIAGONAL-		-6.97 SB27	4.02 SB28								
NORMAL MODE 12		OBSERVED=	0.0 CM-1	CALCULATED=		1402.2 CM-1	ERROR=		0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-		52.29 C1OH	8.34 C1H	8.60 C2OH		9.44 C1C2	3.46 CCO				
FORCE CONSTANTS-		62.80 CCH	14.13 OCH	7.92 CCH		5.04 CCH					
OFF DIAGONAL-		4.99 SB28	-3.05 SB26	-2.06 SB22							
NORMAL MODE 13		OBSERVED=	0.0 CM-1	CALCULATED=		1392.6 CM-1	ERROR=		0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-		71.49 C1CH	9.53 OCHA	10.65 CCH							
FORCE CONSTANTS-		74.27 BC0H	11.79 OCH	1.65 SB27							
OFF DIAGONAL-		3.33 SB28	-2.06 BB39								
NORMAL MODE 14		OBSERVED=	0.0 CM-1	CALCULATED=		1387.6 CM-1	ERROR=		0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-		26.45 C2OH	11.31 C1OH	6.87 OC1H		6.65 OC2H					
FORCE CONSTANTS-		73.26 BC0H	18.55 OCH	5.71 CCH							
OFF DIAGONAL-		3.94 SB28	-3.47 SB27	-2.56 BB39							
NORMAL MODE 15		OBSERVED=	1368.0 CM-1	CALCULATED=		1373.5 CM-1	ERROR=		-5.5 CM-1	OR	-0.4 PERCENT
INTERNAL COORDINATES-		33.99 C4OH	25.35 C3OH	9.80 C5H		9.05 CC3H	1.56 SB26				
FORCE CONSTANTS-		64.45 CCH	16.41 CCH	12.99 OCH							
OFF DIAGONAL-		-2.75 SB27	2.50 BB34	2.32 BB29		-1.91 BB36					
NORMAL MODE 16		OBSERVED=	1363.0 CM-1	CALCULATED=		1352.7 CM-1	ERROR=		10.3 CM-1	OR	0.8 PERCENT
INTERNAL COORDINATES-		11.69 C3OH	10.19 C5H	9.18 CC4H		8.98 CCHB	8.67 HC3C		7.58 HC5C	7.08 OCHB	5.76 C1OH
FORCE CONSTANTS-		42.48 CCH	24.31 CCH	21.63 BC0H		10.38 CO	2.00 BB34		-1.57 SB25		
OFF DIAGONAL-		-4.75 SB27	4.26 BB29	-2.95 SB28		-2.71 BB45					
NORMAL MODE 17		OBSERVED=	1334.0 CM-1	CALCULATED=		1342.5 CM-1	ERROR=		-8.5 CM-1	OR	-0.6 PERCENT
INTERNAL COORDINATES-		19.67 CCH2	11.71 C1C1	10.64 CC2H		9.74 CCH	8.27 C-08		7.94 OC1H		
FORCE CONSTANTS-		32.92 BC0H	84.00 OCH	21.95 CCH		15.52 CCH	3.46 CCO				
OFF DIAGONAL-		4.57 SB27	-4.25 SB28	-3.95 SB25		3.29 BB34	-2.28 BB45		1.87 BB33		
NORMAL MODE 18		OBSERVED=	1330.0 CM-1	CALCULATED=		1335.8 CM-1	ERROR=		-5.8 CM-1	OR	-0.4 PERCENT
INTERNAL COORDINATES-		18.34 CCHA	14.94 HC3C	9.25 CC4H		9.24 HC5C	9.20 CC5H		5.91 C1OH	5.33 HC4C	5.20 OCHA
FORCE CONSTANTS-		66.22 CCH	14.71 OCH	10.61 BC0H		3.49 SB27	-1.66 SB28				
OFF DIAGONAL-		7.83 BB29	-6.02 SB26								
NORMAL MODE 19		OBSERVED=	1311.0 CM-1	CALCULATED=		1311.7 CM-1	ERROR=		-0.7 CM-1	OR	-0.0 PERCENT
INTERNAL COORDINATES-		26.87 HC2C	22.04 CC3H	18.51 OC3H		10.35 OC2H	8.35 C2OH				
FORCE CONSTANTS-		54.43 CCH	30.27 OCH	9.24 BC0H							
OFF DIAGONAL-		-3.65 BB45	2.78 BB34	-2.04 SB28		-1.99 SB27	1.63 BB30				
NORMAL MODE 20		OBSERVED=	1292.0 CM-1	CALCULATED=		1293.2 CM-1	ERROR=		-1.2 CM-1	OR	-0.1 PERCENT
INTERNAL COORDINATES-		16.00 OCHA	14.82 OC4H	13.48 CCHA		12.73 OC8B	11.21 BB34		6.33 HC4C	6.06 OC3H	
FORCE CONSTANTS-		50.59 CCH	34.81 CCH	2.40 SB26							
OFF DIAGONAL-		-3.48 BB45	2.50 BB34								
NORMAL MODE 21		OBSERVED=	1278.0 CM-1	CALCULATED=		1281.4 CM-1	ERROR=		-3.4 CM-1	OR	-0.3 PERCENT
INTERNAL COORDINATES-		37.23 C5H	13.28 CCHB	12.11 OC4H		11.42 CCHB					
FORCE CONSTANTS-		68.99 CCH	9.24 CCH	-2.97 SB26		-2.55 BB29					
OFF DIAGONAL-		4.76 SB27	-3.61 BB45								
NORMAL MODE 22		OBSERVED=	1261.0 CM-1	CALCULATED=		1261.1 CM-1	ERROR=		-0.1 CM-1	OR	-0.0 PERCENT
INTERNAL COORDINATES-		21.69 OC2H	11.36 CC3H	9.38 HC2C		8.65 CC4H	7.12 C-07		6.13 OC3H		
FORCE CONSTANTS-		42.92 CCH	36.24 OCH	7.51 CO							
OFF DIAGONAL-		6.51 SB27	-3.28 BB45	1.73 BB29							
NORMAL MODE 23		OBSERVED=	1238.0 CM-1	CALCULATED=		1245.7 CM-1	ERROR=		-7.7 CM-1	OR	-0.6 PERCENT
INTERNAL COORDINATES-		13.32 OC4H	10.51 CC4H	7.76 HC3C		7.50 HC5C	6.33 OC2H		5.89 C5H		
FORCE CONSTANTS-		42.45 CCH	36.81 OCH	11.30 CO		5.03 CCO	3.07 BB34		1.64 BB43		
OFF DIAGONAL-		8.87 SB27	-3.64 BB29	-3.51 SB25		-3.19 BB45					
NORMAL MODE 24		OBSERVED=	1212.0 CM-1	CALCULATED=		1207.7 CM-1	ERROR=		4.3 CM-1	OR	0.3 PERCENT
INTERNAL COORDINATES-		21.40 CCH	31.80 OC1H	9.52 OC3H		8.16 HC5C	6.94 CC3H		6.02 HC4C		
FORCE CONSTANTS-		54.11 CCH	31.80 OCH	12.24 CO		5.66 BC0H	-1.58 SB28				
OFF DIAGONAL-		-4.33 SB26	-3.52 BB45	-3.22 SB25		-2.64 BB29					
NORMAL MODE 25		OBSERVED=	0.0 CM-1	CALCULATED=		1178.6 CM-1	ERROR=		0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-		12.38 HC5C	11.72 CC1H	9.73 CC5H		8.96 OC1H	6.95 C2C3		6.66 C-06	6.25 CC3H	5.64 C5O
FORCE CONSTANTS-		54.03 CCH	23.22 CCH	17.63 OC2H		11.31 CCH	10.46 CCO		6.70 BC0H	5.01 C-04	5.01 C-04
OFF DIAGONAL-		-7.28 SB28	-5.25 SB25	-4.40 BB29		-3.10 SB28	-3.04 BB45		-2.87 SB22	2.29 BB33	-2.12 BB43 1.56 BB34
NORMAL MODE 26		OBSERVED=	1167.0 CM-1	CALCULATED=		1158.4 CM-1	ERROR=		8.6 CM-1	OR	0.7 PERCENT
INTERNAL COORDINATES-		17.60 CCH2	16.71 C1C1	12.20 C-08		10.22 CCH	8.74 C-08		8.72 HC4C	7.73 OC2H	7.34 C1C2
FORCE CONSTANTS-		18.34 CCH	14.94 CCH	6.11 CCH		5.98 BC0H	5.13 CCH		5.13 CCH	5.13 CCH	6.18 CCH
OFF DIAGONAL-		-12.47 SB26	-6.35 SB25	-6.22 BB27		-4.18 SB28	-3.85 SB21		-2.95 BB43	-2.65 SS18	-2.36 BB45 -1.58 SB22
NORMAL MODE 27		OBSERVED=	1124.0 CM-1	CALCULATED=		1141.1 CM-1	ERROR=		-17.1 CM-1	OR	-1.5 PERCENT
INTERNAL COORDINATES-		41.32 C5H	10.57 C-06	9.28 C5C		6.74 OC8B	5.35 C-04				
FORCE CONSTANTS-		41.32 C5H	22.29 CCO	18.78 CCH		17.90 OCH	9.80 CCH				
OFF DIAGONAL-		-11.85 SB25	-4.66 SB22	2.88 SB27		-2.39 SB28	-2.08 SB26		1.59 BB43		
NORMAL MODE 28		OBSERVED=	1118.0 CM-1	CALCULATED=		1130.3 CM-1	ERROR=		-12.3 CM-1	OR	-1.1 PERCENT
INTERNAL COORDINATES-		37.55 C5C	19.15 C4C5	14.73 C-04		9.73 OCHA	6.97 CCO		6.69 C1OH	5.91 C-08	5.60 CC1C
FORCE CONSTANTS-		65.93 CCH	26.48 OCH	13.63 CCO		12.40 OCH	8.44 BC0H		6.04 CCH	5.60 CCO	
OFF DIAGONAL-		-13.64 SB22	-11.33 SB26	-5.14 SB28		-4.08 SS18	-3.31 SB27		-2.91 BB34	-1.98 SS17	
NORMAL MODE 29		OBSERVED=	1113.0 CM-1	CALCULATED=		1104.2 CM-1	ERROR=		8.8 CM-1	OR	0.8 PERCENT
INTERNAL COORDINATES-		19.88 C3C4	17.30 C-09	13.99 C2C3		10.45 C-08	6.80 C4C5		6.29 C1C2	5.39 OC1C	
FORCE CONSTANTS-		47.07 CCH	43.76 CCH	11.24 CCO		10.04 CCH	6.37 CCH				
OFF DIAGONAL-		-6.33 SB22	-9.16 SB29	-3.52 SS18		-2.86 SB28	1.91 SB27		-1.86 SS17		
NORMAL MODE 30		OBSERVED=	1086.0 CM-1	CALCULATED=		1102.8 CM-1	ERROR=		-16.8 CM-1	OR	-1.5 PERCENT
INTERNAL COORDINATES-		16.82 C1C2	14.36 C2C3	14.20 C5C3		11.90 C-09	16.34 C1C3		6.18 OCHA		
FORCE CONSTANTS-		33.14 CCH	14.98 CCH	13.11 OCH		12.91 CCH	1.42 CCH				
OFF DIAGONAL-		-6.86 SB22	-2.93 SB25	-2.34 SB25		-1.78 BB29	-1.67 SB24		-1.51 SB21		
NORMAL MODE 31		OBSERVED=	1070.0 CM-1	CALCULATED=		1058.0 CM-1	ERROR=		12.0 CM-1	OR	1.1 PERCENT
INTERNAL COORDINATES-		17.10 C-08	48.63 C-08	15.26 OCH		14.38 BC0H	13.12 CCO		11.41 CCF	9.63 CCH	5.94 BBCC 5.84 C3CC
FORCE CONSTANTS-		18.10 CCH	48.63 CCH	10.21 SB28		-8.97 SS18	-5.36 SB25		-4.29 SB22	-3.05 SB26	-2.70 BB36 -2.68 BB34
OFF DIAGONAL-		-12.96 SB27	-11.02 SB21								
NORMAL MODE 32		OBSERVED=	1057.0 CM-1	CALCULATED=		1044.4 CM-1	ERROR=		12.6 CM-1	OR	1.2 PERCENT
INTERNAL COORDINATES-		29.71 C-09	19.80 C-07	16.98 C-04		11.37 C1C2	9.52 C2C3		6.74 C4C5	5.73 C5C	
FORCE CONSTANTS-		69.74 CCH	34.35 CCH	11.95 OCH		11.36 CCH	10.69 BC0H		9.12 CCH	6.60 CCO	
OFF DIAGONAL-		-12.32 SB27	-10.98 SB21	-9.88 SS18		-9.87 SB28	-4.48 SB26		-2.62 SB25	-1.56 SB22	
NORMAL MODE 33		OBSERVED=	1041.0 CM-1	CALCULATED=		1034.8 CM-1	ERROR=		6.3 CM-1	OR	0.6 PERCENT
INTERNAL COORDINATES-		27.78 C-06	29.74 C-08	13.75 C3C4		9.05 C1C2	5.86 CCH2				
FORCE CONSTANTS-		56.11 CCH	25.76 CCH	16.48 CCH		7.97 CCO	7.76 OCH		7.31 BC0H	6.07 CCC	
OFF DIAGONAL-		-7.66 SB28	-5.83 SB22	-4.73 SB24		-4.61 SB21	-3.71 SB27		-3.28 SS18	-2.86 SB25 2.08 SB26	
NORMAL MODE 34		OBSERVED=	1032.0 CM-1	CALCULATED=		1012.2 CM-1	ERROR=		19.8 CM-1	OR	1.9 PERCENT
INTERNAL COORDINATES-		29.22 C-04	16.80 C-07	10.71 C3C4		9.54 C-08	8.61 C5C		5.43 HC4C	5.24 CC4H	
FORCE CONSTANTS-		83.17 CCH	20.16 CCH	22.72 CCH		11.63 CCO	5.83 OCH				
OFF DIAGONAL-		-7.96 SB25	-5.13 SB26	-5.07 SB28		-3.92 SB22	-3.84 BB29		-3.28 SB27	-2.18 SB21	
NORMAL MODE 35		OBSERVED=	1007.0 CM-1	CALCULATED=		957.1 CM-1	ERROR=		49.9 CM-1	OR	4.9 PERCENT
INTERNAL COORDINATES-		13.55 C1C2	16.17 C3C4	8.42 C2C3		7.86 C4C5	6.40 C1C3		6.20 OC1C	5.28 CCHA	5.23 CCHB 5.07 C5O
FORCE CONSTANTS-		33.47 CCH	16.17 CCH	18.62 CCH		12.91 CCH	1.84 SB26				
OFF DIAGONAL-		-5.87 SB22	2.77 SS18	-2.49 SB21		1.84 SB26					

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400										PAGE 2	
MOLECULE 39 -6 NG-1239 BETA MANNOSE GG											
NORMAL MODE 36	OBSERVED=	933.0 CM-1	CALCULATED=	907.9 CM-1	ERROR=	25.1 CM-1	OR	2.7 PERCENT			
INTERNAL COORDINATES-	28.90	C5C4 25.28 C-O*	7.84 C4C5	7.20 HC8C							
FORCE CONSTANTS-	37.32	CC 36.03 CC	14.31 CCH	5.74 CCO							
OFF DIAGONAL-	8.48	SB26 -6.85 SB21	-6.01 SB22	5.44 SS18	-4.39	SB27 -2.71 SB25	-1.74 SB28	1.61 BB43			
NORMAL MODE 37	OBSERVED=	896.0 CM-1	CALCULATED=	898.4 CM-1	ERROR=	-2.4 CM-1	OR	-0.3 PERCENT			
INTERNAL COORDINATES-	15.20	C-O7 11.94 C3C4	9.78 C5O*	6.89 CC3H	5.50	CCO9 5.42 C2C3	5.23 CCH8				
FORCE CONSTANTS-	28.74	CC 25.76 CCH	23.28 CC	14.36 CCO	8.58	CCO 5.24 CC	5.06 CCH				
OFF DIAGONAL-	-6.63	SB22 -5.14 SB21	-3.34 SB27	3.16 SB26	3.09	BB43 1.58 SS18					
NORMAL MODE 38	OBSERVED=	855.0 CM-1	CALCULATED=	843.3 CM-1	ERROR=	11.7 CM-1	OR	1.4 PERCENT			
INTERNAL COORDINATES-	18.99	O7C1 12.50 C1C2	9.53 CCH	8.81 CCH	7.65	CCH8 6.58 C5O*	5.21 C4C5				
FORCE CONSTANTS-	32.54	CC 25.76 CCH	20.10 CC	8.81 CCH	7.65	CCH8 6.58 C5O*	5.21 C4C5				
OFF DIAGONAL-	-6.00	SB23 -4.96 SB24	-3.95 SB21	3.87 SB26	-2.27	SB22 2.05 SS18	1.85 BB43				
NORMAL MODE 39	OBSERVED=	769.0 CM-1	CALCULATED=	776.9 CM-1	ERROR=	-7.9 CM-1	OR	-1.0 PERCENT			
INTERNAL COORDINATES-	15.79	C-O7 15.13 C*CC	8.59 CCO*	7.59 CCO*							
FORCE CONSTANTS-	31.08	CCO 21.49 CC	9.76 CCH	8.37 CCH	6.93	CC 5.15 CCH					
OFF DIAGONAL-	8.14	SB25 5.86 BB43	-2.81 SB27	2.11 SS18	1.88	BB33 -1.72 BB41					
NORMAL MODE 40	OBSERVED=	730.0 CM-1	CALCULATED=	725.8 CM-1	ERROR=	4.2 CM-1	OR	0.6 PERCENT			
INTERNAL COORDINATES-	14.40	CCO6 12.93 O7CC	11.74 CCO8	11.02 CCO7							
FORCE CONSTANTS-	56.74	CCO 12.43 CCH	8.49 CCH	7.84 CCH	-6.36	CC 5.11 CCH					
OFF DIAGONAL-	6.03	BB43 5.83 SB25	-3.99 BB34	-3.72 SB27	-2.07	BB41 1.96 BB33					
NORMAL MODE 41	OBSERVED=	618.0 CM-1	CALCULATED=	677.4 CM-1	ERROR=	-59.4 CM-1	OR	-9.6 PERCENT			
INTERNAL COORDINATES-	19.18	CCO* 9.17 O8CC	8.55 C3C4	7.90 C4C5	6.46	CC5H 5.81 CCO*	5.06 CCO*				
FORCE CONSTANTS-	39.80	CCO 19.41 CCH	16.85 CC	8.88 CC	5.81	CCO 5.54 CCH					
OFF DIAGONAL-	5.21	SB25 5.17 BB43	-4.94 BB34	-2.98 BB29	1.92	SS18 -1.66 SB22					
NORMAL MODE 42	OBSERVED=	599.0 CM-1	CALCULATED=	589.4 CM-1	ERROR=	9.6 CM-1	OR	1.6 PERCENT			
INTERNAL COORDINATES-	15.75	O9CC 15.48 CCO	7.52 C4CC	6.53 CCO*	6.15	CCO* 5.48 CCO*					
FORCE CONSTANTS-	45.48	CCO 15.48 CCO	10.79 CC	8.35 CCH	6.60	CCH 6.53 CCH					
OFF DIAGONAL-	6.76	SB24 -3.17 BB42	-2.11 SB27	2.06 BB43	-1.87	BB34 1.85 SB22	1.83 SB23				
NORMAL MODE 43	OBSERVED=	492.0 CM-1	CALCULATED=	527.8 CM-1	ERROR=	-35.8 CM-1	OR	-7.3 PERCENT			
INTERNAL COORDINATES-	16.94	O8CC 13.30 C4C5	7.59 CCO*	7.45 C4C5	7.37	CCO* 7.01 CCO6					
FORCE CONSTANTS-	64.31	CCO 20.60 CCH	11.88 CC	8.05 CC							
OFF DIAGONAL-	-12.55	BB34 4.51 BB43	-2.78 BB29	2.33 SB25	-2.28	BB42 -2.06 SB24	-1.76 BB41	-1.68 BB33	-1.65 SB22		
NORMAL MODE 44	OBSERVED=	444.0 CM-1	CALCULATED=	476.5 CM-1	ERROR=	-32.5 CM-1	OR	-7.3 PERCENT			
INTERNAL COORDINATES-	7.57	CCO 6.22 C4C5	6.03 C2C3	5.70 C1CC	5.66	C1C2					
FORCE CONSTANTS-	20.52	CCO 18.85 CC	12.84 CC	11.13 CCH	10.26	CCH 7.57 CCO					
OFF DIAGONAL-	5.98	SB22 -4.57 SB26	3.62 SB25	3.54 BB43	3.31	SB21 3.18 SS18	-2.60 SB27	2.33 SB24			
NORMAL MODE 45	OBSERVED=	423.0 CM-1	CALCULATED=	409.2 CM-1	ERROR=	13.8 CM-1	OR	3.3 PERCENT			
INTERNAL COORDINATES-	22.02	CCO9 10.41 C4C5	6.71 O7CC	6.23 C1CC	6.11	CC4H 5.94 HC8C	5.79 HC3C	5.28 CCO8			
FORCE CONSTANTS-	55.86	CCO 22.37 CCH	9.43 CC	9.30 CC							
OFF DIAGONAL-	-10.51	BB34 6.63 BB43	-4.61 BB29	4.59 SB22	-1.95	SB26 -1.59 BB36	1.57 SB21				
NORMAL MODE 46	OBSERVED=	394.0 CM-1	CALCULATED=	395.4 CM-1	ERROR=	-1.4 CM-1	OR	-0.4 PERCENT			
INTERNAL COORDINATES-	19.19	C3C4 12.16 C2CC	9.53 CCO6	8.41 O4CC	7.29	CCO* 6.26 CCO*					
FORCE CONSTANTS-	41.87	CCO 13.48 CCH	10.34 CCO	7.49 CCH	5.49	CCH					
OFF DIAGONAL-	5.95	SB25 -4.47 BB42	4.24 SB21	-3.77 BB34	-3.17	SB22 -2.12 BB41	1.92 SB23				
NORMAL MODE 47	OBSERVED=	370.0 CM-1	CALCULATED=	351.4 CM-1	ERROR=	18.6 CM-1	OR	5.0 PERCENT			
INTERNAL COORDINATES-	19.23	OCC 18.75 CCO6	10.34 O9CC	7.32 CCO8	7.04	CCO*					
FORCE CONSTANTS-	52.58	CCO 19.23 CCO	10.54 CC	5.75 CCH	5.59	CCO					
OFF DIAGONAL-	5.24	SB22 -4.52 BB34	-3.33 BB42								
NORMAL MODE 48	OBSERVED=	326.0 CM-1	CALCULATED=	327.6 CM-1	ERROR=	-1.6 CM-1	OR	-0.5 PERCENT			
INTERNAL COORDINATES-	22.16	O8CC 19.65 CCO8	17.50 O9CC	14.34 CCO7	9.42	CCO9 6.47 TH-3					
FORCE CONSTANTS-	87.71	CCO 11.83 T-OH	5.96 CCH								
OFF DIAGONAL-	-7.07	BB34 -4.37 BB42	1.64 BB41								
NORMAL MODE 49	OBSERVED=	0.0 CM-1	CALCULATED=	306.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	18.10	CCO7 9.17 C7CC	7.06 TH-2	6.84 CCO9	5.86	C3CC 5.04 O*CC					
FORCE CONSTANTS-	55.16	CCO 12.92 T-OH	7.82 CCH	7.70 CCH	6.84	CC					
OFF DIAGONAL-	6.21	SB22 -3.58 BB33	3.37 BB43	-2.73 SB26	-1.86	BB42					
NORMAL MODE 50	OBSERVED=	288.0 CM-1	CALCULATED=	277.2 CM-1	ERROR=	10.8 CM-1	OR	3.7 PERCENT			
INTERNAL COORDINATES-	22.82	CCO* 20.32 TH-5	10.15 C4CC	7.96 O9CC	7.51	CCO6 5.61 TH-1					
FORCE CONSTANTS-	52.23	CCO 28.35 T-OH	10.33 CCH	9.53 CCH							
OFF DIAGONAL-	-6.40	BB34 -2.71 BB42	-2.54 BB33								
NORMAL MODE 51	OBSERVED=	258.0 CM-1	CALCULATED=	261.0 CM-1	ERROR=	-3.0 CM-1	OR	-1.2 PERCENT			
INTERNAL COORDINATES-	24.13	O7CC 19.21 C1CC	9.60 CCO7	5.64 O*CC	5.47	CCO* 5.38 CCO8					
FORCE CONSTANTS-	49.58	CCO 19.88 CCH	11.84 CCH	11.69 T-OH	5.47	CCO					
OFF DIAGONAL-	4.90	SB22 -4.51 BB33	3.86 BB43	-3.81 SB25	-3.16	SB21 -2.20 SB26	-1.83 BB36				
NORMAL MODE 52	OBSERVED=	239.0 CM-1	CALCULATED=	258.0 CM-1	ERROR=	-19.0 CM-1	OR	-7.9 PERCENT			
INTERNAL COORDINATES-	13.64	C4CC 9.98 CCO*	9.55 TH-4	6.15 CCO*							
FORCE CONSTANTS-	30.86	CCO 18.73 T-OH	15.80 CCH	9.46 CCH	6.75	CC 6.15 CCO	5.60 T-CC				
OFF DIAGONAL-	4.22	BB43 3.30 SB22	-3.00 BB34	-2.68 SB26	2.10	SB21 -1.92 BB33					
NORMAL MODE 53	OBSERVED=	0.0 CM-1	CALCULATED=	223.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	55.02	TH-1 14.08 TH-5	9.03 TH-4	8.27 TH-3							
FORCE CONSTANTS-	88.62	T-OH 5.28 CCO									
OFF DIAGONAL-	NONE										
NORMAL MODE 54	OBSERVED=	0.0 CM-1	CALCULATED=	218.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	30.68	TH-3 20.29 TH-1	17.53 TH-4	11.56 TH-2							
FORCE CONSTANTS-	81.69	T-OH 10.16 CCO									
OFF DIAGONAL-	NONE										
NORMAL MODE 55	OBSERVED=	0.0 CM-1	CALCULATED=	214.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	22.95	TH-3 11.74 TH-4									
FORCE CONSTANTS-	85.23	T-OH 11.74 CCO									
OFF DIAGONAL-	NONE										
NORMAL MODE 56	OBSERVED=	0.0 CM-1	CALCULATED=	211.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	52.01	TH-5 9.59 TH-1	9.00 CCO*	7.91 C4CC	5.39						
FORCE CONSTANTS-	67.96	T-OH 17.07 CCO	9.27 CCH								
OFF DIAGONAL-	-2.45	BB34 -1.51 BB42									
NORMAL MODE 57	OBSERVED=	0.0 CM-1	CALCULATED=	209.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	40.43	TH-3 22.36 TH-2	13.44 TH-4	7.19 CCO8							
FORCE CONSTANTS-	78.77	T-OH 19.88 CCO									
OFF DIAGONAL-	-2.14	BB34									
NORMAL MODE 58	OBSERVED=	0.0 CM-1	CALCULATED=	141.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	11.11	CO* 10.68 C4CC	8.98 TCC4	6.11 C1CC	6.13	CCO1 5.98 CCO*	5.78 CCO				
FORCE CONSTANTS-	24.18	CCO 17.79 CCH	17.11 CCO	10.93 T-CC	9.39	T-CC 8.72 CCH	5.78 CCO				
OFF DIAGONAL-	4.28	BB43 -2.08 BB33	-1.97 SB25	-1.64 BB34							
NORMAL MODE 59	OBSERVED=	0.0 CM-1	CALCULATED=	90.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	41.10	C2CC 20.73 TCC5	9.40 TCC2	7.23 C3CC	5.78	C1CC 5.57 TCC1					
FORCE CONSTANTS-	41.10	T-CC 37.48 CCH	15.60 CCO								
OFF DIAGONAL-	-3.86	SB25 -2.93 BB42	-2.30 SB21	1.97 BB41	-1.81	BB34					
NORMAL MODE 60	OBSERVED=	0.0 CM-1	CALCULATED=	74.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	62.83	TCC5 6.39 C2CC	5.05 CCO*								
FORCE CONSTANTS-	67.86	T-CC 12.51 CCH	9.20 CCO	5.05 CCH							
OFF DIAGONAL-	NONE										
NORMAL MODE 61	OBSERVED=	0.0 CM-1	CALCULATED=	71.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	14.33	C3CC 14.32 TCC4	11.97 CCO*	9.89 TCC3	6.82	TCC2 6.56 C1CC	6.18 O*CC				
FORCE CONSTANTS-	33.32	T-CC 31.94 CCO	25.71 CCH	5.59 T-CC							
OFF DIAGONAL-	-3.22	BB42 -2.20 BB34	-1.87 SB25	1.74 BB41							

40. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 12.62

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400									
MOLECULE 40 -6 NG-1238 BETA MANNOSIDE-1-D GG									
PAGE 1									
NORMAL MODE 8	OBSERVED=	1480.0 CM-1	CALCULATED=	1450.1 CM-1	ERROR=	29.9 CM-1	OR	2.0 PERCENT	
INTERNAL COORDINATES--	61.33 HCH	20.21 OCHB	19.69 OCHA						
FORCE CONSTANTS--	61.33 HCH	40.02 OCH							
OFF DIAGONAL--	-4.13 SB27								
NORMAL MODE 9	OBSERVED=	1420.0 CM-1	CALCULATED=	1420.6 CM-1	ERROR=	-0.6 CM-1	OR	-0.0 PERCENT	
INTERNAL COORDINATES--	49.28 C4OH	17.92 OC4H	19.07 HC4C	8.50 C4C5	5.31 CC5H				
FORCE CONSTANTS--	45.02 BC0H	21.18 OCH	21.16 CCH	6.92 CO	6.56 CC				
OFF DIAGONAL--	-6.16 SB26	-5.58 SB27	5.17 SB28	4.06 BB29	2.87 BB36	-2.39 BB39	-2.33 SB25	2.13 BB34	-1.93 SB21
NORMAL MODE 10	OBSERVED=	1405.0 CM-1	CALCULATED=	1406.0 CM-1	ERROR=	-1.0 CM-1	OR	-0.1 PERCENT	
INTERNAL COORDINATES--	34.13 C3OH	17.96 OC3H	8.64 HC3C	8.02 C2OH					
FORCE CONSTANTS--	46.30 BCCH	24.18 OCH	20.48 CCH	5.35 CO					
OFF DIAGONAL--	-5.38 SB27	-3.89 SB28	-3.42 SB26	3.42 BB29	-2.01 BB39	-1.74 BB45	-1.61 SB25	1.57 BB34	
NORMAL MODE 11	OBSERVED=	0.0 CM-1	CALCULATED=	1392.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES--	72.62 C*OH	9.67 OCHA	7.41 OCH	6.34 CC	6.32 CCH				
FORCE CONSTANTS--	69.38 BCCH	7.94 CO	-2.19 SB26	-1.70 BB39	-1.62 SB22				
OFF DIAGONAL--	6.66 SB28	-2.75 SB27							
NORMAL MODE 12	OBSERVED=	0.0 CM-1	CALCULATED=	1398.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES--	46.39 C1OH	18.51 C2OH	6.15 C1C2	5.40 OC2H					
FORCE CONSTANTS--	74.38 BCCH	11.51 OCH	10.80 CCH						
OFF DIAGONAL--	3.33 SB28	-2.04 BB39	-1.57 SB27						
NORMAL MODE 13	OBSERVED=	0.0 CM-1	CALCULATED=	1387.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES--	49.91 C2OH	25.67 C1OH	7.06 OC2H						
FORCE CONSTANTS--	80.93 BCCH	8.67 OCH							
OFF DIAGONAL--	4.25 SB28	-2.10 BB39	-1.63 SB27						
NORMAL MODE 14	OBSERVED=	1373.0 CM-1	CALCULATED=	1373.4 CM-1	ERROR=	-0.4 CM-1	OR	-0.0 PERCENT	
INTERNAL COORDINATES--	34.64 C4OH	25.40 C3OH	9.91 C5H	9.23 CC5H					
FORCE CONSTANTS--	64.50 BCCH	16.36 CCH	13.07 OCH						
OFF DIAGONAL--	-2.76 SB27	2.52 BB34	2.38 BB29	-1.92 BB36	1.62 SB26				
NORMAL MODE 15	OBSERVED=	1348.0 CM-1	CALCULATED=	1353.6 CM-1	ERROR=	-5.6 CM-1	OR	-0.4 PERCENT	
INTERNAL COORDINATES--	11.21 CCH2	10.41 C*C1	9.67 C3OH	6.28 CCHB	6.23 HC3C	6.18 CC4H	6.10 C5H	5.55 HC5C	5.11 OCHB
FORCE CONSTANTS--	41.48 CCH	22.00 BCCH	19.15 CO	18.47 OCH					
OFF DIAGONAL--	-6.83 SB27	-3.51 SB28	3.37 BB34	-2.96 SB25	2.87 BB29	-2.46 BB45			
NORMAL MODE 16	OBSERVED=	1339.0 CM-1	CALCULATED=	1347.4 CM-1	ERROR=	-8.4 CM-1	OR	-0.6 PERCENT	
INTERNAL COORDINATES--	19.33 CCH2	11.27 C*C1	9.77 OC2H	7.98 C1OH	7.48 C*O6	6.90 C5H	5.25 CCHB		
FORCE CONSTANTS--	40.83 CCH	26.22 C*O1	20.65 CO	14.42 BCCH	8.21 CC				
OFF DIAGONAL--	-6.65 SB27	-4.02 SB28	-3.80 SB25	3.60 BB34	-2.78 BB45	2.41 BB29	1.68 BB33		
NORMAL MODE 17	OBSERVED=	0.0 CM-1	CALCULATED=	1335.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES--	66.11 CCH	9.65 HC3C	9.35 HC5C	9.11 CC4H	9.11 CC5H	6.02 C*OH	5.21 OCHA	5.14 HC4C	
FORCE CONSTANTS--	66.11 CCH	14.56 OCH	10.77 BCCH						
OFF DIAGONAL--	7.67 BB29	-5.92 SB26	-3.48 BB29	-3.43 BB45	-1.70 SB28				
NORMAL MODE 18	OBSERVED=	1318.0 CM-1	CALCULATED=	1310.6 CM-1	ERROR=	7.4 CM-1	OR	0.6 PERCENT	
INTERNAL COORDINATES--	26.98 HC2C	1.77 CC3H	18.13 OC3H	15.82 OC2H	7.61 C2OH				
FORCE CONSTANTS--	51.56 CCH	35.52 OCH	7.81 BCCH						
OFF DIAGONAL--	-3.70 BB45	2.59 BB34	-2.18 SB27	1.72 BB30	-1.55 SB28				
NORMAL MODE 19	OBSERVED=	1300.0 CM-1	CALCULATED=	1293.4 CM-1	ERROR=	6.6 CM-1	OR	0.5 PERCENT	
INTERNAL COORDINATES--	15.75 OCHA	15.42 OC4H	13.47 CCHA	11.92 OCHB	10.47 CCHB	6.82 OC3H	6.77 HC4C		
FORCE CONSTANTS--	50.70 OCH	34.64 CCH	2.50 BB34						
OFF DIAGONAL--	-3.47 BB45	2.54 SB26							
NORMAL MODE 20	OBSERVED=	1276.0 CM-1	CALCULATED=	1281.8 CM-1	ERROR=	-3.8 CM-1	OR	-0.3 PERCENT	
INTERNAL COORDINATES--	37.65 C*OH	14.11 CCHB	12.15 CCHB	11.27 OC4H					
FORCE CONSTANTS--	66.76 OCH	27.36 CO							
OFF DIAGONAL--	4.71 SB27	-3.61 BB45	-2.96 SB26	-2.43 BB29					
NORMAL MODE 21	OBSERVED=	0.0 CM-1	CALCULATED=	1257.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES--	46.83 CC4H	12.17 OC3H	12.02 OC2H	10.85 CC3H	7.98 HC2C				
FORCE CONSTANTS--	46.83 CCH	36.88 OCH							
OFF DIAGONAL--	5.48 SB27	-3.47 BB45	1.58 BB34						
NORMAL MODE 22	OBSERVED=	1242.0 CM-1	CALCULATED=	1240.7 CM-1	ERROR=	1.3 CM-1	OR	0.1 PERCENT	
INTERNAL COORDINATES--	13.92 CC3H	12.55 OC4H	12.09 OC2H	10.77 HC3C	7.26 HC5C				
FORCE CONSTANTS--	45.52 CCH	32.40 OCH	13.23 CO	5.87 CCO					
OFF DIAGONAL--	8.47 SB27	-3.99 SB25	-3.91 SB26	-3.16 BB45	-3.07 BB29	2.80 BB34	1.55 BB33		
NORMAL MODE 23	OBSERVED=	1216.0 CM-1	CALCULATED=	1190.4 CM-1	ERROR=	25.6 CM-1	OR	2.1 PERCENT	
INTERNAL COORDINATES--	17.47 HC5C	15.53 CC5H	10.74 HC4C	7.34 CC4H	5.74 C*O*	5.15 C*O8			
FORCE CONSTANTS--	62.46 CCH	15.86 CO	12.58 CCH	9.49 CCO					
OFF DIAGONAL--	-8.24 BB29	7.04 SB27	-5.31 SB25	-4.66 SB26	3.40 BB34	-3.11 BB45	2.52 BB33	-1.55 SB22	
NORMAL MODE 24	OBSERVED=	0.0 CM-1	CALCULATED=	1162.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES--	18.47 O*CI	16.27 C*O6	15.83 C5O	15.16 CCH2	10.68 OC2H	9.15 C*O8	5.14 HC2C		
FORCE CONSTANTS--	61.84 CO	26.20 C*O6	16.82 CCH	10.72 CCO	10.72 BCCH	5.26 CC	5.26 CCC		
OFF DIAGONAL--	-9.28 SB25	-7.40 SB27	-5.81 SB28	-4.98 SB26	-2.49 BB43	-2.41 SB21	-1.77 SS18	-1.63 BB45	
NORMAL MODE 25	OBSERVED=	1130.0 CM-1	CALCULATED=	1141.8 CM-1	ERROR=	-11.8 CM-1	OR	-1.0 PERCENT	
INTERNAL COORDINATES--	20.26 C5O	11.63 C*O6	10.93 C5C	10.89 OCHB	5.80 C*O*	5.32 C*O9			
FORCE CONSTANTS--	22.44 CCH	14.13 CO	4.72 SB27	-2.70 SB28	2.00 BB43	-1.97 SB26			
OFF DIAGONAL--	-11.85 SB25	-4.89 SB22							
NORMAL MODE 26	OBSERVED=	1125.0 CM-1	CALCULATED=	1132.6 CM-1	ERROR=	-7.6 CM-1	OR	-0.7 PERCENT	
INTERNAL COORDINATES--	56.51 C5C	15.77 C*O*	14.00 CC5C	8.92 OCH	7.26 CC6C	7.00 C*OH	6.86 C*O*	6.84 C1C2	
FORCE CONSTANTS--	55.09 CCH	28.65 CO	13.87 OCH	13.06 CCO	10.14 BCCH	7.91 CCH	6.86 CCC		
OFF DIAGONAL--	-11.50 SB22	10.08 SB26	-5.48 SB28	-4.36 SS18	-3.13 SB27	-2.51 SB24	-2.22 BB34		
NORMAL MODE 27	OBSERVED=	1120.0 CM-1	CALCULATED=	1120.6 CM-1	ERROR=	-0.6 CM-1	OR	-0.1 PERCENT	
INTERNAL COORDINATES--	45.07 C2C3	16.89 C1C2	14.21 C3C4	11.63 C*O7	8.35 CCO7	7.66 C4C5	6.22 CC1H		
FORCE CONSTANTS--	87.65 CC	19.05 CO	17.02 CCH	16.64 CCO	6.58 OCH				
OFF DIAGONAL--	-17.71 SB26	-14.42 SB22	-3.54 SB27	-3.47 SS17	-3.40 SS18	-3.05 SB21	-2.67 SB25	-2.38 SB28	2.31 BB33
NORMAL MODE 28	OBSERVED=	1106.0 CM-1	CALCULATED=	1106.4 CM-1	ERROR=	-0.4 CM-1	OR	-0.0 PERCENT	
INTERNAL COORDINATES--	24.59 C*O9	21.46 C3O*	6.03 C*O8	5.88 OCHA	5.35 C1C2				
FORCE CONSTANTS--	60.50 CO	19.04 OCH	10.86 CC	8.66 CCO	8.47 CCH				
OFF DIAGONAL--	-5.74 SB25	-3.02 SB28	-2.61 SS18	-2.52 SB21	-2.24 SB27	-1.53 SB23			
NORMAL MODE 29	OBSERVED=	1080.0 CM-1	CALCULATED=	1072.3 CM-1	ERROR=	7.7 CM-1	OR	0.7 PERCENT	
INTERNAL COORDINATES--	32.42 C*O8	31.06 C*O7	11.25 C3C4	8.44 C1C2	7.00 C*CI	6.58 C4C5	6.27 C3OH	5.22 OC3H	
FORCE CONSTANTS--	29.70 CO	29.70 CCH	11.17 CCH	9.88 CCO	10.19 CCH				
OFF DIAGONAL--	-9.46 SB28	-9.18 SB27	-7.83 SS18	-6.57 SB25	-4.62 SB21	-2.69 SB22	-2.28 BB36		
NORMAL MODE 30	OBSERVED=	1066.0 CM-1	CALCULATED=	1053.2 CM-1	ERROR=	12.8 CM-1	OR	1.2 PERCENT	
INTERNAL COORDINATES--	46.01 CCH	19.53 C3C4	16.00 OCCH	9.85 C4C5	6.02 C*OH	5.88 C4CC	5.84 C1C2	5.63 C3CC	5.42 OC4H
FORCE CONSTANTS--	46.01 CC	33.58 CO	-6.14 SS18	-5.68 SB28	-4.76 SB27	-2.65 SB24			
OFF DIAGONAL--	-12.76 SB21	-6.63 SB22							
NORMAL MODE 31	OBSERVED=	1055.0 CM-1	CALCULATED=	1045.8 CM-1	ERROR=	9.2 CM-1	OR	0.9 PERCENT	
INTERNAL COORDINATES--	30.06 C*O9	13.18 C1C2	11.30 C*O*	9.70 C*O6	9.27 C2C3	7.80 C*O7	5.20 C5C*		
FORCE CONSTANTS--	59.91 CO	32.64 CC	13.10 OCH	11.30 CCH	11.04 BCCH	9.06 CCO	8.28 CCC		
OFF DIAGONAL--	-9.47 SB28	-7.15 SB27	-6.68 SB21	-5.93 SS18	-4.22 SB22	-4.18 SB26	-2.30 SB25	-2.00 BB43	-1.96 SB24
NORMAL MODE 32	OBSERVED=	1033.0 CM-1	CALCULATED=	1021.3 CM-1	ERROR=	11.7 CM-1	OR	1.1 PERCENT	
INTERNAL COORDINATES--	31.23 C*O8	28.34 C*O*	8.70 CC4H	7.04 HC3C	6.17 HC4C	5.25 C*O7	5.00 C4C5		
FORCE CONSTANTS--	69.65 CC	37.51 CCH	10.17 CO	7.31 CCO	6.43 OCH				
OFF DIAGONAL--	-7.69 SB27	-7.06 SB25	-6.16 SB28	-6.12 BB29	-3.52 SB26	-1.92 BB45	-1.84 SB22	-1.65 BB43	
NORMAL MODE 33	OBSERVED=	985.0 CM-1	CALCULATED=	1000.9 CM-1	ERROR=	-15.9 CM-1	OR	-1.6 PERCENT	
INTERNAL COORDINATES--	40.43 C*CIH	35.61 OC1H	9.40 C*O6	5.63 C*O*					
FORCE CONSTANTS--	77.07 CO	20.16 CO	8.20 C*O6	11.07 CC5C					
OFF DIAGONAL--	-3.53 SB27	-3.36 BB37	-2.78 BB45	-2.59 SB24	-1.69 SS18				
NORMAL MODE 34	OBSERVED=	969.0 CM-1	CALCULATED=	953.9 CM-1	ERROR=	15.1 CM-1	OR	1.6 PERCENT	
INTERNAL COORDINATES--	37.91 CC	25.31 C2C3	20.51 CCH	9.70 CCO	5.80 CCO9	5.45 CC3H	5.38 C1C2		
FORCE CONSTANTS--	37.91 CC	25.31 CO	3.11 SB26	2.52 SS18					
OFF DIAGONAL--	-6.80 SB22	-3.32 SB21							
NORMAL MODE 35	OBSERVED=	930.0 CM-1	CALCULATED=	915.8 CM-1	ERROR=	14.2 CM-1	OR	1.5 PERCENT	
INTERNAL COORDINATES--	11.68 C*O*	10.55 OC1H	9.33 C3C4	8.57 CC1H	6.37 C2C3	6.03 CC3H	5.69 C1C2		
FORCE CONSTANTS--	25.49 CCH	23.40 CC	23.19 CO	16.08 OCH	11.32 CCO	5.07 CCC			
OFF DIAGONAL--	-7.91 SB21	-6.49 SB22	2.89 BB43	1.80 SB25	-1.74 SB27				

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400									
MOLECULE 40 -6 NG-1238 BETA MANNOSIDE-1-D GG									
PAGE 2									
NORMAL MODE 36	OBSERVED=	911.0 CM-1	CALCULATED=	907.2 CM-1	ERROR=	3.8 CM-1	OR	0.4 PERCENT	
INTERNAL COORDINATES-	30.93	C50	18.10	C-0*	6.72	CCB	5.93	C4C5	5.58
FORCE CONSTANTS-	39.77	CC	30.89	CC	17.08	CC	8.88	CC	5.67
OFF DIAGONAL-	7.51	SB26	-6.38	SB22	6.23	SS18	-4.73	SB21	-3.52
								SB25	-2.53
								SB27	
NORMAL MODE 37	OBSERVED=	828.0 CM-1	CALCULATED=	850.5 CM-1	ERROR=	-22.5 CM-1	OR	-2.7 PERCENT	
INTERNAL COORDINATES-	16.11	O*CI	10.98	OC1H	22.88	OC	12.07	CC	7.45
FORCE CONSTANTS-	30.78	CC	28.59	CC	17.08	CC	8.88	CC	5.67
OFF DIAGONAL-	-5.69	SB23	-5.36	SB24	4.69	SB27	-3.66	SB21	-2.24
								BB37	2.14
								BB43	-1.96
								SB26	
NORMAL MODE 38	OBSERVED=	790.0 CM-1	CALCULATED=	817.1 CM-1	ERROR=	-27.1 CM-1	OR	-3.4 PERCENT	
INTERNAL COORDINATES-	26.14	CC1H	16.06	OC1H	8.12	C-0*	8.12	CC1H	5.66
FORCE CONSTANTS-	35.44	CC	24.72	OC	15.97	CC	15.63	CC	6.07
OFF DIAGONAL-	5.43	SB26	-3.06	SB27	-2.41	BB33	-1.87	BB45	1.54
								BB37	
NORMAL MODE 39	OBSERVED=	758.0 CM-1	CALCULATED=	764.6 CM-1	ERROR=	-6.6 CM-1	OR	-0.9 PERCENT	
INTERNAL COORDINATES-	18.93	C-0*	9.99	O*CC	6.54	CC1H	5.24	O*CC	6.00
FORCE CONSTANTS-	25.68	CC	25.56	CC	13.60	CC	9.55	CC	6.00
OFF DIAGONAL-	7.85	SB25	5.05	BB43	-3.02	SB27	2.99	SS18	
NORMAL MODE 40	OBSERVED=	725.0 CM-1	CALCULATED=	714.8 CM-1	ERROR=	10.2 CM-1	OR	1.4 PERCENT	
INTERNAL COORDINATES-	15.03	CC06	13.74	CC07	9.57	O*CC	8.51	CC08	5.90
FORCE CONSTANTS-	55.17	CC	13.94	CC	6.71	CC	5.96	CC	5.90
OFF DIAGONAL-	7.05	BB43	5.19	SB25	3.38	BB33	-3.29	BB34	-2.71
								SB27	-1.89
								BB41	
NORMAL MODE 41	OBSERVED=	0.0 CM-1	CALCULATED=	676.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	19.31	CC0*	9.22	OBCC	8.70	C3C4	7.83	C4C5	6.28
FORCE CONSTANTS-	52.26	CC	18.95	CC	12.83	CC	11.05	CC	9.64
OFF DIAGONAL-	5.26	BB43	5.17	SB25	-4.94	BB34	-2.88	BB29	1.97
								SS18	-1.69
								SB22	
NORMAL MODE 42	OBSERVED=	0.0 CM-1	CALCULATED=	587.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	43.03	O*CC	15.52	OC0	10.01	CC	8.18	CC	6.76
FORCE CONSTANTS-	6.51	SB24	-3.16	BB42	-2.55	SB27	2.54	BB43	2.11
OFF DIAGONAL-								SB22	-1.83
								BB34	1.74
								SB23	
NORMAL MODE 43	OBSERVED=	0.0 CM-1	CALCULATED=	527.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	16.93	UBCC	13.82	4C0*	7.98	CC09	7.36	CC0*	7.32
FORCE CONSTANTS-	64.52	CC	21.07	CC	11.72	CC	7.99	CC	6.77
OFF DIAGONAL-	-12.60	BB34	4.54	BB43	-2.80	BB29	-2.24	BB42	2.21
								SB25	-2.02
								SB24	-1.78
								BB41	-1.77
								SB22	-1.74
								BB33	
NORMAL MODE 44	OBSERVED=	0.0 CM-1	CALCULATED=	475.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	7.84	CC	6.05	C2C3	5.83	4C0*	5.61	C1C2	5.56
FORCE CONSTANTS-	20.39	CC	18.95	CC	12.83	CC	11.05	CC	9.64
OFF DIAGONAL-	5.91	SB22	-4.35	SB26	3.67	BB43	3.57	SB25	3.35
								SB21	3.22
								SS18	-2.77
								SB27	2.40
								SB24	
NORMAL MODE 45	OBSERVED=	0.0 CM-1	CALCULATED=	408.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	21.77	CC09	10.61	4C0*	6.81	O*CC	6.18	C1C2	6.15
FORCE CONSTANTS-	10.54	CC	22.24	CC	-4.60	CC	9.40	CC	6.28
OFF DIAGONAL-	-10.54	BB34	6.70	BB43	-4.60	BB29	4.61	SB22	-1.87
								SB26	1.59
								SB21	-1.58
								BB36	
NORMAL MODE 46	OBSERVED=	0.0 CM-1	CALCULATED=	394.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	41.60	C3CC	33.69	C2CC	9.13	CC06	8.53	O*CC	7.27
FORCE CONSTANTS-	5.99	SB25	-4.53	BB42	9.41	CC	7.27	CC	5.31
OFF DIAGONAL-					4.12	SB21	-3.74	BB34	-3.14
								SB22	-2.12
								BB41	1.95
								SB23	
NORMAL MODE 47	OBSERVED=	0.0 CM-1	CALCULATED=	350.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	19.82	CC06	19.09	CC0	8.88	O*CC	7.08	CC08	6.87
FORCE CONSTANTS-	53.08	CC	19.09	CC	10.76	CC	5.76	CC	5.38
OFF DIAGONAL-	5.18	SB22	-4.57	BB34	-3.33	BB42	1.53	BB43	
NORMAL MODE 48	OBSERVED=	0.0 CM-1	CALCULATED=	326.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	22.27	UBCC	20.13	CC08	17.77	O*CC	13.02	CC07	10.12
FORCE CONSTANTS-	87.74	CC	12.09	T-OH	6.22	CC	6.22	CC	6.22
OFF DIAGONAL-	-7.19	BB34	-4.42	BB42	1.84	BB41			
NORMAL MODE 49	OBSERVED=	0.0 CM-1	CALCULATED=	306.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	18.44	CC09	17.92	O*CC	7.34	TH-2	6.27	CC09	5.79
FORCE CONSTANTS-	94.47	CC	19.95	T-OH	8.22	CC	7.62	CC	6.72
OFF DIAGONAL-	6.22	SB22	-3.75	BB33	3.46	BB43	-2.72	SB26	-1.78
								BB42	
NORMAL MODE 50	OBSERVED=	0.0 CM-1	CALCULATED=	277.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	19.43	CC	20.91	TH-5	10.70	CC	9.35	CC	7.06
FORCE CONSTANTS-	52.41	CC	20.69	T-OH	10.70	CC	9.35	CC	7.06
OFF DIAGONAL-	-6.35	BB34	-2.76	BB42	-2.50	BB33			
NORMAL MODE 51	OBSERVED=	0.0 CM-1	CALCULATED=	259.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	23.88	O*CC	14.24	C1CC	9.15	CC07	6.71	C0*CC	5.92
FORCE CONSTANTS-	48.93	CC	19.37	CC	12.29	CC	11.55	T-OH	6.71
OFF DIAGONAL-	-4.51	BB33	4.02	SB22	-3.87	SB25	3.87	BB43	-2.42
								SB21	-2.00
								SB26	-1.86
								BB36	
NORMAL MODE 52	OBSERVED=	0.0 CM-1	CALCULATED=	257.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	13.07	C4CC	10.18	CC0*	9.17	TH-4	5.77	TH-3	6.92
FORCE CONSTANTS-	31.44	CC	19.05	T-OH	16.09	CC	9.80	CC	6.92
OFF DIAGONAL-	4.36	BB43	4.07	SB22	-2.98	SB26	-2.52	BB34	-2.20
								BB33	
NORMAL MODE 53	OBSERVED=	0.0 CM-1	CALCULATED=	223.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	55.84	TH-1	13.61	TH-5	8.67	TH-4	8.05	TH-3	
FORCE CONSTANTS-	85.33	T-OH	9.41	CC					
OFF DIAGONAL-	NONE								
NORMAL MODE 54	OBSERVED=	0.0 CM-1	CALCULATED=	218.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	31.17	TH-3	19.28	TH-1	17.36	TH-4	11.74	TH-2	
FORCE CONSTANTS-	81.19	T-OH	10.11	CC					
OFF DIAGONAL-	NONE								
NORMAL MODE 55	OBSERVED=	0.0 CM-1	CALCULATED=	214.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	45.54	TH-5	39.81	TH-4					
FORCE CONSTANTS-	85.27	T-OH	11.80	CC					
OFF DIAGONAL-	NONE								
NORMAL MODE 56	OBSERVED=	0.0 CM-1	CALCULATED=	210.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	50.95	TH-5	9.66	TH-1	8.85	CC	7.50	C4CC	5.42
FORCE CONSTANTS-	68.17	T-OH	17.17	CC	8.90	CC			
OFF DIAGONAL-	-2.40	BB34							
NORMAL MODE 57	OBSERVED=	0.0 CM-1	CALCULATED=	208.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	39.19	TH-3	21.99	TH-2	13.02	TH-4	6.98	CC08	
FORCE CONSTANTS-	71.21	T-OH	20.07	CC					
OFF DIAGONAL-	-2.19	BB34							
NORMAL MODE 58	OBSERVED=	0.0 CM-1	CALCULATED=	140.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	14.42	CC	10.72	C4CC	9.00	TH-4	6.06	C1C2	6.22
FORCE CONSTANTS-	4.12	BB43	-2.06	BB33	-1.99	SB25	-1.60	BB34	9.51
OFF DIAGONAL-									
NORMAL MODE 59	OBSERVED=	0.0 CM-1	CALCULATED=	90.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	22.79	C2CC	20.81	TCC5	9.48	TCC2	7.31	C3CC	5.72
FORCE CONSTANTS-	41.17	T-CC	37.45	CC	15.61	CC			
OFF DIAGONAL-	-3.86	SB25	-2.94	BB42	-2.30	SB21	1.97	BB41	-1.81
								BB34	
NORMAL MODE 60	OBSERVED=	0.0 CM-1	CALCULATED=	74.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	62.80	TCC5	6.40	C2CC	5.13	C0*CC			
FORCE CONSTANTS-	67.78	T-CC	12.34	CC	9.29	CC	5.13	CC	
OFF DIAGONAL-	NONE								
NORMAL MODE 61	OBSERVED=	0.0 CM-1	CALCULATED=	71.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	14.43	TCC4	14.37	C3CC	11.90	4C0*	9.87	TCC3	6.83
FORCE CONSTANTS-	33.40	T-CC	31.76	CC	25.91	CC	5.60	T-CC	6.22
OFF DIAGONAL-	-3.23	BB42	-2.17	BB34	-1.87	SB25	1.74	BB41	

27. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 9.93

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400									
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NORMAL MODE 8 OBSERVED= 1478.0 CM-1 CALCULATED= 1449.5 CM-1 ERROR= 28.5 CM-1 OR 1.9 PERCENT									
INTERNAL COORDINATES-	59.79	HCH	21.21	OCHA	19.60	OCBH			
FORCE CONSTANTS-	59.79	HCH	41.02	OCH					
OFF DIAGONAL-	-4.09	SB27							
NORMAL MODE 9 OBSERVED= 1428.0 CM-1 CALCULATED= 1428.7 CM-1 ERROR= -0.7 CM-1 OR -0.0 PERCENT									
INTERNAL COORDINATES-	17.71	C4OH	12.76	OC4H	11.91	HC4C	6.93	C5H	6.54
FORCE CONSTANTS-	32.35	OCH	32.00	OC4H	21.45	BCOH	9.44	CO	5.58
OFF DIAGONAL-	-8.36	SB27	-6.30	SB26	5.35	BB34	5.26	BB29	-3.56
NORMAL MODE 10 OBSERVED= 1419.0 CM-1 CALCULATED= 1418.6 CM-1 ERROR= 0.4 CM-1 OR 0.0 PERCENT									
INTERNAL COORDINATES-	38.28	OC1H	18.24	OC1H	18.52	C2OH	7.82	CC1H	7.32
FORCE CONSTANTS-	63.95	OCH	19.32	BCOH	17.92	CCH	8.14	CO	
OFF DIAGONAL-	-10.55	SB27	-3.11	BB45	2.53	SB28	-2.03	BB43	-1.58
NORMAL MODE 11 OBSERVED= 1406.0 CM-1 CALCULATED= 1406.4 CM-1 ERROR= -0.4 CM-1 OR -0.0 PERCENT									
INTERNAL COORDINATES-	30.31	C3OH	16.59	C4OH	13.36	OC3H	6.78	C1H	
FORCE CONSTANTS-	52.79	BCOH	26.43	OCH	13.48	CCH	5.68	CO	
OFF DIAGONAL-	-5.86	SB27	3.32	SB28	-1.99	SB26	-1.96	BB39	
NORMAL MODE 12 OBSERVED= 1402.0 CM-1 CALCULATED= 1402.4 CM-1 ERROR= 0.4 CM-1 OR 0.0 PERCENT									
INTERNAL COORDINATES-	59.15	C1OH	7.51	C1C2	7.19	C2OH	6.61	C1H	
FORCE CONSTANTS-	68.37	BCOH	9.48	OCH	7.76	CC			
OFF DIAGONAL-	5.50	SB28	-2.81	SB26	-2.13	SB22			
NORMAL MODE 13 OBSERVED= 1394.8 CM-1 CALCULATED= 1394.8 CM-1 ERROR= 0.0 CM-1 OR 0.0 PERCENT									
INTERNAL COORDINATES-	36.42	C1OH	9.29	C4OH	7.43	OCHA	6.23	C3OH	5.74
FORCE CONSTANTS-	57.31	BCOH	20.47	OCH	14.73	BCOH	5.69	CCHA	5.56
OFF DIAGONAL-	4.02	SB28	-4.05	SB27	-3.93	SB26	-2.52	BB39	2.22
NORMAL MODE 14 OBSERVED= 1387.5 CM-1 CALCULATED= 1387.5 CM-1 ERROR= 0.0 CM-1 OR 0.0 PERCENT									
INTERNAL COORDINATES-	52.84	C2OH	11.27	C1OH	6.55	OC2H	6.33	OC1H	5.46
FORCE CONSTANTS-	73.81	BCOH	18.41	OCH	11.79	C5H			
OFF DIAGONAL-	3.76	SB28	-3.16	SB27	-2.51	BB39			
NORMAL MODE 15 OBSERVED= 1368.0 CM-1 CALCULATED= 1378.9 CM-1 ERROR= -10.9 CM-1 OR -0.8 PERCENT									
INTERNAL COORDINATES-	30.88	C1OH	19.00	C4OH	10.61	C5H	10.28	C3OH	
FORCE CONSTANTS-	63.51	BCOH	17.26	OCH	14.53	CC			
OFF DIAGONAL-	-3.46	SB27	2.64	BB29	2.12	BB34			
NORMAL MODE 16 OBSERVED= 1363.0 CM-1 CALCULATED= 1364.1 CM-1 ERROR= -1.1 CM-1 OR -0.1 PERCENT									
INTERNAL COORDINATES-	22.90	C3OH	11.39	C4OH	8.82	HC3C	8.54	CC4H	7.07
FORCE CONSTANTS-	40.78	BCOH	36.62	CCH	11.18	OCH			
OFF DIAGONAL-	7.53	BB29	-3.76	SB28	3.55	BB34	-2.83	SB27	-1.86
NORMAL MODE 17 OBSERVED= 1334.0 CM-1 CALCULATED= 1346.2 CM-1 ERROR= -12.2 CM-1 OR -0.9 PERCENT									
INTERNAL COORDINATES-	20.61	CC2H	15.80	O1C1	10.94	C1OH	8.39	C-06	7.55
FORCE CONSTANTS-	28.47	CCH	25.88	OC1	19.56	BCOH	18.85	OCH	6.22
OFF DIAGONAL-	4.92	SB27	-4.45	SB28	-4.24	SB25	4.02	BB34	-1.94
NORMAL MODE 18 OBSERVED= 1330.0 CM-1 CALCULATED= 1328.5 CM-1 ERROR= 1.5 CM-1 OR 0.1 PERCENT									
INTERNAL COORDINATES-	12.86	CC5H	11.78	HC3C	11.48	HC4C	9.55	CC4H	6.98
FORCE CONSTANTS-	35.81	CCH	31.33	OCH	11.79	C5H			
OFF DIAGONAL-	13.98	BB29	-6.02	SB26	-3.63	BB45	-2.19	SB27	-1.56
NORMAL MODE 19 OBSERVED= 1311.0 CM-1 CALCULATED= 1318.3 CM-1 ERROR= -7.3 CM-1 OR -0.6 PERCENT									
INTERNAL COORDINATES-	46.73	CCCH	43.13	OCBH	13.94	HC5C	12.24	C5H	
FORCE CONSTANTS-	46.73	CCCH	43.13	OCBH					
OFF DIAGONAL-	-3.73	BB45	2.68	BB34					
NORMAL MODE 20 OBSERVED= 1292.0 CM-1 CALCULATED= 1311.2 CM-1 ERROR= -19.2 CM-1 OR -1.5 PERCENT									
INTERNAL COORDINATES-	25.04	HC2C	21.47	GC3H	21.37	CC3H	8.49	OC2H	7.81
FORCE CONSTANTS-	53.25	CCCH	31.09	OCH	9.12	BCOH			
OFF DIAGONAL-	-3.62	BB45	2.61	BB34	-2.01	SB28	-1.85	SB27	1.53
NORMAL MODE 21 OBSERVED= 1278.0 CM-1 CALCULATED= 1281.8 CM-1 ERROR= -3.8 CM-1 OR -0.3 PERCENT									
INTERNAL COORDINATES-	27.66	OC4H	26.25	C5H	7.86	OC3H	7.15	HC4C	5.81
FORCE CONSTANTS-	68.19	OCH	26.40	CCH					
OFF DIAGONAL-	-5.57	BB29	-3.67	BB45	2.19	SB27			
NORMAL MODE 22 OBSERVED= 1261.0 CM-1 CALCULATED= 1260.8 CM-1 ERROR= 0.2 CM-1 OR 0.0 PERCENT									
INTERNAL COORDINATES-	22.90	OC2H	12.06	CC3H	9.56	HC2C	7.52	C-07	7.22
FORCE CONSTANTS-	42.43	CCH	31.33	OCH	7.87	CC	5.60	BCOH	
OFF DIAGONAL-	6.46	SB27	-3.26	BB45	-1.66	SB25			
NORMAL MODE 23 OBSERVED= 1238.0 CM-1 CALCULATED= 1242.5 CM-1 ERROR= -4.5 CM-1 OR -0.4 PERCENT									
INTERNAL COORDINATES-	40.44	CCH	39.61	OC4H	10.81	CO	5.41	CCO	
FORCE CONSTANTS-	40.44	CCH	39.61	OC4H					
OFF DIAGONAL-	7.89	SB27	-5.35	BB29	-3.69	SB25	3.38	BB34	-3.15
NORMAL MODE 24 OBSERVED= 1212.0 CM-1 CALCULATED= 1204.7 CM-1 ERROR= 7.3 CM-1 OR 0.6 PERCENT									
INTERNAL COORDINATES-	23.11	CC1H	15.04	OC1H	11.79	OC3H	6.93	OCHA	5.35
FORCE CONSTANTS-	47.71	CCH	40.10	OCH	11.37	CO	6.77	BCOH	
OFF DIAGONAL-	-4.27	SB26	-3.40	BB45	-2.85	SB25	-2.68	BB29	
NORMAL MODE 25 OBSERVED= 1181.0 CM-1 CALCULATED= 1181.5 CM-1 ERROR= -0.5 CM-1 OR 0.0 PERCENT									
INTERNAL COORDINATES-	14.67	C5O	12.07	OCHA	9.30	HC5C	9.09	CC5H	8.07
FORCE CONSTANTS-	38.60	CCH	29.91	CO	27.80	OCH	8.47	CCO	6.77
OFF DIAGONAL-	-5.18	SB25	-4.72	BB29	-2.42	BB45	-1.97	SB26	-1.65
NORMAL MODE 26 OBSERVED= 1167.0 CM-1 CALCULATED= 1159.1 CM-1 ERROR= 7.9 CM-1 OR 0.7 PERCENT									
INTERNAL COORDINATES-	15.39	C-08	15.03	CC2H	12.25	O1C1	9.37	C2C3	8.59
FORCE CONSTANTS-	41.90	CCH	41.90	OCH	10.07	CC	3.75	OCH	3.22
OFF DIAGONAL-	-14.94	SB26	-5.59	SB25	-4.26	SB27	-3.77	SB28	-3.04
NORMAL MODE 27 OBSERVED= 1124.0 CM-1 CALCULATED= 1150.6 CM-1 ERROR= -26.6 CM-1 OR -1.5 PERCENT									
INTERNAL COORDINATES-	17.09	C5O	14.29	C-06	16.28	CC	15.45	OCCH	5.14
FORCE CONSTANTS-	42.43	CCH	31.33	CCO	16.81	CO	15.45	OCH	7.66
OFF DIAGONAL-	-11.26	SB25	-3.57	SB22	3.15	SB27	-3.00	SB28	2.25
NORMAL MODE 28 OBSERVED= 1118.0 CM-1 CALCULATED= 1111.7 CM-1 ERROR= 6.3 CM-1 OR 0.6 PERCENT									
INTERNAL COORDINATES-	26.39	C4C5	15.43	C3C4	21.03	C5C1	20.89	C2C3	
FORCE CONSTANTS-	95.50	CC	15.62	CCO	13.04	CC	6.01	CO	
OFF DIAGONAL-	-17.75	SB22	-8.51	SB26	-3.96	SS17	-2.51	SB27	-2.33
NORMAL MODE 29 OBSERVED= 1113.0 CM-1 CALCULATED= 1102.0 CM-1 ERROR= 11.0 CM-1 OR 1.0 PERCENT									
INTERNAL COORDINATES-	19.41	C-08	16.41	C-09	13.72	C5C1	8.64	C1C2	8.34
FORCE CONSTANTS-	55.45	CO	27.72	CC	9.01	CCH	8.42	CCO	5.40
OFF DIAGONAL-	-5.59	SB22	4.38	SB27	-4.24	SB28	-3.47	SS18	-3.15
NORMAL MODE 30 OBSERVED= 1086.0 CM-1 CALCULATED= 1085.4 CM-1 ERROR= 0.6 CM-1 OR 0.0 PERCENT									
INTERNAL COORDINATES-	27.02	C5O	16.95	C1C2	11.80	C-09	5.73	OCBH	5.57
FORCE CONSTANTS-	48.02	CO	28.09	CC	16.60	CO	15.53	OCCH	9.22
OFF DIAGONAL-	-7.32	SB22	-4.49	SB23	-4.23	SB25	-2.21	SB26	-1.98
NORMAL MODE 31 OBSERVED= 1070.0 CM-1 CALCULATED= 1064.9 CM-1 ERROR= 5.0 CM-1 OR 0.5 PERCENT									
INTERNAL COORDINATES-	41.85	C-08	17.44	C-09	11.93	C2C3	7.81	C4C5	6.82
FORCE CONSTANTS-	91.83	CC	18.00	CC	11.93	BCOH	8.94	CCH	8.19
OFF DIAGONAL-	-9.88	SB27	-9.33	SB28	-6.57	SS18	-5.34	SB21	-4.52
NORMAL MODE 32 OBSERVED= 1057.0 CM-1 CALCULATED= 1051.5 CM-1 ERROR= 5.5 CM-1 OR 0.5 PERCENT									
INTERNAL COORDINATES-	12.42	C-07	22.35	C-08	11.09	OC4H	10.88	BCOH	8.94
FORCE CONSTANTS-	72.42	CC	22.31	CC	-7.19	SB21	-5.32	SB25	-3.57
OFF DIAGONAL-	-9.75	SB28	-7.48	SB27					
NORMAL MODE 33 OBSERVED= 1041.0 CM-1 CALCULATED= 1037.0 CM-1 ERROR= 4.0 CM-1 OR 0.4 PERCENT									
INTERNAL COORDINATES-	29.61	C-07	27.11	C-09	13.15	C2C3	11.93	C1C2	6.55
FORCE CONSTANTS-	59.50	CO	35.02	CC	15.29	OCH	15.04	CC	13.88
OFF DIAGONAL-	-11.38	SB27	-10.53	SB21	-8.85	SB28	-7.09	SS18	-6.48
NORMAL MODE 34 OBSERVED= 1032.0 CM-1 CALCULATED= 1033.7 CM-1 ERROR= -1.7 CM-1 OR -0.2 PERCENT									
INTERNAL COORDINATES-	29.17	C-06	22.39	C-08	17.00	C3C4	6.17	CC2H	
FORCE CONSTANTS-	61.44	CC	22.12	CC	13.39	CCH	8.22	OCH	
OFF DIAGONAL-	-6.79	SB28	-5.74	SB21	-4.97	SB22	-4.34	SB24	-3.48
NORMAL MODE 35 OBSERVED= 1007.0 CM-1 CALCULATED= 978.3 CM-1 ERROR= 28.6 CM-1 OR 2.8 PERCENT									
INTERNAL COORDINATES-	27.61	C5C1	17.44	C-09	10.16	C4C5	7.49	C3C4	5.01
FORCE CONSTANTS-	61.44	CC	44.63	CC	16.16	CCH	14.90	CCO	5.00
OFF DIAGONAL-	-13.69	SB22	-5.73	SB26	-5.51	SB21	-2.88	BB29	-2.21

TABLE XXXIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 400									
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NORMAL MODE 36	OBSERVED=	933.0 CM-1		CALCULATED=	934.2 CM-1	ERROR=	-1.2 CM-1	OR	-0.1 PERCENT
INTERNAL COORDINATES-	16.76	C3C4 13.94	C-U7	11.20 C2C3	9.35 C6C8	7.88	0.1 C1	7.58 CCO9	6.99 C-06
FORCE CONSTANTS-	31.06	CCO 26.92	CC	24.58 CCH	12.97 CCO	5.44	CC	5.53 CCH	
OFF DIAGONAL-	-6.77	SB22 -4.27	SB21	4.19 SB26	-4.03 SB24	-3.35	SB25	-2.37 BB34	2.36 SS18 2.02 BB43 -1.53 SB23
NORMAL MODE 37	OBSERVED=	896.0 CM-1		CALCULATED=	858.9 CM-1	ERROR=	37.1 CM-1	OR	4.1 PERCENT
INTERNAL COORDINATES-	25.08	01C1 11.92	CCHB	10.68 C4C5	9.26 CCO	6.22	CCH	6.08 C5C1	
FORCE CONSTANTS-	10.11	CCH 26.92	CC	-3.45 SB23	-3.08 SB22	-3.08	BB29	-3.03 SB24	1.66 BB43
OFF DIAGONAL-	-5.30	SB21 4.67	SB26						
NORMAL MODE 38	OBSERVED=	855.0 CM-1		CALCULATED=	838.5 CM-1	ERROR=	16.5 CM-1	OR	1.9 PERCENT
INTERNAL COORDINATES-	13.90	C-U7 12.51	CCHA	9.75 CCHB	7.43 01C1	7.16	C1C2	5.94 HC5C	
FORCE CONSTANTS-	40.05	CCH 28.48	CO	17.61 CC	10.20 CCO	5.94	CCH		
OFF DIAGONAL-	-5.64	BB29 -5.10	SB22	-3.51 SB21	3.44 SS18	2.17	BB43	1.95 SB26	
NORMAL MODE 39	OBSERVED=	769.0 CM-1		CALCULATED=	768.5 CM-1	ERROR=	0.5 CM-1	OR	0.1 PERCENT
INTERNAL COORDINATES-	18.21	01CC 12.53	CCO7	10.88 C-U7	5.36 01C1				
FORCE CONSTANTS-	35.12	CCO 17.56	CC	11.45 CCH	9.47 CCH	8.83	CC		
OFF DIAGONAL-	8.08	SB25 5.77	BB43	-3.77 SB27	2.21 BB33	-1.73	BB41	-1.57 SB22	1.53 SS18
NORMAL MODE 40	OBSERVED=	730.0 CM-1		CALCULATED=	722.1 CM-1	ERROR=	7.9 CM-1	OR	1.1 PERCENT
INTERNAL COORDINATES-	14.18	CCO6 12.97	07CC	10.19 CCO8	9.07 C3C4	7.55	CCO7	5.45 HC2C	
FORCE CONSTANTS-	49.57	CCO 14.24	CC	11.90 CCH	8.51 CC	7.23	CCC	6.79 CCH	
OFF DIAGONAL-	5.20	BB43 4.64	SB25	-3.55 BB34	-2.68 SB27	-2.34	SB21	-1.74 BB41	-1.69 SB26
NORMAL MODE 41	OBSERVED=	618.0 CM-1		CALCULATED=	663.5 CM-1	ERROR=	-45.5 CM-1	OR	-7.4 PERCENT
INTERNAL COORDINATES-	18.07	UCO 11.20	CCO*	9.27 C-U7	7.83 CCO				
FORCE CONSTANTS-	35.39	CCO 11.97	CCO	14.08 CCH	3.20 CCO	5.46	CCH	5.25 CCH	
OFF DIAGONAL-	5.41	SB25 5.26	SB24	-4.12 SB27			SB22	-1.85 BB42	-1.77 BB34
NORMAL MODE 42	OBSERVED=	599.0 CM-1		CALCULATED=	546.0 CM-1	ERROR=	53.0 CM-1	OR	8.8 PERCENT
INTERNAL COORDINATES-	27.17	0B2C 13.04	C4CC	9.95 CCO9	8.28 CC4H	7.84	4CO*	6.27 HC3C	6.04 CCO6
FORCE CONSTANTS-	60.03	CCO 33.84	CCH	14.60 CCC					
OFF DIAGONAL-	-15.00	BB34 8.90	BB43	-6.80 BB29	-3.84 SB21				
NORMAL MODE 43	OBSERVED=	492.0 CM-1		CALCULATED=	510.0 CM-1	ERROR=	-18.0 CM-1	OR	-3.7 PERCENT
INTERNAL COORDINATES-	19.30	CCO*	8.70 09CC	7.55 C4C5	7.50 HC5C	5.74	C3C4	5.03 C5C*	
FORCE CONSTANTS-	36.02	CCO 21.59	CC	18.01 CCH	6.50 CC	5.11	CCC		
OFF DIAGONAL-	-7.72	BB34 6.62	SB21	5.74 BB43	-3.71 BB29	2.27	SS18	-1.99 SB26	1.88 SB22 -1.57 SB24
NORMAL MODE 44	OBSERVED=	444.0 CM-1		CALCULATED=	468.9 CM-1	ERROR=	-24.9 CM-1	OR	-5.6 PERCENT
INTERNAL COORDINATES-	12.68	CCO 9.47	C1CC	7.94 4CO*	6.68 CCO*	6.59	CCO*	6.02 C1C2	5.59 CCO8
FORCE CONSTANTS-	27.37	CCO 19.46	CCC	12.68 CCO	11.83 CC	11.06	CCO	9.08 CCH	6.59 CCO
OFF DIAGONAL-	-3.91	SB26 3.66	BB43	1.26 SB21	3.22 SB22	-2.83	BB34	2.18 SB24	-2.07 SB27 2.01 SB25 -1.83 BB41
NORMAL MODE 45	OBSERVED=	423.0 CM-1		CALCULATED=	416.7 CM-1	ERROR=	6.3 CM-1	OR	1.5 PERCENT
INTERNAL COORDINATES-	10.39	CCO6 10.12	07CC	8.19 CCO*	7.56 CCO*	7.26	CCO*		
FORCE CONSTANTS-	49.16	CCO 15.00	CCO	10.35 CCH	7.26 CCO	6.13	CCO		
OFF DIAGONAL-	4.11	SB25 3.87	BB34	2.33 SB22	-2.85 SB27	2.72	SB25	2.17 SB21	1.97 BB43 -1.64 BB29
NORMAL MODE 46	OBSERVED=	394.0 CM-1		CALCULATED=	403.1 CM-1	ERROR=	-9.1 CM-1	OR	0.7 PERCENT
INTERNAL COORDINATES-	19.14	C3C6 13.60	C2CC	11.68 09CC	10.04 CCO8	6.66	01CC	5.18 CCO	
FORCE CONSTANTS-	43.97	CCO 36.16	CCC	7.18 CC	5.08 CCO	5.01	CCH		
OFF DIAGONAL-	6.39	SB25 -5.21	BB42	-4.65 BB34	3.44 SB21	-2.13	BB41	-2.01 SB22	
NORMAL MODE 47	OBSERVED=	370.0 CM-1		CALCULATED=	370.5 CM-1	ERROR=	-0.5 CM-1	OR	-0.1 PERCENT
INTERNAL COORDINATES-	23.48	CCO9 14.87	4CO*	11.29 CCO*	7.19 07CC	6.60	CCO7	5.83 HC4C	
FORCE CONSTANTS-	67.71	CCO 19.97	CCH	5.36 SB22	-4.08 BB29	-3.03	SB25		
OFF DIAGONAL-	-9.99	BB34 5.93	BB43						
NORMAL MODE 48	OBSERVED=	326.0 CM-1		CALCULATED=	328.9 CM-1	ERROR=	-2.9 CM-1	OR	-0.9 PERCENT
INTERNAL COORDINATES-	24.67	09CC 18.06	CCO9	13.32 08CC	8.42 CCO8	7.34	CCO7	5.84 TH-4	5.76 CCO6
FORCE CONSTANTS-	81.00	CCO 9.84	T-OH	5.22 CC	5.15 CCH				
OFF DIAGONAL-	-6.43	BB34 -4.66	BB42	-1.86 SB21	1.78 BB41				
NORMAL MODE 49	OBSERVED=	0.0 CM-1		CALCULATED=	316.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	14.31	CCO8 11.86	CCO6	10.75 CCO	6.83 CCO7	6.31	C2C3	6.02 08CC	
FORCE CONSTANTS-	49.13	CCO 11.95	T-OH	11.36 CC	10.75 CCO	5.99	CCO		
OFF DIAGONAL-	5.60	SB22 -3.01	BB42	-2.24 BB34	1.85 SB24	1.79	SB21	1.75 SB25	
NORMAL MODE 50	OBSERVED=	288.0 CM-1		CALCULATED=	290.6 CM-1	ERROR=	-2.6 CM-1	OR	-0.9 PERCENT
INTERNAL COORDINATES-	15.69	CCO 12.27	08CC	11.83 T-OH	8.55 CCC		07CC	5.31 09CC	
FORCE CONSTANTS-	56.37	CCO 16.34	CCH	4.89 SB22	-2.73 BB29	-2.53	BB33	-2.32 SB25	-2.04 SB21
OFF DIAGONAL-	6.86	BB43 -6.39	BB34						
NORMAL MODE 51	OBSERVED=	258.0 CM-1		CALCULATED=	263.4 CM-1	ERROR=	-5.4 CM-1	OR	-2.1 PERCENT
INTERNAL COORDINATES-	21.41	07CC 11.20	C1CC	8.76 TH-1	6.39 CCO7	5.91	01CC	5.41 TH-3	5.25 CCO8
FORCE CONSTANTS-	47.08	CCO 18.52	CCC	18.37 T-OH	9.29 CCH				
OFF DIAGONAL-	-3.80	BB33 3.71	SB22	-3.64 SB21	-2.12 SB25	2.12	BB43	-1.92 BB42	-1.53 BB34
NORMAL MODE 52	OBSERVED=	239.0 CM-1		CALCULATED=	238.8 CM-1	ERROR=	0.2 CM-1	OR	0.1 PERCENT
INTERNAL COORDINATES-	59.90	TH-5 5.89	CCO*	5.61 C4CC					
FORCE CONSTANTS-	64.31	T-OH 19.77	CCO	10.92 CCC					
OFF DIAGONAL-	-1.99	BB34 -1.61	SB25						
NORMAL MODE 53	OBSERVED=	0.0 CM-1		CALCULATED=	225.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	38.69	TH-4 24.60	TH-3	14.33 TH-1	8.79 TH-2	8.01	TH-5		
FORCE CONSTANTS-	94.42	T-OH							
OFF DIAGONAL-	NONE								
NORMAL MODE 54	OBSERVED=	0.0 CM-1		CALCULATED=	218.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	68.89	TH-0 0.0 CM-1	TH-3	6.78 TH-4					
FORCE CONSTANTS-	85.59	T-OH 9.06	CCO						
OFF DIAGONAL-	NONE								
NORMAL MODE 55	OBSERVED=	0.0 CM-1		CALCULATED=	214.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	49.57	TH-2 29.00	TH-4	6.09 TH-3					
FORCE CONSTANTS-	85.61	T-OH 12.46	CCO						
OFF DIAGONAL-	NONE								
NORMAL MODE 56	OBSERVED=	0.0 CM-1		CALCULATED=	209.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	44.96	TH-3 23.13	TH-2	11.79 TH-4	8.02 CCO8				
FORCE CONSTANTS-	79.91	T-OH 18.84	CCO						
OFF DIAGONAL-	-1.81	BB34							
NORMAL MODE 57	OBSERVED=	0.0 CM-1		CALCULATED=	192.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	23.28	C4CC 21.71	TH-5	12.88 TCC5					
FORCE CONSTANTS-	29.09	CCO 23.87	T-OH	18.09 CCO	14.31 T-CC	5.11	T-CCO		
OFF DIAGONAL-	-2.10	BB42 -1.98	SB25						
NORMAL MODE 58	OBSERVED=	0.0 CM-1		CALCULATED=	146.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	30.41	CCO 22.84	COC	9.91 CCO4	5.36 CCO				
FORCE CONSTANTS-	48.15	CCO 22.84	COC	9.05 CCH	5.37 T-CC	6.77	CCC	6.00 T-CCO	5.36 CCO
OFF DIAGONAL-	-9.05	BB34 -3.72	SB25	-2.03 BB42	1.60 BB43				
NORMAL MODE 59	OBSERVED=	0.0 CM-1		CALCULATED=	94.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	34.92	TCC5 12.32	TCC4	10.66 C1CC					
FORCE CONSTANTS-	54.47	T-CC 22.80	CCC	16.36 CCO					
OFF DIAGONAL-	-2.30	SB25 -1.84	BB42	-1.82 BB34					
NORMAL MODE 60	OBSERVED=	0.0 CM-1		CALCULATED=	82.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	18.05	C2CC 17.59	C3CC	15.84 TCC2	12.05 TCC5	6.04	CCO9	5.14 TCC3	
FORCE CONSTANTS-	36.16	CCO 35.18	T-CC	22.05 CCO					
OFF DIAGONAL-	-3.86	SB25 -3.77	BB42	-2.08 BB34	1.93 BB41				
NORMAL MODE 61	OBSERVED=	0.0 CM-1		CALCULATED=	66.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	32.04	TCC5 9.56	4CO*	8.61 TCC4	5.95 C3CC	5.75	TCC3	5.18 C1CC	5.05 C4CC
FORCE CONSTANTS-	19.91	T-CC 19.91	CCO	17.25 C1C	9.05 T-CCO				
OFF DIAGONAL-	-2.29	BB34 -1.97	BB42						

40. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 10.26

TABLE XXXV

CORRELATION MATRIX — GLUCOSE FORCE FIELD

Explanation of the table:

1. This matrix was obtained from a single cycle linear refinement of the final glucose field (Table XI, page 47) obtained by the FPM.
2. The matrix elements are listed row-wise. As an example, under the heading "Row 6" the seventh element in the first row (0.2952) is the element between constants 6 and 7. The third element in the second row (0.2902 is the element between constants 6 and 12.
3. More detailed discussions of this matrix may be found in References 6 and 32.

TABLE XXXV

CORRELATION MATRIX - GLUCOSE FORCE FIELD

CORRELATION MATRIX ON CYCLE 1

SINGLE CYCLE LINEAR GLUCOSE REFINEMENT FOR PURPOSE OF OBTAINING
STATISTICAL PARAMETERS
15 JUNE 1976

ROW 1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ROW 2	0.0	1.0000	0.3998	0.2827	0.1369	0.5342	0.4079	0.0708	0.4604
0.3080	0.2105	0.4649	0.2448	0.0826	0.4451	0.2587	-0.0342	-0.1622	
-0.0867	-0.0846	-0.2538	-0.2493	-0.2408	-0.2213	-0.4449	-0.2706	-0.2335	
-0.0234	0.1355	-0.0183	0.1600	-0.2045	0.3141	-0.4523	-0.0502	-0.2917	
0.0897	-0.0555	0.0560	0.4105	-0.1869	-0.0114	-0.0297	-0.0396	-0.4085	
-0.0654	0.7114	0.1445							
ROW 3	0.0	0.3998	1.0000	0.6537	0.2267	0.2017	0.3658	0.0415	0.4502
0.7105	0.4232	0.7213	0.4217	0.1267	0.4061	0.4404	-0.1689	-0.5840	
-0.2541	-0.2719	-0.5367	-0.5252	-0.3845	-0.5602	-0.7745	-0.3300	-0.3924	
-0.6105	-0.0934	0.0847	0.3461	-0.4459	0.3679	-0.2502	0.3747	0.1405	
0.1441	-0.0410	0.1232	0.7901	-0.4900	-0.4900	0.1973	-0.0554	-0.3665	
-0.0330	0.6703	0.0091							
ROW 4	0.0	0.2827	0.6537	1.0000	0.1519	0.2134	0.2191	0.0325	0.2624
0.7411	0.3756	0.6740	0.4369	0.0882	0.2394	0.3541	-0.5408	-0.6336	
0.0675	-0.0134	-0.6762	-0.9172	-0.2094	-0.4615	-0.3573	-0.4140	-0.3574	
-0.4237	-0.0355	0.0429	0.5221	-0.3453	0.2763	0.0096	0.2024	0.1020	
0.0482	-0.0249	0.0997	0.8504	-0.4481	-0.5829	0.1768	-0.0144	-0.1957	
-0.0241	0.5467	0.0262							
ROW 5	0.0	0.1369	0.2267	0.1519	1.0000	0.0448	0.1977	0.0096	0.2489
0.2355	0.0985	0.1800	0.0928	0.0372	0.1751	0.1418	0.0014	-0.1557	
-0.1469	-0.0873	-0.2053	-0.0977	-0.0614	-0.0867	-0.2154	-0.0958	0.0061	
-0.1455	-0.0302	0.0445	0.1475	-0.1010	0.1482	-0.1437	0.2419	-0.0424	
0.0	-0.1822	0.0755	0.2329	-0.1657	-0.1400	-0.0620	-0.0208	-0.2374	
-0.0085	0.1679	-0.0588							
ROW 6	0.0	0.5342	0.2017	0.2134	0.0448	1.0000	0.2952	0.0173	0.3110
0.2206	0.0776	0.2902	0.1144	0.0395	0.3112	0.1170	-0.0870	-0.1419	
-0.0454	-0.0425	-0.1645	-0.1950	-0.0985	-0.0904	-0.2612	-0.2599	-0.2676	
0.1249	0.1944	-0.0961	0.0567	-0.1543	0.2126	-0.2740	0.0311	-0.2435	
0.1514	-0.0394	-0.1529	0.2757	-0.1358	-0.0849	0.0816	0.0201	-0.3111	
-0.0157	0.3772	-0.0497							
ROW 7	0.0	0.4079	0.3658	0.2191	0.1977	0.2952	1.0000	0.3480	0.6933
0.2382	0.1239	0.3859	0.2439	0.1035	0.7577	0.3064	-0.0691	-0.1987	
-0.2228	-0.1111	-0.1625	-0.1393	-0.2594	-0.1210	-0.4806	-0.4394	-0.5042	
-0.0770	0.3042	-0.0581	0.1344	-0.1688	0.3195	-0.5752	0.1116	0.0223	
0.3993	-0.4555	-0.0082	0.3427	-0.1942	-0.0836	0.2606	0.1444	-0.8424	
-0.3473	0.5199	-0.0050							
ROW 8	0.0	0.0708	0.0415	0.0325	0.0096	0.0173	0.3480	1.0000	0.0452
0.0401	0.0153	0.0320	0.0128	0.0050	0.0234	0.0241	-0.0011	-0.0300	
-0.0024	0.0051	-0.0277	-0.0260	-0.0006	-0.0191	-0.0316	-0.0273	-0.2196	
-0.0157	0.0079	-0.0169	0.0054	-0.0242	0.0274	-0.0192	0.0116	0.0050	
0.0071	-0.0140	-0.0332	0.0374	-0.0209	-0.0183	0.1232	0.7040	-0.0085	
-0.9995	0.2853	0.0038							
ROW 9	0.0	0.4604	0.4502	0.2624	0.2489	0.3110	0.6933	0.0452	1.0000
0.2848	0.2006	0.4753	0.2343	0.1454	0.7351	0.4574	-0.0981	-0.1957	
-0.2397	-0.1918	-0.1806	-0.1627	-0.2270	-0.1775	-0.5361	-0.6649	-0.3730	
-0.1936	0.4838	-0.0605	0.2293	-0.2568	0.3914	-0.6624	0.2276	0.0727	
0.1132	-0.1923	0.1324	0.3761	-0.2395	-0.0826	0.1569	0.0485	-0.9271	
-0.0456	0.4934	0.0134							

TABLE XXXV (Continued)

ROW 10									
0.0	0.3080	0.7105	0.7411	0.2355	0.2206	0.2382	0.0401	0.2648	
1.0000	0.4540	0.6850	0.3965	0.1452	0.3030	0.4371	-0.1526	-0.7043	
0.0252	0.0276	-0.7887	-0.5541	-0.1953	-0.3856	-0.4456	-0.2157	-0.4133	
-0.4894	-0.0487	0.0130	0.3259	-0.4465	0.2077	-0.0055	0.2092	0.1003	
0.0252	-0.0175	0.1254	0.8924	-0.6452	-0.5823	0.0440	-0.0370	-0.2023	
-0.0327	0.5510	0.0223							
ROW 11									
0.0	0.2105	0.4232	0.3756	0.0985	0.0776	0.1239	0.0153	0.2006	
0.4540	1.0000	0.5674	0.4047	0.2012	0.1764	0.5862	-0.0358	-0.1824	
0.1762	-0.0540	-0.3490	-0.2981	-0.3293	-0.5166	-0.0974	-0.1115	-0.1710	
-0.2457	-0.1070	0.0306	0.2142	-0.1149	0.1077	0.0754	0.1635	0.0819	
-0.0012	0.0117	0.0620	0.4525	-0.3969	-0.3867	-0.1673	-0.1266	-0.0772	
-0.0104	0.4320	0.0674							
ROW 12									
0.0	0.4649	0.7213	0.6740	0.1800	0.2902	0.3859	0.0320	0.4753	
0.6850	0.5674	1.0000	0.5597	0.2220	0.4559	0.5820	-0.2781	-0.3651	
-0.1870	-0.1821	-0.4401	-0.6068	-0.3824	-0.3272	-0.5935	-0.3905	-0.3140	
-0.3061	-0.0587	0.0741	0.2993	-0.2272	0.3841	-0.1532	0.2000	0.0298	
0.1275	-0.0293	0.0342	0.8019	-0.6989	-0.4848	-0.1060	-0.0759	-0.3709	
-0.0221	0.6923	0.0305							
ROW 13									
0.0	0.2448	0.4217	0.4369	0.0928	0.1144	0.2439	0.0126	0.2343	
0.3965	0.4047	0.5597	1.0000	0.1270	0.2413	0.2866	-0.2903	-0.0953	
-0.0075	-0.0022	-0.1464	-0.4161	-0.6280	-0.2095	-0.2651	-0.2398	-0.1439	
-0.2278	-0.0513	-0.0002	0.4405	-0.1428	0.3468	-0.0153	0.1063	0.0723	
0.1772	-0.1156	0.0381	0.5353	-0.5956	-0.1728	-0.1944	-0.1117	-0.1685	
-0.0100	0.4323	0.0502							
ROW 14									
0.0	0.0826	0.1267	0.0882	0.0372	0.0395	0.1035	0.0050	0.1454	
0.1452	0.2012	0.2220	0.1270	1.0000	0.1397	0.2752	0.0020	-0.0195	
-0.0053	0.0261	-0.0757	-0.0624	-0.1113	-0.0909	-0.0800	-0.0688	-0.0561	
-0.0582	0.0117	0.0380	0.0242	-0.0147	0.0224	-0.0136	0.0433	0.0309	
0.0174	-0.0274	0.0165	0.0977	-0.0835	-0.1170	-0.0453	-0.0445	-0.1048	
-0.0035	0.1408	0.0049							
ROW 15									
0.0	0.4451	0.4061	0.2394	0.1751	0.3112	0.7577	0.0234	0.7351	
0.3030	0.1764	0.4559	0.2413	0.1397	1.0000	0.3201	-0.0764	-0.2470	
-0.1319	-0.1044	-0.1744	-0.0988	-0.3113	-0.1274	-0.5540	-0.5212	-0.5832	
-0.0865	0.4753	-0.0466	0.1278	-0.2170	0.3342	-0.6676	0.1171	0.0094	
0.2621	-0.1602	-0.0265	0.3987	-0.2021	-0.0669	0.1912	-0.1342	-0.7900	
-0.0227	0.5085	0.0300							
ROW 16									
0.0	0.2587	0.4404	0.3541	0.1418	0.1170	0.3064	0.0241	0.4574	
0.4371	0.5862	0.5820	0.2866	0.2252	0.3201	1.0000	-0.0270	-0.2087	
-0.1320	-0.0830	-0.3337	-0.2624	-0.2138	-0.2355	-0.2595	-0.2900	-0.1582	
-0.2181	0.0045	0.1140	0.1746	-0.1655	0.2347	-0.1522	0.1795	0.0806	
0.1128	-0.0429	0.0773	0.4356	-0.3338	-0.2811	-0.0895	-0.0114	-0.3661	
-0.0184	0.4147	0.0334							
ROW 17									
0.0	-0.0342	-0.1689	-0.5408	0.0014	-0.0870	-0.0691	-0.0011	-0.0981	
-0.1526	-0.0358	-0.2781	-0.2903	0.0020	-0.0764	-0.0270	1.0000	0.1844	
0.0299	0.0891	-0.1182	0.5071	0.1309	0.0725	0.2268	0.3578	0.0954	
0.1398	-0.0301	0.0219	-0.1300	0.2211	-0.2515	-0.0853	-0.1989	-0.0229	
-0.0064	0.0216	-0.0269	-0.3035	0.3520	0.4426	-0.2372	0.0051	0.0941	
0.0029	-0.0216	-0.0287							
ROW 18									
0.0	-0.1622	-0.5840	-0.6336	-0.1557	-0.1419	-0.1987	-0.0300	-0.1957	
-0.7043	-0.1824	-0.3651	-0.0953	-0.0195	-0.2470	-0.2087	0.1844	1.0000	
0.0297	0.0247	0.6419	0.4054	0.0649	0.3057	0.3488	0.2701	0.4686	
0.4207	-0.0339	0.0197	-0.2757	0.3920	-0.2168	0.0500	-0.1764	-0.0781	
-0.0657	0.0150	-0.1103	-0.6462	0.3787	0.4981	-0.2550	0.0188	0.1879	
0.0247	-0.2587	0.0013							
ROW 19									
0.0	-0.0867	-0.2541	0.0675	-0.1469	-0.0454	-0.2228	-0.0024	-0.2397	
0.0252	0.1762	-0.1870	-0.0075	-0.0053	-0.1319	-0.1320	0.0299	0.0297	
1.0000	0.4056	-0.0985	-0.1056	0.1035	-0.3129	0.4810	0.0933	0.0668	
-0.0130	0.0426	-0.1327	-0.0299	0.0610	-0.3007	0.2867	-0.1312	0.0347	
-0.1737	0.0614	-0.0150	-0.0522	0.1434	0.1371	-0.1359	-0.0085	0.2758	
0.0020	0.0005	0.0248							

TABLE XXXV (Continued)

ROW 20									
0.0	-0.0846	-0.2719	-0.0134	-0.0873	-0.0425	-0.1111	0.0051	-0.1918	
0.0276	-0.0540	-0.1821	-0.0022	0.0261	-0.1044	-0.0830	0.0891	0.0247	
0.4056	1.0000	-0.0882	0.0429	-0.1569	0.1447	0.3111	0.1785	0.0289	
0.0397	0.0352	0.0302	-0.0392	-0.0002	-0.0395	0.1959	-0.0818	-0.0272	
0.0076	0.0491	0.0027	-0.0750	0.1138	0.1110	-0.1565	-0.0643	0.2024	
-0.0062	-0.0484	0.0104							
ROW 21									
0.0	-0.2538	-0.5367	-0.6762	-0.2053	-0.1645	-0.1625	-0.0277	-0.1806	
-0.7887	-0.3490	-0.4401	-0.1464	-0.0757	-0.1744	-0.3337	-0.1182	0.6419	
-0.0985	-0.0882	1.0000	0.5482	0.0945	0.4442	0.2305	0.0766	0.3183	
0.3649	0.0510	-0.0349	-0.1534	0.2747	-0.0823	0.0625	-0.0989	-0.0587	
-0.0041	0.0279	-0.1276	-0.7446	0.2032	0.3713	-0.0784	0.0346	0.1210	
0.0191	-0.5197	-0.0179							
ROW 22									
0.0	-0.2493	-0.5252	-0.9172	-0.0977	-0.1950	-0.1393	-0.0260	-0.1627	
-0.5541	-0.2981	-0.6068	-0.4161	-0.0624	-0.0988	-0.2624	0.5071	0.4054	
-0.1056	0.0429	0.5482	1.0000	0.1707	0.4677	0.2536	0.3656	0.2015	
0.3413	0.1073	-0.0511	-0.1849	0.2517	-0.2600	-0.0582	-0.1340	-0.1048	
-0.0393	0.0436	-0.0897	-0.7374	0.2876	0.4732	-0.1525	-0.0013	0.1010	
0.0177	-0.5277	-0.0214							
ROW 23									
0.0	-0.2408	-0.3845	-0.2094	-0.0614	-0.0985	-0.2594	-0.0006	-0.2270	
-0.1953	-0.3293	-0.3824	-0.6280	-0.1113	-0.3113	-0.2138	0.1309	0.0649	
0.1035	-0.1564	0.0945	0.1707	1.0000	0.2301	0.4079	0.0902	0.1224	
0.1322	0.0231	-0.0403	-0.2754	0.1551	-0.3567	0.1819	-0.1971	-0.0367	
-0.3198	0.0071	0.0053	-0.3609	0.2093	0.0809	0.0802	0.2459	0.1642	
-0.0005	-0.4119	-0.0325							
ROW 24									
0.0	-0.2213	-0.5602	-0.4615	-0.0867	-0.0904	-0.1210	-0.0191	-0.1775	
-0.3856	-0.5166	-0.3272	-0.2095	-0.0909	-0.1274	-0.2355	0.0725	0.3057	
-0.3129	0.1447	0.4442	0.4677	0.2301	1.0000	0.2139	0.1432	0.2033	
0.3883	0.0934	-0.0438	-0.1404	0.2099	-0.1001	0.0970	-0.2003	-0.0838	
-0.0112	0.0489	-0.0938	-0.4781	0.0500	0.2566	-0.1708	0.0678	0.1004	
0.0153	-0.4694	-0.0567							
ROW 25									
0.0	-0.4449	-0.7745	-0.3573	-0.2154	-0.2612	-0.4806	-0.0316	-0.5361	
-0.4456	-0.0974	-0.5935	-0.2651	-0.0800	-0.5540	-0.2595	0.2268	0.3488	
0.4810	0.3111	0.2305	0.2536	0.4079	0.2139	1.0000	0.3670	0.2898	
0.3708	-0.0556	-0.0725	-0.1970	0.3642	-0.4638	0.5211	-0.3535	-0.0172	
-0.1760	0.0613	-0.0111	-0.5950	0.3762	0.3414	-0.2720	0.0807	0.5134	
0.0261	-0.5668	-0.0115							
ROW 26									
0.0	-0.2706	-0.3300	-0.4140	-0.0958	-0.2599	-0.4394	-0.0273	-0.6649	
-0.2157	-0.1115	-0.3905	-0.2398	-0.0688	-0.5212	-0.2900	0.3578	0.2701	
0.0933	0.1785	0.0766	0.3656	0.0902	0.1432	0.3670	1.0000	0.3726	
0.1280	-0.5489	-0.0473	-0.1917	0.0090	-0.3948	0.2958	-0.1850	0.0203	
-0.1562	0.0564	0.1130	-0.3519	0.2525	0.2180	-0.3613	-0.1070	0.6292	
0.0245	-0.2866	-0.0024							
ROW 27									
0.0	-0.2335	-0.3924	-0.3574	0.0061	-0.2676	-0.5042	-0.2196	-0.3730	
-0.4133	-0.1710	-0.3140	-0.1439	-0.0561	-0.5832	-0.1582	0.0954	0.4686	
0.0668	0.0289	0.3183	0.2015	0.1224	0.2033	0.2898	0.3726	1.0000	
0.2292	-0.5046	0.1705	-0.1189	0.2761	-0.1644	0.2574	-0.0505	-0.0646	
-0.2704	0.0332	-0.0558	-0.4224	0.2507	0.2914	-0.4756	-0.1873	0.4286	
0.2216	-0.2960	-0.0012							
ROW 28									
0.0	-0.0234	-0.6105	-0.4237	-0.1455	0.1249	-0.0770	-0.0157	-0.1936	
-0.4894	-0.2457	-0.3061	-0.2278	-0.0582	-0.0865	-0.2181	0.1398	0.4207	
-0.0130	0.0397	0.3649	0.3413	0.1322	0.3883	0.3708	0.1280	0.2292	
1.0000	0.0783	0.0058	-0.2527	0.4931	-0.0964	-0.0888	-0.5278	-0.5432	
-0.0367	-0.0086	-0.4824	-0.4525	0.2902	0.3209	-0.0808	-0.0178	0.1212	
0.0126	-0.2586	-0.0000							
ROW 29									
0.0	0.1355	-0.0934	-0.0355	-0.0302	0.1944	0.3042	0.0079	0.4838	
-0.0487	-0.1070	-0.0587	-0.0513	0.0117	0.4753	0.0045	-0.0301	-0.0339	
0.0426	0.0352	0.0510	0.1073	0.0231	0.0934	-0.0556	-0.5489	-0.5046	
0.0783	1.0000	-0.0897	-0.0180	0.0658	0.1391	-0.3145	-0.0202	0.0238	
0.0895	0.0156	0.0626	-0.0127	0.0847	0.0661	0.2519	0.0554	-0.4875	
-0.0169	-0.0098	-0.0118							

TABLE XXXV (Continued)

ROW 30									
U.0	-0.0183	0.0847	0.0429	0.0445	-0.0961	-0.0581	-0.0169	-0.0605	
U.0150	0.0306	0.0741	-0.0002	0.0380	-0.0466	0.1140	0.0219	0.0197	
-C.1327	0.0302	-0.0349	-0.0511	-0.0403	-0.0438	-0.0725	-0.0473	0.1705	
-C.0058	-0.0897	1.0000	0.0331	0.0120	0.1246	-0.0094	-0.0016	-0.0193	
-C.0099	0.0442	-0.1538	0.0361	-0.0084	-0.0484	-0.0818	-0.2082	0.0712	
U.0247	0.0586	-0.0207							
ROW 31									
U.0	0.1600	0.3461	0.2821	0.1475	0.0567	0.1344	0.0054	0.2293	
C.3259	0.2142	0.2993	0.4405	0.0242	0.1278	0.1746	-0.1300	-0.2757	
-U.0299	-0.0392	-0.1534	-0.1849	-0.2754	-0.1404	-0.1970	-0.1917	-0.1189	
-C.2527	-0.0180	0.0331	1.0000	-0.2326	0.2383	-0.0593	0.1243	0.0424	
U.0338	-0.0124	0.0546	0.2952	-0.4062	-0.0577	-0.1345	-0.0248	-0.1615	
-U.0030	0.2410	0.0156							
ROW 32									
U.0	-0.2045	-0.4459	-0.3453	-0.1010	-0.1543	-0.1688	-0.0242	-0.2568	
-C.4465	-0.1149	-0.2272	-0.1428	-0.0147	-0.2170	-0.1655	0.2211	0.3920	
U.0610	-0.0002	0.2747	0.2517	0.1551	0.2099	0.3642	0.0090	0.2761	
-C.4931	-0.0658	0.0120	-0.2326	1.0000	-0.2039	0.1003	-0.2964	-0.2924	
-U.0324	-0.0247	-0.3297	-0.4015	0.2066	0.2495	-0.1122	-0.0384	0.2101	
U.0258	-0.2970	-0.0001							
ROW 33									
U.0	0.3141	0.3679	0.2763	0.1482	0.2126	0.3195	0.0274	0.3914	
C.2077	0.1077	0.3841	0.3468	0.0224	0.3342	0.2347	-0.2515	-0.2168	
-U.3007	-0.0395	-0.0823	-0.2600	-0.3567	-0.1001	-0.4638	-0.3948	-0.1644	
-C.0964	0.1391	0.1246	0.2383	-0.2039	1.0000	-0.3681	0.1608	-0.0292	
U.1773	-0.1980	-0.0197	0.3499	-0.2437	-0.1366	0.0775	-0.0938	-0.3624	
-U.0243	0.3637	0.0363							
ROW 34									
U.0	-0.4523	-0.2502	0.0096	-0.1437	-0.2740	-0.5752	-0.0192	-0.6624	
-C.0055	0.0754	-0.1532	-0.0153	-0.0136	-0.6676	-0.1522	-0.0853	0.0500	
U.02867	0.1959	0.0625	-0.0582	0.1819	0.0970	0.5211	0.2958	0.2574	
-U.0888	-0.3145	-0.0094	-0.0593	0.1003	-0.3681	1.0000	0.0176	0.1084	
-0.1113	0.1181	0.0065	-0.1625	-0.1207	-0.1575	-0.2665	0.0596	0.6950	
U.0182	-0.4092	-0.0093							
ROW 35									
U.0	-0.0502	0.3747	0.2024	0.2419	0.0311	0.1116	0.0116	0.2226	
C.2092	0.1635	0.2000	0.1063	0.0433	0.1171	0.1795	-0.1989	-0.1764	
-0.1312	-0.0818	-0.0989	-0.1340	-0.1971	-0.2003	-0.3535	-0.1850	-0.0505	
-0.5278	-0.0202	-0.0016	0.1243	-0.2964	0.1608	0.0176	1.0000	0.3614	
U.1371	0.0644	0.0689	0.2133	-0.1745	-0.1970	0.0057	0.0147	-0.1726	
-C.0088	0.1291	-0.0071							
ROW 36									
U.0	-0.2917	0.1405	0.1020	-0.0424	-0.2435	0.0223	0.0050	0.0722	
U.1003	0.0819	0.0298	0.0723	0.0309	0.0094	0.0806	-0.0229	-0.0781	
U.0347	-0.0222	-0.0587	-0.1048	-0.0367	-0.0838	-0.0172	0.0203	-0.0646	
-0.5432	0.0238	-0.0193	0.0424	-0.2924	-0.0292	0.1084	0.3614	1.0000	
-0.0071	-0.0212	0.2609	0.0622	-0.0386	-0.0651	-0.0163	0.0014	-0.0515	
-U.0041	-0.0373	-0.0145							
ROW 37									
U.0	0.0897	0.1441	0.0482	0.0	0.1514	0.3993	0.0071	0.1132	
C.0252	-0.0012	0.1275	0.1772	0.0174	0.2621	0.1128	-0.0064	-0.0657	
-U.1737	0.0076	-0.0041	-0.0393	-0.3198	-0.0112	-0.1760	-0.1562	-0.2704	
-C.0367	0.0895	-0.0099	0.0338	-0.0324	0.1773	-0.1113	0.1371	-0.0071	
1.0000	-0.0453	0.0461	0.0846	-0.0625	-0.0413	0.1598	-0.0155	-0.2684	
-U.0061	0.0987	0.0016							
ROW 38									
U.0	-0.0555	-0.0410	-0.0249	-0.1822	-0.0394	-0.4555	-0.0140	-0.1923	
-0.0175	0.0117	-0.0293	-0.1156	-0.0279	-0.1602	-0.0429	0.0216	0.0150	
U.0614	0.0491	0.0279	0.0436	0.0071	0.0489	0.0613	0.0564	0.0332	
-0.0088	0.0156	0.0442	-0.0124	-0.0247	-0.1980	0.1181	0.0644	-0.0212	
-0.0453	1.0000	0.0185	-0.0692	-0.0095	0.0542	-0.0788	-0.0035	0.3685	
0.0155	-0.0520	0.0356							
ROW 39									
U.0	0.0560	0.1232	0.0997	0.0755	-0.1529	-0.0082	-0.0332	0.1324	
U.1254	0.0620	0.0342	0.0381	0.0165	-0.0265	0.0773	-0.0269	-0.1103	
-0.0150	0.0027	-0.1276	-0.0897	0.0053	-0.0938	-0.0111	0.1130	-0.0558	
-C.4824	0.0626	-0.1538	0.0546	-0.3297	-0.0192	0.0065	0.0689	0.2609	
U.0461	0.0185	1.0000	0.0917	-0.0204	-0.0420	-0.1410	0.0318	-0.0810	
U.0285	0.0387	0.0167							

TABLE XXXV (Continued)

ROW 40								
0.0	0.4105	0.7901	0.8504	0.2329	0.2757	0.3427	0.0374	0.3761
0.6924	0.4525	0.8019	0.5353	0.0977	0.3987	0.4356	-0.3035	-0.6462
-0.0522	-0.0750	-0.7446	-0.7374	-0.3609	-0.4781	-0.5950	-0.3514	-0.4224
-0.4525	-0.0127	0.0361	0.2952	-0.4015	0.3499	-0.1625	0.2133	0.0622
0.0846	-0.0692	0.0917	1.0000	-0.5958	-0.6051	0.1333	-0.0704	-0.3045
-0.0293	0.6781	0.0346						
ROW 41								
0.0	-0.1869	-0.4900	-0.4481	-0.1657	-0.1358	-0.1942	-0.0209	-0.2395
-0.6452	-0.3969	-0.6989	-0.5956	-0.0835	-0.2021	-0.3338	0.3520	0.3787
0.1434	0.1138	0.2032	0.2876	0.2093	0.0500	0.3762	0.2525	0.2507
0.2902	0.0847	-0.0084	-0.4062	0.2066	-0.2437	-0.1207	-0.1745	-0.0386
-0.0625	-0.0095	-0.0204	-0.5958	1.0000	0.5301	0.1075	0.0276	0.1773
0.0172	-0.2614	0.0046						
ROW 42								
0.0	-0.0114	-0.4900	-0.5829	-0.1400	-0.0849	-0.0836	-0.0183	-0.0826
-0.5823	-0.3867	-0.4848	-0.1728	-0.1170	-0.0669	-0.2811	0.4426	0.4981
0.1371	0.1110	0.3713	0.4732	0.0809	0.2566	0.3414	0.2180	0.2914
0.3209	0.0661	-0.0484	-0.0577	0.2495	-0.1366	-0.1575	-0.1970	-0.0651
-0.0413	0.0542	-0.0420	-0.6051	0.5301	1.0000	-0.4042	0.0114	0.0784
0.0177	-0.0952	0.0177						
ROW 43								
0.0	-0.0297	0.1973	0.1768	-0.0620	0.0816	0.2606	0.1232	0.1569
0.0440	-0.1673	-0.1060	-0.1944	-0.0453	0.1912	-0.0895	-0.2372	-0.2550
-0.1359	-0.1565	-0.0784	-0.1525	0.0802	-0.1708	-0.2720	-0.3613	-0.4756
-0.0808	0.2519	-0.0818	-0.1345	-0.1122	-0.0775	-0.2665	0.0057	-0.0163
0.1598	-0.0788	-0.1410	0.1333	0.1075	-0.4042	1.0000	0.1740	-0.2661
-0.1254	-0.0418	-0.0278						
ROW 44								
0.0	-0.0396	-0.0554	-0.0144	-0.0208	0.0201	0.1444	0.7040	0.0485
-0.0370	-0.1266	-0.0759	-0.1117	-0.0445	-0.1342	-0.0114	0.0051	0.0188
-0.0085	-0.0643	0.0346	-0.0013	0.2459	0.0678	0.0807	-0.1070	-0.1873
-0.0178	0.0554	-0.2082	-0.0248	-0.0384	-0.0938	0.0596	0.0147	0.0014
-0.0155	-0.0035	0.0318	-0.0704	0.0276	0.0114	0.1740	1.0000	-0.0256
-0.7059	0.0402	-0.0092						
ROW 45								
0.0	-0.4085	-0.3665	-0.1957	-0.2374	-0.3111	-0.8424	-0.0085	-0.9271
-0.2023	-0.0772	-0.3709	-0.1685	-0.1048	-0.7900	-0.3661	0.0941	0.1879
0.2758	0.2024	0.1210	0.1010	0.1642	0.1004	0.5134	0.6292	0.4286
0.1212	-0.4875	0.0712	-0.1615	0.2101	-0.3624	0.6950	-0.1726	-0.0515
-0.2684	0.3685	-0.0810	-0.3045	0.1773	0.0784	-0.2661	-0.0256	1.0000
0.0096	-0.3863	0.0021						
ROW 46								
0.0	-0.0654	-0.0330	-0.0241	-0.0085	-0.0157	-0.3473	-0.9995	-0.0456
-0.0327	-0.0104	-0.0221	-0.0100	-0.0035	-0.0227	-0.0184	0.0029	0.0247
0.0020	-0.0062	0.0191	0.0177	-0.0005	0.0153	0.0261	0.0245	0.2216
0.0126	-0.0169	0.0247	-0.0030	0.0258	-0.0243	0.0182	-0.0088	-0.0041
-0.0061	0.0155	0.0285	-0.0293	0.0172	0.0177	-0.1254	-0.7059	0.0096
1.0000	-0.2731	-0.0040						
ROW 47								
0.0	0.7114	0.6703	0.5467	0.1879	0.3772	0.5199	0.2853	0.4934
0.5510	0.4320	0.6923	0.4323	0.1408	0.5085	0.4147	-0.0216	-0.2587
0.0005	-0.0484	-0.5197	-0.5277	-0.4119	-0.4694	-0.5668	-0.2868	-0.2960
-0.2586	-0.0098	0.0586	0.2410	-0.2970	0.3637	-0.4092	0.1291	-0.0373
0.0987	-0.0520	0.0387	0.6781	-0.2614	-0.0952	-0.0418	0.0402	-0.3863
-0.2731	1.0000	0.0626						
ROW 48								
0.0	0.1445	0.0091	0.0262	-0.0588	-0.0497	-0.0050	0.0038	0.0134
0.0223	0.0674	0.0305	0.0502	0.0049	0.0300	0.0334	-0.0287	0.0013
0.0248	0.0104	-0.0179	-0.0214	-0.0325	-0.0587	-0.0115	-0.0024	-0.0012
-0.0000	-0.0118	-0.0207	0.0156	-0.0001	0.0363	-0.0093	-0.0071	-0.0145
0.0016	0.0356	0.0167	0.0346	0.0046	0.0177	-0.0278	-0.0092	0.0021
-0.0040	0.0626	1.0000						
SQUARE ROOTS OF THE DIAGONAL TERMS OF THE NORMAL EQUATIONS.								
1.0000	0.0123	0.6464	0.6037	0.6739	3.8803	5.1991	4.4512	6.3589
0.4129	0.1328	0.8878	0.1378	1.8013	0.6782	0.2613	0.6186	0.8386
0.2363	0.1870	0.7826	1.0663	0.2054	0.2666	0.8939	1.4605	1.4188
1.0127	4.4861	1.7718	0.3157	0.9935	0.4692	1.7909	0.7766	0.9801
0.3346	0.3306	2.8459	1.1390	1.0190	0.7551	1.8941	2.4850	9.7478
8.3900	0.3244							

APPENDIX III

NORMAL COORDINATE ANALYSIS OF METHANOL AND ETHANOL

INTRODUCTION

As discussed in Chapter I, a number of previous carbohydrate normal coordinate calculations have employed hydroxyl bending constants with values which do not seem appropriate to the hydrogen bonded hydroxyl groups in solid carbohydrates. Since most atoms in monosaccharides are no more than twice removed from hydroxyl oxygens, good estimates for the constants associated with the hydroxyl group would seem critical to construction of a carbohydrate force field. We were unsatisfied with the initial estimates of these values available to us, and thus interrupted our study of the hexose sugars to study the two simplest alcohols in hopes of developing a better set of initial estimates for the hexose force field.

There is a substantial consensus of agreement concerning vibrational assignments for methanol, although a few minor points remain unresolved (42-44,90-92). The next member of the series, ethanol, still provokes substantial disagreement on assignments despite the availability of rather extensive experimental data (50,93). The data for the higher aliphatic alcohols are less extensive, and thus the assignments are more vague (41).

The existing consensus for methanol was reached only as a result of multiple normal coordinate calculations, and these studies indicated that even for so simple a system assignments could not be made reliably without calculations. This indicates the desirability of calculations to clarify the ethanol assignments. We have also restudied methanol, despite the many earlier reports, but as a test of the software and to make use of the matrix isolation data recently published by Barnes and Hallam (92). These authors (92) have also raised some minor

assignment questions based on differences between gas and matrix data, and the calculations provide a chance to clarify these.

DATA

Extensive spectral data for assorted isotopic variations of methanol and ethanol in all states have been published. Our primary sources are listed below:

Methanol:

Gas — Margottin-Maclou (42)

Matrix isolated — Barnes and Hallam (B&H) (92)

Liquid — Falk and Whalley (90)

Ethanol:

Gas — Perchard and Josien (P&J) (50)

Matrix isolated — Barnes and Hallam (93)

Liquid — Perchard and Josien (50)

Falk and Whalley (90), and more recently Timedi and Zerbi (43), have summarized the rather extensive methanol literature. P&J (50) have likewise summarized the work on ethanol, but their work is much more comprehensive than any of its predecessors. Several other minor sources of recent origin were utilized to fill some gaps in the data (1,57,94).

COMPUTATIONS

SOFTWARE

The software package has been described in the first chapter of this thesis.

GEOMETRIC MODEL

Our geometric model for these alcohols was rather idealized in light of the intended force field transfer to carbohydrates. The only directly determined value employed was the 1.428 Å C-O bond length determined by electron diffraction (95). For all other structural parameters, we have used the same set of averaged values used in our carbohydrate calculations. These values, summarized in Table XXXVI, were primarily derived from the neutron diffraction work of Brown and Levy (10,33) for glucose and sucrose. Although derived primarily from another class of compounds, this model is probably as satisfactory as any we might have chosen, since the values in Table XXXVI can be accommodated within the uncertainty of the available structural data for methanol and ethanol (96-99). A plane of symmetry was assumed for each molecule. This is fairly obvious for methanol but must be justified for ethanol, and this will be discussed in a later section. In this point group, C_s , a set of redundant symmetry coordinates may be obtained by inspection, using simple combinations of the internal coordinates which are symmetric or antisymmetric with respect to the symmetry plane. By a slightly more complex transformation, each redundancy may be isolated in a single symmetry coordinate and then dropped from the calculations. The methanol redundancy was isolated and eliminated in this way, using the symmetry coordinates first published by Margottin-Maclou (42). For ethanol, the redundant symmetry coordinates were used throughout the calculations. The details of the geometric model, the internal coordinates, and the symmetry coordinates are given in Appendix IV.

TABLE XXXVI
STRUCTURAL PARAMETERS FOR ALCOHOLS

Bond Lengths

C-H	1.110 A
O-H	0.986 A
C-C	1.540 A
C-O	1.428 A methanol
	1.420 A ethanol

Bond Angles

HCH angle — methylene group — 108°

All other unspecified angles — tetrahedral

Assumed point group: C_s

POTENTIAL ENERGY MODEL

Our potential energy model is an extension of the well known quadratic valence force field approximation (100). This model, sometimes known as a modified valence force field (101), adds selected off-diagonal interaction terms to the diagonal terms of the valence field. We have used this study of the alcohols to provide guidelines for inclusion of off-diagonal terms in the carbohydrate calculations. While the number of interaction constants needed to produce a good fit to the experimental frequencies is a function of the system being investigated, some general guidelines emerge from the results of past studies. Many authors have found that in aliphatic systems, interaction terms between stretching coordinates sharing a common atom and between stretch-bend or bend-bend coordinate pairs with two common atoms are sufficient to give a good frequency fit. A smaller number of studies have considered interactions where a stretching coordinate shares only the central atom of a bending coordinate,

and a few have dealt with more distant interactions. We have investigated only the first four types mentioned.

Since not all members of these general classes of constants may be necessary to reproduce the frequencies, and since it is desirable to reduce the number of force constants to a minimum for statistical reasons, some screening procedure must be used. The most commonly used screening procedure is to perform a regression analysis to evaluate whether the decrease in average error associated with each additional off-diagonal constant justifies the associated decrease in degrees of freedom. Such an analysis is available within Schachtschneider's (32) LLS refinement program and was our first approach. Unfortunately, it failed, since the force field proved to be highly correlated. In practice, constants were accepted into the refinement roughly in the order of their correlation matrix elements with diagonal or previously included off-diagonal constants. This in turn increased the singularity of the $\underline{JZ}$ matrix and thus destabilized the LLS refinement.

After a number of such trial refinements, it became apparent that several classes of interaction constants were unstable on linear refinement due to very high correlations with diagonals. These correlations are summarized in Table XXXVII. The correlations in the first two groups are probably a reflection of the distribution of experimental frequencies, while those in the third are due most likely to the coordinate redundancies. All interaction constants of these three types were fixed at zero and excluded from further refinements. They were also excluded in the construction of the initial carbohydrate field described in Chapter I.

Initial values for the remaining constants in the methanol refinement were taken from the work of Timedi and Zerbi (43). For ethanol, the refined

TABLE XXXVII

CONSTANTS EXCLUDED FROM REFINEMENT DUE TO CORRELATION

Interacting Coordinates		Correlation Matrix Elements ^a
Class X-X, X-H		
15	C-O, O-H	1(.98), 27(.98)
16	C-O, C-H	23(.88), 4(.65)
17	C-C, C-H	5(.87)
Class H-X-X, X-X		
27	H-O-C, H-O	1(.98), 15(.98)
28	H-C-C, H-C	2(.84), 18(.83)
29	H-C-O, H-C	2(.95), 18(.95)
30	H-C-H, H-C	40(.73)
Class X-Y, H-Y-Z		
48	O-C, HCC	22(.86), 25(.76), 49(.79)
49	C-C, HCO	22(.65), 25(.87), 48(.79)

^aThese matrix elements (for ethanol) are represented as follows:

1(.98) means that the constant listed has a matrix element of 0.98 with constant No. 1.

methanol values were augmented by the results of Snyder and Schachtschneider (45) for aliphatic hydrocarbons, of Snyder and Zerbi (46) for aliphatic ethers, and of Wieser, et al. (49) for diethyl ether. The initial fields for the liquid refinements were constructed by changing the hydroxyl stretching and bending constants in the refined gas or matrix field to the values found by Dempster and Zerbi (44) for solid methanol. The description of the force constants employed and their initial values may be found in Table XLI (p. 309).

REFINEMENT STRATEGY

As mentioned above, correlation within the force field is a serious destabilizing influence in LLS refinement. Some of these problems can be eliminated by arbitrarily setting off-diagonals to zero, but correlations between diagonal elements are more troublesome. For small, acyclic, symmetric molecules, the redundancies can be isolated and eliminated in the transformation to symmetry coordinates if the latter are properly chosen. When this is done, examination of the factored $\underline{Z}$ matrix will yield a series of linear relations between the force constants known as the redundancy conditions. These relations have an excess of unknowns over equations and thus no unique solution. If, however, a sufficient number of the constants are arbitrarily fixed so that the solution does become unique, successful LLS refinement is generally possible. The redundancy conditions then provide a relation between the refined yield and all other force fields giving the same eigenvalues. This approach was used for methanol, fixing constant number 34 at zero during the refinement.

For larger symmetric molecules, the redundancy conditions are more complex, and correlations due to sources other than coordinate redundancy are likely to be more severe. If symmetry is lacking, the conditions are even more complex and depend on the values of the force constants. They thus change on each refinement cycle and cannot be incorporated as an invariant constraint upon the refinement process. Some attempts have been made to develop general expressions for the redundancy conditions in such cases, but these efforts have not advanced to the point where they can provide practical assistance in fixing constants (102). When it is no longer practical to specify what constants to refine in terms of redundancy conditions, the process becomes one of trial and error, using the correlation matrix to identify constants whose removal seems likely to decrease the $\underline{JZ}$ singularity.

At this point, the nonlinear FPM refinement procedure becomes an attractive alternative, since it does not employ the inverse JZ matrix and thus does not require the fixing of constants. The slower convergence rate of the FPM is more than offset by the elimination of the need for multiple trial refinements. Our experience indicates that the FPM has less tendency to oscillate wildly when refining correlated fields, and, when the redundancy conditions are known, the FPM solutions have been found to be equivalent to the LLS solutions. This approach was used for ethanol.

ASSIGNMENTS

As in the carbohydrate calculations, our assignments were based primarily on the correspondence of the initial calculations and the experimental spectra, with consideration given to the reasonableness of the potential energy distributions. The assumed plane of symmetry provides a valuable additional constraint on the acceptability of assignments by defining the band properties expected for the two symmetry classes. Modes belonging to the A' representation (symmetric with respect to the plane) give partially polarized Raman bands while those in the A'' (antisymmetric to plane) give polarized bands. Since the only hydroxyl internal coordinate which can contribute to an A'' normal coordinate is the torsion, A'' modes above about 500 cm^{-1} will be insensitive to isotopic substitution at the hydroxyl group or changes in association at that site. In many cases, the combination of depolarization ratio and insensitivity to phase change or hydroxyl deuteration allows identification of the A'' modes by simple inspection of the experimental data. Conversely, the presence of such bands in the proper numbers can be taken as evidence of a plane of symmetry. We have not attempted to use band shape information to assist in the assignments, since the original spectra were not available to us.

The suggestion of Fermi resonance in the C-H stretching region is even stronger for these alcohols than was true in the carbohydrate case, so only a few assignments were made here and they should be regarded with caution. There is likewise some doubt about the fundamental frequencies of the hydroxyl stretch and the various torsions, and caution is merited with respect to these assignments as well. Fortunately, all of these regions are rather isolated, and uncertainties within them will have little impact on our primary objective, the assignment of the 1500-300 cm^{-1} region.

REFINEMENT

Force field refinement for methanol was begun using the Barnes and Hallam (92) matrix data and assignments and the Timidi and Zerbi force field (43). After four cycles of undamped LLS refinement, all corrections to the force constants were less than 0.002, and the refinement was terminated at an overall average error of 3.2 cm^{-1} . Table XXXVIII shows some statistics of the fit in comparison to earlier modified valence force field studies. These suggest that the use of Barnes and Hallam matrix data and assignments has allowed an improvement over the solutions proposed previously. In the 1500-300 cm^{-1} region we have improved on Margottin-Maclou's (42) frequency fit while using only one more parameter than Timidi and Zerbi (43). At this point, the Dempster and Zerbi (44) condensed phase hydroxyl constants were substituted in the refined matrix field, and the resulting field was refined with the liquid methanol experimental data. After eight cycles of undamped LLS, all corrections were less than 0.0004 and the average error for the assigned frequencies was 2.7 cm^{-1} . Statistics of the fit are given in Table XXXIX and shown graphically in Fig. 53-62.

TABLE XXXVIII

COMPARISON OF METHANOL CALCULATIONS

Errors for Assigned Bands Below 1500 cm^{-1} Except Torsion

	This Study, cm^{-1}	Margottin-Maclou, cm^{-1}	Timidi and Zerbi, cm^{-1}
Average Errors			
CH_3OH	3.0	5.1	7.0
CH_3OD	3.5	5.9	8.0
CD_3OH	6.9	3.8	8.5
CD_3OD	5.4	5.3	14.7
Overall	4.6	5.1	9.4
Error Distributions			
cm^{-1}			
0- 5.9	19	15	5
6.0-10.9	7	9	7
11.0-20.9	1	3	9
21.0-30.9	0	0	0
>30.9	0	0	1
Parameters	14	21	13

TABLE XXXIX
SUMMARY OF METHANOL RESULTS

Matrix Data	Error, cm^{-1}	Number of Frequencies
CH_3OH	2.33	9
$\text{C}^{13}\text{H}_3\text{OH}$	1.87	8
CH_3OD	3.49	7
$\text{CH}_3\text{O}^{18}\text{D}$	4.76	6
CD_3OH	4.66	9
CD_3OD	<u>4.36</u>	<u>9</u>
Average = 3.2		Total = 48
Gas Data		
CH_3OH	3.75	9
CH_3OD	3.50	7
CD_3OH	4.20	7
CD_3OD	<u>5.32</u>	<u>8</u>
Average = 4.2		Total = 31
Liquid Data		
CH_3OH	3.63	7
CH_3OD	1.78	7
CD_3OH	2.16	5
CD_3OD	<u>3.07</u>	<u>6</u>
Average = 2.7		Total = 25

CH3OH (MATRIX)

CALCULATED

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM.-1)

Figure 53. Assigned and Calculated Frequencies for Matrix Isolated Methanol, CH₃OH

C(13)H3OH (MATRIX)

CALCULATED

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM. -1)

Figure 54. Assigned and Calculated Frequencies for Matrix Isolated Methanol, C¹³H₃OH

CH3OD (MATRIX)

CALCULATED

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM.⁻¹)

Figure 55. Assigned and Calculated Frequencies for Matrix Isolated Methanol, CH₃OD

CH3O(18)D (MATRIX)

CALCULATED

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM.-1)

Figure 56. Assigned and Calculated Frequencies for Matrix Isolated Methanol, CH₃O¹⁸D

CD3OH (MATRIX)

CALCULATED

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM.-1)

Figure 57. Assigned and Calculated Frequencies for Matrix Isolated Methanol, CD₃OH

CD30D (MATRIX)

CALCULATED

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM.⁻¹)

Figure 58. Assigned and Calculated Frequencies for Matrix Isolated Methanol, CD₃OD

CH3OH LIQUID

CALCULATED

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM.⁻¹)

Figure 59. Assigned and Calculated Frequencies for Liquid Methanol, CH₃OH

CH3OD LIQUID

CALCULATED

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM.⁻¹)

Figure 60. Assigned and Calculated Frequencies for Liquid Methanol, CH₃OD

CD3OH LIQUID

CALCULATED

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM.-1)

Figure 61. Assigned and Calculated Frequencies for Liquid Methanol, CD₃OH

CD3OD LIQUID

CALCULATED

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM.-1)

Figure 62. Assigned and Calculated Frequencies for Liquid Methanol, CD₃OD

Initial calculations for gaseous ethanol with a composite of the refined methanol matrix field and the Snyder and Zerbi (46) ether field produced a recognizable spectral pattern, but some of the A' assignments were ambiguous. After trial refinements with a number of force field variations, the initial field shown in Table XL was formulated. This field was refined by the FPM for 34 cycles, with reconsideration of assignments after 21 cycles. The refinement was terminated when the ratio of sums of squared errors had been greater than 0.995 on six cycles. The average error at this point was 7.9 cm^{-1} . A liquid field was formulated by the same procedure used for methanol and gave good initial agreement. This agreement was improved to 6.7 cm^{-1} in 15 cycles of FPM refinement, using the same convergence criteria. The statistics of fit are given in Table XLI, and the agreement is shown graphically in Fig. 63-86.

Potential energy distributions, displacement coordinates, and normal mode drawings were prepared in the same manner as for glucose, and they were placed on magnetic tape for permanent retention. The potential energy distributions are summarized in Appendix V. The same calculations were subsequently performed for the gauche conformations of both the gas and liquid using the fields refined for the trans (C_s) forms.

RESULTS AND DISCUSSION

THE REFINED FORCE FIELDS

Table XL compares the refined force fields to earlier fields developed for methanol and the aliphatic ethers. Since the force constant correlation and the differing geometric and assignment assumptions are reflected in the final values, precise comparison is difficult. Two major conclusions which are important to the question of transferability can be drawn from the general trends. First, there is no discontinuity in the overlapping constants between the alcohol

and ether fields, justifying to some extent the use of composite fields from both sources in the study of higher alcohols and polyols. Second, the influence of hydrogen bonding is limited primarily to the diagonal constants for the hydroxyl group. Since there is good reason to assume that a simple function form can approximate the relationship between these constants and the strengths of the hydrogen bonds (103), it may be possible to treat systems with varying hydrogen bond strengths using a tractable number of force constants and some constraint functions.

TABLE XL
SUMMARY OF ETHANOL RESULTS

	Gas		Liquid	
	Error, cm ⁻¹	Frequencies	Error, cm ⁻¹	Frequencies
CH ₃ CH ₂ OH	7.53	16	5.97	13
CH ₃ CH ₂ OD	8.43	13	5.32	12
CH ₃ CD ₂ OH	5.33	15	7.21	12
CH ₃ CD ₂ OD	8.36	13	6.11	12
CD ₃ CH ₂ OH	7.63	12	6.43	10
CD ₃ CH ₂ OD	7.83	10	6.63	13
CD ₃ CD ₂ OH	8.13	11	10.07	11
CD ₃ CD ₂ OD	11.16	12	6.66	10
CH ₃ CHDOH	5.27	13	6.06	13
CH ₃ CHDOD	8.20	12	5.63	14
CD ₃ CHDOH	13.25	10	7.29	13
CD ₃ CHDOD	<u>7.06</u>	<u>9</u>	<u>7.33</u>	<u>13</u>
Av. = 7.98	sum = 146		Av. = 6.69	sum = 146

TABLE XLI
SUMMARY OF ALCOHOL FORCE CONSTANTS^a

Description ^b	Code ^c	Methanol					Ethanol		Ethers	
		Matrix ^d	Gas ^e	Gas ^g	Liq. ^d	X-tal ^g	Gas ^d	Liq. ^d	Ether ^h	Ether ⁱ
Bond Stretching										
1. OH	O-H	7.50	7.63	7.53	6.22	5.80	7.54	6.22	-	-
2. CH	C-H	4.68	4.75	4.82 ^j	4.68	4.67	4.65	4.63	4.66	4.65
3. Dummy	C6-H	-	-	-	-	-	-	-	-	-
4. CO	C-O	5.18	5.22	5.26	5.14	4.88	5.15	5.16	5.09	5.04
5. CC	C-C	-	-	-	-	-	4.40	4.44	4.26	4.18
Bond Angle Bending										
6. COH	COH	0.80	0.76	0.76	0.96	0.98	0.77	0.95	-	-
7. OCH	OCH	0.90	0.85	0.91 ^j	0.91	0.87	0.89	0.91	0.90	0.86
8. HCH 1°	HC6H	0.53	0.53	0.55 ^j	0.57	0.53	0.49	0.49	0.54	0.54
9. HCH 2°	HC3H	-	-	-	-	-	0.56	0.57	0.47	0.52
10. CCO	CCO	-	-	-	-	-	1.26	1.33	1.18	1.22
11. CCH 1°	CC6H	-	-	-	-	-	0.62	0.62	0.65	0.65
12. CCH 2°	CC3H	-	-	-	-	-	0.63	0.62	0.75	0.70
Torsions										
13. C-O	TC-O	0.02	0.01	0.03	0.02	0.01	0.02	0.02	0.03	0.04
14. C-C	TC-C	-	-	-	-	-	0.10	0.10	0.02	0.01
Stretch - Stretch Interaction										
18. H-C-H	SS18	-0.01	0.01	-0.01	-0.01	0.01	0.02	0.02	-0.05	0.04
19. Dummy	SS19	-	-	-	-	-	-	-	-	-
20. C-C-O	SS20	-	-	-	-	-	0.13	0.24	0.10	0.10
Stretch - Bend Interaction										
21. CO, COH	SB21	0.25	0.25	0.38	0.35	0.27	0.41	0.43	-	-
22. CO, OCH	SB22	0.47	0.44	0.46	0.47	0.43	0.49	0.47	0.39	0.30
23. CO, CCO	SB23	-	-	-	-	-	0.62	0.59	0.62	0.61
24. CO, CCH 1°	SB24	-	-	-	-	-	0.24	0.25	0.33	0.31
25. CO, CCH 2°	SB25	-	-	-	-	-	0.32	0.34	0.48	0.48
26. CO, CCO	SB26	-	-	-	-	-	0.37	0.33	0.40	0.05
Bend - Bend Interaction										
31. H-O-C-H (g)	BB31	0.0	-0.01	-0.01	0.02	0.03	0.05	0.03	-	-
32. H-O-C-H (t)	BB32	0.10	0.09	0.09	0.08	0.10	0.10	0.10	-	-
33. H-(C-O)-H	BB33	-0.04	-0.03	0.09	0.03	0.03	0.08	0.08	-0.01	-0.01
34. H-(C-H)-H	BB34	0.0	0.0	0.0	0.0	0.0	-0.03	-0.03	0.0	0.0
35. H-(C-C)-H	BB35	-	-	-	-	-	-0.04	-0.05	0.10	0.10
36. H-C-C-H (g)	BB36	-	-	-	-	-	0.01	0.01	0.0	0.0
37. H-C-C-H (t)	BB37	-	-	-	-	-	0.06	0.06	0.12	0.14
38. O-(C-H)-H	BB38	-0.01	0.0	0.07	0.04	0.0	0.03	0.04	0.0	0.0
39. O-(C-H)-C	BB39	-	-	-	-	-	0.0	-0.01	0.01	0.01
40. C-(C-H)-H	BB40	-	-	-	-	-	-0.05	-0.06	0.0	0.0
43. O-(C-C)-H	BB43	-	-	-	-	-	0.01	-0.03	-0.03	-0.03
44. O-C-C-H (g)	BB44	-	-	-	-	-	-0.12	-0.17	-0.11	-0.11
45. O-C-C-H (t)	BB45	-	-	-	-	-	0.07	0.07	0.03	0.0
46. C-(C-O)-H	BB46	-	-	-	-	-	0.04	0.07	-0.03	-0.03
47. C-C-O-H (t)	BB47	-	-	-	-	-	-0.01	-0.03	-	-

TABLE XLI (Continued)

^aThis is a partial listing of a 49 parameter field. Several groups of constants which were not refined may be found in Table XXXVII.

^bConventions for descriptions are as in Table XI.

^cForce constant code used in potential energy distributions.

^dValues from this work.

^eFrom Reference 43.

^f(gas) From Reference 42.

^g(xtal) From Reference 44.

^hFrom Reference 46.

ⁱFrom Reference 49.

^jAverage value. The constant was subdivided into several parameters.

^kUnits for the force constants are given in Table XI.

CH₃CH₂OH (TRANS GAS)

CALCULATED

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM.⁻¹)

Figure 63. Assigned and Calculated Frequencies for Gaseous Ethanol, CH₃CH₂OH

CH₃CH₂OD (TRANS GAS)

CALCULATED

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM. -1)

Figure 64. Assigned and Calculated Frequencies for Gaseous Ethanol, CH₃CH₂OD

CH₃CD₂OH (TRANS GAS)

CALCULATED

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM.-1)

Figure 65. Assigned and Calculated Frequencies for Gaseous Ethanol, CH₃CD₂OH

CH₃CD₂OD (TRANS GAS)

CALCULATED

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM.-1)

Figure 66. Assigned and Calculated Frequencies for Gaseous Ethanol, CH₃CD₂OD

CD3CH2OH (TRANS GAS)

CALCULATED

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM.-1)

Figure 67. Assigned and Calculated Frequencies for Gaseous Ethanol, CD₃CH₂OH

CD3CH2OD (TRANS GAS)

CALCULATED

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM.⁻¹)

Figure 68. Assigned and Calculated Frequencies for Gaseous Ethanol, CD₃CH₂OD

CD3CD2OH (TRANS GAS)

CALCULATED

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM.-1)

Figure 69. Assigned and Calculated Frequencies for Gaseous Ethanol, CD₃CD₂OH

CD3CD2OD (TRANS GAS)

CALCULATED

OBSERVED

Figure 70. Assigned and Calculated Frequencies for Gaseous Ethanol, CD₃CD₂OD

CH₃CHDOH (TRANS GAS)

CALCULATED

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM.-1)

Figure 71. Assigned and Calculated Frequencies for Gaseous Ethanol, CH₃CHDOH

CH3CHD00 (TRANS GAS)

CALCULATED

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM.-1)

Figure 72. Assigned and Calculated Frequencies for Gaseous Ethanol, CH₃CHDOD

CD₃CHDOH (TRANS GAS)

CALCULATED

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM. -1)

Figure 73. Assigned and Calculated Frequencies for Gaseous Ethanol, CD₃CHDOH

CD₃CHDOD (TRANS GAS)

CALCULATED

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM.-1)

Figure 74. Assigned and Calculated Frequencies for Gaseous Ethanol, CD₃CHDOD

CH₃CH₂OH (TRANS LIQUID)

CALCULATED

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM.⁻¹)

Figure 75. Assigned and Calculated Frequencies for Liquid Ethanol, CH₃CH₂OH

CH3CH2OD (TRANS LIQUID)

CALCULATED

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM. -1)

Figure 76. Assigned and Calculated Frequencies for Liquid Ethanol, CH₃CH₂OD

CH₃CD₂OH (TRANS LIQUID)

CALCULATED

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM.⁻¹)

Figure 77. Assigned and Calculated Frequencies for Liquid Ethanol, CH₃CD₂OH

CH3CD2OD (TRANS LIQUID)

CALCULATED

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM.⁻¹)

Figure 78. Assigned and Calculated Frequencies for Liquid Ethanol, CH₃CD₂OD

CD₃CH₂OH (TRANS LIQUID)

CALCULATED

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM.⁻¹)

Figure 79. Assigned and Calculated Frequencies for Liquid Ethanol, CD₃CH₂OH

CD3CH2OD (TRANS LIQUID)

CALCULATED

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM.-1)

Figure 80. Assigned and Calculated Frequencies for Liquid Ethanol, CD₃CH₂OD

CD3CD2OH (TRANS LIQUID)

CALCULATED

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM.-1)

Figure 81. Assigned and Calculated Frequencies for Liquid Ethanol, CD₃CD₂OH

CD3CD2OD (TRANS LIQUID)

CALCULATED

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM.-1)

Figure 82. Assigned and Calculated Frequencies for Liquid Ethanol, CD₃CD₂OD

CH₃CHDOH (TRANS LIQUID)

CALCULATED

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM.⁻¹)

Figure 83. Assigned and Calculated Frequencies for Liquid Ethanol, CH₃CHDOH

CH3CHD00 (TRANS LIQUID)

CALCULATED

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM.-1)

Figure 84. Assigned and Calculated Frequencies for Liquid Ethanol, CH3CHDOD

CD₃CHDOH (TRANS LIQUID)

CALCULATED

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM. -1)

Figure 85. Assigned and Calculated Frequencies for Liquid Ethanol, CD₃CHDOH

CD3CHD00 (TRANS LIQUID)

CALCULATED

OBSERVED

VIBRATIONAL ENERGY LEVEL (CM.-1)

Figure 86. Assigned and Calculated Frequencies for Liquid Ethanol, CD₃CHDOD

FINAL ASSIGNMENTS AND NORMAL MODES

Methanol

Since our results for methanol in the vapor and matrix isolated states differ only slightly from previous reports, we will only summarize the points of divergence. The B&H (92) assignment of the symmetric methyl deformation at 1451 cm^{-1} can be supported by normal coordinate calculations as well as or better than the more widely reported 1425 cm^{-1} value can (42,43). In addition to the absence of the 1425 cm^{-1} band in the matrix spectra, the assignment is supported by the observed isotope data. In the matrix spectrum of methanol- C^{13} , only the 1451 cm^{-1} band of the higher frequency deformations is found to have been shifted measurably from the values for ordinary methanol. A shift of the proper magnitude is calculated only for the symmetric methyl deformation.

A few assignments remain clouded by the fact that B&H (92) observed the CD_3OH and CD_3OD spectra only as a mixture and by the fact that the $10\text{ }\mu\text{m}$ region in the gas spectra of these compounds is poorly resolved. Timidi and Zerbi's (43) assignment of the A'' methyl twisting mode to 1031 cm^{-1} in CD_3OH and to 1083 cm^{-1} in CD_3OD does not seem defensible in light of the previously discussed coupling restrictions. Our calculations favor the 1055 cm^{-1} band for this mode rather than the 1068 cm^{-1} chosen by B&H (92), but with such a small difference the issue can only be settled by better data. For these same isotopic species, we agree with the earlier calculations (42,43) in favoring 895 cm^{-1} over B&H's 865 cm^{-1} for the A'' methyl rocking mode.

Dempster and Zerbi's (44) calculations for crystalline CH_3OH and CH_3OD are in complete agreement with our liquid calculations and provide greater insight by considering intermolecular effects. No calculations have appeared for CD_3OH and CD_3OD in condensed phases, and the precalculation assignments

have been summarized by Falk and Whalley (90). We differ with these authors primarily with respect to the A'' deformation assignments, placing them at 1060 and 895 cm^{-1} by analogy to the gas and matrix results.

Ethanol

The ethanol assignment problem is somewhat more difficult, since the increased number of atoms aggravates band overlap in all phases, and since there are no prior ethanol calculations suitable as starting points. In such a situation, we cannot expect that the assignments will be as reliable as for methanol, and some assignments must remain unsettled. Still, the good overall agreement between our calculations and the substantial mass of isotopic data reported by P&J (50) suggests that our assignments are largely valid.

The most satisfactory situation exists for ordinary ethanol and ethanol-O-d, since these have been studied by B&H (93) in argon matrices. We generally favor the assignments of B&H over those of P&J with a few minor exceptions. We do not support B&H's proposal that the methylene wagging and methyl symmetric deformation exchange positions upon deuteration of the hydroxyl group. Some movement of the wagging mode is expected since it is calculated to be coupled with the hydroxyl deformation, but a 30 cm^{-1} shift in the methyl mode is rather extreme considering its distance from the point of exchange. B&H based their assignment on apparent changes in relative intensities of these bands on deuteration. Our interpretation of the spectra suggests that the relative intensities of the 1370 cm^{-1} band and the three highest frequency deformations are more or less constant. The major change is the shift and extreme sharpening of the wagging mode upon removal of the hydroxyl contribution.

The key difference between the B&H and P&J assignments is the location of several of the A'' deformations. We regard B&H's value of 1250 cm^{-1} for the

methylene twist as low, in view of the Raman liquid frequency of 1280 cm^{-1} . Perhaps the weak band at 1250 cm^{-1} is associated with the hydroxyl deformation, and the methylene twist has near vanishing infrared intensity. The A'' methyl rocking mode at 1055 cm^{-1} is more obvious in light of the depolarization ratios of the various bands in the region, if one accepts the C_s symmetry.

For the other isotopic species of ethanol our calculations generally agree with P&J's assignments for the internal modes above 1200 cm^{-1} and below 800 cm^{-1} . Between these two limits, many of the modes are highly coupled combinations of heavy atom stretching with proton and deuteron deformations and thus do not correspond very well with P&J's group frequency assignments. We would hesitate, however, to suggest that our calculations provide a final assignment for this region or even that they are in all cases superior to P&J's assignments. The region is difficult to assign due to the close spacing of bands and the resulting overlap problems, particularly in the vapor. We would therefore suggest that the assignments in this region cannot be finalized until better data, preferably matrix isolation and vapor phase Raman, are available.

In some cases, the calculations in this region seem suspect. The worst example is found in the heavy atom stretching assignments. With the deuteromethylene group present, strong infrared bands are observed at 1160 and 960 cm^{-1} . These bands are insensitive to change of state or hydroxyl deuteration, but their depolarization ratios suggest that they belong to the A' representation. P&J have assigned them as stretching motions of the CCO group, and the calculations concur. The difficulty lies in the large calculated COH deformation contributions to these modes which prevent the calculated spectra from reproducing the phase and hydroxyl deuteration insensitivity of the experimental data. Weaker bands are found near the calculated positions of 1200 and 1229 cm^{-1} for $\text{CH}_3\text{CD}_2\text{OD}$

and $\text{CD}_3\text{CD}_2\text{OD}$, respectively, but intensity considerations suggest that the true fundamentals are at the unshifted 1160 cm^{-1} frequency. These discrepancies suggest that perhaps the solution reached in the refinement overestimates the degree of coupling between CO stretching and COH bending.

ETHANOL CONFORMATIONS

The two distinguishable fully staggered ethanol conformers are normally described in terms of the trans or gauche relationship between the hydroxyl proton and the methyl carbon (93). Microwave studies of the gas have supported the presence of both, with the trans form apparently predominant (98,99). In the vibrational spectra, coupling between the methylene twisting or rocking modes and the hydroxyl in plane deformation constitutes evidence for the presence of the gauche form, while adherence to the C_s coupling restrictions argues for the trans form. Our assignments for these two methylene modes are summarized in Table XLII. The evidence is mixed, but it seems to favor the trans form as dominant in all phases.

The matrix spectra seem to offer the most definite evidence for the trans form, since the isolated and easily assigned rocking mode is found at identical frequency in both $\text{CH}_3\text{CH}_2\text{OH}$ and $\text{CH}_3\text{CH}_2\text{OD}$. This fact also casts doubt on the B&H assignments for the weaker twisting mode at 1250 and 1259 cm^{-1} , respectively, in these molecules. The dilute solution and condensed phase data also seem in reasonable agreement with the C_s rules, particularly with respect to the more readily assigned rocking modes. The gas data are the most difficult to evaluate, both in light of their sparsity and the probability that many of the fundamentals will have multiple Q branches (104). The gas data are not by themselves conclusive, but other information can be used to further the argument. Since all the other states seem to be dominated by the trans, the presence of the gauche

TABLE XLII

METHYLENE TWISTING (T) AND ROCKING (R) MODES IN ETHANOL

Mode	Calculated (Gas)	Gas	Matrix	Dilute Solution	Liquid	ρ	Crystal
CH₃CH₂OH							
T	1275	a	1250.8?	a	1276.0	>0.8	1278.0
R	795	801.0	812.1	800.0	803.0	b	805.0
CH₃CH₂OD							
T	1275	a	1259.4?	1290.0	1277.0	>0.8	a
R	795	790.0	812.1	802.0	798.0	b	798.0
CD₃CH₂OH							
T	1270	1338.?	c	1325.?	1323.?	b	1318.?
R	974	a	c	a	a	b	a
CD₃CH₂OD							
T	1270	a	c	1280.?	a	b	a
R	974	956.?	c	958.?	979.0	b	979.0
CH₃CD₂OH							
T	914	890.?	c	890.?	912.0	0.8	912.0
R	667	a	c	671.0	676.0	b	676.0
CH₃CD₂OD							
T	914	a	c	a	908.0	b	911.0
R	667	a	c	670.0	675.0	b	673.0
CD₃CD₂OH							
T	923	902.7	c	897.0	901.0	0.7	904.0
R	866	878.4	c	878.0	a	b	876.0
CD₃CD₂OD							
T	923	902.1	c	904.0	904.0	>0.8	911.0
R	866	a	c	a	875.0	b	874.0

^aNot observed due to band weakness or overlap.

^bNot determined due to band weakness or overlap.

^cNo data in literature.

form in the gas would presume a shift of the hydroxyl deformation relative to its position in either the matrix or dilute solution. In fact, such shifts tend to be quite small, arguing that the trans form is also dominant in the gas.

At first glance, the spectra of $\text{CD}_3\text{CH}_2\text{OH}$ and $-\text{OD}$ seem to fit the expected gauche pattern well. The 1325 cm^{-1} band assigned by P&J to coupled methylene twist and hydroxyl deformation in $\text{CD}_3\text{CH}_2\text{OH}$ is near the position calculated for the gauche form, and a band is observed near the uncoupled frequency of 1280 cm^{-1} in the $-\text{OD}$ compound. On closer examination of the data, however, one notes that the 1325 cm^{-1} band is also present in the condensed phases, and the assignment is discredited. Comparison of the calculated trans and gauche spectra to the gas and dilute solution data does reveal some bands which apparently belong to the gauche structure, but these bands always tend to be weaker than their trans counterparts.

Since the spectral data offer some support for and never clearly contradict the dominance of the trans form in all phases, and in view of the microwave results, we feel that the trans form of ethanol is the more appropriate geometric model for normal coordinate calculations. The manifestation of the gauche form in the experimental data, particularly the gas data, is not excluded and may result in some misassignments. Both the assignment and conformation questions could profitably be pursued further by obtaining matrix infrared data for the remaining isotopic species and, if possible, gas and matrix Raman data.

APPENDIX IV
COMPUTER INPUT — ALCOHOLS*

The information reported in this appendix is as follows:

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* For details of the input or programs, see References 6 or 32.

TABLE XLIII

MODIFIED VALENCE FORCE FIELD FOR METHANOL AND ETHANOL

Diagonal Force Constants

Force Constant Number	Atomic Grouping	Description Code
<u>Stretch</u>		
1	O-H	O-H
2	C-H Methyl	C6-H
3	C-H Methylene	C3-H
4	C-O	C-O
5	C-C	C-C
<u>Bend</u>		
6	COH	COH
7	OCH	OCH
8	HCH Methyl	HC6H
9	HCH Methylene	HC3H
10	CCO	CCO
11	CCH Methyl	CC6H
12	CCH Methylene	CC3H
<u>Torsion</u>		
13	C-O	TC-O
14	C-C	TC-C

TABLE XLIII (Continued)

MODIFIED VALENCE FORCE FIELD FOR METHANOL AND ETHANOL

Off-Diagonal (Interaction) Force Constants

Force Constant Number	Atomic Grouping	Description Code
<u>Stretch-Stretch</u>		
15	OH,CO	SS15
16	CH,CO	SS16
17	CH,CC	SS17
18	CH,CH Methyl	SS18
19	CH,CH Methylene	SS19
20	CO,CC	SS20
<u>Stretch-Bend</u>		
21	CO,COH	SB21
22	CO,OCH	SB22
23	CO,CCO	SB23
24	CC,CCH Methyl	SB24
25	CC,CCH Methylene	SB25
26	CC,CCO	SB26
27	OH,COH	SB27
28	CH,CCH	SB28
29	CH,OCH	SB29
30	CH,HCH	SB30
<u>Bend-Bend</u>		
31	COH,OCH Gauche	BB31
32	COH,OCH Trans	BB32
33	H-(C-O)-H	BB33
34	H-(C-H)-H	BB34
35	H-(C-C)-H	BB35
36	H-C-C-H Gauche	BB36
37	H-C-C-H Trans	BB37
38	O-(C-H)-H	BB38
39	O-(C-H)-C	BB39
40	H-(C-H)-C	BB40

TABLE XLIII (Continued)

MODIFIED VALENCE FORCE FIELD FOR METHANOL AND ETHANOL

Off-Diagonal (Interaction) Force Constants

Force Constant Number	Atomic Grouping	Description Code
	<u>Bend-Bend</u>	
41	O-C-C-O Gauche	BB41
42	O-C-C-O Trans	BB42
43	O-(C-C)-H	BB43
44	O-C-C-H Gauche	BB44
45	O-C-C-H Trans	BB45
46	C-(C-O)-H	BB46
47	C-C-O-H Trans	BB47

TABLE XLIV

DESCRIPTION OF THE INTERNAL COORDINATES
USED TO DESCRIBE METHANOL

Description Code			Description Code		
<u>Bond Stretching Coordinates</u>					
1.	H1-O2	O-H	4.	C3-H5	C-HB
2.	O2-C3	C-O	5.	C3-H6	C-HC
3.	C3-H4	C-HA			
<u>Valence Angle Bending Coordinates</u>					
6.	H1-O2-C3	HOC	10.	H4-C3-H5	HAHB
7.	O2-C3-H4	HACO	11.	H5-C3-H6	HBHC
8.	O2-C3-H5	HBCO	12.	H4-C3-H6	HAHC
9.	O2-C3-H6	HCCO			
<u>Torsional Coordinate</u>					
13.	Linear combination of:				T
	H1-O2-C3-H4				
	H1-O2-C3-H5				
	H1-O2-C3-H6				

TABLE XLV

SYMMETRY COORDINATES FOR METHANOL

Symmetry Coordinate Number	Contributing Internal Coordinates
<u>A' Representation</u>	
1	(1)
2	(2)
3	(3)+(4)+(5)
4	2(5)-(3)-(4)
5	(6)
6	2(9)-(7)-(8)
7	2(10)-(11)-(12)
8	(10)+(11)+(12)-(7)-(8)-(9)
(13) (Redundant)	(7)+(8)+(9)+(10)+(11)+(12)
<u>A'' Representation</u>	
9	(4)-(3)
10	(7)-(8)
11	(11)-(12)
12	(13)

TABLE XLVI
DESCRIPTION OF THE INTERNAL COORDINATES
USED TO DESCRIBE ETHANOL

		Description Code			Description Code
<u>Bond Stretching Coordinates</u>					
1.	H1-O2	O-H	5.	C3-H5	C-H5
2.	O2-C3	C-O	6.	C6-H7	C-H7
3.	C3-C6	C-C	7.	C6-H8	C-H8
4.	C3-H4	C-H4	8.	C6-H9	C-H9
<u>Valence Angle Bending Coordinates</u>					
9.	H1-O2-C3	HOC	16.	C3-C6-H7	CCH7
10.	O2-C3-H4	OCH4	17.	C3-C6-H8	CCH8
11.	O2-C3-H5	OCH5	18.	C3-C6-H9	CCH9
12.	H4-C3-H5	HCH	19.	H7-C6-H8	H7H8
13.	H4-C3-C6	H4CC	20.	H8-C6-H9	H8H9
14.	H5-C3-C6	H5CC	21.	H7-C6-H9	H7H9
15.	O2-C3-C6	OCC			
<u>Torsional Coordinates</u>					
22.	Linear combination of:				T-CO
	H1-O2-C3-H4				
	H1-O2-C3-H5				
	H1-O2-C3-C6				
23.	Linear combination of:				T-CC
	O2-C3-C6-H7				
	O2-C3-C6-H8				
	O2-C3-C6-H9				

TABLE XLVII

SYMMETRY COORDINATES FOR ETHANOL

Symmetry Coordinate Number	Contributing Internal Coordinates
-------------------------------	--------------------------------------

A' Representation

1	(1)
2	(2)
3	(3)
4	(4)+(5)
5	(6)+(7)+(8)
6	(6)+(7)-2(8)
7	(9)
8	(10)+(11)
9	(12)
10	(13)+(14)
11	(15)
12	(16)+(17)+(18)
13	2(18)-(16)-(17)
14	(19)+(20)+(21)
15	2(19)-(20)-(21)

A'' Representation

16	(4)-(5)
17	(7)-(6)
18	(10)-(11)
19	(13)-(14)
20	(16)-(17)
21	(20)-(21)
22	(22)
23	(23)

TABLE XLVIII

COMPUTER INPUT - METHANOL

```

      PAMOLE INPUT      . . . .      METHANOL
-9   10   3   1 -3.80  C.50  0.21
-6   NG= 79      METHANOL, CH3OH
SCALE 2.000 0 0.0
      C   .290   .27H   .12D   .03
H1     0.0     0.0     0.0   02
O2     0.986   0.0     0.0   C3
C3     1.462   1.346   0.0   H4   H5   H6
H4     1.092   1.870  -0.9C6C3
H5     1.092   1.870   0.9C6C3
H6     2.572   1.346   0.0   C3
VIEW  10. 10. -10.
VIEW  10. -10. 10.
VIEW -10. 10. 10.

```

```

      PAM1 INPUT      . . . .      METHANOL
-09 12   4   0.10  1.0  0 1 2.5  2.0  4
-9   6   2   1   0.0  .5  .21
      METHANOL
SCALE 2.0
SIZES C   .290   .27H   .12D   .03
H1     0.000   0.000   0.0C002
O2     0.986   0.000   0.0C0C3
C3     1.462   1.346   0.0C0H4   H5   H6
H4     1.092   1.870  -0.9C6C3
H5     1.092   1.870   0.9C6C3
H6     2.572   1.346   0.0C0C3
D7
D8
D9
D10
D11
D12
VIEW  -3   10   0
VIEW  -10  10  10
999

```

TABLE XLVIII (Continued)

```

-09          CART INPUT      ...      METHANOL
-09          6      5      -1
METHANOL, C-O = 1.428 (K. KIMURA, ELECTRON DIFFRACTION DATA). ANGLES
ALL TETRA. C-H, O-H LENGTHS FROM NEUTRON DATA (BROWN-SUCROSE). 7/8/75 .
1          1          0.984          1.00000
2          2          1.428          12.00000
3          3          1.11C          0.00
4          3          2          1          1.11C          0.00          60.000          1.00000
5          3          3          2          1          1.11C          0.00          -60.000          1.00000
6          3          3          3          2          1          1.11C          0.00          180.000          1.00000
-06          1          3          12          METHANOL, C(13)H3OH          1.007825          1.007825          1.007825
-06          1.007825          15.99491C          13.003350          1.007825          1.007825          1.007825
-06          2          0.14005          METHANOL, CH3OD          1.007825          1.007825          1.007825
-06          1          3          12          METHANOL, CH3O(18)D          1.007825          1.007825          1.007825
-06          2.014005          18.00000C          12.00000C          1.007825          1.007825          1.007825
-06          1          3          12          METHANOL, CD3OH          2.0140          2.0140          2.0140
-06          1.007825          15.99491C          12.00000C          2.0140          2.0140          2.0140
-06          2.014005          15.99491C          12.00000C          2.0140          2.0140          2.0140
999

```

```

-09          GMAT INPUT      ...      METHANOL
-09          200      6      13      1      1
METHANOL, NO REDUNDANCY, SUMMED TORSIONS.
23 JUNE 1975, C-O=1.42A, C-O-H=110. DEG.
1          2          0.986000          1          3          1.461959          2          3          1.346331          1          4          1.091998
2          4          1.864589          3          4          -0.906310          1          5          1.091998          2          5          1.869589
3          5          0.906310          1          6          2.571998          2          6          1.346330          -1          0          0.0
4          1          1          3          0          0          2          1          2          3          0          0          3          1          3          4          0          0
5          1          3          3          0          0          2          1          3          6          0          0          6          2          1          2          3          0
7          2          4          3          0          0          8          2          2          3          6          0          9          2          2          3          6          0
10         2          4          3          0          0          11         2          2          3          6          0          12         2          2          4          3          6          0
13         4          1          2          3          6          3          0          4          1          2          3          4          3          0          4          1          2          3          5          3
-02
-06          1          3          12          METHANOL, CH3OH          1.007825          1.007825          1.007825
-06          1.007825          15.99491C          12.00000C          1.007825          1.007825          1.007825
1          1          3          12          2          2          1.0          3          3          1.0          4          4          1.0          5          5          1.0          6          6          1.0          7          7          1.0          8          8          1.0          9          9          1.0          10         10         1.0          11         11         1.0          12         12         1.0          13         13         1.0
5          6          1.0          6          7          -1.0          6          8          -1.0          6          9          -1.0          6          10         -1.0          6          11         -1.0          6          12         -1.0          6          13         -1.0
7          10         2.0          7          11         -1.0          7          12         -1.0          7          13         -1.0
8          8          -1.0          8          9          -1.0          8          10         -1.0          8          11         -1.0          8          12         -1.0          8          13         -1.0
12         3          -1.0          10         7          1.0          10         8          -1.0
11         11         1.0          11         12         -1.0          12         13         1.0          -03          8          -1.0
1          9          13
-06          1          3          12          METHANOL, C(13)H3OH          1.007825          1.007825          1.007825
-06          1.007825          15.99491C          13.003350          1.007825          1.007825          1.007825
1          9          13
-06          2          0.14005          METHANOL, CH3OD          1.007825          1.007825          1.007825
-06          1          3          12          METHANOL, CH3O(18)D          1.007825          1.007825          1.007825
-06          2.014005          18.00000C          12.00000C          1.007825          1.007825          1.007825
1          9          13
-06          1          3          12          METHANOL, CD3OH          2.0140          2.0140          2.0140
-06          1.007825          15.99491C          12.00000C          2.0140          2.0140          2.0140
1          9          13
-06          2          0.14005          METHANOL, CD3OD          2.0140          2.0140          2.0140
-06          1          3          12          2.014005          15.99491C          12.00000C          2.0140          2.0140          2.0140
1          9          13
999

```

```

UNFACTORED Z MATRIX      ..      METHANOL
1          1          1          1.000000          1          2          15          1.000000          1          6          27          1.000000          2          2          4          1.000000
2          3          22          1.000000          2          4          16          1.000000          2          5          16          1.000000          2          6          21          1.000000
3          4          18          1.000000          3          5          18          1.000000          3          7          29          1.000000          3          10         30          1.000000
4          12         30          1.000000          4          4          2          1.000000          4          5          18          1.000000          4          8          29          1.000000
5          10         30          1.000000          4          11         30          1.000000          5          5          2          1.000000          5          9          29          1.000000
6          11         30          1.000000          5          12         30          1.000000          6          6          6          1.000000          6          7          31          1.000000
7          8          31          1.000000          6          7          32          1.000000          7          7          7          1.000000          7          8          33          1.000000
8          9          33          1.000000          7          10         38          1.000000          7          12         38          1.000000          8          8          7          1.000000
9          11         38          1.000000          8          10         38          1.000000          8          11         38          1.000000          9          9          7          1.000000
10         12         34          1.000000          9          12         38          1.000000          10         10         8          1.000000          10         11         34          1.000000
11         12         34          1.000000          11         11         8          1.000000          11         12         34          1.000000          12         12         8          1.000000
13         13         13          1.000000          -2

```

```

-09          ZSYM INPUT      ...      METHANOL
-09          13      47      12      3
METHANOL -47 PARAMETER Z-MATRIX
10 APRIL 1975      --      REDUNDANCY      REMOVED
1          1          1.000000          1          15          1.000000          1          6          27          1.000000          2          2          4          1.000000
2          3          16          1.000000          2          4          16          1.000000          2          5          16          1.000000          2          6          21          1.000000
3          4          22          1.000000          3          5          22          1.000000          3          7          29          1.000000          3          10         30          1.000000
4          12         30          1.000000          4          4          2          1.000000          4          5          18          1.000000          4          8          29          1.000000
5          10         30          1.000000          4          11         30          1.000000          5          5          2          1.000000          5          9          29          1.000000
6          11         30          1.000000          5          12         30          1.000000          6          6          6          1.000000          6          7          31          1.000000
7          8          31          1.000000          6          7          32          1.000000          7          7          7          1.000000          7          8          33          1.000000
8          9          33          1.000000          7          10         38          1.000000          7          12         38          1.000000          8          8          7          1.000000
9          11         38          1.000000          8          10         38          1.000000          8          11         38          1.000000          9          9          7          1.000000
10         12         34          1.000000          9          12         38          1.000000          10         10         8          1.000000          10         11         34          1.000000
11         12         34          1.000000          11         11         8          1.000000          11         12         34          1.000000          12         12         8          1.000000
13         13         13          1.000000          -2
1          1          1.0          2          2          1.0          3          3          1.0          3          4          1.0
2          3          1.0          4          3          -1.0          4          4          -1.0          4          5          2.0
3          5          1.0          6          7          -1.0          6          8          -1.0          6          9          2.0
4          6          1.0          7          11         -1.0          7          12         -1.0          7          13         -1.0
5          8          -1.0          8          9          -1.0          8          10         -1.0          8          11         1.0
6          12         1.0
7          9          -1.0          10         7          1.0          10         8          -1.0
8          12         1.0          11         12         -1.0          12         13         1.0          -03          8          -1.0
9          3          1.0          11         12         -1.0          12         13         1.0
1          11         1.0          11         12         -1.0          12         13         1.0
1          9          13
999

```

TABLE XLIX

COMPUTER INPUT - ETHANOL

```

      PAMOLE INPUT      ..:. ETHANOL
-9  15  2  1  0.0  C.50  0.21
-6  NG= 201  ETHANOL, CH3CH2OH
SCALE 1.700.0 0.0
      C .290 .27H .12D .03
H1    0.0  0.0  0.0  02
O2    0.986 0.0  0.0  C3
C3    1.459 1.339 0.0  H4      H5      C6
H4    1.079 1.866 -0.9C0C3
H5    1.079 1.866 0.9C0C3
C6    2.999 1.339 0.0  C3      H7      H8      H9
H7    3.369 0.815 -0.9C6C6
H8    3.369 0.815 0.9C6C6
H9    3.369 2.385 0.0  C6
VIEW -3. 10. 0.
VIEW-10. 10. 10.
  
```

```

      PAM1 INPUT      :.:. ETHANOL
-09 21  6  0.10  1:0  0  1 2.5  3.0 12
-9  9  2  1  0.0  C.2 .21
      ETHANOL
SCALE 1.7
SIZES C .290 .27H .12D .03
H1    0.000 0.000 0.0C002
O2    0.986 0.000 0.0C0C3
C3    1.459 1.339 0.0C0H4      H5      C6
H4    1.079 1.866 -0.9C0C3
H5    1.079 1.866 0.9C0C3
C6    3.000 1.339 0.0C0C3      H7      H8      H9
H7    3.370 0.815 -0.9C6C6
H8    3.369 0.815 0.9C6C6
H9    3.369 2.385 0.0C0C6
D10   H1
D11   O2
D12   C3
D13   H4
D14   H5
D15   C6
D16   H7
D17   H8
D18   H9
VIEW -3. 10. 0.
VIEW-10. 10. 10.
999
  
```

TABLE XLIX (Continued)

CART INPUT ... ETHANOL (TRANS)											
ETHANOL, TRANS CONFORMATION (C1 NONTETRAHEDRAL)											
29 OCT. 75 C-i= 1.42 COH ANGLE TETRAHEDRAL											
1	2	3	4	5	6	7	8	9	10	ETCT	10
1	1									1.007825	10
2	1									15.994910	20
3	2	1								12.000000	30
4	3	2	1							1.007825	40
5	3	2	1							1.007825	50
6	3	2	1							1.007825	60
7	6	3	2	1						1.007825	70
8	6	3	2	1						1.007825	80
9	6	3	2	1						1.007825	90
10	6	3	2	1						1.007825	100
11	6	3	2	1						1.007825	110
12	6	3	2	1						1.007825	120
13	6	3	2	1						1.007825	130
14	6	3	2	1						1.007825	140
15	6	3	2	1						1.007825	150
16	6	3	2	1						1.007825	160
17	6	3	2	1						1.007825	170
18	6	3	2	1						1.007825	180
19	6	3	2	1						1.007825	190
20	6	3	2	1						1.007825	200
21	6	3	2	1						1.007825	210
22	6	3	2	1						1.007825	220
23	6	3	2	1						1.007825	230
24	6	3	2	1						1.007825	240
25	6	3	2	1						1.007825	250
26	6	3	2	1						1.007825	260
27	6	3	2	1						1.007825	270
28	6	3	2	1						1.007825	280
29	6	3	2	1						1.007825	290
30	6	3	2	1						1.007825	300
31	6	3	2	1						1.007825	310
32	6	3	2	1						1.007825	320
33	6	3	2	1						1.007825	330
34	6	3	2	1						1.007825	340
35	6	3	2	1						1.007825	350
36	6	3	2	1						1.007825	360
37	6	3	2	1						1.007825	370
38	6	3	2	1						1.007825	380
39	6	3	2	1						1.007825	390
40	6	3	2	1						1.007825	400
41	6	3	2	1						1.007825	410
42	6	3	2	1						1.007825	420
43	6	3	2	1						1.007825	430
44	6	3	2	1						1.007825	440
45	6	3	2	1						1.007825	450
46	6	3	2	1						1.007825	460
47	6	3	2	1						1.007825	470
48	6	3	2	1						1.007825	480
49	6	3	2	1						1.007825	490
50	6	3	2	1						1.007825	500
51	6	3	2	1						1.007825	510
52	6	3	2	1						1.007825	520
53	6	3	2	1						1.007825	530
54	6	3	2	1						1.007825	540
55	6	3	2	1						1.007825	550
56	6	3	2	1						1.007825	560
57	6	3	2	1						1.007825	570
58	6	3	2	1						1.007825	580
59	6	3	2	1						1.007825	590
60	6	3	2	1						1.007825	600
61	6	3	2	1						1.007825	610
62	6	3	2	1						1.007825	620
63	6	3	2	1						1.007825	630
64	6	3	2	1						1.007825	640
65	6	3	2	1						1.007825	650
66	6	3	2	1						1.007825	660
67	6	3	2	1						1.007825	670
68	6	3	2	1						1.007825	680
69	6	3	2	1						1.007825	690
70	6	3	2	1						1.007825	700
71	6	3	2	1						1.007825	710
72	6	3	2	1						1.007825	720
73	6	3	2	1						1.007825	730
74	6	3	2	1						1.007825	740
75	6	3	2	1						1.007825	750
76	6	3	2	1						1.007825	760
77	6	3	2	1						1.007825	770
78	6	3	2	1						1.007825	780
79	6	3	2	1						1.007825	790
80	6	3	2	1						1.007825	800
81	6	3	2	1						1.007825	810
82	6	3	2	1						1.007825	820
83	6	3	2	1						1.007825	830
84	6	3	2	1						1.007825	840
85	6	3	2	1						1.007825	850
86	6	3	2	1						1.007825	860
87	6	3	2	1						1.007825	870
88	6	3	2	1						1.007825	880
89	6	3	2	1						1.007825	890
90	6	3	2	1						1.007825	900
91	6	3	2	1						1.007825	910
92	6	3	2	1						1.007825	920
93	6	3	2	1						1.007825	930
94	6	3	2	1						1.007825	940
95	6	3	2	1						1.007825	950
96	6	3	2	1						1.007825	960
97	6	3	2	1						1.007825	970
98	6	3	2	1						1.007825	980
99	6	3	2	1						1.007825	990

CART INPUT ... ETHANOL (GAUCHE)											
ETHANOL, GAUCHE CONFORMATION											
21 NOV. 1975											
1	2	3	4	5	6	7	8	9	10	EGCT	10
1	1									1.007825	10
2	1									15.994910	20
3	2	1								12.000000	30
4	3	2	1							1.007825	40
5	3	2	1							1.007825	50
6	3	2	1							1.007825	60
7	6	3	2	1						1.007825	70
8	6	3	2	1						1.007825	80
9	6	3	2	1						1.007825	90
10	6	3	2	1						1.007825	100
11	6	3	2	1						1.007825	110
12	6	3	2	1						1.007825	120
13	6	3	2	1						1.007825	130
14	6	3	2	1						1.007825	140
15	6	3	2	1						1.007825	150
16	6	3	2	1						1.007825	160
17	6	3	2	1						1.007825	170
18	6	3	2	1						1.007825	180
19	6	3	2	1						1.007825	190
20	6	3	2	1						1.007825	200
21	6	3	2	1						1.007825	210
22	6	3	2	1						1.007825	220
23	6	3	2	1						1.007825	230
24	6	3	2	1						1.007825	240
25	6	3	2	1						1.007825	250
26	6	3	2	1						1.007825	260
27	6	3	2	1						1.007825	270
28	6	3	2	1						1.007825	280
29	6	3	2	1						1.007825	290
30	6	3	2	1						1.007825	300
31	6	3	2	1						1.007825	310
32	6	3	2	1						1.007825	320
33	6	3	2	1						1.007825	330
34	6	3	2	1						1.007825	340
35	6	3	2	1						1.007825	350
36	6	3	2	1						1.007825	360
37	6	3	2	1						1.007825	370
38	6	3	2	1						1.007825	380
39	6	3	2	1						1.007825	390
40	6	3	2	1						1.007825	400
41	6	3	2	1						1.007825	410
42	6	3	2	1						1.007825	420
43	6	3	2	1						1.007825	430
44	6	3	2	1						1.007825	440
45	6	3	2	1						1.007825	450
46	6	3	2	1						1.007825	460
47	6	3	2	1						1.007825	470

GMAT INPUT ... ETHANOL (TRANS)															ETGM	10
-09	300	9	23	1	1	1	GMAT INPUT ... ETHANOL (TRANS) NORMALIZED TORSIONS, NONREDUNDANT								ETGM	20
GMAT	COORDINATES	INPUT	TRANS	C-O	ETHANOL	ETHANOL	UPDATED 1 NOV. 75								ETGM	30
1	2	0.986	0.000	1	3	1.459332	2	3	1.338787	1	4	1.078930	1	0.000000	ETGM	40
2	4	1.865724	1	3	4	-0.998950	1	5	1.078930	2	5	1.865724	1	0.000000	ETGM	50
3	5	0.899850	1	6	5	-2.999331	2	6	1.338786	1	7	3.369328	1	0.000000	ETGM	60
4	6	0.815526	1	7	6	-0.406312	1	8	3.369328	2	8	0.155226	1	0.000000	ETGM	70
5	7	0.908309	1	8	7	-3.369329	2	9	2.385303	-1	0	0.000000	1	0.000000	ETGM	80
6	8	0.000000	2	9	8	2.385303	3	10	1.338787	1	3	0.000000	0	0.000000	ETGM	90
7	9	0.000000	3	10	9	1.338787	4	11	1.078930	2	1	0.000000	0	0.000000	ETGM	100
8	10	0.000000	4	11	10	-0.998950	5	12	1.865724	1	2	0.000000	0	0.000000	ETGM	110
9	11	0.000000	5	12	11	-2.999331	6	13	3.369328	2	2	0.000000	0	0.000000	ETGM	120
10	12	0.000000	6	13	12	-0.406312	7	14	2.385303	1	3	0.000000	0	0.000000	ETGM	130
11	13	0.000000	7	14	13	3.369329	8	15	1.338787	2	3	0.000000	0	0.000000	ETGM	140
12	14	0.000000	8	15	14	1.338787	9	16	1.078930	1	4	0.000000	0	0.000000	ETGM	150
13	15	0.000000	9	16	15	-0.998950	10	17	1.865724	2	4	0.000000	0	0.000000	ETGM	160
14	16	0.000000	10	17	16	-2.999331	11	18	3.369328	1	5	0.000000	0	0.000000	ETGM	170
15	17	0.000000	11	18	17	-0.406312	12	19	2.385303	2	5	0.000000	0	0.000000	ETGM	180
16	18	0.000000	12	19	18	3.369329	13	20	1.338787	1	6	0.000000	0	0.000000	ETGM	190
17	19	0.000000	13	20	19	1.338787	14	21	1.078930	2	6	0.000000	0	0.000000	ETGM	200
18	20	0.000000	14	21	20	-0.998950	15	22	1.865724	1	7	0.000000	0	0.000000	ETGM	210
19	21	0.000000	15	22	21	-2.999331	16	23	3.369328	2	7	0.000000	0	0.000000	ETGM	220
20	22	0.000000	16	23	22	-0.406312	17	24	2.385303	1	8	0.000000	0	0.000000	ETGM	230
21	23	0.000000	17	24	23	3.369329	18	25	1.338787	2	8	0.000000	0	0.000000	ETGM	240
22	24	0.000000	18	25	24	1.338787	19	26	1.078930	1	9	0.000000	0	0.000000	ETGM	250
23	25	0.000000	19	26	25	-0.998950	20	27	1.865724	2	9	0.000000	0	0.000000	ETGM	260
24	26	0.000000	20	27	26	-2.999331	21	28	3.369328	1	10	0.000000	0	0.000000	ETGM	270
25	27	0.000000	21	28	27	-0.406312	22	29	2.385303	2	10	0.000000	0	0.000000	ETGM	280
26	28	0.000000	22	29	28	3.369329	23	30	1.338787	1	11	0.000000	0	0.000000	ETGM	290
27	29	0.000000	23	30	29	1.338787	24	31	1.078930	2	11	0.000000	0	0.000000	ETGM	300
28	30	0.000000	24	31	30	-0.998950	25	32	1.865724	1	12	0.000000	0	0.000000	ETGM	310
29	31	0.000000	25	32	31	-2.999331	26	33	3.369328	2	12	0.000000	0	0.000000	ETGM	320
30	32	0.000000	26	33	32	-0.406312	27	34	2.385303	1	13	0.000000	0	0.000000	ETGM	330
31	33	0.000000	27	34	33	3.369329	28	35	1.338787	2	13	0.000000	0	0.000000	ETGM	340
32	34	0.000000	28	35	34	1.338787	29	36	1.078930	1	14	0.000000	0	0.000000	ETGM	350
33	35	0.000000	29	36	35	-0.998950	30	37	1.865724	2	14	0.000000	0	0.000000	ETGM	360
34	36	0.000000	30	37	36	-2.999331	31	38	3.369328	1	15	0.000000	0	0.000000	ETGM	370
35	37	0.000000	31	38	37	-0.406312	32	39	2.385303	2	15	0.000000	0	0.000000	ETGM	380
36	38	0.000000	32	39	38	3.369329	33	40	1.338787	1	16	0.000000	0	0.000000	ETGM	390
37	39	0.000000	33	40	39	1.338787	34	41	1.078930	2	16	0.000000	0	0.000000	ETGM	400
38	40	0.000000	34	41	40	-0.998950	35	42	1.865724	1	17	0.000000	0	0.000000	ETGM	410
39	41	0.000000	35	42	41	-2.999331	36	43	3.369328	2	17	0.000000	0	0.000000	ETGM	420
40	42	0.000000	36	43	42	-0.406312	37	44	2.385303	1	18	0.000000	0	0.000000	ETGM	430
41	43	0.000000	37	44	43	3.369329	38	45	1.338787	2	18	0.000000	0	0.000000	ETGM	440
42	44	0.000000	38	45	44	1.338787	39	46	1.078930	1	19	0.000000	0	0.000000	ETGM	450
43	45	0.000000	39	46	45	-0.998950	40	47	1.865724	2	19	0.000000	0	0.000000	ETGM	460
44	46	0.000000	40	47	46	-2.999331	41	48	3.369328	1	20	0.000000	0	0.000000	ETGM	470
45	47	0.000000	41	48	47	-0.406312	42	49	2.385303	2	20	0.000000	0	0.000000	ETGM	480
46	48	0.000000	42	49	48	3.369329	43	50	1.338787	1	21	0.000000	0	0.000000	ETGM	490
47	49	0.000000	43	50	49	1.338787	44	51	1.078930	2	21	0.000000	0	0.000000	ETGM	500
48	50	0.000000	44	51	50	-0.998950	45	52	1.865724	1	22	0.000000	0	0.000000	ETGM	510
49	51	0.000000	45	52	51	-2.999331	46	53	3.369328	2	22	0.000000	0	0.000000	ETGM	520
50	52	0.000000	46	53	52	-0.406312	47	54	2.385303	1	23	0.000000	0	0.000000	ETGM	530
51	53	0.000000	47	54	53	3.369329	48	55	1.338787	2	23	0.000000	0	0.000000	ETGM	540
52	54	0.000000	48	55	54	1.338787	49	56	1.078930	1	24	0.000000	0	0.000000	ETGM	550
53	55	0.000000	49	56	55	-0.998950	50	57	1.865724	2	24	0.000000	0	0.000000	ETGM	560
54	56	0.000000	50	57	56	-2.999331	51	58	3.369328	1	25	0.000000	0	0.000000	ETGM	570
55	57	0.000000	51	58	57	-0.406312	52	59	2.385303	2	25	0.000000	0	0.000000	ETGM	580
56	58	0.000000	52	59	58	3.369329	53	60	1.338787	1	26	0.000000	0	0.000000	ETGM	590
57	59	0.000000	53	60	59	1.338787	54	61	1.078930	2	26	0.000000	0	0.000000	ETGM	600
58	60	0.000000	54	61	60	-0.998950	55	62	1.865724	1	27	0.000000	0	0.000000	ETGM	610
59	61	0.000000	55	62	61	-2.999331	56	63	3.369328	2	27	0.000000	0	0.000000	ETGM	620
60	62	0.000000	56	63	62	-0.406312	57	64	2.385303	1	28	0.000000	0	0.000000	ETGM	630
61	63	0.000000	57	64	63	3.369329	58	65	1.338787	2	28	0.000000	0	0.000000	ETGM	640
62	64	0.000000	58	65	64	1.338787	59	66	1.078930	1	29	0.000000	0	0.000000	ETGM	650
63	65	0.000000	59	66	65	-0.998950	60	67	1.865724	2	29	0.000000	0	0.000000	ETGM	660
64	66	0.000000	60	67	66	-2.999331	61	68	3.369328	1	30	0.000000	0	0.000000	ETGM	670
65	67	0.000000	61	68	67	-0.406312	62	69	2.385303	2	30	0.000000	0	0.000000	ETGM	680
66	68	0.000000	62	69	68	3.369329	63	70	1.338787	1	31	0.000000	0	0.000000	ETGM	690
67	69	0.000000	63	70	69	1.338787	64	71	1.078930	2	31	0.000000	0	0.000000	ETGM	700
68	70	0.000000	64	71	70	-0.998950	65	72	1.865724	1	32	0.000000	0	0.000000	ETGM	710
69	71	0.000000	65	72	71	-2.999331	66	73	3.369328	2	32	0.000000	0	0.000000	ETGM	720
70	72	0.000000	66	73	72	-0.406312	67	74	2.385303	1	33	0.000000	0	0.000000	ETGM	730
71	73	0.000000	67	74	73	3.369329	68	75	1.338787	2	33	0.000000	0	0.000000	ETGM	740
72	74	0.000000	68	75	74	1.338787	69	76	1.078930	1	34	0.000000	0	0.000000	ETGM	750
73	75	0.000000	69	76	75	-0.998950	70	77	1.865724	2	34	0.000000	0	0.000000	ETGM	760
74	76	0.000000	70	77	76	-2.999331	71	78	3.369328	1	35	0.000000	0	0.000000	ETGM	770
75	77	0.000000	71	78	77	-0.406312	72	79	2.385303	2	35	0.000000	0	0.000000	ETGM	780
76	78	0.000000	72	79	78	3.369329	73	80	1.338787	1	36	0.000000	0	0.000000	ETGM	790
77	79	0.000000	73	80	79	1.338787	74	81	1.078930	2	36	0.000000	0	0.000000	ETGM	800
78	80	0.000000	74	81	80	-0.998950	75	82	1.865724	1	37	0.000000	0	0.000000	ETGM	810
79	81	0.000000	75	82	81	-2.999331	76	83	3.369328	2	37	0.000000	0	0.000000	ETGM	820
80	82	0.000000	76	83	82	-0.406312	77	84	2.385303	1	38	0.000000	0	0.000000	ETGM	830
81	83	0.000000	77	84	83	3.369329	78	85	1.338787	2						

[illegible]

APPENDIX V

POTENTIAL ENERGY DISTRIBUTIONS FOR METHANOL AND ETHANOL

The information reported in this appendix is as follows:

Content	Description of Content	Page
1. Table L	Potential Energy Distribution for Matrix Isolated Methanol	357
2. Table LI	Potential Energy Distribution for Liquid Methanol	364
3. Table LII	Potential Energy Distribution for Gaseous Ethanol (Trans)	369
4. Table LIII	Potential Energy Distribution for Liquid Ethanol (Trans)	382
5. Table LIV	Potential Energy Distribution for Gaseous Ethanol (Gauche)	395
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TABLE L

POTENTIAL ENERGY DISTRIBUTION FOR MATRIX ISOLATED METHANOL

Explanation of the table:

This table is presented in the same format as Table XXXIV except that the force constant and internal coordinate description codes are found in Tables XLIII and XLIV, respectively.

TABLE I

POTENTIAL ENERGY DISTRIBUTION FOR MATRIX ISOLATED METHANOL

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 200	PAGE	1
MOLECULE 1 -6 NG= 79 METHANOL, CH3OH		
NORMAL MODE 5 OBSERVED= 1474.1 CM-1 CALCULATED= 1475.8 CM-1 ERROR= -1.7 CM-1 OR -0.1 PERCENT		
INTERNAL COORDINATES- 37.12 HAHB 23.14 HCCO 14.17 HBHC 14.14 HAHB		
FORCE CONSTANTS- 65.44 HC6H 27.50 OCH		
OFF DIAGONAL- 2.08 B832		
NORMAL MODE 6 OBSERVED= 1465.8 CM-1 CALCULATED= 1469.3 CM-1 ERROR= -3.5 CM-1 OR -0.2 PERCENT		
INTERNAL COORDINATES- 38.07 HAHB 38.04 HBHC 10.97 HBCCO 10.96 HACO		
FORCE CONSTANTS- 76.11 HC6H 21.93 OCH		
OFF DIAGONAL - NONE		
NORMAL MODE 7 OBSERVED= 1451.4 CM-1 CALCULATED= 1454.9 CM-1 ERROR= -3.5 CM-1 OR -0.2 PERCENT		
INTERNAL COORDINATES- 24.30 HACO 24.30 HBCCO 23.56 HAHB 19.21 HCCO 9.37 HBHC 9.37 HAHB		
FORCE CONSTANTS- 67.81 OCH 42.30 HC6H		
OFF DIAGONAL- -10.46 SB22 -5.92 B833 2.48 B838		
NORMAL MODE 8 OBSERVED= 1335.0 CM-1 CALCULATED= 1335.6 CM-1 ERROR= -0.6 CM-1 OR -0.0 PERCENT		
INTERNAL COORDINATES- 61.39 HOC 10.57 HAHB 5.51 HCCO 5.07 HBHC 5.07 HAHB		
FORCE CONSTANTS- 61.39 COH 20.70 HC6H 13.39 OCH		
OFF DIAGONAL- 4.39 B832 -1.51 SB21		
NORMAL MODE 9 OBSERVED= 1157.0 CM-1 CALCULATED= 1159.3 CM-1 ERROR= -2.3 CM-1 OR -0.2 PERCENT		
INTERNAL COORDINATES- 36.79 HACO 36.78 HBCCO 11.81 HBHC 11.81 HAHB		
FORCE CONSTANTS- 73.57 OCH 23.62 HC6H		
OFF DIAGONAL- 3.22 B833		
NORMAL MODE 10 OBSERVED= 1076.7 CM-1 CALCULATED= 1073.2 CM-1 ERROR= 3.5 CM-1 OR 0.3 PERCENT		
INTERNAL COORDINATES- 32.86 HOC 32.12 HCCO 18.03 C-O 9.16 HBCCO 9.16 HACO 6.86 HAHB		
FORCE CONSTANTS- 50.45 OCH 32.86 COH 18.03 C-O 11.12 HC6H		
OFF DIAGONAL- -7.76 B832 -6.09 SB21 2.20 B833		
NORMAL MODE 11 OBSERVED= 1034.0 CM-1 CALCULATED= 1039.9 CM-1 ERROR= -5.9 CM-1 OR -0.6 PERCENT		
INTERNAL COORDINATES- 89.41 C-O 8.13 HCCO		
FORCE CONSTANTS- 89.41 C-O 8.38 OCH		
OFF DIAGONAL- -8.77 SB22 5.02 SB21		
NORMAL MODE 12 OBSERVED= 240.0 CM-1 CALCULATED= 240.0 CM-1 ERROR= 0.0 CM-1 OR 0.0 PERCENT		
INTERNAL COORDINATES- 99.97 T		
FORCE CONSTANTS- 99.97 TC-O		
OFF DIAGONAL - NONE		

9. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 2.33

TABLE L (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR	PROBLEM 200	PAGE 1
MOLECULE 5	-6 NG= 79	
	METHANOL, C(13)H3OH	
NORMAL MODE 5	OBSERVED= 1473.0 CM-1	
INTERNAL COORDINATES-	38.76 HAHB 21.95 HCCO 13.41 HAHB 13.40 HBHC	ERROR= -2.7 CM-1 OR -0.2 PERCENT
FORCE CONSTANTS-	65.57 HC6H 27.28 OCH	
OFF DIAGONAL-	2.03 BB32	
NORMAL MODE 6	OBSERVED= 1465.8 CM-1	
INTERNAL COORDINATES-	37.82 HBHC 37.82 HAHB 11.19 HACO 11.19 HBHC	ERROR= -3.1 CM-1 OR -0.2 PERCENT
FORCE CONSTANTS-	75.64 HC6H 22.38 OCH	
OFF DIAGONAL -	NONE	
NORMAL MODE 7	OBSERVED= 1445.8 CM-1	
INTERNAL COORDINATES-	23.70 HACO 23.70 HBHC 21.61 HAHB 20.22 HCCO 9.99 HBHC	ERROR= -2.8 CM-1 OR -0.2 PERCENT
FORCE CONSTANTS-	67.63 OCH 41.58 HC6H	
OFF DIAGONAL-	-8.88 SB22 -5.91 BB33 2.47 BB38	
NORMAL MODE 8	OBSERVED= 1327.0 CM-1	
INTERNAL COORDINATES-	63.06 HOC 10.39 HAHB	ERROR= -1.6 CM-1 OR -0.1 PERCENT
FORCE CONSTANTS-	63.06 COH 20.35 HC6H 12.34 OCH	
OFF DIAGONAL-	4.23 BB32 -1.67 SB21	
NORMAL MODE 9	OBSERVED= 0.0 CM-1	
INTERNAL COORDINATES-	36.58 HACO 36.58 HBHC	ERROR= 0.0 CM-1 OR 0.0 PERCENT
FORCE CONSTANTS-	73.16 OCH 24.13 HC6H	
OFF DIAGONAL-	3.21 BB33	
NORMAL MODE 10	OBSERVED= 1070.2 CM-1	
INTERNAL COORDINATES-	35.66 HCCO 33.57 HOC	ERROR= 1.6 CM-1 OR 0.1 PERCENT
FORCE CONSTANTS-	54.99 OCH 33.57 COH 12.55 HC6H 9.79 C-O	
OFF DIAGONAL-	-8.26 BB32 -4.53 SB21 2.41 BB33	
NORMAL MODE 11	OBSERVED= 1018.5 CM-1	
INTERNAL COORDINATES-	98.45 C-O 5.33 HCCO	ERROR= -3.1 CM-1 OR -0.3 PERCENT
FORCE CONSTANTS-	98.45 C-O 5.35 OCH	
OFF DIAGONAL-	-10.92 SB22 3.58 SB21	
NORMAL MODE 12	OBSERVED= 240.0 CM-1	
INTERNAL COORDINATES-	99.97 T	ERROR= 0.0 CM-1 OR 0.0 PERCENT
FORCE CONSTANTS-	99.97 TC-O	
OFF DIAGONAL -	NONE	

8. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 1.87

TABLE I (Continued)

CONDENSED POTENTIAL MOLECULE	2	ENERGY DISTRIBUTIONS	FOR PROBLEM	200	PAGE	1
		-6 NG= 79	METHANOL, CH3OD			
NORMAL MODE 5		OBSERVED= 1472.7 CM-1	CALCULATED= 1470.0 CM-1	ERROR= 2.6 CM-1	OR	0.2 PERCENT
INTERNAL COORDINATES-		49.00 HAHB 15.80 HCCO	12.48 HBHC 12.45 HAHC			
FORCE CONSTANTS-		73.93 HC6H 23.38 OCH				
OFF DIAGONAL -		NONE				
NORMAL MODE 6		OBSERVED= 1465.8 CM-1	CALCULATED= 1469.3 CM-1	ERROR= -3.5 CM-1	OR	-0.2 PERCENT
INTERNAL COORDINATES-		38.07 HAHB 38.04 HBHC	10.97 HBHC 10.96 HACO			
FORCE CONSTANTS-		76.11 HC6H 21.93 OCH				
OFF DIAGONAL -		NONE				
NORMAL MODE 7		OBSERVED= 1451.4 CM-1	CALCULATED= 1453.8 CM-1	ERROR= -2.4 CM-1	OR	-0.2 PERCENT
INTERNAL COORDINATES-		23.72 HCCO 23.00 HBHC	22.99 HACO 14.42 HAHB 13.50 HBHC	13.49 HAHC		
FORCE CONSTANTS-		69.71 OCH 41.41 HC6H				
OFF DIAGONAL -		-10.68 SB22 -6.11 BB33	2.54 BB33			
NORMAL MODE 8		OBSERVED= 1227.3 CM-1	CALCULATED= 1218.3 CM-1	ERROR= 9.0 CM-1	OR	0.7 PERCENT
INTERNAL COORDINATES-		34.44 HCCO 16.40 HOC	14.86 HAHB 9.06 HACO	9.05 HBHC		
FORCE CONSTANTS-		52.55 OCH 22.74 HC6H	16.40 COH			
OFF DIAGONAL -		5.67 BB32 2.30 BB33				
NORMAL MODE 9		OBSERVED= 1160.0 CM-1	CALCULATED= 1159.3 CM-1	ERROR= 0.7 CM-1	OR	0.1 PERCENT
INTERNAL COORDINATES-		36.79 HBHC 36.78 HACO	11.81 HBHC 11.81 HAHC			
FORCE CONSTANTS-		73.57 OCH 23.62 HC6H				
OFF DIAGONAL -		3.22 BB33				
NORMAL MODE 10		OBSERVED= 1042.8 CM-1	CALCULATED= 1048.6 CM-1	ERROR= -5.8 CM-1	OR	-0.5 PERCENT
INTERNAL COORDINATES-		103.10 C-O 5.09 HOC				
FORCE CONSTANTS-		103.10 C-O 5.09 COH				
OFF DIAGONAL -		-8.46 SB22 -5.73 SB21				
NORMAL MODE 11		OBSERVED= 864.9 CM-1	CALCULATED= 864.4 CM-1	ERROR= 0.5 CM-1	OR	0.1 PERCENT
INTERNAL COORDINATES-		80.68 HOC 13.30 HCCO				
FORCE CONSTANTS-		80.68 COH 17.08 OCH				
OFF DIAGONAL -		-7.82 BB32 4.06 SB21				
NORMAL MODE 12		OBSERVED= 0.0 CM-1	CALCULATED= 190.6 CM-1	ERROR= 0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-		99.97 T				
FORCE CONSTANTS-		99.97 TC-O				
OFF DIAGONAL -		NONE				
7. EXPERIMENTAL FREQUENCIES				AVERAGE ERROR = 3.49		

TABLE I, (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 200	PAGE	1
MOLECULE 6 -6 NG= 79 METHANOL, CH3O(18)D		
NORMAL MODE 5 OBSERVED= 1472.7 CM-1 CALCULATED= 1469.2 CM-1	3.5 CM-1	OR
INTERNAL COORDINATES- 49.16 HAHB 15.66 HCCO 12.68 HBHC 12.68 HAHC		
FORCE CONSTANTS- 74.52 HC6H 22.93 OCH		
OFF DIAGONAL - NONE		
ERROR=		0.2 PERCENT
NORMAL MODE 6 OBSERVED= 1465.8 CM-1 CALCULATED= 1468.6 CM-1	-2.8 CM-1	OR
INTERNAL COORDINATES- 38.24 HAHB 38.23 HBHC 10.79 HACO 10.79 HBHC		
FORCE CONSTANTS- 76.47 HC6H 21.59 OCH		
OFF DIAGONAL - NONE		
ERROR=		-0.2 PERCENT
NORMAL MODE 7 OBSERVED= 1451.4 CM-1 CALCULATED= 1453.4 CM-1	-2.0 CM-1	OR
INTERNAL COORDINATES- 23.63 HCCO 23.10 HBHC 23.10 HACO 14.73 HAHB 13.38 HBHC 13.38 HAHC		
FORCE CONSTANTS- 69.82 OCH 41.48 HC6H		
OFF DIAGONAL - -11.13 SB22 -6.12 BB33 2.54 BB38		
ERROR=		-0.1 PERCENT
NORMAL MODE 8 OBSERVED= 1227.3 CM-1 CALCULATED= 1212.2 CM-1	15.1 CM-1	OR
INTERNAL COORDINATES- 35.44 HCCO 15.08 HOC 14.47 HAHB 9.62 HACO 9.61 HBHC		
FORCE CONSTANTS- 54.67 OCH 22.45 HC6H 15.08 COH		
OFF DIAGONAL - 5.52 BB32 2.39 BB33		
ERROR=		1.2 PERCENT
NORMAL MODE 9 OBSERVED= 0.0 CM-1 CALCULATED= 1156.6 CM-1	0.0 CM-1	OR
INTERNAL COORDINATES- 36.96 HBHC 36.95 HACO 11.63 HBHC 11.63 HAHC		
FORCE CONSTANTS- 73.91 OCH 23.27 HC6H		
OFF DIAGONAL - 3.24 BB33		
ERROR=		0.0 PERCENT
NORMAL MODE 10 OBSERVED= 1017.3 CM-1 CALCULATED= 1020.7 CM-1	-3.4 CM-1	OR
INTERNAL COORDINATES- 104.28 C-0 5.19 HOC		
FORCE CONSTANTS- 104.28 C-0 5.19 COH		
OFF DIAGONAL - -8.10 SB22 -5.82 SB21		
ERROR=		-0.3 PERCENT
NORMAL MODE 11 OBSERVED= 860.9 CM-1 CALCULATED= 862.6 CM-1	-1.7 CM-1	OR
INTERNAL COORDINATES- 81.95 HOC 12.93 HCCO		
FORCE CONSTANTS- 81.95 COH 16.64 OCH		
OFF DIAGONAL - -7.77 BB32 3.73 SB21		
ERROR=		-0.2 PERCENT
NORMAL MODE 12 OBSERVED= 0.0 CM-1 CALCULATED= 189.6 CM-1	0.0 CM-1	OR
INTERNAL COORDINATES- 99.97 T		
FORCE CONSTANTS- 99.97 TC-0		
OFF DIAGONAL - NONE		
ERROR=		0.0 PERCENT

6. EXPERIMENTAL FREQUENCIES AVERAGE ERROR = 4.76

TABLE L (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR	PROBLEM 200	PAGE 1
MOLECULE 3	METHANOL, CD3OH	
	-6 NG= 79	
NORMAL MODE 5	OBSERVED= 1293.3 CM-1	
INTERNAL COORDINATES-	87.78 HOC 5.69 HCCO	
FORCE CONSTANTS-	87.78 COH 6.86 OCH	
OFF DIAGONAL -	5.34 8832 -3.60 8821	
		ERROR= -0.9 CM-1 OR -0.1 PERCENT
	CALCULATED= 1294.2 CM-1	
NORMAL MODE 6	OBSERVED= 1132.7 CM-1	
INTERNAL COORDINATES-	43.79 C-O 21.50 HACO	
FORCE CONSTANTS-	59.64 OCH 43.79 C-O	
OFF DIAGONAL -	-38.30 8822 -5.20 8833 2.16 8838	
		ERROR= 10.9 CM-1 OR 1.0 PERCENT
	CALCULATED= 1121.8 CM-1	
NORMAL MODE 7	OBSERVED= 1055.0 CM-1	
INTERNAL COORDINATES-	39.56 HBHC 39.54 HAHC	
FORCE CONSTANTS-	79.11 HC6H 18.99 OCH	
OFF DIAGONAL -	NONE	
		ERROR= 8.3 CM-1 OR 0.8 PERCENT
	CALCULATED= 1046.7 CM-1	
NORMAL MODE 8	OBSERVED= 0.0 CM-1	
INTERNAL COORDINATES-	55.98 HAHC 14.14 HAHC	
FORCE CONSTANTS-	84.22 HC6H 13.70 OCH	
OFF DIAGONAL -	NONE	
		ERROR= 0.0 CM-1 OR 0.0 PERCENT
	CALCULATED= 1043.9 CM-1	
NORMAL MODE 9	OBSERVED= 988.0 CM-1	
INTERNAL COORDINATES-	63.42 C-O 5.92 HCCO	
FORCE CONSTANTS-	63.42 C-O 11.37 OCH	
OFF DIAGONAL -	19.80 8822	
		ERROR= 5.9 CM-1 OR 0.6 PERCENT
	CALCULATED= 982.1 CM-1	
NORMAL MODE 10	OBSERVED= 894.7 CM-1	
INTERNAL COORDINATES-	37.88 HACO 37.88 HBHC	
FORCE CONSTANTS-	75.76 OCH 19.98 HC6H	
OFF DIAGONAL -	3.32 8833	
		ERROR= -8.3 CM-1 OR -0.9 PERCENT
	CALCULATED= 903.0 CM-1	
NORMAL MODE 11	OBSERVED= 865.8 CM-1	
INTERNAL COORDINATES-	49.94 HCCO 12.46 HOC	
FORCE CONSTANTS-	74.60 OCH 14.72 HC6H	
OFF DIAGONAL -	-5.96 8832 3.27 8833	
		ERROR= 7.1 CM-1 OR 0.8 PERCENT
	CALCULATED= 858.7 CM-1	
NORMAL MODE 12	OBSERVED= 0.0 CM-1	
INTERNAL COORDINATES-	99.92 T	
FORCE CONSTANTS-	99.92 TC-O	
OFF DIAGONAL -	NONE	
		ERROR= 0.0 CM-1 OR 0.0 PERCENT
	CALCULATED= 227.4 CM-1	

9. EXPERIMENTAL FREQUENCIES AVERAGE ERROR = 4.66

TABLE L (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 200				PAGE 1	
MOLECULE 4	-6	NG= 79	METHANOL, CD30D		
NORMAL MODE 5	OBSERVED= 1132.7 CM-1	CALCULATED= 1128.8 CM-1	ERROR= 3.9 CM-1	OR	0.3 PERCENT
INTERNAL COORDINATES-	49.84 C-O 27.63 HCCO	13.00 HBCH 13.00 HACO	10.59 HBCH 10.59 HAHB	9.60 HAHB	5.78 HOC
FORCE CONSTANTS-	53.62 OCH 49.84 C-O 30.78 HC6H	5.78 COH			
OFF DIAGONAL-	-38.15 SB22 -4.46 BB33	-4.25 SB21 3.02 BB32	1.89 BB38		
NORMAL MODE 6	OBSERVED= 1068.1 CM-1	CALCULATED= 1066.7 CM-1	ERROR= 1.4 CM-1	OR	0.1 PERCENT
INTERNAL COORDINATES-	29.14 HOC 18.01 HAHB	17.38 HBCH 17.38 HACO	10.45 HCCO		
FORCE CONSTANTS-	45.22 OCH 29.14 COH	18.05 HC6H			
OFF DIAGONAL-	4.17 BB32 1.81 SB22				
NORMAL MODE 7	OBSERVED= 1055.2 CM-1	CALCULATED= 1046.7 CM-1	ERROR= 8.5 CM-1	OR	0.8 PERCENT
INTERNAL COORDINATES-	39.56 HBCH 39.55 HAHB	9.49 HACO	9.49 HBCH		
FORCE CONSTANTS-	79.11 HC6H 18.99 OCH				
OFF DIAGONAL -	NONE				
NORMAL MODE 8	OBSERVED= 1031.3 CM-1	CALCULATED= 1033.7 CM-1	ERROR= -2.4 CM-1	OR	-0.2 PERCENT
INTERNAL COORDINATES-	40.71 HAHB 18.32 HAHB	18.31 HBCH 17.24 HOC			
FORCE CONSTANTS-	77.33 HC6H 17.24 COH				
OFF DIAGONAL-	1.92 SB22 -1.63 SB21				
NORMAL MODE 9	OBSERVED= 983.4 CM-1	CALCULATED= 970.2 CM-1	ERROR= 13.2 CM-1	OR	1.3 PERCENT
INTERNAL COORDINATES-	55.63 C-O 15.91 HCCO	6.72 HAHB			
FORCE CONSTANTS-	55.63 C-O 16.19 OCH	7.28 HC6H			
OFF DIAGONAL-	15.32 SB22 2.21 SB21				
NORMAL MODE 10	OBSERVED= 894.7 CM-1	CALCULATED= 903.0 CM-1	ERROR= -8.3 CM-1	OR	-0.9 PERCENT
INTERNAL COORDINATES-	37.88 HACO 37.88 HBCH	9.99 HBCH 9.99 HAHB			
FORCE CONSTANTS-	75.76 OCH 19.98 HC6H				
OFF DIAGONAL-	3.32 BB33				
NORMAL MODE 11	OBSERVED= 775.8 CM-1	CALCULATED= 776.0 CM-1	ERROR= -0.2 CM-1	OR	-0.0 PERCENT
INTERNAL COORDINATES-	48.48 HOC 32.06 HCCO	8.14 HBCH 5.00 HAHB			
FORCE CONSTANTS-	48.48 COH 48.34 OCH	7.58 HC6H			
OFF DIAGONAL-	-9.41 BB32 2.12 BB33	1.73 SB21			
NORMAL MODE 12	OBSERVED= 0.0 CM-1	CALCULATED= 174.6 CM-1	ERROR= 0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	99.92 T				
FORCE CONSTANTS-	99.92 TC-O				
OFF DIAGONAL -	NONE				

AVERAGE ERROR = 4.36

9. EXPERIMENTAL FREQUENCIES

TABLE LI

POTENTIAL ENERGY DISTRIBUTION FOR LIQUID METHANOL

Explanation of the table:

This table is presented in the same format as Table XXXIV except that the force constant and internal coordinate description codes are found in Tables XLIII and XLIV, respectively.

TABLE LI

POTENTIAL ENERGY DISTRIBUTION FOR LIQUID METHANOL

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 200	PAGE 1
MOLECULE 1 -6 NG= 79 METHANOL, CH3OH	
NORMAL MODE 5 OBSERVED= 1480.0 CM-1 CALCULATED= 1472.7 CM-1 ERROR= 7.0 CM-1 OR 0.5 PERCENT	
INTERNAL COORDINATES- 64.06 HAHB 14.67 HAHB 14.46 HBHC 6.08 HCCO	
FORCE CONSTANTS- 92.93 HC6H 10.69 OCH	
OFF DIAGONAL- -3.44 BB38	
NORMAL MODE 6 OBSERVED= 1469.0 CM-1 CALCULATED= 1473.0 CM-1 ERROR= -3.7 CM-1 OR -0.3 PERCENT	
INTERNAL COORDINATES- 46.57 HBHC 46.36 HAHB 5.36 HACO 5.33 HBHC	
FORCE CONSTANTS- 93.19 HC6H 10.39 OCH	
OFF DIAGONAL- -3.40 BB38	
NORMAL MODE 7 OBSERVED= 1455.0 CM-1 CALCULATED= 1456.8 CM-1 ERROR= -1.8 CM-1 OR -0.1 PERCENT	
INTERNAL COORDINATES- 30.63 HCCO 17.11 HBHC 17.11 HACO 13.51 HBHC 13.51 HAHB 7.35 HOC	
FORCE CONSTANTS- 64.85 OCH 40.04 HC6H 7.35 COH	
OFF DIAGONAL- -11.03 BB38-10.19 SB22 3.97 BB33 2.66 BB32	
NORMAL MODE 8 OBSERVED= 1420.0 CM-1 CALCULATED= 1419.5 CM-1 ERROR= 0.5 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES- 75.31 HOC 8.83 HACO 8.82 HBHC	
FORCE CONSTANTS- 75.31 COH 19.41 OCH 5.41 HC6H	
OFF DIAGONAL- 2.04 BB32 -1.78 BB31	
NORMAL MODE 9 OBSERVED= 1162.0 CM-1 CALCULATED= 1164.2 CM-1 ERROR= -2.2 CM-1 OR -0.2 PERCENT	
INTERNAL COORDINATES- 46.28 HACO 46.28 HBHC	
FORCE CONSTANTS- 92.57 OCH 7.05 HC6H	
OFF DIAGONAL- -2.92 BB33 2.79 BB38	
NORMAL MODE 10 OBSERVED= 1112.0 CM-1 CALCULATED= 1109.5 CM-1 ERROR= 2.5 CM-1 OR 0.2 PERCENT	
INTERNAL COORDINATES- 53.92 HCCO 19.43 HOC 12.86 HBHC 12.86 HACO	
FORCE CONSTANTS- 79.64 OCH 19.43 COH 5.89 HC6H	
OFF DIAGONAL- -5.74 BB32 -2.51 BB33 2.36 BB38	
NORMAL MODE 11 OBSERVED= 1029.0 CM-1 CALCULATED= 1036.7 CM-1 ERROR= -7.7 CM-1 OR -0.8 PERCENT	
INTERNAL COORDINATES- 109.47 C-O	
FORCE CONSTANTS- 109.47 C-O	
OFF DIAGONAL- -10.92 SB22 -2.48 SB21	
NORMAL MODE 12 OBSERVED= 0.0 CM-1 CALCULATED= 240.0 CM-1 ERROR= 0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES- 99.97 T	
FORCE CONSTANTS- 99.97 TC-O	
OFF DIAGONAL - NONE	

7. EXPERIMENTAL FREQUENCIES AVERAGE ERROR = 3.63

TABLE II (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 200	PAGE	1
MOLECULE 2	-6 NG= 79	METHANOL, CH300
NORMAL MODE 5	OBSERVED= 1472.0 CM-1	CALCULATED= 1472.5 CM-1
INTERNAL COORDINATES-	64.10 HAHB 14.75 HAHB	14.33 HBHC 6.06 HCCO
FORCE CONSTANTS-	92.93 HC6H 10.69 OCH	
OFF DIAGONAL-	-3.44 BB38	
		ERROR= -1.0 CM-1 OR -0.1 PERCENT
NORMAL MODE 6	OBSERVED= 1469.0 CM-1	CALCULATED= 1473.0 CM-1
INTERNAL COORDINATES-	46.68 HBHC 46.25 HAHB	5.37 HACO 5.32 HBCC
FORCE CONSTANTS-	93.18 HC6H 10.39 OCH	
OFF DIAGONAL-	-3.40 BB38	
		ERROR= -3.5 CM-1 OR -0.2 PERCENT
NORMAL MODE 7	OBSERVED= 1452.0 CM-1	CALCULATED= 1453.2 CM-1
INTERNAL COORDINATES-	25.04 HCCO 22.84 HBCC	22.84 HACO 15.84 HBHC 15.84 HAHB
FORCE CONSTANTS-	70.71 OCH 44.63 HC6H	
OFF DIAGONAL-	-12.27 BB38-10.29 SB22	4.46 BB33
		ERROR= -1.2 CM-1 OR -0.1 PERCENT
NORMAL MODE 8	OBSERVED= 1235.0 CM-1	CALCULATED= 1232.1 CM-1
INTERNAL COORDINATES-	43.12 HCCO 24.84 HOC	11.17 HBCC 11.17 HACO
FORCE CONSTANTS-	65.47 OCH 24.84 COH	
OFF DIAGONAL-	5.80 BB32 -2.07 BB33	1.92 BB38 -1.69 SB21
		ERROR= 2.9 CM-1 OR 0.2 PERCENT
NORMAL MODE 9	OBSERVED= 1162.0 CM-1	CALCULATED= 1164.2 CM-1
INTERNAL COORDINATES-	46.28 HACO 46.28 HBCC	
FORCE CONSTANTS-	92.57 OCH 7.05 HC6H	
OFF DIAGONAL-	-2.92 BB33 2.79 BB38	
		ERROR= -2.2 CM-1 OR -0.2 PERCENT
NORMAL MODE 10	OBSERVED= 1038.0 CM-1	CALCULATED= 1039.0 CM-1
INTERNAL COORDINATES-	103.05 C-O 8.96 HOC	
FORCE CONSTANTS-	103.05 C-O 8.96 COH	5.98 OCH
OFF DIAGONAL-	-9.67 SB22 -9.54 SB21	
		ERROR= -1.0 CM-1 OR -0.1 PERCENT
NORMAL MODE 11	OBSERVED= 942.0 CM-1	CALCULATED= 942.6 CM-1
INTERNAL COORDINATES-	68.81 HOC 17.98 HCCO	5.72 C-O
FORCE CONSTANTS-	68.81 COH 23.48 OCH	5.72 C-O
OFF DIAGONAL-	-6.23 BB32 6.22 SB21	
		ERROR= -0.6 CM-1 OR -0.1 PERCENT
NORMAL MODE 12	OBSERVED= 0.0 CM-1	CALCULATED= 190.6 CM-1
INTERNAL COORDINATES-	99.97 T	
FORCE CONSTANTS-	99.97 TC-O	
OFF DIAGONAL-	NONE	
		ERROR= 0.0 CM-1 OR 0.0 PERCENT

7. EXPERIMENTAL FREQUENCIES AVERAGE ERROR = 1.78

TABLE II (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 200			PAGE 1	
MOLECULE 3	-6 NG= 79	METHANOL, CD3OH		
NORMAL MODE 5	OBSERVED= 1391.0 CM-1	CALCULATED= 1391.8 CM-1	ERROR= -0.8 CM-1	OR -0.1 PERCENT
INTERNAL COORDINATES-	94.57 HOC			
FORCE CONSTANTS-	94.57 COH			
OFF DIAGONAL-	2.52 BB32 -2.39 SB21			
NORMAL MODE 6	OBSERVED= 1122.0 CM-1	CALCULATED= 1117.1 CM-1	ERROR= 4.9 CM-1	OR 0.4 PERCENT
INTERNAL COORDINATES-	42.19 C-O 21.09 HACO	21.09 HBCO 20.64 HCCO 13.70 HBHC 13.70 HAHC 12.21 HAHB		
FORCE CONSTANTS-	62.82 OCH 42.19 C-O 39.61 HC6H			
OFF DIAGONAL-	-39.26 SB22-10.90 BB38 3.97 BB33			
NORMAL MODE 7	OBSERVED= 1060.0 CM-1	CALCULATED= 1058.3 CM-1	ERROR= 1.8 CM-1	OR 0.2 PERCENT
INTERNAL COORDINATES-	48.88 HBHC 48.77 HAHC			
FORCE CONSTANTS-	97.65 HC6H			
OFF DIAGONAL-	-2.10 BB38			
NORMAL MODE 8	OBSERVED= 0.0 CM-1	CALCULATED= 1057.2 CM-1	ERROR= 0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	66.03 HAHB 15.30 HAHC			
FORCE CONSTANTS-	96.53 HC6H 5.11 OCH			
OFF DIAGONAL-	-2.42 BB38			
NORMAL MODE 9	OBSERVED= 982.0 CM-1	CALCULATED= 979.5 CM-1	ERROR= 2.5 CM-1	OR 0.3 PERCENT
INTERNAL COORDINATES-	68.39 C-O			
FORCE CONSTANTS-	68.39 C-O 9.26 OCH 5.85 HC6H			
OFF DIAGONAL-	19.07 SB22 -2.27 SB21 -1.60 BB38			
NORMAL MODE 10	OBSERVED= 898.0 CM-1	CALCULATED= 898.8 CM-1	ERROR= -0.8 CM-1	OR -0.1 PERCENT
INTERNAL COORDINATES-	49.36 HBCO 49.35 HACO			
FORCE CONSTANTS-	98.71 OCH			
OFF DIAGONAL-	-3.12 BB33			
NORMAL MODE 11	OBSERVED= 0.0 CM-1	CALCULATED= 868.4 CM-1	ERROR= 0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	62.81 HCCO 15.88 HBHC	15.88 HACO 6.51 HOC		
FORCE CONSTANTS-	94.57 OCH 6.51 COH			
OFF DIAGONAL-	-3.58 BB32 -2.98 BB33 1.55 BB38			
NORMAL MODE 12	OBSERVED= 0.0 CM-1	CALCULATED= 227.4 CM-1	ERROR= 0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	99.91 T			
FORCE CONSTANTS-	99.91 TC-O			
OFF DIAGONAL -	NONE			
5. EXPERIMENTAL FREQUENCIES			AVERAGE ERROR = 2.16	

TABLE II (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 200	PAGE	1
MOLECULE 4 -6 NG= 79 METHANOL, CD300		
NORMAL MODE 5 OBSERVED= 1124.0 CM-1 CALCULATED= 1121.8 CM-1 ERROR= 2.3 CM-1 OR 0.2 PERCENT		
INTERNAL COORDINATES- 44.08 C-O 27.96 HCCO 17.87 HAHB 16.90 HOC 10.73 HACO 10.73 HBCCO 6.68 HBHC 6.68 HAHC		
FORCE CONSTANTS- 49.41 OCH 44.08 C-O 31.23 HC6H 16.90 COH		
OFF DIAGONAL- -34.60 SB22 -8.57 SB21 -7.86 BB38 3.85 BB32 2.86 BB33		
NORMAL MODE 6 OBSERVED= 1097.0 CM-1 CALCULATED= 1098.8 CM-1 ERROR= -1.8 CM-1 OR -0.2 PERCENT		
INTERNAL COORDINATES- 47.22 HOC 12.97 HACO 12.97 HBCCO 12.43 HBHC 12.43 HAHC		
FORCE CONSTANTS- 47.22 COH 26.90 HC6H 25.96 OCH		
OFF DIAGONAL- -3.26 SB22 2.25 SB21 -1.71 BB31 -1.57 BB38		
NORMAL MODE 7 OBSERVED= 1060.0 CM-1 CALCULATED= 1058.3 CM-1 ERROR= 1.8 CM-1 OR 0.2 PERCENT		
INTERNAL COORDINATES- 48.83 HBHC 48.82 HAHC		
FORCE CONSTANTS- 97.65 HC6H		
OFF DIAGONAL- -2.10 BB38		
NORMAL MODE 8 OBSERVED= 0.0 CM-1 CALCULATED= 1051.6 CM-1 ERROR= 0.0 CM-1 OR 0.0 PERCENT		
INTERNAL COORDINATES- 59.02 HAHB 9.98 HAHC 9.97 HBHC 7.83 HOC 6.42 HCCO		
FORCE CONSTANTS- 78.98 HC6H 15.47 OCH 7.83 COH		
OFF DIAGONAL- -3.85 BB38		
NORMAL MODE 9 OBSERVED= 979.0 CM-1 CALCULATED= 970.8 CM-1 ERROR= 8.3 CM-1 OR 0.8 PERCENT		
INTERNAL COORDINATES- 64.42 C-O 11.81 HCCO		
FORCE CONSTANTS- 64.42 C-O 12.68 OCH		
OFF DIAGONAL- 16.81 SB22		
NORMAL MODE 10 OBSERVED= 898.0 CM-1 CALCULATED= 898.8 CM-1 ERROR= -0.8 CM-1 OR -0.1 PERCENT		
INTERNAL COORDINATES- 49.35 HACO 49.35 HBCCO		
FORCE CONSTANTS- 98.71 OCH		
OFF DIAGONAL- -3.12 BB33		
NORMAL MODE 11 OBSERVED= 818.0 CM-1 CALCULATED= 814.4 CM-1 ERROR= 3.6 CM-1 OR 0.4 PERCENT		
INTERNAL COORDINATES- 46.33 HCCO 30.12 HOC 12.44 HBCCO 12.44 HACO		
FORCE CONSTANTS- 71.21 OCH 30.12 COH		
OFF DIAGONAL- -6.62 BB32 -2.25 BB33		
NORMAL MODE 12 OBSERVED= 0.0 CM-1 CALCULATED= 174.6 CM-1 ERROR= 0.0 CM-1 OR 0.0 PERCENT		
INTERNAL COORDINATES- 99.92 T		
FORCE CONSTANTS- 99.92 TC-O		
OFF DIAGONAL - NONE		

6. EXPERIMENTAL FREQUENCIES AVERAGE ERROR = 3.07

TABLE LII

POTENTIAL ENERGY DISTRIBUTIONS FOR GASEOUS ETHANOL (TRANS)

Explanation of the table:

This table is presented in the same format as Table XXXIV except that the force constant and internal coordinate description codes are found in Tables XLIII and XLIV, respectively.

TABLE LII

POTENTIAL ENERGY DISTRIBUTIONS FOR GASEOUS ETHANOL (TRANS)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 300					PAGE 1	
MOLECULE 1		-6 NG= 202		ETHANOL, CH3CHDOH (TRANS)		
NORMAL MODE 7	OBSERVED=	1465.0 CM-1	CALCULATED=	1458.8 CM-1	ERROR=	6.1 CM-1 OR 0.4 PERCENT
INTERNAL COORDINATES-	50.08	H7H8 15.28 H8H9	8.93	H7H9 7.48 CCH9		
FORCE CONSTANTS-	74.29	HC6H 11.87 CC6H				
OFF DIAGONAL-	5.52	BB40 4.82 BB34				
NORMAL MODE 8	OBSERVED=	1448.0 CM-1	CALCULATED=	1454.8 CM-1	ERROR=	-6.8 CM-1 OR -0.5 PERCENT
INTERNAL COORDINATES-	42.26	H7H9 35.74 H8H9	5.57	CCH8		
FORCE CONSTANTS-	78.26	HC6H 10.33 CC6H				
OFF DIAGONAL-	5.35	BB40 5.09 BB34				
NORMAL MODE 9	OBSERVED=	1384.0 CM-1	CALCULATED=	1384.0 CM-1	ERROR=	0.0 CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	17.91	CCH7 16.59 CCH8	15.26	H8H9 14.73 H7H9 13.23	CCH9 11.77 C-C 8.46	H7H8
FORCE CONSTANTS-	47.73	CC6H 38.45 HC6H	11.77	C-C 5.15 OCH		
OFF DIAGONAL-	15.88	BB40-11.95 SB24	-5.95	BB35 -4.88 BB34 -3.11	SB25 2.00	BB37
NORMAL MODE 10	OBSERVED=	1347.0 CM-1	CALCULATED=	1357.1 CM-1	ERROR=	-10.1 CM-1 OR -0.8 PERCENT
INTERNAL COORDINATES-	32.96	UCH5 32.26 H5CC	12.81	HOC 5.12 C-C		
FORCE CONSTANTS-	35.32	CC3H 35.11 OCH	12.81	COH 5.85 CC6H 5.47	HC6H 5.12 C-C	
OFF DIAGONAL-	-6.41	SB25 -5.72 SB22	4.16	BB40 -2.83 BB31 2.66	SB24 2.64 SB21 -1.84	BB35 1.52 BB33
NORMAL MODE 11	OBSERVED=	1332.0 CM-1	CALCULATED=	1334.0 CM-1	ERROR=	-2.0 CM-1 OR -0.1 PERCENT
INTERNAL COORDINATES-	59.47	HCH 31.88 UCH5				
FORCE CONSTANTS-	59.47	HC3H 33.07 OCH				
OFF DIAGONAL-	-4.20	BB38 2.60 BB40	-2.25	SB22		
NORMAL MODE 12	OBSERVED=	1243.0 CM-1	CALCULATED=	1236.5 CM-1	ERROR=	6.5 CM-1 OR 0.5 PERCENT
INTERNAL COORDINATES-	60.86	HOC 12.98 H5CC	6.56	HCH		
FORCE CONSTANTS-	60.86	COH 13.17 CC3H	6.56	HC3H		
OFF DIAGONAL-	3.56	SB21 2.60 SB25				
NORMAL MODE 13	OBSERVED=	1132.0 CM-1	CALCULATED=	1120.8 CM-1	ERROR=	11.2 CM-1 OR 1.0 PERCENT
INTERNAL COORDINATES-	51.63	C-O 16.33 CCH9	15.04	HOC 8.57 OCH4 6.83	H7H8 5.60 H4CC	
FORCE CONSTANTS-	51.63	C-O 20.40 CC6H	15.04	COH 10.99 OCH 7.95	HC6H 5.61 CC3H	
OFF DIAGONAL-	-11.46	SB21 -7.26 SB23	-4.38	SB22 -2.25 BB40 -1.82	SB25 1.60	BB44
NORMAL MODE 14	OBSERVED=	1046.0 CM-1	CALCULATED=	1043.3 CM-1	ERROR=	2.7 CM-1 OR 0.3 PERCENT
INTERNAL COORDINATES-	27.18	CCH7 20.10 C-C	10.78	H4CC 7.71 CCH9 6.81	HOC 6.00 CCH8 5.86	H8H9
FORCE CONSTANTS-	40.89	CC6H 20.10 C-C	12.64	CC3H 8.85 HC6H 6.81	COH	
OFF DIAGONAL-	-3.28	SB25 -3.22 BB40	3.05	BB37 3.05 BB35 -2.83	SB26 1.54	BB44
NORMAL MODE 15	OBSERVED=	1021.0 CM-1	CALCULATED=	1009.7 CM-1	ERROR=	11.3 CM-1 OR 1.1 PERCENT
INTERNAL COORDINATES-	29.84	CCH8 23.23 C-C	10.12	CCH9 5.82 H7H9 5.53	C-O	
FORCE CONSTANTS-	44.63	CC6H 23.23 C-C	8.53	HC6H 5.53 C-O		
OFF DIAGONAL-	-3.48	BB40 2.83 BB35	-2.35	SB26 -2.16 SB21 1.91	BB37 1.91 SB25 1.78	SB23
NORMAL MODE 16	OBSERVED=	940.0 CM-1	CALCULATED=	939.1 CM-1	ERROR=	0.9 CM-1 OR 0.1 PERCENT
INTERNAL COORDINATES-	57.68	UCH4 16.03 C-O	12.14	H4CC 5.04 UCH5		
FORCE CONSTANTS-	62.72	UCH 16.03 C-O	12.14	CC3H		
OFF DIAGONAL-	9.48	SB22 -3.08 BB33				
NORMAL MODE 17	OBSERVED=	865.0 CM-1	CALCULATED=	860.9 CM-1	ERROR=	4.1 CM-1 OR 0.5 PERCENT
INTERNAL COORDINATES-	35.26	C-O 34.32 C-C	16.81	CCH9 6.48 OCH4 5.90	CCH7	
FORCE CONSTANTS-	35.26	C-O 34.32 C-C	24.16	CC6H 6.53 OCH		
OFF DIAGONAL-	-7.24	SB22 4.77 SB25	-2.75	SB23 1.85 SS20 -1.81	BB40 -1.75	SB26
NORMAL MODE 18	OBSERVED=	716.0 CM-1	CALCULATED=	710.9 CM-1	ERROR=	5.1 CM-1 OR 0.7 PERCENT
INTERNAL COORDINATES-	35.20	H4CC 20.47 H5CC	11.39	CCH7 10.92 CCH8 9.03	UCH5 8.50 OCH4	
FORCE CONSTANTS-	55.67	CC3H 22.32 CC6H	17.54	UCH		
OFF DIAGONAL-	-7.02	BB37 4.62 BB35	-1.58	BB33		
NORMAL MODE 19	OBSERVED=	427.0 CM-1	CALCULATED=	428.8 CM-1	ERROR=	-1.8 CM-1 OR -0.4 PERCENT
INTERNAL COORDINATES-	87.55	UCC 6.90 CCH9	5.35	H4CC 5.07 CCH8		
FORCE CONSTANTS-	87.55	CCD 16.40 CC6H	8.73	CC3H		
OFF DIAGONAL-	-11.31	BB44 -3.93 BB45	3.28	SB26 -1.83 BB37 -1.77	SB25 -1.71	SB23
NORMAL MODE 20	OBSERVED=	0.0 CM-1	CALCULATED=	245.1 CM-1	ERROR=	0.0 CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	98.46	T-CC				
FORCE CONSTANTS-	98.46	TC-C				
OFF DIAGONAL -	NONE					
NORMAL MODE 21	OBSERVED=	0.0 CM-1	CALCULATED=	207.9 CM-1	ERROR=	0.0 CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	98.90	T-CO				
FORCE CONSTANTS-	98.90	TC-O				
OFF DIAGONAL -	NONE					

13. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 5.28

TABLE LII (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 300
 MOLECULE 2 -6 NG= 202 ETHANOL, CH3CHDO (TRANS)

PAGE 1

NORMAL MODE 7	OBSERVED= 1465.0 CM-1	CALCULATED= 1458.8 CM-1	ERROR= 6.2 CM-1 OR 0.4 PERCENT
INTERNAL COORDINATES-	50.12 H7H8 15.41 H8H9	8.86 H7H9 7.48 CCH9	
FORCE CONSTANTS-	74.38 HC6H 11.86 CC6H		
OFF DIAGONAL-	5.53 BB40 4.83 BB34		
NORMAL MODE 8	OBSERVED= 1448.0 CM-1	CALCULATED= 1454.8 CM-1	ERROR= -6.8 CM-1 OR -0.5 PERCENT
INTERNAL COORDINATES-	42.35 H7H9 35.62 H8H9	5.59 CCH8	
FORCE CONSTANTS-	78.26 HC6H 10.33 CC6H		
OFF DIAGONAL-	5.35 BB40 5.09 BB34		
NORMAL MODE 9	OBSERVED= 1386.0 CM-1	CALCULATED= 1383.5 CM-1	ERROR= 2.5 CM-1 OR 0.2 PERCENT
INTERNAL COORDINATES-	18.41 CCH7 17.33 CCH8	15.53 H8H9 15.13 H7H9 13.93 CCH9 10.24 C-C 9.23 H7H8	
FORCE CONSTANTS-	49.67 CC6H 39.90 HC6H	10.24 C-C	
OFF DIAGONAL-	16.47 BB40-11.38 SB24	-6.13 BB35 -5.08 BB34 -2.27 SB25 1.60 BB37	
NORMAL MODE 10	OBSERVED= 1348.0 CM-1	CALCULATED= 1347.3 CM-1	ERROR= 0.7 CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	58.31 OCH5 30.96 H5CC		
FORCE CONSTANTS-	61.01 OCH 32.84 CC3H		
OFF DIAGONAL-	-7.96 SB22 -4.61 SB25	2.27 BB33 1.72 SB24	
NORMAL MODE 11	OBSERVED= 1336.0 CM-1	CALCULATED= 1328.8 CM-1	ERROR= 7.1 CM-1 OR 0.5 PERCENT
INTERNAL COORDINATES-	68.33 HCH 12.33 H5CC	9.24 OCH5	
FORCE CONSTANTS-	68.33 HC3H 14.35 CC3H	9.71 OCH	
OFF DIAGONAL-	7.14 BB40 -3.15 SB25	-2.49 BB38	
NORMAL MODE 12	OBSERVED= 1110.0 CM-1	CALCULATED= 1141.5 CM-1	ERROR= -31.5 CM-1 OR -2.8 PERCENT
INTERNAL COORDINATES-	41.56 C-O 22.62 C-C	13.67 OCH4 8.41 H4CC 6.12 CCH9	
FORCE CONSTANTS-	41.56 C-O 22.62 C-C	16.03 OCH 11.13 CC3H 8.59 CC6H	
OFF DIAGONAL-	-6.18 SB22 2.85 SB21	-2.26 SB25 -1.74 SB23 -1.63 SS20 1.62 SB24	
NORMAL MODE 13	OBSERVED= 1066.0 CM-1	CALCULATED= 1080.4 CM-1	ERROR= -14.4 CM-1 OR -1.3 PERCENT
INTERNAL COORDINATES-	21.17 C-C 20.64 CCH9	13.57 CCH7 13.19 HOC 11.15 OCC 8.70 C-O 5.93 H7H8	
FORCE CONSTANTS-	34.33 CC6H 21.17 C-C	13.19 COH 11.15 CCO 9.20 HC6H 8.70 C-O	
OFF DIAGONAL-	-4.82 SB26 -4.80 SB23	-4.40 SB21 3.73 BB44 -3.32 BB40 2.50 SB22 2.42 BB45 2.31 BB35	
NORMAL MODE 14	OBSERVED= 0.0 CM-1	CALCULATED= 1018.8 CM-1	ERROR= 0.0 CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	35.47 CCH8 18.34 CCH7	8.39 H4CC 7.04 H7H9 5.66 C-C	
FORCE CONSTANTS-	56.49 CC6H 11.33 HC6H	9.02 CC3H 5.66 C-C	
OFF DIAGONAL-	-4.22 BB40 4.16 BB37	3.74 BB35 1.91 SB25	
NORMAL MODE 15	OBSERVED= 952.0 CM-1	CALCULATED= 941.8 CM-1	ERROR= 10.2 CM-1 OR 1.1 PERCENT
INTERNAL COORDINATES-	45.57 OCH4 23.62 C-O	9.11 H4CC 7.98 HOC 5.29 OCH5	
FORCE CONSTANTS-	50.86 OCH 23.62 C-O	9.12 CC3H 7.98 COH	
OFF DIAGONAL-	9.58 SB22 -5.64 SB21	-2.80 BB33 1.72 SB25	
NORMAL MODE 16	OBSERVED= 882.0 CM-1	CALCULATED= 893.3 CM-1	ERROR= -11.3 CM-1 OR -1.3 PERCENT
INTERNAL COORDINATES-	46.54 HOC 19.77 C-O	18.45 OCH4 15.10 CCH9 5.08 H4CC	
FORCE CONSTANTS-	46.54 COH 22.36 CC6H	19.77 C-O 18.45 OCH 6.29 CC3H	
OFF DIAGONAL-	-12.47 SB21 -8.37 SB22	3.18 BB31 1.81 SB25 -1.75 BB40	
NORMAL MODE 17	OBSERVED= 831.0 CM-1	CALCULATED= 829.9 CM-1	ERROR= 1.1 CM-1 OR 0.1 PERCENT
INTERNAL COORDINATES-	35.85 C-C 32.48 HOC	14.72 C-O 5.08 CCH9	
FORCE CONSTANTS-	35.85 C-C 32.48 COH	14.72 C-O 7.02 CC6H	
OFF DIAGONAL-	8.99 SB21		
NORMAL MODE 18	OBSERVED= 707.0 CM-1	CALCULATED= 710.8 CM-1	ERROR= -3.8 CM-1 OR -0.5 PERCENT
INTERNAL COORDINATES-	35.34 H4CC 20.45 H5CC	11.36 CCH7 10.97 CCH8 9.04 OCH5 8.49 OCH4	
FORCE CONSTANTS-	55.79 CC3H 22.33 CC6H	17.53 OCH	
OFF DIAGONAL-	-7.03 BB37 4.63 BB35	-1.58 BB33	
NORMAL MODE 19	OBSERVED= 424.0 CM-1	CALCULATED= 421.1 CM-1	ERROR= 2.8 CM-1 OR 0.7 PERCENT
INTERNAL COORDINATES-	87.31 OCC 6.76 CCH9	5.11 H4CC	
FORCE CONSTANTS-	87.31 CCO 16.07 CC6H	8.44 CC3H	
OFF DIAGONAL-	-11.19 BB44 -3.88 BB45	2.99 SB26 -1.78 BB37 -1.59 SB25 -1.51 SB23	
NORMAL MODE 20	OBSERVED= 0.0 CM-1	CALCULATED= 245.0 CM-1	ERROR= 0.0 CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	98.55 T-CC		
FORCE CONSTANTS-	98.55 TC-C		
OFF DIAGONAL -	NONE		
NORMAL MODE 21	OBSERVED= 0.0 CM-1	CALCULATED= 153.7 CM-1	ERROR= 0.0 CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	99.03 T-CO		
FORCE CONSTANTS-	99.03 TC-O		
OFF DIAGONAL -	NONE		

12. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 8.20

TABLE LII (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 300				PAGE 1			
MOLECULE 3		-6 NG= 202		ETHANOL, C03CHDOH (TRANS)			
NORMAL MODE 7	OBSERVED=	1386.0 CM-1	CALCULATED=	1358.5 CM-1	ERROR=	27.5 CM-1	OR 2.0 PERCENT
INTERNAL COORDINATES-	42.58	OCH5 33.47 H5CC	13.26	HOC 11.63 C-C			
FORCE CONSTANTS-	45.58	OCH 36.91 CC3H	13.26	COH 11.63 C-C			
OFF DIAGONAL-	-9.93	S825 -8.07 S822	3.30	S821 -3.30 B831	2.04	B833 1.69 B840	
NORMAL MODE 8	OBSERVED=	1328.0 CM-1	CALCULATED=	1335.3 CM-1	ERROR=	-7.3 CM-1	OR -0.5 PERCENT
INTERNAL COORDINATES-	62.33	HCH 28.23 OCH5					
FORCE CONSTANTS-	62.33	HC3H 29.34 OCH					
OFF DIAGONAL-	-4.06	B838 3.33 B840	-2.23	S822			
NORMAL MODE 9	OBSERVED=	1259.0 CM-1	CALCULATED=	1235.1 CM-1	ERROR=	23.9 CM-1	OR 1.9 PERCENT
INTERNAL COORDINATES-	56.85	HOC 13.53 H5CC	6.65	HCH 5.81 C-C			
FORCE CONSTANTS-	56.85	COH 13.63 CC3H	6.65	HC3H 5.81 C-C	5.80	OCH	
OFF DIAGONAL-	4.12	S821 3.08 S825	1.76	B840			
NORMAL MODE 10	OBSERVED=	1130.0 CM-1	CALCULATED=	1132.7 CM-1	ERROR=	-2.7 CM-1	OR -0.2 PERCENT
INTERNAL COORDINATES-	29.71	C-O 28.08 C-C	23.86	HOC 9.44 CCH7 9.27	CCH8 8.29 H7H8		
FORCE CONSTANTS-	29.71	C-O 28.08 C-C	23.86	COH 19.55 CC6H 14.14	HC6H 5.42 OCH		
OFF DIAGONAL-	-10.94	S821 -10.87 S824	5.85	B840 -3.21 S825 -2.83	S822 -2.37 S823 -1.83	B835 -1.64 B834 -1.53	SS20
NORMAL MODE 11	OBSERVED=	1060.0 CM-1	CALCULATED=	1072.8 CM-1	ERROR=	-12.8 CM-1	OR -1.2 PERCENT
INTERNAL COORDINATES-	26.21	C-O 24.65 CCH9	21.74	H8H9 11.96 H7H9 7.74	C-C		
FORCE CONSTANTS-	35.40	HC6H 28.42 CC6H	26.21	C-O 7.74 C-C			
OFF DIAGONAL-	8.95	B840 -6.21 S824	-2.97	S823 -2.93 S822 -2.11	S821 -1.90 B835 1.63	S825	
NORMAL MODE 12	OBSERVED=	1045.0 CM-1	CALCULATED=	1041.3 CM-1	ERROR=	3.7 CM-1	OR 0.4 PERCENT
INTERNAL COORDINATES-	47.47	H7H9 30.75 H8H9					
FORCE CONSTANTS-	80.14	HC6H 7.84 CC6H					
OFF DIAGONAL-	5.21	B834 4.70 B840					
NORMAL MODE 13	OBSERVED=	0.0 CM-1	CALCULATED=	1021.9 CM-1	ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	56.15	H7H8 15.56 C-O	7.81	OCH4 7.81 H8H9 5.01	CCH7		
FORCE CONSTANTS-	64.68	HC6H 15.56 C-O	7.95	OCH 7.24 CC6H			
OFF DIAGONAL-	-4.21	S822 3.24 B834	3.08	B840 -2.38 S821 -1.95	S823		
NORMAL MODE 14	OBSERVED=	985.0 CM-1	CALCULATED=	958.1 CM-1	ERROR=	26.9 CM-1	OR 2.7 PERCENT
INTERNAL COORDINATES-	22.90	OCH4 20.59 H4CC	15.01	C-O 8.88 C-C 7.55	CCH7 6.99 OCC		
FORCE CONSTANTS-	23.90	CC3H 22.90 OCH	15.01	C-O 8.88 C-C 8.10	CC6H 6.99 CCO 6.31	HC6H	
OFF DIAGONAL-	8.28	S822 -4.99 S823	-3.08	S825 -2.47 S826 1.99	B844 1.72 S824		
NORMAL MODE 15	OBSERVED=	911.0 CM-1	CALCULATED=	913.6 CM-1	ERROR=	-2.6 CM-1	OR -0.3 PERCENT
INTERNAL COORDINATES-	31.94	OCH4 14.87 C-C	12.87	CCH7 8.49 OCH5 5.72	H8H9		
FORCE CONSTANTS-	40.43	OCH 14.87 C-C	13.87	CC6H 5.99 HC6H			
OFF DIAGONAL-	3.87	S824 3.67 S825	-2.97	B833 2.50 S822 -2.36	S826 2.28 B844 1.96	S823	
NORMAL MODE 16	OBSERVED=	0.0 CM-1	CALCULATED=	879.8 CM-1	ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	27.72	CCH8 16.44 H4CC	11.19	C-C 7.02 OCH4 6.53	H7H9		
FORCE CONSTANTS-	32.20	CC6H 20.54 CC3H	11.19	C-C 10.54 OCH 6.75	HC6H		
OFF DIAGONAL-	4.96	B837 2.65 B835	2.59	S825 2.23 S824 -2.00	S826 1.92 B844		
NORMAL MODE 17	OBSERVED=	744.0 CM-1	CALCULATED=	738.2 CM-1	ERROR=	5.8 CM-1	OR 0.8 PERCENT
INTERNAL COORDINATES-	40.49	CCH9 17.56 C-O	15.88	C-C 5.94 H7H8			
FORCE CONSTANTS-	46.82	CC6H 17.56 C-O	15.88	C-C 5.99 HC6H			
OFF DIAGONAL-	-4.66	S822 3.39 S824	2.42	S823 2.33 B835 -1.51	B840		
NORMAL MODE 18	OBSERVED=	609.0 CM-1	CALCULATED=	618.6 CM-1	ERROR=	-9.6 CM-1	OR -1.6 PERCENT
INTERNAL COORDINATES-	28.38	CCH7 25.39 CCH8	20.71	H4CC 13.17 H5CC			
FORCE CONSTANTS-	53.78	CC6H 33.88 CC3H	9.14	OCH 6.52 HC6H			
OFF DIAGONAL-	-8.50	B837 5.29 B835	-3.34	B840			
NORMAL MODE 19	OBSERVED=	0.0 CM-1	CALCULATED=	382.1 CM-1	ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	80.28	OCC 11.64 CCH9	8.36	CCH8 7.36 CCH7 5.00	H4CC		
FORCE CONSTANTS-	80.28	CCO 27.36 CC6H	8.36	CC3H			
OFF DIAGONAL-	-13.94	B844 -4.88 B845	3.02	S826 -2.91 S823 -2.30	B837 -1.77 B840 -1.67	S825	
NORMAL MODE 20	OBSERVED=	0.0 CM-1	CALCULATED=	207.4 CM-1	ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	97.56	T-CO					
FORCE CONSTANTS-	97.56	TC-O					
OFF DIAGONAL -	NONE						
NORMAL MODE 21	OBSERVED=	0.0 CM-1	CALCULATED=	186.2 CM-1	ERROR=	0.0 CM-1	OR 0.0 PERCENT
INTERNAL COORDINATES-	97.75	T-CC					
FORCE CONSTANTS-	97.75	TC-C					
OFF DIAGONAL -	NONE						

10. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR =12.30

TABLE LII (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 300
MOLECULE 4 -6 NG= 202 ETHANOL, CD3CHDOO (TRANS)

PAGE 1

NORMAL MODE 7	OBSERVED=	1352.0 CM-1	CALCULATED=	1348.5 CM-1	ERROR=	3.5 CM-1	OR	0.3 PERCENT
INTERNAL COORDINATES-	67.67	OCH5 28.44 H5CC	6.88	C-C 5.15 C-O				
FORCE CONSTANTS-	71.13	OCH 30.31 CC3H	6.88	C-C 5.15 C-O				
OFF DIAGONAL-	-10.14	S822 -6.70 SB25	2.76	BB33 -1.65 BB40				
NORMAL MODE 8	OBSERVED=	1328.0 CM-1	CALCULATED=	1329.0 CM-1	ERROR=	-1.0 CM-1	OR	-0.1 PERCENT
INTERNAL COORDINATES-	67.46	HCH 16.06 H5CC	5.17	OCH5				
FORCE CONSTANTS-	67.46	HC3H 18.63 CC3H	5.47	OCH				
OFF DIAGONAL-	8.13	BB40 -4.08 SB25	-1.87	BB38				
NORMAL MODE 9	OBSERVED=	1151.0 CM-1	CALCULATED=	1160.9 CM-1	ERROR=	-9.9 CM-1	OR	-0.9 PERCENT
INTERNAL COORDINATES-	41.17	C-C 26.41 C-O	8.67	OCH4 7.66 CCH8 6.16	H7H8 5.91 CCH7			
FORCE CONSTANTS-	41.17	C-C 26.41 C-O	14.45	CC6H 11.06 OCH 10.77	HC6H 6.66 CC3H			
OFF DIAGONAL-	-11.48	S824 4.36 BB40	-3.18	S822 2.12 SB21 -1.75	SS20			
NORMAL MODE 10	OBSERVED=	1079.0 CM-1	CALCULATED=	1072.4 CM-1	ERROR=	6.6 CM-1	OR	0.6 PERCENT
INTERNAL COORDINATES-	26.28	C-O 24.64 CCH9	21.76	H8H9 11.87 H7H9 7.56	C-C			
FORCE CONSTANTS-	35.52	HC6H 28.16 CC6H 26.28	C-O 7.56	C-C				
OFF DIAGONAL-	8.85	BB40 -6.05 SB24	-3.06	S823 -2.92 SB22 -2.22	SB21 -1.82 BB35 1.63 SB25			
NORMAL MODE 11	OBSERVED=	1051.0 CM-1	CALCULATED=	1041.3 CM-1	ERROR=	9.6 CM-1	OR	0.9 PERCENT
INTERNAL COORDINATES-	46.17	H7H9 30.61 H8H9	5.40	CCH8				
FORCE CONSTANTS-	79.85	HC6H 7.64 CC6H						
OFF DIAGONAL-	5.17	BB34 4.63 BB40						
NORMAL MODE 12	OBSERVED=	0.0 CM-1	CALCULATED=	1028.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	46.28	H7H8 12.95 CCH7	9.65	OCH4 6.12 H4CC 5.70	HOC			
FORCE CONSTANTS-	49.97	HC6H 17.00 CC6H 9.70	OCH 7.23	CC3H 5.70	COH			
OFF DIAGONAL-	6.41	BB40 -2.04 SB22	1.57	SB21				
NORMAL MODE 13	OBSERVED=	0.0 CM-1	CALCULATED=	1000.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	28.93	C-O 28.27 HOC	12.26	H7H8 11.81 OCC 9.38	H8H9 6.13 C-C			
FORCE CONSTANTS-	28.93	C-O 28.27 COH 26.54	HC6H 11.81	CCO 6.13	C-C 5.21 CC3H 5.05 CC6H			
OFF DIAGONAL-	-11.75	SB21 -9.00 SB23	3.40	SB22 -2.67 SB26 2.58	BB44 1.52 BB34			
NORMAL MODE 14	OBSERVED=	919.0 CM-1	CALCULATED=	924.5 CM-1	ERROR=	-5.5 CM-1	OR	-0.6 PERCENT
INTERNAL COORDINATES-	44.57	OCH4 13.82 H4CC	7.97	C-O				
FORCE CONSTANTS-	48.46	OCH 14.09 CC3H	7.97	C-O				
OFF DIAGONAL-	5.88	S822 3.50 SB25	-2.38	BB33 1.92 SB21 1.68	SB24			
NORMAL MODE 15	OBSERVED=	0.0 CM-1	CALCULATED=	890.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	19.82	H4CC 16.81 CCH8	12.79	CCH7 9.83 OCH4 8.39	HOC 8.06 OCH5 7.02 H5CC			
FORCE CONSTANTS-	29.67	CC6H 26.84 CC3H 17.89	OCH 8.39	COH 6.32	HC6H			
OFF DIAGONAL-	5.58	BB37 3.24 BB35	-2.01	BB40 -1.61	BB33			
NORMAL MODE 16	OBSERVED=	825.0 CM-1	CALCULATED=	835.6 CM-1	ERROR=	-10.6 CM-1	OR	-1.3 PERCENT
INTERNAL COORDINATES-	54.37	HOC 15.97 C-C	8.73	CCH8 5.36 CCH9				
FORCE CONSTANTS-	54.37	COH 16.14 CC6H 15.97	C-C					
OFF DIAGONAL-	-2.67	SB21 2.42 SB24	-2.39	SB26 2.33 BB44 1.56	BB31			
NORMAL MODE 17	OBSERVED=	750.0 CM-1	CALCULATED=	733.6 CM-1	ERROR=	16.4 CM-1	OR	2.2 PERCENT
INTERNAL COORDINATES-	37.82	CCH9 18.74 C-C	17.00	C-O 5.64 H7H8				
FORCE CONSTANTS-	43.13	CC6H 18.74 C-C	17.00	C-O 5.73 HC6H				
OFF DIAGONAL-	-4.20	S822 3.81 SB24	2.14	SB23 2.07 BB35 1.52	SB21			
NORMAL MODE 18	OBSERVED=	619.0 CM-1	CALCULATED=	618.5 CM-1	ERROR=	0.5 CM-1	OR	0.1 PERCENT
INTERNAL COORDINATES-	28.32	CCH7 25.46 CCH8	20.79	H4CC 13.18 H5CC				
FORCE CONSTANTS-	53.79	CC6H 33.97 CC3H 9.15	OCH 6.52	HC6H				
OFF DIAGONAL-	-8.52	BB37 5.30 BB35	-3.34	BB40				
NORMAL MODE 19	OBSERVED=	0.0 CM-1	CALCULATED=	375.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	80.44	OCC 11.41 CCH9	8.14	CCH8 7.20 CCH7				
FORCE CONSTANTS-	80.44	CCO 26.75 CC6H	8.16	CC3H				
OFF DIAGONAL-	-13.78	BB44 -4.84 BB45	2.80	S826 -2.71 SB23 -2.25	BB37 -1.76 BB40 -1.52 SB25			
NORMAL MODE 20	OBSERVED=	0.0 CM-1	CALCULATED=	186.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	97.98	T-CC						
FORCE CONSTANTS-	97.98	TC-C						
OFF DIAGONAL -	NONE							
NORMAL MODE 21	OBSERVED=	0.0 CM-1	CALCULATED=	152.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	98.25	T-CO						
FORCE CONSTANTS-	98.25	TC-O						
OFF DIAGONAL -	NONE							

9. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 7.06

TABLE I,II (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 300									
MOLECULE 5 -6 NG= 201 ETHANOL, CH3CH2OH (TRANS)									
PAGE 1									
NORMAL MODE 7	OBSERVED=	1490.0 CM-1	CALCULATED=	1498.7 CM-1	ERROR=	-8.7 CM-1	OR	-0.6 PERCENT	
INTERNAL COORDINATES-	69.88	HCH 6.07 OCH5	6.07	OC4					
FORCE CONSTANTS-	69.88	HC3H 12.13 OCH	8.76	CC3H					
OFF DIAGONAL-	6.55	BB40 -3.33 BB38							
NORMAL MODE 8	OBSERVED=	1462.0 CM-1	CALCULATED=	1457.5 CM-1	ERROR=	4.5 CM-1	OR	0.3 PERCENT	
INTERNAL COORDINATES-	46.40	H7H8 10.76 H7H9	10.74	H8H9 6.87 CCH9					
FORCE CONSTANTS-	67.89	HC6H 11.09 CC6H							
OFF DIAGONAL-	6.10	BB40 4.41 BB34							
NORMAL MODE 9	OBSERVED=	1445.0 CM-1	CALCULATED=	1455.3 CM-1	ERROR=	-10.3 CM-1	OR	-0.7 PERCENT	
INTERNAL COORDINATES-	39.04	H8H9 39.02 H7H9	5.28	CCH7 5.28 CCH8					
FORCE CONSTANTS-	78.07	HC6H 10.56 CC6H							
OFF DIAGONAL-	5.40	BB40 5.07 BB34							
NORMAL MODE 10	OBSERVED=	1390.0 CM-1	CALCULATED=	1400.5 CM-1	ERROR=	-10.5 CM-1	OR	-0.8 PERCENT	
INTERNAL COORDINATES-	24.24	UCH4 24.24 OCH5	13.92	H4CC 13.91 H5CC 12.35	C-C 6.10	H8H9 6.10	H7H9		
FORCE CONSTANTS-	48.49	UCH 27.83 CC3H	12.35	C-C 12.33 HC6H 8.93	CC6H				
OFF DIAGONAL-	-9.99	SB25 -8.43 SB22	-5.26	SB24 4.37 BB33 2.81	BB37 -2.75	BB35 -2.35	BB31 2.12	BB40 1.73	SB21
NORMAL MODE 11	OBSERVED=	1390.0 CM-1	CALCULATED=	1376.9 CM-1	ERROR=	13.1 CM-1	OR	0.9 PERCENT	
INTERNAL COORDINATES-	15.50	H7H8 14.92 CCH8	14.92	CCH7 14.72 CCH9 10.16	H8H9 10.16	H7H9 5.61	UCH4 5.61	UCH5	
FORCE CONSTANTS-	44.55	CC6H 35.82 HC6H	11.23	UCH 5.66 CC3H					
OFF DIAGONAL-	14.80	BB40 -5.80 BB35	-4.58	BB34 -4.19 SB24 -2.62	BB37 1.59	SB25			
NORMAL MODE 12	OBSERVED=	1280.0 CM-1	CALCULATED=	1275.8 CM-1	ERROR=	4.2 CM-1	OR	0.3 PERCENT	
INTERNAL COORDINATES-	33.23	UCH4 33.23 OCH5	17.23	H4CC 17.23 H5CC					
FORCE CONSTANTS-	66.46	UCH 34.45 CC3H							
OFF DIAGONAL-	-5.99	BB33 2.17 BB35							
NORMAL MODE 13	OBSERVED=	1241.0 CM-1	CALCULATED=	1239.1 CM-1	ERROR=	1.9 CM-1	OR	0.2 PERCENT	
INTERNAL COORDINATES-	76.48	HOC 6.05 C-C							
FORCE CONSTANTS-	76.48	COH 6.05 C-C	5.34	CC3H					
OFF DIAGONAL-	3.06	SB25 2.12 SB21	1.87	BB31					
NORMAL MODE 14	OBSERVED=	1089.0 CM-1	CALCULATED=	1107.1 CM-1	ERROR=	-18.1 CM-1	OR	-1.7 PERCENT	
INTERNAL COORDINATES-	58.89	C-O 19.96 CCH9	7.89	H7H8 6.54 HOC 6.23	OCC				
FORCE CONSTANTS-	58.89	C-O 25.21 CC6H	9.37	HC6H 6.54 COH 6.23	CCO				
OFF DIAGONAL-	-9.33	SB23 -8.07 SB21	3.96	SB22 -2.66 BB40 2.25	BB44 1.78	BB45			
NORMAL MODE 15	OBSERVED=	1065.0 CM-1	CALCULATED=	1060.5 CM-1	ERROR=	4.5 CM-1	OR	0.4 PERCENT	
INTERNAL COORDINATES-	22.76	CCH8 22.75 CCH7	12.49	UCH4 12.49 OCH5 7.37	H4CC 7.37	H5CC 5.30	H8H9 5.30	H7H9	
FORCE CONSTANTS-	45.51	CC6H 24.98 OCH	14.74	CC3H 10.60 HC6H					
OFF DIAGONAL-	5.21	BB37 -4.13 BB40	3.68	BB35 -2.25 BB33					
NORMAL MODE 16	OBSERVED=	1027.0 CM-1	CALCULATED=	1024.9 CM-1	ERROR=	2.1 CM-1	OR	0.2 PERCENT	
INTERNAL COORDINATES-	51.27	C-C 14.05 HOC	12.60	CCH9 9.08 C-O 5.00	OCC				
FORCE CONSTANTS-	51.27	C-C 19.75 CC6H	14.05	COH 9.08 C-O					
OFF DIAGONAL-	-5.02	SB26 -4.64 SB21	3.28	SB23 2.35 BB44 -1.98	SB22 -1.59	BB40			
NORMAL MODE 17	OBSERVED=	879.0 CM-1	CALCULATED=	867.6 CM-1	ERROR=	11.4 CM-1	OR	1.3 PERCENT	
INTERNAL COORDINATES-	42.39	C-O 31.85 C-C	18.39	CCH9					
FORCE CONSTANTS-	42.39	C-O 31.85 C-C	25.79	CC6H					
OFF DIAGONAL-	-4.75	SB22 -3.23 SB23	2.81	SB25 1.95	SS20 -1.80	SB26 -1.79	BB40 1.52	BB35	
NORMAL MODE 18	OBSERVED=	801.0 CM-1	CALCULATED=	795.8 CM-1	ERROR=	5.2 CM-1	OR	0.6 PERCENT	
INTERNAL COORDINATES-	22.20	H4CC 22.20 H5CC	18.99	CCH7 18.99 CCH8 8.69	UCH4 8.69	UCH5			
FORCE CONSTANTS-	44.40	CC3H 37.99 CC6H	17.38	UCH 5.51 HC6H					
OFF DIAGONAL-	-8.26	BB37 5.02 BB35	-2.72	BB40 -1.57 BB33					
NORMAL MODE 19	OBSERVED=	419.0 CM-1	CALCULATED=	431.5 CM-1	ERROR=	-12.5 CM-1	OR	-3.0 PERCENT	
INTERNAL COORDINATES-	87.39	OCC 6.92 CCH9							
FORCE CONSTANTS-	87.39	CCO 16.45 CC6H	7.99	CC3H					
OFF DIAGONAL-	-11.33	BB44 -3.93 BB45	3.52	SB26 -1.83	SB25 -1.76	BB37 -1.52	SB23		
NORMAL MODE 20	OBSERVED=	243.0 CM-1	CALCULATED=	249.0 CM-1	ERROR=	-6.0 CM-1	OR	-2.5 PERCENT	
INTERNAL COORDINATES-	99.08	TC-C							
FORCE CONSTANTS-	99.08	TC-C							
OFF DIAGONAL-	NONE								
NORMAL MODE 21	OBSERVED=	201.0 CM-1	CALCULATED=	208.1 CM-1	ERROR=	-7.1 CM-1	OR	-3.5 PERCENT	
INTERNAL COORDINATES-	98.89	TC-C							
FORCE CONSTANTS-	98.89	TC-C							
OFF DIAGONAL-	NONE								

16. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 7.53

TABLE LII (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 300										PAGE 1
MOLECULE 6		-6 NG= 201		ETHANOL, CH ₃ CH ₂ OD (TRANS)						
NORMAL MODE 7	OBSERVED=	1490.0 CM-1		CALCULATED=	1497.2 CM-1		ERROR=	-7.2 CM-1 OR -0.5 PERCENT		
INTERNAL COORDINATES-	69.92	HCH	6.69 OCH5	6.69	OCCH4					
FORCE CONSTANTS-	69.92	HC3H	13.37 OCH	8.05	CC3H					
OFF DIAGONAL-	6.36	BB40	-3.49 BB38	-1.60	SB22					
NORMAL MODE 8	OBSERVED=	1462.0 CM-1		CALCULATED=	1456.8 CM-1		ERROR=	5.1 CM-1 OR 0.3 PERCENT		
INTERNAL COORDINATES-	46.48	H7H8	10.89 H7H9	10.82	H8H9	6.80 CCH9				
FORCE CONSTANTS-	68.19	HC6H	10.90 CC6H							
OFF DIAGONAL-	6.15	BB40	4.43 BB34							
NORMAL MODE 9	OBSERVED=	1445.0 CM-1		CALCULATED=	1455.3 CM-1		ERROR=	-10.3 CM-1 OR -0.7 PERCENT		
INTERNAL COORDINATES-	39.07	H8H9	39.00 H7H9	5.29	CCH7	5.28 CCH8				
FORCE CONSTANTS-	78.07	HC6H	10.56 CC6H							
OFF DIAGONAL-	5.40	BB40	5.07 BB34							
NORMAL MODE 10	OBSERVED=	1401.0 CM-1		CALCULATED=	1396.3 CM-1		ERROR=	4.7 CM-1 OR 0.3 PERCENT		
INTERNAL COORDINATES-	21.60	OCCH4	21.60 OCH5	13.95	H4CC	13.95 H5CC	12.48 C-C	7.60 H8H9	7.60 H7H9	5.50 CCH7
FORCE CONSTANTS-	43.19	OCCH	27.89 CC3H	15.25	HC6H	14.03 CC6H	12.48 C-C			5.50 CCH8
OFF DIAGONAL-	-10.05	SB25	-7.63 SB22	-6.63	SB24	4.27 BB40	3.90 BB33	3.52 BB37	-3.37 BB35	
NORMAL MODE 11	OBSERVED=	1389.0 CM-1		CALCULATED=	1375.3 CM-1		ERROR=	13.7 CM-1 OR 1.0 PERCENT		
INTERNAL COORDINATES-	15.16	H7H8	13.69 CCH9	12.94	CCH8	12.93 CCH7	8.74 OCH4	8.74 OCH5	8.48 H8H9	8.48 H7H9
FORCE CONSTANTS-	39.56	CC6H	32.12 HC6H	17.47	OCCH	10.18 CC3H				5.09 H4CC
OFF DIAGONAL-	13.16	BB40	-5.46 BB35	-4.05	BB34	-3.27 BB37	-2.93 SB24	-1.76 SB22	1.58 SB25	1.58 BB33
NORMAL MODE 12	OBSERVED=	1280.0 CM-1		CALCULATED=	1275.8 CM-1		ERROR=	4.2 CM-1 OR 0.3 PERCENT		
INTERNAL COORDINATES-	33.23	OCCH4	33.23 OCH5	17.23	H4CC	17.23 H5CC				
FORCE CONSTANTS-	66.47	OCCH	34.45 CC3H							
OFF DIAGONAL-	-6.00	BB33	2.17 BB35							
NORMAL MODE 13	OBSERVED=	1135.0 CM-1		CALCULATED=	1111.4 CM-1		ERROR=	23.6 CM-1 OR 2.1 PERCENT		
INTERNAL COORDINATES-	60.08	C-O	13.73 C-C	12.19	CCH9	5.42 H7H8				
FORCE CONSTANTS-	60.08	C-O	14.78 CC6H	13.73	C-C	6.19 HC6H				
OFF DIAGONAL-	-5.67	SB23	3.87 SB22	1.75	SB26	-1.52 SS20				
NORMAL MODE 14	OBSERVED=	0.0 CM-1		CALCULATED=	1080.1 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT		
INTERNAL COORDINATES-	42.77	C-C	15.76 CCH9	15.60	HOC	10.68 OCC				
FORCE CONSTANTS-	42.77	C-C	22.83 CC6H	15.60	COH	10.68 CCO	5.71 HC6H			
OFF DIAGONAL-	-6.70	SB26	3.87 SB25	3.41	BB44	-2.15 BB40	2.07 BB45			
NORMAL MODE 15	OBSERVED=	1065.0 CM-1		CALCULATED=	1060.4 CM-1		ERROR=	4.6 CM-1 OR 0.4 PERCENT		
INTERNAL COORDINATES-	22.76	CCH7	22.76 CCH8	12.49	OCCH4	12.49 OCH5	7.37 H4CC	7.37 H5CC	5.30 H8H9	5.30 H7H9
FORCE CONSTANTS-	45.52	CC6H	24.97 OCH	14.74	CC3H	10.61 HC6H				
OFF DIAGONAL-	5.21	BB37	-4.14 BB40	3.68	BB35	-2.25 BB33				
NORMAL MODE 16	OBSERVED=	898.0 CM-1		CALCULATED=	904.1 CM-1		ERROR=	-6.1 CM-1 OR -0.7 PERCENT		
INTERNAL COORDINATES-	52.77	HOC	36.37 C-O	18.07	CCH9					
FORCE CONSTANTS-	52.77	COH	36.37 C-O	26.95	CC6H					
OFF DIAGONAL-	-18.01	SB21	-5.16 SB22	-1.88	BB40	1.57 BB35	1.54 BB31			
NORMAL MODE 17	OBSERVED=	850.0 CM-1		CALCULATED=	831.4 CM-1		ERROR=	18.5 CM-1 OR 2.2 PERCENT		
INTERNAL COORDINATES-	35.33	C-C	34.42 HOC	13.99	C-O	5.19 CCH9				
FORCE CONSTANTS-	35.33	C-C	34.42 COH	13.99	C-O	6.73 CC6H				
OFF DIAGONAL-	9.02	SB21								
NORMAL MODE 18	OBSERVED=	790.0 CM-1		CALCULATED=	795.7 CM-1		ERROR=	-5.7 CM-1 OR -0.7 PERCENT		
INTERNAL COORDINATES-	22.22	H4CC	22.22 H5CC	18.99	CCH7	18.99 CCH8	8.70 OCH4	8.70 OCH5		
FORCE CONSTANTS-	44.44	CC3H	37.99 CC6H	17.40	OCCH	5.51 HC6H				
OFF DIAGONAL-	-8.27	BB37	5.02 BB35	-2.72	BB40	-1.57 BB33				
NORMAL MODE 19	OBSERVED=	423.0 CM-1		CALCULATED=	423.8 CM-1		ERROR=	-0.8 CM-1 OR -0.2 PERCENT		
INTERNAL COORDINATES-	87.13	OCC	6.78 CCH9							
FORCE CONSTANTS-	87.13	CCO	16.13 CC6H	7.79	CC3H					
OFF DIAGONAL-	-11.20	BB44	-3.89 BB45	3.20	SB26	-1.72 BB37	-1.64 SB25			
NORMAL MODE 20	OBSERVED=	244.0 CM-1		CALCULATED=	249.0 CM-1		ERROR=	-5.0 CM-1 OR -2.0 PERCENT		
INTERNAL COORDINATES-	99.11	T-CC								
FORCE CONSTANTS-	99.11	TC-C								
OFF DIAGONAL -	NONE									
NORMAL MODE 21	OBSERVED=	0.0 CM-1		CALCULATED=	154.0 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT		
INTERNAL COORDINATES-	98.97	T-CO								
FORCE CONSTANTS-	98.97	TC-O								
OFF DIAGONAL -	NONE									

13. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 8.43

TABLE LII (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 300										PAGE 1
MOLECULE 7		-6 NG= 201		ETHANOL, CH3CD2OH (TRANS)						
NORMAL MODE 7	OBSERVED=	1465.0 CM-1	CALCULATED=	1457.4 CM-1	ERROR=	7.6 CM-1	OR	0.5 PERCENT		
INTERNAL COORDINATES-	51.13 H7H8	12.44 H7H9	12.40 H8H9	7.42 CCH9						
FORCE CONSTANTS-	75.97 HC6H	11.45 CC6H								
OFF DIAGONAL-	5.53 BB40	4.94 BB34								
NORMAL MODE 8	OBSERVED=	1448.0 CM-1	CALCULATED=	1454.3 CM-1	ERROR=	-6.3 CM-1	OR	-0.4 PERCENT		
INTERNAL COORDINATES-	39.30 H8H9	39.26 H7H9	5.08 CCH7	5.07 CCH8						
FORCE CONSTANTS-	78.56 HC6H	10.14 CC6H								
OFF DIAGONAL-	5.31 BB40	5.10 BB34								
NORMAL MODE 9	OBSERVED=	1377.0 CM-1	CALCULATED=	1381.9 CM-1	ERROR=	-4.9 CM-1	OR	-0.3 PERCENT		
INTERNAL COORDINATES-	18.73 CCH7	18.73 CCH8	15.45 CCH9	15.13 H7H9	15.12 H8H9	11.89 H7H8	8.74 C-C			
FORCE CONSTANTS-	52.91 CC6H	42.14 HC6H	8.74 C-C							
OFF DIAGONAL-	17.70 BB40	-10.85 SB24	-6.47 BB35	-5.45 BB34						
NORMAL MODE 10	OBSERVED=	1284.0 CM-1	CALCULATED=	1289.8 CM-1	ERROR=	-5.8 CM-1	OR	-0.4 PERCENT		
INTERNAL COORDINATES-	59.09 HOC	16.84 C-C	6.71 C-O							
FORCE CONSTANTS-	59.09 COH	16.84 C-C	9.49 OCH	8.69 CC3H	6.71 C-O					
OFF DIAGONAL-	8.18 SB21	-6.52 SB25	-5.00 SB22	-3.68 BB31						
NORMAL MODE 11	OBSERVED=	1169.0 CM-1	CALCULATED=	1152.1 CM-1	ERROR=	16.9 CM-1	OR	1.4 PERCENT		
INTERNAL COORDINATES-	40.02 C-O	24.28 HOC	13.75 CCH9	10.80 OCH5	10.80 OCH4	8.90 HCH	6.72 H7H8			
FORCE CONSTANTS-	40.02 C-O	24.28 COH	21.60 OCH	16.50 CC6H	8.90 HC3H	7.66 HC6H	6.90 CC3H			
OFF DIAGONAL-	-18.42 SB22	-12.81 SB21	-6.21 SB23	-3.75 BB40	3.56 BB31	-2.45 SB25	1.95 BB33	-1.58 BB38		
NORMAL MODE 12	OBSERVED=	1092.0 CM-1	CALCULATED=	1088.3 CM-1	ERROR=	3.7 CM-1	OR	0.3 PERCENT		
INTERNAL COORDINATES-	53.17 HCH	16.60 HOC	13.49 C-C	7.57 H4CC	7.57 H5CC					
FORCE CONSTANTS-	53.17 HC3H	16.60 COH	15.15 CC3H	13.49 C-C						
OFF DIAGONAL-	-7.70 SB25	6.94 BB40	-1.62 SB26							
NORMAL MODE 13	OBSERVED=	1016.0 CM-1	CALCULATED=	1024.5 CM-1	ERROR=	-8.5 CM-1	OR	-0.8 PERCENT		
INTERNAL COORDINATES-	31.23 CCH7	31.23 CCH8	8.54 H4CC	8.54 H5CC	6.21 H8H9	6.21 H7H9				
FORCE CONSTANTS-	62.46 CC6H	17.08 CC3H	12.42 HC6H							
OFF DIAGONAL-	6.57 BB37	-5.24 BB40	4.86 BB35							
NORMAL MODE 14	OBSERVED=	1006.0 CM-1	CALCULATED=	1012.1 CM-1	ERROR=	-6.1 CM-1	OR	-0.6 PERCENT		
INTERNAL COORDINATES-	21.74 CCH9	19.19 C-C	11.46 HCH	10.33 OCH4	10.33 OCH5	5.14 CCH8	5.14 CCH7	5.11 OCC		
FORCE CONSTANTS-	32.02 CC6H	20.66 OCH	19.19 C-C	11.46 HC3H	6.18 HC6H	5.11 CCO				
OFF DIAGONAL-	-3.11 SB26	2.84 BB44	-2.72 BB40	1.96 BB35	1.86 BB33	-1.76 BB38	1.68 BB45			
NORMAL MODE 15	OBSERVED=	966.0 CM-1	CALCULATED=	958.2 CM-1	ERROR=	7.8 CM-1	OR	0.8 PERCENT		
INTERNAL COORDINATES-	36.74 C-O	9.77 OCH5	9.75 OCH4	7.29 H5CC	7.28 H4CC	5.54 C-C				
FORCE CONSTANTS-	36.74 C-O	19.52 OCH	14.57 CC3H	5.54 C-C						
OFF DIAGONAL-	16.77 SB22	4.84 SB25	-3.16 SB21	1.76 BB33						
NORMAL MODE 16	OBSERVED=	915.0 CM-1	CALCULATED=	914.4 CM-1	ERROR=	0.6 CM-1	OR	0.1 PERCENT		
INTERNAL COORDINATES-	45.20 OCH4	45.18 OCH5	6.47 H4CC	6.47 H5CC						
FORCE CONSTANTS-	90.38 OCH	12.94 CC3H								
OFF DIAGONAL-	-8.15 BB33									
NORMAL MODE 17	OBSERVED=	845.0 CM-1	CALCULATED=	848.8 CM-1	ERROR=	-3.8 CM-1	OR	-0.4 PERCENT		
INTERNAL COORDINATES-	39.50 C-C	30.33 C-O	13.86 CCH9							
FORCE CONSTANTS-	39.50 C-C	30.33 C-O	19.03 CC6H	5.72 CC3H						
OFF DIAGONAL-	8.10 SB25	-7.64 SB22	-2.34 SB23	1.84 SS20	-1.72 SB26					
NORMAL MODE 18	OBSERVED=	670.0 CM-1	CALCULATED=	667.3 CM-1	ERROR=	2.7 CM-1	OR	0.4 PERCENT		
INTERNAL COORDINATES-	31.43 H4CC	31.43 H5CC	9.43 CCH7	9.43 CCH8	8.60 OCH4	8.60 OCH5				
FORCE CONSTANTS-	62.85 CC3H	18.86 CC6H	17.20 OCH							
OFF DIAGONAL-	-6.93 BB37	4.97 BB35	-1.55 BB33							
NORMAL MODE 19	OBSERVED=	421.0 CM-1	CALCULATED=	426.3 CM-1	ERROR=	-5.3 CM-1	OR	-1.3 PERCENT		
INTERNAL COORDINATES-	87.87 OCC	6.89 CCH9								
FORCE CONSTANTS-	87.87 CCO	16.36 CC6H	9.22 CC3H							
OFF DIAGONAL-	-11.32 BB44	-3.93 BB45	3.09 SB26	-1.88 SB23	-1.88 BB37	-1.72 SB25				
NORMAL MODE 20	OBSERVED=	0.0 CM-1	CALCULATED=	242.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	97.95 T-CC									
FORCE CONSTANTS-	97.95 TC-C									
OFF DIAGONAL -	NONE									
NORMAL MODE 21	OBSERVED=	0.0 CM-1	CALCULATED=	207.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	98.89 T-CO									
FORCE CONSTANTS-	98.89 TC-O									
OFF DIAGONAL -	NONE									

15. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 5.33

TABLE LII (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 300					PAGE 1	
MOLECULE	8	-6 NG= 201	ETHANOL, CH3CD2OD (TRANS)			
NORMAL MODE 7	OBSERVED=	1470.0 CM-1	CALCULATED=	1457.4 CM-1	ERROR=	12.6 CM-1 OR 0.9 PERCENT
INTERNAL COORDINATES-	51.17	H7H8 12.44 H7H9	12.43	H8H9 7.42 CCH9		
FORCE CONSTANTS-	76.04	HC6H 11.44 CC6H				
OFF DIAGONAL-	5.53	BB40 4.94 BB34				
NORMAL MODE 8	OBSERVED=	1448.0 CM-1	CALCULATED=	1454.3 CM-1	ERROR=	-6.3 CM-1 OR -0.4 PERCENT
INTERNAL COORDINATES-	39.28	H8H9 39.28 H7H9	5.07	CCH7 5.07 CCH8		
FORCE CONSTANTS-	78.56	HC6H 10.14 CC6H				
OFF DIAGONAL-	5.31	BB40 5.10 BB34				
NORMAL MODE 9	OBSERVED=	1378.0 CM-1	CALCULATED=	1381.8 CM-1	ERROR=	-3.8 CM-1 OR -0.3 PERCENT
INTERNAL COORDINATES-	18.76	CCH7 18.76 CCH8	15.50	CCH9 15.11 H8H9 15.11	H7H9 12.00 H7H8 8.41	C-C
FORCE CONSTANTS-	53.03	CC6H 42.23 HC6H	8.41	C-C		
OFF DIAGONAL-	17.74	BB40-10.66 SB24	-6.49	BB35 -5.46 BB34		
NORMAL MODE 10	OBSERVED=	1201.0 CM-1	CALCULATED=	1210.2 CM-1	ERROR=	-9.2 CM-1 OR -0.8 PERCENT
INTERNAL COORDINATES-	32.53	C-C 29.67 C-O	13.26	OCH4 13.26 OCH5 11.52	H4CC 11.52 H5CC	
FORCE CONSTANTS-	32.53	C-C 29.67 C-O	26.51	OCH 23.03 CC3H		
OFF DIAGONAL-	-17.57	SB22-14.75 SB25	4.76	SB21 2.49 SB24 2.39	BB33 -1.70 BB31 -1.65	SS20
NORMAL MODE 11	OBSERVED=	1120.0 CM-1	CALCULATED=	1121.1 CM-1	ERROR=	-1.1 CM-1 OR -0.1 PERCENT
INTERNAL COORDINATES-	46.79	HCH 12.49 C-O	11.40	CCH9 8.36 OCC 8.07	C-C 5.83 HOC	
FORCE CONSTANTS-	46.79	HC3H 15.05 CC6H	12.49	C-O 8.36 CCO 8.07	C-C 6.70 OCH 5.86	HC6H 5.83 COH
OFF DIAGONAL-	-5.73	SB22 -4.98 SB23	-3.51	SB21 -2.58 SB26 -2.28	SB25 2.17 BB44 -2.02	BB38 1.56 BB45
NORMAL MODE 12	OBSERVED=	1044.0 CM-1	CALCULATED=	1028.9 CM-1	ERROR=	15.1 CM-1 OR 1.4 PERCENT
INTERNAL COORDINATES-	26.97	HCH 16.57 CCH9	8.21	OCH4 8.21 OCH5 7.60	HOC 7.45 C-C	
FORCE CONSTANTS-	26.97	HC3H 23.68 CC6H	16.41	OCH 7.60 COH 7.45	C-C	
OFF DIAGONAL-	4.33	SB22 -2.40 BB38	2.26	SB25 2.11 BB44 -1.93	SB21 -1.74 BB31 -1.73	SB26 -1.67 SB23
NORMAL MODE 13	OBSERVED=	1016.0 CM-1	CALCULATED=	1024.5 CM-1	ERROR=	-8.5 CM-1 OR -0.8 PERCENT
INTERNAL COORDINATES-	31.24	CCH7 31.23 CCH8	8.54	H4CC 8.54 H5CC 6.21	H8H9 6.21 H7H9	
FORCE CONSTANTS-	62.46	CC6H 17.08 CC3H	12.42	HC6H		
OFF DIAGONAL-	6.57	BB37 -5.24 BB40	4.86	BB35		
NORMAL MODE 14	OBSERVED=	963.0 CM-1	CALCULATED=	958.6 CM-1	ERROR=	4.4 CM-1 OR 0.4 PERCENT
INTERNAL COORDINATES-	39.03	C-O 7.95 C-C	7.69	OCH4 7.69 OCH5 6.11	H4CC 6.11 H5CC 5.18	HOC
FORCE CONSTANTS-	39.03	C-O 15.37 OCH	12.21	CC3H 7.95 C-C 5.18	COH	
OFF DIAGONAL-	15.34	SB22 -5.84 SB21	5.31	SB25		
NORMAL MODE 15	OBSERVED=	915.0 CM-1	CALCULATED=	914.4 CM-1	ERROR=	0.6 CM-1 OR 0.1 PERCENT
INTERNAL COORDINATES-	45.19	OCH4 45.19 OCH5	6.47	H4CC 6.47 H5CC		
FORCE CONSTANTS-	90.38	OCH 12.94 CC3H				
OFF DIAGONAL-	-8.15	BB33				
NORMAL MODE 16	OBSERVED=	854.0 CM-1	CALCULATED=	884.4 CM-1	ERROR=	-30.4 CM-1 OR -3.6 PERCENT
INTERNAL COORDINATES-	55.54	HOC 13.43 C-O	11.67	CCH9 5.78 OCH5 5.78	OCH4 5.50 H5CC 5.50	H4CC
FORCE CONSTANTS-	55.54	COH 17.19 CC6H	13.43	C-O 11.57 OCH 10.99	CC3H	
OFF DIAGONAL-	-11.23	SB21 -7.81 SB22	3.94	BB31 2.65 SB25 -1.57	BB37	
NORMAL MODE 17	OBSERVED=	813.0 CM-1	CALCULATED=	825.5 CM-1	ERROR=	-12.5 CM-1 OR -1.5 PERCENT
INTERNAL COORDINATES-	39.88	C-C 25.54 HOC	16.73	C-O 5.41 CCH9		
FORCE CONSTANTS-	39.88	C-C 25.54 COH	16.73	C-O 6.99 CC6H		
OFF DIAGONAL-	8.50	SB21 2.61 SB25	-1.72	SB22		
NORMAL MODE 18	OBSERVED=	670.0 CM-1	CALCULATED=	667.2 CM-1	ERROR=	2.8 CM-1 OR 0.4 PERCENT
INTERNAL COORDINATES-	31.46	H4CC 31.45 H5CC	9.43	CCH7 9.43 CCH8 8.61	OCH4 8.61 OCH5	
FORCE CONSTANTS-	62.91	CC3H 18.87 CC6H	17.22	OCH		
OFF DIAGONAL-	-6.93	BB37 4.97 BB35	-1.55	BB33		
NORMAL MODE 19	OBSERVED=	420.0 CM-1	CALCULATED=	418.7 CM-1	ERROR=	1.3 CM-1 OR 0.3 PERCENT
INTERNAL COORDINATES-	87.63	OCC 6.75 CCH9				
FORCE CONSTANTS-	87.63	CCO 16.03 CC6H	8.87	CC3H		
OFF DIAGONAL-	-11.19	BB44 -3.89 BB45	2.81	SB26 -1.83 BB37 -1.69	SB23 -1.54 SB25	
NORMAL MODE 20	OBSERVED=	0.0 CM-1	CALCULATED=	242.2 CM-1	ERROR=	0.0 CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	98.11	T-C				
FORCE CONSTANTS-	98.11	TC-C				
OFF DIAGONAL -	NONE					
NORMAL MODE 21	OBSERVED=	0.0 CM-1	CALCULATED=	153.4 CM-1	ERROR=	0.0 CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	99.08	T-CO				
FORCE CONSTANTS-	99.08	TC-O				
OFF DIAGONAL -	NONE					

13. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 8.36

TABLE LII (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 300										PAGE 1
MOLECULE 9		-6 NG= 201		ETHANOL, C03CH2OH (TRANS)						
NORMAL MODE 7	OBSERVED=	1490.0 CM-1		CALCULATED=		1496.5 CM-1		ERROR=	-6.5 CM-1 OR -0.4 PERCENT	
INTERNAL COORDINATES-	73.55	HCH	5.64 OCH5	5.64 OCH4		5.17 H4CC	5.17 H5CC			
FORCE CONSTANTS-	73.55	HC3H	11.27 OCH	10.34 CC3H						
OFF DIAGONAL-	6.88	BB40	-3.29 BB38	-1.75 SB25						
NORMAL MODE 8	OBSERVED=	1380.0 CM-1		CALCULATED=		1397.3 CM-1		ERROR=	-17.3 CM-1 OR -1.3 PERCENT	
INTERNAL COORDINATES-	30.83	UCH4	30.83 OCH5	17.78 H4CC		17.78 H5CC	8.67 C-C	6.73 HOC		
FORCE CONSTANTS-	61.66	UCH	35.55 CC3H	8.67 C-C		6.73 COH				
OFF DIAGONAL-	-10.75	SB22	-9.46 SB25	5.56 BB33		-3.16 BB31	2.33 SB21	-2.13 BB35		
NORMAL MODE 9	OBSERVED=	1270.0 CM-1		CALCULATED=		1271.2 CM-1		ERROR=	-1.2 CM-1 OR -0.1 PERCENT	
INTERNAL COORDINATES-	35.46	UCH4	35.46 OCH5	16.16 H4CC		16.16 H5CC				
FORCE CONSTANTS-	70.93	UCH	32.32 CC3H							
OFF DIAGONAL-	-6.40	BB33	1.97 BB35							
NORMAL MODE 10	OBSERVED=	1230.0 CM-1		CALCULATED=		1238.0 CM-1		ERROR=	-8.0 CM-1 OR -0.6 PERCENT	
INTERNAL COORDINATES-	73.09	HOC	7.19 C-C							
FORCE CONSTANTS-	73.09	COH	7.19 C-C	5.66 CC3H						
OFF DIAGONAL-	3.44	SB25	2.95 SB21	2.10 BB31						
NORMAL MODE 11	OBSERVED=	1138.0 CM-1		CALCULATED=		1126.3 CM-1		ERROR=	11.7 CM-1 OR 1.0 PERCENT	
INTERNAL COORDINATES-	30.69	C-C	27.30 C-O	16.82 HOC		11.21 CCH7	11.21 CCH8	10.47 H7H8		
FORCE CONSTANTS-	30.69	C-C	27.30 C-O	24.28 CC6H		18.30 HC6H	16.82 COH			
OFF DIAGONAL-	-13.03	SB24	-8.81 SB21	7.59 BB40		-2.50 BB35	-2.17 BB34	-2.16 SB23	1.58 BB44 -1.54 SS20	
NORMAL MODE 12	OBSERVED=	1058.0 CM-1		CALCULATED=		1071.0 CM-1		ERROR=	-13.0 CM-1 OR -1.2 PERCENT	
INTERNAL COORDINATES-	31.61	C-O	23.20 CCH9	15.88 H8H9		15.87 H7H9	6.56 C-C	5.01 H7H8		
FORCE CONSTANTS-	36.76	HC6H	31.61 C-O	24.49 CC6H		6.56 C-C				
OFF DIAGONAL-	7.72	BB40	-4.80 SB24	-3.83 SB23		-1.84 SB21				
NORMAL MODE 13	OBSERVED=	1045.0 CM-1		CALCULATED=		1041.9 CM-1		ERROR=	3.0 CM-1 OR 0.3 PERCENT	
INTERNAL COORDINATES-	37.70	H7H9	37.69 H8H9	5.44 CCH7		5.44 CCH8				
FORCE CONSTANTS-	75.39	HC6H	10.89 CC6H							
OFF DIAGONAL-	5.39	BB40	4.90 BB34							
NORMAL MODE 14	OBSERVED=	1022.0 CM-1		CALCULATED=		1014.1 CM-1		ERROR=	7.9 CM-1 OR 0.8 PERCENT	
INTERNAL COORDINATES-	54.48	H7H8	32.37 C-O							
FORCE CONSTANTS-	61.84	HC6H	32.37 C-O	5.28 CC6H						
OFF DIAGONAL-	-4.65	SB23	3.20 BB34	-3.18 SB21		1.89 BB40				
NORMAL MODE 15	OBSERVED=	0.0 CM-1		CALCULATED=		974.1 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	19.34	H4CC	19.34 H5CC	15.62 OCH4		15.62 OCH5	7.32 CCH7	7.32 CCH8		
FORCE CONSTANTS-	38.69	CC3H	31.23 OCH	14.64 CC6H		9.56 HC6H				
OFF DIAGONAL-	4.79	BB37	3.24 BB35	-2.82 BB33		-2.23 BB40				
NORMAL MODE 16	OBSERVED=	925.0 CM-1		CALCULATED=		923.0 CM-1		ERROR=	2.0 CM-1 OR 0.2 PERCENT	
INTERNAL COORDINATES-	36.80	C-C	12.71 OCC	9.80 CCH7		9.80 CCH8				
FORCE CONSTANTS-	36.80	C-C	20.90 CC6H	12.71 CCO		9.48 HC6H				
OFF DIAGONAL-	9.07	SB24	-6.78 SB26	6.19 BB44		2.52 SB25	1.81 BB40			
NORMAL MODE 17	OBSERVED=	751.0 CM-1		CALCULATED=		742.1 CM-1		ERROR=	8.9 CM-1 OR 1.2 PERCENT	
INTERNAL COORDINATES-	41.83	CCH9	19.13 C-O	14.53 C-C		5.96 H7H8				
FORCE CONSTANTS-	48.45	CC6H	19.13 C-O	14.53 C-C		5.96 HC6H				
OFF DIAGONAL-	-3.68	SB22	3.15 SB24	2.59 SB23		2.47 BB35	-1.62 BB40			
NORMAL MODE 18	OBSERVED=	668.0 CM-1		CALCULATED=		661.8 CM-1		ERROR=	6.2 CM-1 OR 0.9 PERCENT	
INTERNAL COORDINATES-	34.58	CCH7	34.58 CCH8	10.47 H4CC		10.47 H5CC				
FORCE CONSTANTS-	69.16	CC6H	20.94 CC3H	8.54 HC6H		6.38 OCH				
OFF DIAGONAL-	-7.66	BB37	5.51 BB35	-4.57 BB40						
NORMAL MODE 19	OBSERVED=	390.0 CM-1		CALCULATED=		384.2 CM-1		ERROR=	5.8 CM-1 OR 1.5 PERCENT	
INTERNAL COORDINATES-	80.04	OCC	11.63 CCH9	7.93 CCH8		7.93 CCH7				
FORCE CONSTANTS-	80.04	CCO	27.49 CC6H	7.72 CC3H						
OFF DIAGONAL-	-13.99	BB44	-4.88 BB45	3.21 SB26		-2.78 SB23	-2.23 BB37	-1.81 BB40 -1.71 SB25		
NORMAL MODE 20	OBSERVED=	0.0 CM-1		CALCULATED=		207.5 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	97.39	T-CO								
FORCE CONSTANTS-	97.39	TC-O								
OFF DIAGONAL -	NONE									
NORMAL MODE 21	OBSERVED=	0.0 CM-1		CALCULATED=		190.7 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	98.01	T-CC								
FORCE CONSTANTS-	98.01	TC-C								
OFF DIAGONAL -	NONE									

12. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 7.63

TABLE LII (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 300				PAGE 1	
MOLECULE 10		-6 NG= 201 ETHANOL, C03CH20D (TRANS)			
NORMAL MODE 7	OBSERVED=	1490.0 CM-1	CALCULATED=	1494.8 CM-1	ERROR= -4.8 CM-1 OR -0.3 PERCENT
INTERNAL COORDINATES-	74.37	HCH 6.29 OCH5	6.29	UCH4	
FORCE CONSTANTS-	74.37	HC3H 12.59 OCH	9.69	CC3H	
OFF DIAGONAL-	6.70	BB40 -3.49 BB38			
NORMAL MODE 8	OBSERVED=	1385.0 CM-1	CALCULATED=	1390.9 CM-1	ERROR= -5.9 CM-1 OR -0.4 PERCENT
INTERNAL COORDINATES-	31.20	UCH4 31.20 OCH5	20.00	H4CC 20.00 H5CC	7.85 C-C
FORCE CONSTANTS-	62.39	UCH 40.01 CC3H	7.85	C-C	
OFF DIAGONAL-	-10.55	SB22 -9.55 SB25	5.63	BB33 -2.39 BB35	
NORMAL MODE 9	OBSERVED=	1270.0 CM-1	CALCULATED=	1271.2 CM-1	ERROR= -1.2 CM-1 OR -0.1 PERCENT
INTERNAL COORDINATES-	35.47	UCH5 35.46 UCH4	16.16	H4CC 16.16 H5CC	
FORCE CONSTANTS-	70.93	UCH 32.32 CC3H			
OFF DIAGONAL-	-6.40	BB33 1.97 BB35			
NORMAL MODE 10	OBSERVED=	1138.0 CM-1	CALCULATED=	1145.3 CM-1	ERROR= -7.3 CM-1 OR -0.6 PERCENT
INTERNAL COORDINATES-	45.57	C-C 23.12 C-O	8.95	CCH7 8.95 CCH8	8.67 H7H8
FORCE CONSTANTS-	45.57	C-C 23.12 C-O	20.44	CC6H 15.95 HC6H	
OFF DIAGONAL-	-14.92	SB24 6.67 BB40	2.81	SB25 -2.30 BB35	1.99 SB22 -1.93 BB34 -1.72 SS20 1.59 SB21
NORMAL MODE 11	OBSERVED=	1058.0 CM-1	CALCULATED=	1071.3 CM-1	ERROR= -13.3 CM-1 OR -1.3 PERCENT
INTERNAL COORDINATES-	34.78	C-O 22.16 CCH9	14.25	H8H9 14.24 H7H9	6.46 H7H8 6.06 C-C
FORCE CONSTANTS-	34.95	HC6H 34.78 C-O	22.57	CC6H 6.06 C-C	
OFF DIAGONAL-	6.85	BB40 -4.71 SB23	-4.29	SB21 -4.03 SB24	
NORMAL MODE 12	OBSERVED=	1045.0 CM-1	CALCULATED=	1041.9 CM-1	ERROR= 3.0 CM-1 OR 0.3 PERCENT
INTERNAL COORDINATES-	37.70	H8H9 37.70 H7H9	5.44	CCH7 5.44 CCH8	
FORCE CONSTANTS-	75.39	HC6H 10.88 CC6H			
OFF DIAGONAL-	5.39	BB40 4.90 BB34			
NORMAL MODE 13	OBSERVED=	0.0 CM-1	CALCULATED=	1014.2 CM-1	ERROR= 0.0 CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	55.39	H7H8 29.99 C-O			
FORCE CONSTANTS-	60.09	HC6H 29.99 C-O	8.15	CC6H	
OFF DIAGONAL-	-3.45	SB23 3.13 BB40	2.66	BB34	
NORMAL MODE 14	OBSERVED=	0.0 CM-1	CALCULATED=	994.7 CM-1	ERROR= 0.0 CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	38.36	HOC 11.84 C-C	11.21	OC	7.58 CCH7 7.57 CCH8 6.77 H7H9 6.76 H8H9
FORCE CONSTANTS-	38.36	COH 15.19 CC6H	13.54	HC6H 11.84 C-C	11.21 CO
OFF DIAGONAL-	5.72	SB24 5.12 BB44	-4.92	SB21 -3.61 SB26 -3.15 SB23	2.72 BB40 2.65 SB25
NORMAL MODE 15	OBSERVED=	0.0 CM-1	CALCULATED=	974.1 CM-1	ERROR= 0.0 CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	19.35	H4CC 19.35 H5CC	15.62	UCH4 15.62 UCH5	7.33 CCH7 7.33 CCH8
FORCE CONSTANTS-	38.70	CC3H 31.23 OCH	14.65	CC6H 9.55 HC6H	
OFF DIAGONAL-	4.79	BB37 3.24 BB35	-2.82	BB33 -2.23 BB40	
NORMAL MODE 16	OBSERVED=	827.0 CM-1	CALCULATED=	839.5 CM-1	ERROR= -12.5 CM-1 OR -1.5 PERCENT
INTERNAL COORDINATES-	59.69	HOC 15.87 C-C			
FORCE CONSTANTS-	59.69	COH 15.87 C-C	14.46	CC6H	
OFF DIAGONAL-	-3.95	SB21 2.46 SB24	-2.33	SB26 2.25 BB44	
NORMAL MODE 17	OBSERVED=	758.0 CM-1	CALCULATED=	736.7 CM-1	ERROR= 21.3 CM-1 OR, 2.8 PERCENT
INTERNAL COORDINATES-	38.59	CCH9 18.07 C-O	17.81	C-C 5.63 H7H8	
FORCE CONSTANTS-	43.90	CC6H 18.07 C-O	17.81	C-C 5.66 HC6H	
OFF DIAGONAL-	3.64	SB24 -3.33 SB22	2.24	SB23 2.15 BB35	1.81 SB21
NORMAL MODE 18	OBSERVED=	668.0 CM-1	CALCULATED=	661.7 CM-1	ERROR= 6.3 CM-1 OR 0.9 PERCENT
INTERNAL COORDINATES-	34.58	CCH7 34.58 CCH8	10.49	H4CC 10.49 H5CC	
FORCE CONSTANTS-	69.17	CC6H 20.99 CC3H	8.54	HC6H 6.40 OCH	
OFF DIAGONAL-	-7.67	BB37 5.51 BB35	-4.58	BB40	
NORMAL MODE 19	OBSERVED=	380.0 CM-1	CALCULATED=	377.4 CM-1	ERROR= 2.6 CM-1 OR 0.7 PERCENT
INTERNAL COORDINATES-	80.19	UCC 11.42 CCH9	7.74	CCH8 7.74 CCH7	
FORCE CONSTANTS-	80.19	CCO 26.90 CC6H	7.59	CC3H	
OFF DIAGONAL-	-13.83	BB44 -4.84 BB45	2.97	SB26 -2.58 SB23 -2.18 BB37	-1.79 BB40 -1.57 SB25
NORMAL MODE 20	OBSERVED=	0.0 CM-1	CALCULATED=	191.1 CM-1	ERROR= 0.0 CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	98.76	T-CC			
FORCE CONSTANTS-	98.76	TC-C			
OFF DIAGONAL -	NONE				
NORMAL MODE 21	OBSERVED=	0.0 CM-1	CALCULATED=	152.9 CM-1	ERROR= 0.0 CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	98.46	T-CO			
FORCE CONSTANTS-	98.46	TC-O			
OFF DIAGONAL -	NONE				

10. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 7.83

TABLE LII (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 300										PAGE 1
MOLECULE 11 -6 NG= 201 ETHANOL, CD3CD2OH (TRANS)										
NORMAL MODE 7	OBSERVED=	1286.0 CM-1	CALCULATED=	1291.3 CM-1	ERROR=	-5.3 CM-1	OR	-0.4 PERCENT		
INTERNAL COORDINATES-	56.59	HOC 21.78 C-C	7.60 C-O							
FORCE CONSTANTS-	56.59	COH 21.78 C-C	9.95 OCH 8.73 CC3H 7.60 C-O							
OFF DIAGONAL-	8.53	SB21 -7.43 SB25	-5.45 SB22 -3.69 BB31 -2.11 SB24							
NORMAL MODE 8	OBSERVED=	1155.0 CM-1	CALCULATED=	1151.3 CM-1	ERROR=	3.7 CM-1	OR	0.3 PERCENT		
INTERNAL COORDINATES-	34.95	C-O 33.89 HOC	16.82 C-C 8.63 OCH4 8.63 OCH5 6.26 HCH 6.05 CCH7 6.05 CCH8							
FORCE CONSTANTS-	34.95	C-O 33.89 COH	17.27 OCH 16.82 C-C 12.16 CC6H 6.77 HC6H 6.26 HC3H							
OFF DIAGONAL-	-15.39	SB22-14.15 SB21	-5.59 SB24 -4.87 SB25 3.76 BB31 -3.68 SB23 1.75 BB44 1.64 SB26 1.56 BB33							
NORMAL MODE 9	OBSERVED=	1120.0 CM-1	CALCULATED=	1097.8 CM-1	ERROR=	22.2 CM-1	OR	2.0 PERCENT		
INTERNAL COORDINATES-	43.80	HCH 16.03 C-C	11.40 CCH9 6.51 H8H9 6.50 H7H9							
FORCE CONSTANTS-	43.80	HC3H 16.03 C-C	13.87 CC6H 13.02 HC6H 8.38 OCH							
OFF DIAGONAL-	7.27	BB40 -6.54 SB24	-3.94 SB25 -3.90 SB22 -2.19 BB38 1.90 SB21 -1.75 SB26							
NORMAL MODE 10	OBSERVED=	1064.0 CM-1	CALCULATED=	1065.8 CM-1	ERROR=	-1.8 CM-1	OR	-0.2 PERCENT		
INTERNAL COORDINATES-	18.08	HCH 13.87 CCH9	9.79 H8H9 9.79 H7H9 8.62 H5CC 8.62 H4CC 8.17 C-O 6.73 HOC							5.65 CCH8
FORCE CONSTANTS-	25.17	CC6H 21.28 HC6H	18.08 HC3H 17.23 CC3H 8.17 C-O 6.73 COH							
OFF DIAGONAL-	12.75	BB40 -3.91 BB35	-3.05 SB21 -2.93 SB24 -2.81 BB37 2.65 SB25 -2.41 SB22 -2.33 BB34							
NORMAL MODE 11	OBSERVED=	1052.0 CM-1	CALCULATED=	1041.3 CM-1	ERROR=	10.7 CM-1	OR	1.0 PERCENT		
INTERNAL COORDINATES-	40.38	H8H9 40.38 H7H9								
FORCE CONSTANTS-	80.76	HC6H 7.46 CC6H								
OFF DIAGONAL-	5.25	BB34 4.62 BB40								
NORMAL MODE 12	OBSERVED=	0.0 CM-1	CALCULATED=	1032.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	57.26	H7H8 7.00 H7H9	6.98 H8H9 5.84 OCH5 5.84 OCH4							
FORCE CONSTANTS-	71.24	HC6H 11.69 OCH								
OFF DIAGONAL-	4.29	BB34 2.50 BB40	-1.62 SB22							
NORMAL MODE 13	OBSERVED=	965.0 CM-1	CALCULATED=	964.6 CM-1	ERROR=	0.4 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	41.84	C-O 12.18 OCH4	12.17 OCH5 6.24 H7H8							
FORCE CONSTANTS-	41.84	C-O 24.35 OCH	8.32 HC6H 5.56 CC3H							
OFF DIAGONAL-	20.00	SB22 -7.03 SB23	2.20 BB33 -1.81 SB25							
NORMAL MODE 14	OBSERVED=	904.0 CM-1	CALCULATED=	923.0 CM-1	ERROR=	-19.0 CM-1	OR	-2.1 PERCENT		
INTERNAL COORDINATES-	30.70	UCH4 30.70 UCH5	17.04 H4CC 17.04 H5CC							
FORCE CONSTANTS-	61.40	UCH 34.08 CC3H								
OFF DIAGONAL-	-5.54	BB33 2.57 BB37	2.36 BB35							
NORMAL MODE 15	OBSERVED=	889.0 CM-1	CALCULATED=	885.1 CM-1	ERROR=	3.9 CM-1	OR	0.4 PERCENT		
INTERNAL COORDINATES-	29.26	C-C 8.93 CCH7	8.93 CCH8 8.86 OCC							
FORCE CONSTANTS-	29.26	C-C 22.03 CC6H	8.86 CCO 8.00 CC3H 5.81 HC6H							
OFF DIAGONAL-	8.24	SB25 6.21 SB24	-5.05 SB26 4.94 BB44 2.40 BB37 1.62 BB40 1.51 SB23							
NORMAL MODE 16	OBSERVED=	878.0 CM-1	CALCULATED=	866.5 CM-1	ERROR=	11.5 CM-1	OR	1.3 PERCENT		
INTERNAL COORDINATES-	18.00	CCH7 17.99 CCH8	17.58 UCH4 17.58 UCH5 7.93 H5CC 7.92 H4CC							
FORCE CONSTANTS-	35.99	CC6H 35.16 UCH	15.85 CC3H 7.39 HC6H							
OFF DIAGONAL-	4.81	BB37 3.17 BB35	-3.17 BB33 -3.07 BB40							
NORMAL MODE 17	OBSERVED=	744.0 CM-1	CALCULATED=	733.9 CM-1	ERROR=	10.1 CM-1	OR	1.3 PERCENT		
INTERNAL COORDINATES-	39.02	CCH9 17.89 C-C	16.43 C-O 5.96 H7H8							
FORCE CONSTANTS-	44.15	CC6H 17.89 C-C	16.43 C-O 6.00 HC6H							
OFF DIAGONAL-	-5.35	SB22 3.76 SB24	2.38 SB25 2.27 SB23 2.07 BB35 1.53 SB26							
NORMAL MODE 18	OBSERVED=	589.0 CM-1	CALCULATED=	589.6 CM-1	ERROR=	-0.6 CM-1	OR	-0.1 PERCENT		
INTERNAL COORDINATES-	23.20	CCH7 23.20 CCH8	21.28 H4CC 21.28 H5CC 5.07 UCH4 5.07 UCH5							
FORCE CONSTANTS-	46.39	CC6H 42.55 CC3H	10.13 UCH 5.59 HC6H							
OFF DIAGONAL-	-8.94	BB37 5.42 BB35	-3.03 BB40							
NORMAL MODE 19	OBSERVED=	0.0 CM-1	CALCULATED=	380.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	80.62	OCC 11.66 CCH9	7.79 CCH8 7.79 CCH7							
FORCE CONSTANTS-	80.62	CCO 27.24 CC6H	8.81 CC3H							
OFF DIAGONAL-	-13.91	BB44 -4.90 BB45	-3.02 SB23 2.86 SB26 -2.36 BB37 -1.74 BB40 -1.62 SB25							
NORMAL MODE 20	OBSERVED=	0.0 CM-1	CALCULATED=	207.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	97.67	T-CO								
FORCE CONSTANTS-	97.67	TC-O								
OFF DIAGONAL -	NONE									
NORMAL MODE 21	OBSERVED=	0.0 CM-1	CALCULATED=	182.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	97.53	T-CC								
FORCE CONSTANTS-	97.53	TC-C								
OFF DIAGONAL -	NONE									

11. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 8.13

TABLE LII (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 300

PAGE 1

MOLECULE 12 -6 NG= 201 ETHANOL, C03C020D (TRANS)

NORMAL MODE 7	OBSERVED=	1229.0 CM-1	CALCULATED=	1218.0 CM-1	ERROR=	11.0 CM-1	OR	0.9 PERCENT
INTERNAL COORDINATES-	46.76	C-C 27.22 C-O	11.78	OCH4 11.78 OCH5	9.70	H4CC 9.70 H5CC		
FORCE CONSTANTS-	46.76	C-C 27.22 C-O	23.56	OCH 19.40 CC3H	6.55	CC6H		
OFF DIAGONAL-	-16.23	SB25-15.86 SB22	-7.32	SB24 4.35 SB21	2.56	BB40 2.27 BB37	2.13 BB33 -1.89 SS20	-1.60 BB35
NORMAL MODE 8	OBSERVED=	1130.0 CM-1	CALCULATED=	1110.9 CM-1	ERROR=	19.1 CM-1	OR	1.7 PERCENT
INTERNAL COORDINATES-	57.40	HCH 15.83 C-O	5.52	OCH5 5.52 OCH4				
FORCE CONSTANTS-	57.40	HC3H 15.83 C-O	11.05	OCH 6.22 CC6H				
OFF DIAGONAL-	-8.28	SB22 4.38 BB40	-4.24	SB23 -3.35 SB21	-2.88	BB38 -1.78 SB25		
NORMAL MODE 9	OBSERVED=	1068.0 CM-1	CALCULATED=	1075.0 CM-1	ERROR=	-7.0 CM-1	OR	-0.7 PERCENT
INTERNAL COORDINATES-	19.96	CCH9 15.00 H7H9	14.99	H8H9 10.10 CCH8	10.10	CCH7 7.99 C-C		
FORCE CONSTANTS-	40.16	CC6H 33.64 HC6H	7.99	C-C 7.93 CC3H	5.07	OCH		
OFF DIAGONAL-	14.44	BB40 -8.93 SB24	-5.20	BB35 4.29 SB25	-3.87	BB34 -2.83 SB22	-2.55	BB37
NORMAL MODE 10	OBSERVED=	1052.0 CM-1	CALCULATED=	1041.3 CM-1	ERROR=	10.7 CM-1	OR	1.0 PERCENT
INTERNAL COORDINATES-	40.39	H8H9 40.37 H7H9						
FORCE CONSTANTS-	80.76	HC6H 7.46 CC6H						
OFF DIAGONAL-	5.25	BB34 4.62 BB40						
NORMAL MODE 11	OBSERVED=	1019.0 CM-1	CALCULATED=	1034.6 CM-1	ERROR=	-15.6 CM-1	OR	-1.5 PERCENT
INTERNAL COORDINATES-	52.14	H7H8 8.27 HCH	7.24	H7H9 7.23 H8H9	5.86	OCH4 5.85 OCH5		
FORCE CONSTANTS-	66.62	HC6H 11.71 OCH	8.27	HC3H				
OFF DIAGONAL-	4.11	BB34 2.74 BB40						
NORMAL MODE 12	OBSERVED=	965.0 CM-1	CALCULATED=	983.0 CM-1	ERROR=	-18.0 CM-1	OR	-1.9 PERCENT
INTERNAL COORDINATES-	46.03	C-O 24.30 HOC	9.25	H7H8 7.29 OCC	5.29	OCH4 5.29 OCH5		
FORCE CONSTANTS-	46.03	C-O 24.30 COH	13.17	HC6H 10.59 OCH	7.29	CCO		
OFF DIAGONAL-	13.83	SB22-13.75 SB21	-8.92	SB23 -2.49 BB31				
NORMAL MODE 13	OBSERVED=	915.0 CM-1	CALCULATED=	923.0 CM-1	ERROR=	-8.0 CM-1	OR	-0.9 PERCENT
INTERNAL COORDINATES-	30.71	OCH4 30.71 OCH5	17.04	H4CC 17.04 H5CC				
FORCE CONSTANTS-	61.42	OCH 34.08 CC3H						
OFF DIAGONAL-	-5.54	BB33 2.57 BB37	2.36	BB35				
NORMAL MODE 14	OBSERVED=	904.0 CM-1	CALCULATED=	915.7 CM-1	ERROR=	-11.7 CM-1	OR	-1.3 PERCENT
INTERNAL COORDINATES-	15.57	HOC 9.84 H4CC	9.84	H5CC 7.91 C-C	5.33	C-O		
FORCE CONSTANTS-	19.68	CC3H 15.57 COH	9.76	OCH 7.91 C-C	7.86	CC6H 5.33 C-O		
OFF DIAGONAL-	6.72	SB25 4.52 SB22	3.74	SB21 2.71 BB40	2.57	SB24 2.42 BB37	1.91 BB31	1.69 SB23 1.60 BB44
NORMAL MODE 15	OBSERVED=	878.0 CM-1	CALCULATED=	866.4 CM-1	ERROR=	11.5 CM-1	OR	1.3 PERCENT
INTERNAL COORDINATES-	18.00	CCH7 18.00 CCH8	17.57	OCH4 17.57 OCH5	7.93	H4CC 7.93 H5CC		
FORCE CONSTANTS-	36.01	CC6H 35.14 OCH	15.86	CC3H 7.39 HC6H				
OFF DIAGONAL-	4.81	BB37 3.17 BB35	-3.17	BB33 -3.07 BB40				
NORMAL MODE 16	OBSERVED=	819.0 CM-1	CALCULATED=	833.6 CM-1	ERROR=	-14.6 CM-1	OR	-1.8 PERCENT
INTERNAL COORDINATES-	53.55	HOC 16.80 C-C	5.89	CCH9 5.14 CCH8	5.14	CCH7		
FORCE CONSTANTS-	53.55	COH 16.80 C-C	16.18	CC6H				
OFF DIAGONAL-	-2.54	SB26 2.52 SB24	2.49	BB44 -2.30 SB21	1.80	BB31		
NORMAL MODE 17	OBSERVED=	736.0 CM-1	CALCULATED=	729.9 CM-1	ERROR=	6.1 CM-1	OR	0.8 PERCENT
INTERNAL COORDINATES-	36.78	CCH9 20.39 C-C	16.18	C-O 5.68 H7H8				
FORCE CONSTANTS-	41.13	CC6H 20.39 C-C	16.18	C-O 5.76 HC6H				
OFF DIAGONAL-	-4.86	SB22 4.11 SB24	2.24	SB25 2.05 SB23	1.87	BB35		
NORMAL MODE 18	OBSERVED=	589.0 CM-1	CALCULATED=	589.5 CM-1	ERROR=	-0.5 CM-1	OR	-0.1 PERCENT
INTERNAL COORDINATES-	23.20	CCH7 23.20 CCH8	21.32	H4CC 21.32 H5CC	5.08	OCH4 5.08 OCH5		
FORCE CONSTANTS-	46.41	CC6H 42.64 CC3H	10.16	OCH 5.59 HC6H				
OFF DIAGONAL-	-8.95	BB37 5.43 BB35	-3.03	BB40				
NORMAL MODE 19	OBSERVED=	0.0 CM-1	CALCULATED=	373.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	80.78	OCC 11.41 CCH9	7.61	CCH8 7.60 CCH7				
FORCE CONSTANTS-	80.78	CCO 26.62 CC6H	8.56	CC3H				
OFF DIAGONAL-	-13.76	BB44 -4.85 BB45	-2.93	SB23 2.65 SB26	-2.30	BB37 -1.71 BB40		
NORMAL MODE 20	OBSERVED=	0.0 CM-1	CALCULATED=	183.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	97.27	T-CC						
FORCE CONSTANTS-	97.27	TC-C						
OFF DIAGONAL -	NONE							
NORMAL MODE 21	OBSERVED=	0.0 CM-1	CALCULATED=	152.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	97.98	T-CO						
FORCE CONSTANTS-	97.98	TC-O						
OFF DIAGONAL -	NONE							

12. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR =11.16

TABLE LIII

POTENTIAL ENERGY DISTRIBUTIONS FOR LIQUID ETHANOL (TRANS)

Explanation of the table:

This table is presented in the same format as Table XXXIV except that the force constant and internal coordinate description codes are found in Tables XLIII and XLIV, respectively.

TABLE LIII

POTENTIAL ENERGY DISTRIBUTIONS FOR LIQUID ETHANOL (TRANS)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 300										PAGE 1	
MOLECULE 1		-6 NG= 202		ETHANOL, CH3CHDOH (TRANS)							
NORMAL MODE 7	OBSERVED=	1460.0 CM-1	CALCULATED=	1457.1 CM-1	ERROR=	2.9 CM-1	OR	0.2 PERCENT			
INTERNAL COORDINATES-	49.10 H7H8	14.70 H8H9	8.19 H7H9	8.01 CCH9							
FORCE CONSTANTS-	72.00 HC6H	13.16 CC6H									
OFF DIAGONAL-	6.28 BB40	4.25 BB34									
NORMAL MODE 8	OBSERVED=	1447.0 CM-1	CALCULATED=	1452.2 CM-1	ERROR=	-5.2 CM-1	OR	-0.4 PERCENT			
INTERNAL COORDINATES-	41.78 H7H9	34.98 H8H9	6.00 CCH8	5.01 CCH7							
FORCE CONSTANTS-	77.06 HC6H	11.06 CC6H									
OFF DIAGONAL-	6.04 BB40	4.56 BB34									
NORMAL MODE 9	OBSERVED=	1398.0 CM-1	CALCULATED=	1411.6 CM-1	ERROR=	-13.6 CM-1	OR	-1.0 PERCENT			
INTERNAL COORDINATES-	62.57 HOC	12.53 H5CC	10.46 C-C	10.33 OCH5							
FORCE CONSTANTS-	62.57 COH	14.80 CC3H	12.02 OCH	10.46 C-C							
OFF DIAGONAL-	-6.59 SB25	3.38 SB21	-2.64 BB31	-2.17 SB22	2.07 BB40						
NORMAL MODE 10	OBSERVED=	1374.0 CM-1	CALCULATED=	1380.7 CM-1	ERROR=	-6.7 CM-1	OR	-0.5 PERCENT			
INTERNAL COORDINATES-	18.22 CCH7	17.66 CCH8	15.68 H8H9	15.19 H7H9	13.60 CCH9	8.79 H7H8					
FORCE CONSTANTS-	49.48 CC6H	39.65 HC6H									
OFF DIAGONAL-	17.97 BB40	-8.03 BB35	-7.84 SB24	-4.58 BB34	2.01 BB44						
NORMAL MODE 11	OBSERVED=	1333.0 CM-1	CALCULATED=	1325.5 CM-1	ERROR=	7.5 CM-1	OR	0.6 PERCENT			
INTERNAL COORDINATES-	57.16 OCH5	34.38 HCH									
FORCE CONSTANTS-	58.86 OCH	34.38 HC3H									
OFF DIAGONAL-	-6.21 BB38	-5.85 SB22	1.78 BB33								
NORMAL MODE 12	OBSERVED=	1313.0 CM-1	CALCULATED=	1298.8 CM-1	ERROR=	14.3 CM-1	OR	1.1 PERCENT			
INTERNAL COORDINATES-	32.69 H5CC	31.70 HCH	23.10 HOC								
FORCE CONSTANTS-	33.85 CC3H	31.70 HC3H	23.10 COH								
OFF DIAGONAL-	7.56 BB40										
NORMAL MODE 13	OBSERVED=	1130.0 CM-1	CALCULATED=	1131.7 CM-1	ERROR=	-1.7 CM-1	OR	-0.1 PERCENT			
INTERNAL COORDINATES-	51.07 C-O	16.91 CCH9	9.75 OCH4	8.59 H7H8	6.22 H4CC						
FORCE CONSTANTS-	51.07 C-O	20.49 CC6H	13.24 OCH	9.82 HC6H	6.40 CC3H						
OFF DIAGONAL-	-6.74 SB23	-5.39 SB21	-3.87 SB22	-2.64 BB40	1.99 BB44	-1.72 SB25	1.65 BB35				
NORMAL MODE 14	OBSERVED=	1044.0 CM-1	CALCULATED=	1051.3 CM-1	ERROR=	-7.3 CM-1	OR	-0.7 PERCENT			
INTERNAL COORDINATES-	37.54 C-C	19.11 CCH7	9.19 H4CC	8.72 CCH9	5.45 OCC						
FORCE CONSTANTS-	37.54 C-C	30.45 CC6H	10.45 CC3H	7.72 HC6H	6.42 OCH	5.45 CCO					
OFF DIAGONAL-	-4.72 SB25	-3.91 SB26	3.03 BB35	-2.95 BB40	2.38 BB44	2.04 BB37	-1.75 SB22				
NORMAL MODE 15	OBSERVED=	0.0 CM-1	CALCULATED=	1014.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	30.77 CCH8	18.18 C-C	11.52 CCH7	6.83 C-O	6.77 H7H9						
FORCE CONSTANTS-	47.27 CC6H	18.18 C-C	10.61 HC6H	6.83 C-O							
OFF DIAGONAL-	-4.33 BB40	4.13 BB35	2.98 BB37	2.11 SB25							
NORMAL MODE 16	OBSERVED=	943.0 CM-1	CALCULATED=	937.3 CM-1	ERROR=	5.7 CM-1	OR	0.6 PERCENT			
INTERNAL COORDINATES-	58.01 OCH4	16.05 C-O	12.78 H4CC								
FORCE CONSTANTS-	61.84 OCH	16.05 C-O	12.79 CC3H								
OFF DIAGONAL-	9.78 SB22	-2.69 BB33									
NORMAL MODE 17	OBSERVED=	870.0 CM-1	CALCULATED=	873.2 CM-1	ERROR=	-3.2 CM-1	OR	-0.4 PERCENT			
INTERNAL COORDINATES-	33.29 C-O	30.62 C-C	18.83 CCH9	6.30 CCH7	6.08 OCH4						
FORCE CONSTANTS-	33.29 C-O	30.62 C-C	27.24 CC6H	6.12 OCH							
OFF DIAGONAL-	-6.59 SB22	4.25 SB25	3.14 SS20	-2.37 BB40	-2.14 SB23	2.06 BB35					
NORMAL MODE 18	OBSERVED=	724.0 CM-1	CALCULATED=	716.2 CM-1	ERROR=	7.8 CM-1	OR	1.1 PERCENT			
INTERNAL COORDINATES-	33.94 H4CC	19.84 H5CC	10.55 CCH7	10.11 CCH8	9.67 OCH4	9.52 OCH5					
FORCE CONSTANTS-	53.78 CC3H	20.66 CC6H	19.19 OCH								
OFF DIAGONAL-	-6.88 BB37	5.89 BB35	-1.73 BB33	1.54 BB36							
NORMAL MODE 19	OBSERVED=	432.0 CM-1	CALCULATED=	432.8 CM-1	ERROR=	-0.8 CM-1	OR	-0.2 PERCENT			
INTERNAL COORDINATES-	87.67 OCC	7.07 CCH9	6.43 CCH8	5.79 CCH7							
FORCE CONSTANTS-	87.67 CCO	19.29 CC6H	5.81 CC3H								
OFF DIAGONAL-	-17.14 BB44	-3.79 BB45	-3.38 BB46	3.03 SB26	2.04 BB43	-1.75 BB37	-1.62 SB25				
NORMAL MODE 20	OBSERVED=	0.0 CM-1	CALCULATED=	245.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	98.46 T-CC										
FORCE CONSTANTS-	98.46 TC-C										
OFF DIAGONAL -	NONE										
NORMAL MODE 21	OBSERVED=	0.0 CM-1	CALCULATED=	207.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	98.91 T-CO										
FORCE CONSTANTS-	98.91 TC-O										
OFF DIAGONAL -	NONE										

13. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 6.06

TABLE LIII (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 300										PAGE 1	
MOLECULE 2		-6, NG= 202		ETHANOL, CH3CHDOO (TRANS)							
NORMAL MODE 7	OBSERVED=	1462.0 CM-1		CALCULATED=		1457.1 CM-1		ERROR=	4.9 CM-1	OR	0.3 PERCENT
INTERNAL COORDINATES-	49.17	H7H8	14.90	H8H9	8.09	H7H9	8.00	CCH9			
FORCE CONSTANTS-	72.17	HC6H	13.14	CC6H							
OFF DIAGONAL -	6.30	BB40	4.26	BB34							
NORMAL MODE 8	OBSERVED=	1446.0 CM-1		CALCULATED=		1452.2 CM-1		ERROR=	-6.2 CM-1	OR	-0.4 PERCENT
INTERNAL COORDINATES-	41.96	H7H9	34.78	H8H9	6.02	CCH8					
FORCE CONSTANTS-	77.06	HC6H	11.07	CC6H							
OFF DIAGONAL -	6.04	BB40	4.56	BB34							
NORMAL MODE 9	OBSERVED=	1376.0 CM-1		CALCULATED=		1383.2 CM-1		ERROR=	-7.2 CM-1	OR	-0.5 PERCENT
INTERNAL COORDINATES-	17.95	CCH7	16.19	CCH8	15.61	H8H9	14.73	H7H9	11.88	CCH9	10.15 C-C 6.92 H7H8 6.20 OCH5
FORCE CONSTANTS-	46.02	CC6H	37.26	HC6H	10.15	C-C	6.69	UCH	5.08	CC3H	
OFF DIAGONAL -	16.69	BB40	-11.23	SB24	-7.66	BB35	-4.22	BB34	-3.64	SB25	2.47 BB37 -1.59 SB22
NORMAL MODE 10	OBSERVED=	1344.0 CM-1		CALCULATED=		1344.3 CM-1		ERROR=	-0.3 CM-1	OR	-0.0 PERCENT
INTERNAL COORDINATES-	40.91	UCH5	36.50	H5CC							
FORCE CONSTANTS-	42.55	UCH	38.90	CC3H	7.81	CC6H	6.74	HC6H			
OFF DIAGONAL -	-5.39	SB22	-4.91	SB25	4.71	BB40	-2.64	BB35	2.24	SB24	-1.72 BB37
NORMAL MODE 11	OBSERVED=	1328.0 CM-1		CALCULATED=		1320.4 CM-1		ERROR=	7.6 CM-1	OR	0.6 PERCENT
INTERNAL COORDINATES-	67.03	HCH	23.97	UCH5							
FORCE CONSTANTS-	67.03	HC3H	25.02	UCH							
OFF DIAGONAL -	-5.80	BB38	4.73	BB40	-1.99	SB22					
NORMAL MODE 12	OBSERVED=	1159.0 CM-1		CALCULATED=		1141.2 CM-1		ERROR=	17.8 CM-1	OR	1.5 PERCENT
INTERNAL COORDINATES-	31.25	C-O	26.36	C-C	14.41	UCH4	8.78	H4CC	7.09	HOC	
FORCE CONSTANTS-	31.25	C-O	26.36	C-C	16.45	UCH	12.19	CC3H	7.09	COH	6.39 CC6H
OFF DIAGONAL -	5.70	SB21	-5.70	SB22	-2.82	SS20	-2.31	SB25			
NORMAL MODE 13	OBSERVED=	1120.0 CM-1		CALCULATED=		1117.8 CM-1		ERROR=	2.2 CM-1	DR	0.2 PERCENT
INTERNAL COORDINATES-	26.21	HOC	19.06	CCH9	17.44	C-O	13.62	C-C	11.33	OCC	8.18 H7H8 5.36 CCH7
FORCE CONSTANTS-	26.21	COH	24.99	CC6H	17.44	C-O	13.62	C-C	11.33	CCO	10.05 HC6H
OFF DIAGONAL -	-8.18	SB21	-6.33	SB23	3.83	BB44	-3.40	SB26	-2.91	BB40	2.58 SB22 2.24 BB45 2.04 SB25 1.91 BB35
NORMAL MODE 14	OBSERVED=	1016.0 CM-1		CALCULATED=		1020.7 CM-1		ERROR=	-4.7 CM-1	DR	-0.5 PERCENT
INTERNAL COORDINATES-	31.42	CCH8	25.03	CCH7	9.17	H4CC	7.10	H7H9	6.12	H8H9	
FORCE CONSTANTS-	56.90	CC6H	13.28	HC6H	10.11	CC3H					
OFF DIAGONAL -	5.12	BB35	-5.09	BB40	4.55	BB37					
NORMAL MODE 15	OBSERVED=	968.0 CM-1		CALCULATED=		963.1 CM-1		ERROR=	4.9 CM-1	OR	0.5 PERCENT
INTERNAL COORDINATES-	41.47	HOC	30.41	C-O	12.84	C-C	9.66	CCH9	5.47	UCH4	
FORCE CONSTANTS-	41.47	COH	30.41	C-O	15.19	CC6H	12.84	C-C	9.28	UCH	
OFF DIAGONAL -	-13.59	SB21	-1.94	SS20							
NORMAL MODE 16	OBSERVED=	916.0 CM-1		CALCULATED=		923.1 CM-1		ERROR=	-7.1 CM-1	OR	-0.8 PERCENT
INTERNAL COORDINATES-	57.58	UCH4	15.46	HOC	14.28	H4CC					
FORCE CONSTANTS-	58.68	UCH	15.46	COH	14.65	CC3H	8.02	CC6H			
OFF DIAGONAL -	1.90	BB31									
NORMAL MODE 17	OBSERVED=	868.0 CM-1		CALCULATED=		856.0 CM-1		ERROR=	12.0 CM-1	OR	1.4 PERCENT
INTERNAL COORDINATES-	37.38	C-C	27.57	C-O	11.90	CCH9	8.53	HOC			
FORCE CONSTANTS-	37.38	C-C	27.57	C-O	17.04	CC6H	8.53	COH			
OFF DIAGONAL -	5.87	SB21	3.15	SS20	-2.40	SB22	-2.08	SB23	1.68	SB25	
NORMAL MODE 18	OBSERVED=	716.0 CM-1		CALCULATED=		716.1 CM-1		ERROR=	-0.1 CM-1	OR	-0.0 PERCENT
INTERNAL COORDINATES-	34.02	H4CC	19.83	H5CC	10.53	CCH7	10.14	CCH8	9.67	UCH4	9.53 UCH5
FORCE CONSTANTS-	53.86	CC3H	20.67	CC6H	19.20	UCH					
OFF DIAGONAL -	-6.89	BB37	5.89	BB35	-1.73	BB33	1.54	BB36			
NORMAL MODE 19	OBSERVED=	427.0 CM-1		CALCULATED=		425.4 CM-1		ERROR=	1.6 CM-1	OR	0.4 PERCENT
INTERNAL COORDINATES-	87.62	UCH	6.95	CCH9	6.30	CCH8	5.72	CCH7			
FORCE CONSTANTS-	87.62	CCO	18.97	CC6H	5.59	CC3H					
OFF DIAGONAL -	-16.99	BB44	-3.75	BB45	-3.46	BB46	2.79	SB26	2.00	BB43	-1.70 BB37
NORMAL MODE 20	OBSERVED=	0.0 CM-1		CALCULATED=		245.0 CM-1		ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	98.55	T-CC									
FORCE CONSTANTS-	98.55	TC-C									
OFF DIAGONAL -	NONE										
NORMAL MODE 21	OBSERVED=	0.0 CM-1		CALCULATED=		153.7 CM-1		ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	99.05	T-CO									
FORCE CONSTANTS-	99.05	TC-O									
OFF DIAGONAL -	NONE										

14. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 5.63

TABLE LIII (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 300										PAGE 1	
MOLECULE 3		-6 NG= 202		ETHANOL, CD3CHDOH (TRANS)							
NORMAL MODE 7	OBSERVED=	1420.0	CM-1	CALCULATED=	1410.5	CM-1	ERROR=	9.5	CM-1	OR	0.7 PERCENT
INTERNAL COORDINATES-	65.39	HOC	11.94	H5CC	10.18	OCH5	9.02	C-C			
FORCE CONSTANTS-	65.39	COH	14.21	CC3H	11.87	OCH	9.02	C-C			
OFF DIAGONAL-	-6.01	SB25	3.43	SB21	-2.69	BB31	-2.14	SB22	1.79	BB40	
NORMAL MODE 8	OBSERVED=	1328.0	CM-1	CALCULATED=	1327.9	CM-1	ERROR=	0.1	CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	59.43	OCH5	38.44	HCH							
FORCE CONSTANTS-	61.45	OCH	38.44	HC3H							
OFF DIAGONAL-	-7.13	SB22	-6.77	BB38	1.98	BB33	-1.89	BB40			
NORMAL MODE 9	OBSERVED=	1298.0	CM-1	CALCULATED=	1296.6	CM-1	ERROR=	1.4	CM-1	OR	0.1 PERCENT
INTERNAL COORDINATES-	33.72	H5CC	29.39	HCH	24.70	HOC					
FORCE CONSTANTS-	35.13	CC3H	29.39	HC3H	24.70	COH					
OFF DIAGONAL-	7.30	BB40	-1.96	SB25							
NORMAL MODE 10	OBSERVED=	1142.0	CM-1	CALCULATED=	1140.8	CM-1	ERROR=	1.2	CM-1	OR	0.1 PERCENT
INTERNAL COORDINATES-	38.57	C-O	31.69	C-C	9.30	CCH8	9.07	CCH7	7.92	H7H8	7.77
FORCE CONSTANTS-	38.57	C-O	31.69	C-C	18.58	CC6H	12.51	HC6H	9.43	OCH	6.26
OFF DIAGONAL-	-11.03	SB24	-5.95	SB21	5.57	BB40	-4.02	SB22	-3.48	SB25	-3.43
										SS20	-2.64
										SB23	2.12
										BB44	-1.78
										BB35	
NORMAL MODE 11	OBSERVED=	1065.0	CM-1	CALCULATED=	1076.3	CM-1	ERROR=	-11.3	CM-1	OR	-1.1 PERCENT
INTERNAL COORDINATES-	25.82	CCH9	22.41	C-O	20.13	H8H9	13.43	C-C	11.97	H7H9	
FORCE CONSTANTS-	32.60	HC6H	30.70	CC6H	22.41	C-O	13.43	C-C			
OFF DIAGONAL-	10.41	BB40	-8.98	SB24	-2.97	BB35	-2.91	SB23	2.08	SB25	-1.88
										SB22	1.70
										SS20	-1.55
										BB44	
NORMAL MODE 12	OBSERVED=	1049.0	CM-1	CALCULATED=	1038.8	CM-1	ERROR=	10.2	CM-1	OR	1.0 PERCENT
INTERNAL COORDINATES-	46.46	H7H9	30.39	H8H9	5.16	CCH8					
FORCE CONSTANTS-	78.56	HC6H	8.90	CC6H							
OFF DIAGONAL-	5.44	BB40	4.65	BB34							
NORMAL MODE 13	OBSERVED=	1005.0	CM-1	CALCULATED=	1018.9	CM-1	ERROR=	-13.9	CM-1	OR	-1.4 PERCENT
INTERNAL COORDINATES-	57.76	H7H8	13.05	C-O	8.37	H8H9	7.56	OCH4	5.18	CCH7	
FORCE CONSTANTS-	67.24	HC6H	13.05	C-O	7.65	OCH	7.04	CC6H			
OFF DIAGONAL-	-3.81	SB22	3.54	BB40	3.19	BB34	-1.59	SB23			
NORMAL MODE 14	OBSERVED=	943.0	CM-1	CALCULATED=	962.7	CM-1	ERROR=	-19.7	CM-1	OR	-2.1 PERCENT
INTERNAL COORDINATES-	17.89	C-C	16.36	H4CC	15.31	OCH4	10.48	CCH7	10.04	OCC	6.65
FORCE CONSTANTS-	19.16	CC3H	17.89	C-C	16.34	OCH	11.21	CC6H	10.16	HC6H	10.04
OFF DIAGONAL-	5.48	SB22	4.56	BB44	4.24	SB24	-4.05	SB25	-3.68	SB23	-3.66
										SB26	-2.10
										BB46	
NORMAL MODE 15	OBSERVED=	917.0	CM-1	CALCULATED=	924.8	CM-1	ERROR=	-7.8	CM-1	OR	-0.9 PERCENT
INTERNAL COORDINATES-	31.44	OCH4	14.04	C-C	12.10	C-O	6.50	H4CC	5.47	OCH5	
FORCE CONSTANTS-	36.91	OCH	14.04	C-C	12.10	C-O	7.84	CC6H	6.92	CC3H	
OFF DIAGONAL-	4.90	SB22	4.84	SB25	3.64	SB24	2.51	SB23	-2.37	BB33	2.27
										BB44	-1.64
										SB26	-1.61
										SB21	
NORMAL MODE 16	OBSERVED=	0.0	CM-1	CALCULATED=	883.3	CM-1	ERROR=	0.0	CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	23.04	CCH8	15.77	OCH4	14.60	H4CC	6.94	CCH7	6.81	H5CC	6.44
FORCE CONSTANTS-	30.73	CC6H	21.52	OCH	21.40	CC3H	8.10	HC6H		H7H9	5.75
OFF DIAGONAL-	5.26	BB37	3.98	BB35	-2.55	BB40	-1.72	BB33		OCH5	
NORMAL MODE 17	OBSERVED=	746.0	CM-1	CALCULATED=	744.1	CM-1	ERROR=	1.9	CM-1	OR	0.3 PERCENT
INTERNAL COORDINATES-	40.76	CCH9	16.45	C-O	14.42	C-C	7.12	H7H8			
FORCE CONSTANTS-	46.54	CC6H	16.45	C-O	14.42	C-C	7.15	HC6H			
OFF DIAGONAL-	-4.55	SB22	3.52	SB24	3.00	BB35	2.31	SB23	-1.85	BB40	1.55
										BB44	1.51
										SS20	
NORMAL MODE 18	OBSERVED=	619.0	CM-1	CALCULATED=	624.2	CM-1	ERROR=	-5.2	CM-1	OR	-0.8 PERCENT
INTERNAL COORDINATES-	27.29	CCH7	24.61	CCH8	19.76	H4CC	12.49	H5CC			
FORCE CONSTANTS-	51.91	CC6H	32.25	CC3H	9.83	OCH	7.36	HC6H			
OFF DIAGONAL-	-8.45	BB37	6.77	BB35	-3.84	BB40	1.90	BB36			
NORMAL MODE 19	OBSERVED=	388.0	CM-1	CALCULATED=	383.6	CM-1	ERROR=	4.4	CM-1	OR	1.1 PERCENT
INTERNAL COORDINATES-	80.34	OCC	11.63	CCH9	10.01	CCH8	9.04	CCH7			
FORCE CONSTANTS-	80.34	CCO	30.68	CC6H	5.67	CC3H	5.21	HC6H			
OFF DIAGONAL-	-20.48	BB44	-4.65	BB45	-2.83	BB46	2.76	SB26	-2.16	BB37	1.94
										BB43	-1.60
										BB40	-1.56
										SB23	-1.52
										SB25	
NORMAL MODE 20	OBSERVED=	0.0	CM-1	CALCULATED=	207.4	CM-1	ERROR=	0.0	CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	97.58	T-CO									
FORCE CONSTANTS-	97.58	TC-O									
OFF DIAGONAL-	NONE										
NORMAL MODE 21	OBSERVED=	0.0	CM-1	CALCULATED=	186.2	CM-1	ERROR=	0.0	CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	97.75	T-CC									
FORCE CONSTANTS-	97.75	TC-C									
OFF DIAGONAL-	NONE										

13. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 7.29

TABLE LIII (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 300										PAGE 1
MOLECULE 4		-6 NG= 202		ETHANOL, CD3CHDOO (TRANS)						
NORMAL MODE 7	OBSERVED=	1350.0 CM-1		CALCULATED=	1347.1 CM-1	ERROR=	2.9 CM-1	OR	0.2 PERCENT	
INTERNAL COORDINATES-	52.93	OCH5	38.73 H5CC	8.30	C-C					
FORCE CONSTANTS-	55.38	OCH	41.59 CC3H	8.30	C-C					
OFF DIAGONAL-	-9.20	SB25	-8.05 SB22	2.06	BB33 -1.67	BB35				
NORMAL MODE 8	OBSERVED=	1327.0 CM-1		CALCULATED=	1321.8 CM-1	ERROR=	5.2 CM-1	OR	0.4 PERCENT	
INTERNAL COORDINATES-	69.56	HCH	20.17 OCH5	5.46	H5CC					
FORCE CONSTANTS-	69.56	HC3H	21.15 OCH	6.86	CC3H					
OFF DIAGONAL-	5.69	BB40	-5.46 BB38	-1.97	SB22 -1.66	SB25				
NORMAL MODE 9	OBSERVED=	1146.0 CM-1		CALCULATED=	1156.6 CM-1	ERROR=	-10.6 CM-1	OR	-0.9 PERCENT	
INTERNAL COORDINATES-	41.64	C-C	22.88 C-O	9.83	OCH4	7.10 CCH8	5.52	H7H8	5.35 CCH7	
FORCE CONSTANTS-	41.64	C-C	22.88 C-O	13.16	CC6H	12.26 OCH	9.70	HC6H	7.50 CC3H	
OFF DIAGONAL-	-11.31	SB24	4.29 BB40	3.76	SB21 -3.25	SB22 -3.03	SS20			
NORMAL MODE 10	OBSERVED=	1081.0 CM-1		CALCULATED=	1086.1 CM-1	ERROR=	-5.1 CM-1	OR	-0.5 PERCENT	
INTERNAL COORDINATES-	37.79	C-O	25.77 HOC	15.19	CCH9	8.40 C-C	6.87	OCC	6.53 H8H9	
FORCE CONSTANTS-	37.79	C-O	25.77 COH	16.07	CC6H	13.71 HC6H	8.40	C-C	6.87 CCO	
OFF DIAGONAL-	-11.95	SB21	-7.26 SB23	3.62	BB40 -2.55	SB24 2.25	SB25 -2.08	SB26 1.75	SS20 1.55 BB45	
NORMAL MODE 11	OBSERVED=	1068.0 CM-1		CALCULATED=	1057.9 CM-1	ERROR=	10.0 CM-1	OR	0.9 PERCENT	
INTERNAL COORDINATES-	26.99	HOC	17.53 H8H9	9.96	CCH7	9.88 CCH9	8.65	CCCH8	7.15 H7H9 7.12 OCH4	
FORCE CONSTANTS-	28.49	CC6H	26.99 COH	26.54	HC6H	7.18 OCH				
OFF DIAGONAL-	10.42	BB40	-4.31 BB35	2.99	BB44 -2.43	BB34 -2.40	SB24			
NORMAL MODE 12	OBSERVED=	1045.0 CM-1		CALCULATED=	1038.6 CM-1	ERROR=	6.4 CM-1	OR	0.6 PERCENT	
INTERNAL COORDINATES-	48.98	H7H9	27.91 H8H9	5.00	CCH7					
FORCE CONSTANTS-	78.01	HC6H	9.40 CC6H							
OFF DIAGONAL-	5.58	BB40	4.59 BB34							
NORMAL MODE 13	OBSERVED=	1000.0 CM-1		CALCULATED=	1017.3 CM-1	ERROR=	-17.3 CM-1	OR	-1.7 PERCENT	
INTERNAL COORDINATES-	56.60	H7H8	15.93 C-O	11.33	H8H9					
FORCE CONSTANTS-	70.54	HC6H	15.93 C-O							
OFF DIAGONAL-	3.79	BB34	-2.99 SB22	-2.92	SB23 -2.80	SB21 1.89	BB40			
NORMAL MODE 14	OBSERVED=	922.0 CM-1		CALCULATED=	928.5 CM-1	ERROR=	-6.5 CM-1	OR	-0.7 PERCENT	
INTERNAL COORDINATES-	40.33	OCH4	19.26 H4CC	14.92	C-O					
FORCE CONSTANTS-	42.21	OCH	19.29 CC3H	14.92	C-O					
OFF DIAGONAL-	8.29	SB22	2.83 SB25	-1.58	BB33 1.54	BB37				
NORMAL MODE 15	OBSERVED=	891.0 CM-1		CALCULATED=	902.5 CM-1	ERROR=	-11.5 CM-1	OR	-1.3 PERCENT	
INTERNAL COORDINATES-	22.15	HOC	17.75 CCH7	13.47	H4CC	9.64 C-C	9.10	OCH5	6.38 H8H9 5.08 H5CC	
FORCE CONSTANTS-	22.15	COH	20.77 CC6H	18.55	CC3H	12.69 OCH	9.64	C-C	6.82 HC6H	
OFF DIAGONAL-	3.15	BB37	2.75 BB35	-1.77	SB25 1.74	SB24 1.54	BB44			
NORMAL MODE 16	OBSERVED=	874.0 CM-1		CALCULATED=	872.2 CM-1	ERROR=	1.8 CM-1	OR	0.2 PERCENT	
INTERNAL COORDINATES-	20.28	CCH8	16.80 HOC	16.29	C-C	16.05 OCH4	6.13	H7H9		
FORCE CONSTANTS-	23.62	CC6H	17.32 OCH	16.80	COH	16.29 C-C	7.05	CC3H	6.32 HC6H	
OFF DIAGONAL-	2.96	BB44	2.59 SB24	-2.30	SB26 2.12	BB35 2.06	BB37 -1.61	BB40		
NORMAL MODE 17	OBSERVED=	744.0 CM-1		CALCULATED=	740.0 CM-1	ERROR=	3.9 CM-1	OR	0.5 PERCENT	
INTERNAL COORDINATES-	39.12	CCH9	16.56 C-O	16.38	C-C	6.84 H7H8				
FORCE CONSTANTS-	44.35	CC6H	16.56 C-O	16.38	C-C	6.89 HC6H				
OFF DIAGONAL-	-4.18	SB22	3.80 SB24	2.81	BB35 2.12	SB23 1.62	SS20 -1.62	BB40		
NORMAL MODE 18	OBSERVED=	618.0 CM-1		CALCULATED=	624.0 CM-1	ERROR=	-6.0 CM-1	OR	-1.0 PERCENT	
INTERNAL COORDINATES-	27.25	CCH7	24.66 CCH8	19.82	H4CC	12.50 H5CC				
FORCE CONSTANTS-	51.92	CC6H	32.32 CC3H	9.85	OCH	7.36 HC6H				
OFF DIAGONAL-	-8.46	BB37	6.77 BB35	-3.84	BB40 1.90	BB36				
NORMAL MODE 19	OBSERVED=	0.0 CM-1		CALCULATED=	377.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	80.62	OCC	11.43 CCH9	9.79	CCH8	8.88 CCH7				
FORCE CONSTANTS-	80.62	CCO	30.09 CC6H	5.50	CC3H	5.10 HC6H				
OFF DIAGONAL-	-20.31	BB44	-4.62 BB45	-2.91	BB46 2.57	SB26 -2.11	BB37 1.91	BB43 -1.58	BB40	
NORMAL MODE 20	OBSERVED=	0.0 CM-1		CALCULATED=	186.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	97.98	T-CC								
FORCE CONSTANTS-	97.98	TC-C								
OFF DIAGONAL -	NONE									
NORMAL MODE 21	OBSERVED=	0.0 CM-1		CALCULATED=	152.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	98.26	T-CO								
FORCE CONSTANTS-	98.26	TC-O								
OFF DIAGONAL -	NONE									

13. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 7.33

TABLE LIII (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 300										PAGE 1
MOLECULE 5		-6 NG= 201		ETHANOL, CH ₃ CH ₂ OH (TRANS)						
NORMAL MODE 7	OBSERVED=	1480.0 CM-1			CALCULATED=	1493.2 CM-1			ERROR=	-13.2 CM-1 OR -0.9 PERCENT
INTERNAL COORDINATES-	65.46	HCH	6.47	H4CC	6.47	H5CC	5.69	HOC		
FORCE CONSTANTS-	65.46	HC3H	12.95	CC3H	5.69	COH	5.58	OCH		
OFF DIAGONAL-	8.46	BB40	-3.23	BB38	-2.83	SB25				
NORMAL MODE 8	OBSERVED=	0.0 CM-1			CALCULATED=	1456.9 CM-1			ERROR=	0.0 CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	42.81	H7H8	8.71	H7H9	8.70	H8H9	6.80	CCH9		
FORCE CONSTANTS-	60.22	HC6H	12.34	CC6H	6.10	CC3H				
OFF DIAGONAL-	6.60	BB40	3.54	BB34	-1.76	SB25	-1.58	SB22		
NORMAL MODE 9	OBSERVED=	1454.0 CM-1			CALCULATED=	1452.8 CM-1			ERROR=	1.2 CM-1 OR 0.1 PERCENT
INTERNAL COORDINATES-	38.43	H8H9	38.42	H7H9	5.66	CCH7	5.66	CCH8		
FORCE CONSTANTS-	76.85	HC6H	11.31	CC6H						
OFF DIAGONAL-	6.10	BB40	4.54	BB34						
NORMAL MODE 10	OBSERVED=	1420.0 CM-1			CALCULATED=	1417.9 CM-1			ERROR=	2.1 CM-1 OR 0.1 PERCENT
INTERNAL COORDINATES-	31.14	HOC	21.34	OCH4	21.34	OCH5	7.56	HCH	7.43	C-C 5.16 H4CC 5.16 H5CC
FORCE CONSTANTS-	42.67	OCH	31.14	COH	11.17	HC6H	10.33	CC3H	7.56	HC3H 7.43 C-C
OFF DIAGONAL-	-5.67	SB22	-5.00	SB25	3.85	BB33	-3.81	BB31	3.04	SB21 -3.04 BB38 -2.02 SB24 -1.56 BB40
NORMAL MODE 11	OBSERVED=	1390.0 CM-1			CALCULATED=	1380.2 CM-1			ERROR=	9.8 CM-1 OR 0.7 PERCENT
INTERNAL COORDINATES-	16.90	CCH8	16.89	CCH7	13.58	H8H9	13.58	H7H9	12.89	CCH9 11.31 HOC 9.87 H7H8
FORCE CONSTANTS-	46.68	CC6H	37.03	HC6H	11.31	COH				
OFF DIAGONAL-	17.16	BB40	-7.59	BB35	-6.13	SB24	-4.34	BB34	2.00	BB44
NORMAL MODE 12	OBSERVED=	1331.0 CM-1			CALCULATED=	1325.9 CM-1			ERROR=	5.1 CM-1 OR 0.4 PERCENT
INTERNAL COORDINATES-	43.63	HOC	11.34	OCH4	11.34	OCH5	11.02	H4CC	11.02	H5CC
FORCE CONSTANTS-	43.63	COH	22.69	OCH	22.03	CC3H	5.32	CC6H	5.13	HC6H
OFF DIAGONAL-	-3.79	SB22	-3.29	SB21	3.29	BB31	-2.49	BB35	2.47	SB25 2.23 BB40 2.05 BB33
NORMAL MODE 13	OBSERVED=	1276.0 CM-1			CALCULATED=	1281.0 CM-1			ERROR=	-5.0 CM-1 OR -0.4 PERCENT
INTERNAL COORDINATES-	32.87	OCH4	32.87	OCH5	17.16	H4CC	17.16	H5CC		
FORCE CONSTANTS-	65.74	OCH	34.31	CC3H						
OFF DIAGONAL-	-5.93	BB33	2.87	BB35						
NORMAL MODE 14	OBSERVED=	1095.0 CM-1			CALCULATED=	1113.7 CM-1			ERROR=	-18.7 CM-1 OR -1.7 PERCENT
INTERNAL COORDINATES-	53.52	C-O	20.67	CCH9	9.71	H7H8	6.91	OCC		
FORCE CONSTANTS-	53.52	C-O	25.59	CC6H	6.91	CCO				
OFF DIAGONAL-	-8.67	SB23	5.99	SB22	-3.15	BB40	3.05	BB44	-3.04	SB21 1.92 BB35 1.82 BB45
NORMAL MODE 15	OBSERVED=	1051.0 CM-1			CALCULATED=	1058.5 CM-1			ERROR=	-7.5 CM-1 OR -0.7 PERCENT
INTERNAL COORDINATES-	22.55	CCH8	22.54	CCH7	12.19	OCH4	12.19	OCH5	7.31	H4CC 7.31 H5CC 6.00 H8H9 6.00 H7H9
FORCE CONSTANTS-	45.09	CC6H	24.38	OCH	14.63	CC3H	12.00	HC6H		
OFF DIAGONAL-	5.36	BB37	4.86	BB35	-4.81	BB40	-2.20	BB33		
NORMAL MODE 16	OBSERVED=	1032.0 CM-1			CALCULATED=	1038.9 CM-1			ERROR=	-6.9 CM-1 OR -0.7 PERCENT
INTERNAL COORDINATES-	63.99	C-C	14.58	C-O	8.27	CCH9	7.83	HOC		
FORCE CONSTANTS-	63.99	C-C	14.58	C-O	12.29	CC6H	7.83	COH		
OFF DIAGONAL-	-4.85	SB26	-4.09	SB21	3.81	SB23	-3.36	SB22	-3.00	SS20 2.33 BB44
NORMAL MODE 17	OBSERVED=	884.0 CM-1			CALCULATED=	879.1 CM-1			ERROR=	4.9 CM-1 OR 0.6 PERCENT
INTERNAL COORDINATES-	40.53	C-O	28.01	C-C	20.09	CCH9				
FORCE CONSTANTS-	40.53	C-O	28.51	CC6H	28.01	C-C				
OFF DIAGONAL-	-4.05	SB22	3.31	SS20	-2.52	SB23	-2.31	BB40	2.27	BB35 2.20 SB25
NORMAL MODE 18	OBSERVED=	803.0 CM-1			CALCULATED=	802.2 CM-1			ERROR=	0.8 CM-1 OR 0.1 PERCENT
INTERNAL COORDINATES-	21.36	H4CC	21.36	H5CC	17.97	CCH7	17.97	CCH8	9.34	OCH4 9.34 OCH5
FORCE CONSTANTS-	42.71	CC3H	35.94	CC6H	18.68	OCH	6.04	HC6H		
OFF DIAGONAL-	-8.17	BB37	6.39	BB35	-3.05	BB40	1.83	BB36	-1.69	BB33
NORMAL MODE 19	OBSERVED=	433.0 CM-1			CALCULATED=	435.3 CM-1			ERROR=	-2.3 CM-1 OR -0.5 PERCENT
INTERNAL COORDINATES-	87.50	UCC	7.10	CCH9	6.13	CCH8	6.13	CCH7		
FORCE CONSTANTS-	87.50	CCO	19.36	CC6H	5.32	CC3H				
OFF DIAGONAL-	-17.15	BB44	-3.79	BB45	-3.36	BB46	3.20	SB26	1.97	BB43 -1.68 BB37 -1.65 SB25
NORMAL MODE 20	OBSERVED=	0.0 CM-1			CALCULATED=	249.0 CM-1			ERROR=	0.0 CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	99.08	T-CC								
FORCE CONSTANTS-	99.08	TC-C								
OFF DIAGONAL -	NONE									
NORMAL MODE 21	OBSERVED=	0.0 CM-1			CALCULATED=	208.1 CM-1			ERROR=	0.0 CM-1 OR 0.0 PERCENT
INTERNAL COORDINATES-	98.90	T-CO								
FORCE CONSTANTS-	98.90	TC-O								
OFF DIAGONAL -	NONE									

13. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 5.97

TABLE LIII (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 300
 MOLECULE 6 -6 NG= 201 ETHANOL, CH3CH2OD (TRANS)

PAGE 1

NORMAL MODE 7	OBSERVED=	1479.0 CM-1	CALCULATED=	1488.9 CM-1	ERROR=	-9.9 CM-1	OR	-0.7 PERCENT	
INTERNAL COORDINATES-	67.76	HCH 5.03 H4CC	5.03 H5CC						
FORCE CONSTANTS-	67.76	HC3H 10.05 CC3H	9.48 OCH 7.02 HC6H						
OFF DIAGONAL-	7.91	BB40 -4.29 BB38	-1.71 SB25						
NORMAL MODE 8	OBSERVED=	0.0 CM-1	CALCULATED=	1454.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	44.06	H7H8 9.18 H7H9	9.14 H8H9 6.68 HCH 6.56 CCH9						
FORCE CONSTANTS-	62.38	HC6H 11.73 CC6H	6.68 HC3H 5.77 CC3H						
OFF DIAGONAL-	7.30	BB40 3.67 BB34							
NORMAL MODE 9	OBSERVED=	1451.0 CM-1	CALCULATED=	1452.8 CM-1	ERROR=	-1.8 CM-1	OR	-0.1 PERCENT	
INTERNAL COORDINATES-	38.44	H8H9 38.41 H7H9	5.66 CCH7 5.65 CCH8						
FORCE CONSTANTS-	76.85	HC6H 11.31 CC6H							
OFF DIAGONAL-	6.10	BB40 4.54 BB34							
NORMAL MODE 10	OBSERVED=	1392.0 CM-1	CALCULATED=	1397.3 CM-1	ERROR=	-5.3 CM-1	OR	-0.4 PERCENT	
INTERNAL COORDINATES-	19.33	UCH4 19.33 OCH5	10.39 C-C 10.26 H4CC 10.26 H5CC 10.24 H8H9 10.24 H7H9 7.49 CCH7 7.49 CCH8						
FORCE CONSTANTS-	38.67	UCH 20.60 HC6H	20.53 CC3H 19.35 CC6H 10.39 C-C						
OFF DIAGONAL-	-8.34	SB25 -7.34 SB24	-6.81 SB22 5.61 BB40 -4.75 BB35 3.66 BB37 3.49 BB33						
NORMAL MODE 11	OBSERVED=	1365.0 CM-1	CALCULATED=	1366.1 CM-1	ERROR=	-1.1 CM-1	OR	-0.1 PERCENT	
INTERNAL COORDINATES-	14.00	H7H8 12.95 OCH5	12.95 OCH4 12.31 CCH9 10.87 CCH7 10.87 CCH8 6.89 H8H9 6.89 H7H9 6.61 H4CC						
FORCE CONSTANTS-	34.05	CC6H 27.78 HC6H	25.90 OCH 13.23 CC3H						
OFF DIAGONAL-	11.98	BB40 -6.62 BB35	-3.54 BB37 -3.14 BB34 -2.78 SB22 2.34 BB33 -1.63 BB36						
NORMAL MODE 12	OBSERVED=	1277.0 CM-1	CALCULATED=	1281.0 CM-1	ERROR=	-4.0 CM-1	OR	-0.3 PERCENT	
INTERNAL COORDINATES-	32.87	UCH4 32.87 OCH5	17.16 H4CC 17.16 H5CC						
FORCE CONSTANTS-	65.74	UCH 34.31 CC3H							
OFF DIAGONAL-	-5.94	BB33 2.87 BB35							
NORMAL MODE 13	OBSERVED=	1139.0 CM-1	CALCULATED=	1125.6 CM-1	ERROR=	13.4 CM-1	OR	1.2 PERCENT	
INTERNAL COORDINATES-	28.83	HOC 18.66 C-C	18.39 CCH9 15.33 C-O 12.42 OCC 8.21 H7H8						
FORCE CONSTANTS-	28.83	COH 22.81 CC6H	18.66 C-C 15.33 C-O 12.42 CCO 9.64 HC6H						
OFF DIAGONAL-	-8.05	SB21 -6.22 SB23	-4.16 SB26 3.88 BB44 -2.77 BB40 2.30 BB45 2.25 SB25 2.14 SB22 -1.71 SB24						
NORMAL MODE 14	OBSERVED=	1106.0 CM-1	CALCULATED=	1104.5 CM-1	ERROR=	1.5 CM-1	OR	0.1 PERCENT	
INTERNAL COORDINATES-	43.75	C-O 31.39 C-C	5.77 HOC						
FORCE CONSTANTS-	43.75	C-O 31.39 C-C	5.77 COH 5.15 CC6H						
OFF DIAGONAL-	6.08	SB21 -3.64 SS20	3.06 SB22 2.65 SB25						
NORMAL MODE 15	OBSERVED=	1057.0 CM-1	CALCULATED=	1058.5 CM-1	ERROR=	-1.5 CM-1	OR	-0.1 PERCENT	
INTERNAL COORDINATES-	22.55	CCH7 22.55 CCH8	12.19 OCH4 12.19 OCH5 7.31 H4CC 7.31 H5CC 6.00 H8H9 6.00 H7H9						
FORCE CONSTANTS-	45.11	CC6H 24.37 OCH	14.63 CC3H 12.00 HC6H						
OFF DIAGONAL-	5.36	BB37 4.86 BB35	-4.81 BB40 -2.20 BB33						
NORMAL MODE 16	OBSERVED=	957.0 CM-1	CALCULATED=	956.1 CM-1	ERROR=	0.9 CM-1	OR	0.1 PERCENT	
INTERNAL COORDINATES-	57.12	HOC 21.65 C-O	14.74 CCH9 8.81 C-C						
FORCE CONSTANTS-	57.12	COH 22.23 CC6H	21.65 C-O 8.81 C-C						
OFF DIAGONAL-	-13.46	SB21 -4.92 SB22	-1.91 BB40 -1.84 SB25 1.72 BB35						
NORMAL MODE 17	OBSERVED=	877.0 CM-1	CALCULATED=	858.6 CM-1	ERROR=	18.4 CM-1	OR	2.1 PERCENT	
INTERNAL COORDINATES-	36.49	C-C 28.01 C-O	12.31 CCH9 9.50 HOC						
FORCE CONSTANTS-	36.49	C-C 28.01 C-O	17.04 CC6H 9.50 COH						
OFF DIAGONAL-	6.24	SB21 3.14 SS20	-2.10 SB23 -1.85 SB22						
NORMAL MODE 18	OBSERVED=	798.0 CM-1	CALCULATED=	802.1 CM-1	ERROR=	-4.1 CM-1	OR	-0.5 PERCENT	
INTERNAL COORDINATES-	21.38	H4CC 21.38 H5CC	17.97 CCH7 17.97 CCH8 9.35 OCH4 9.35 OCH5						
FORCE CONSTANTS-	42.76	CC3H 35.94 CC6H	18.69 OCH 6.04 HC6H						
OFF DIAGONAL-	-8.17	BB37 6.39 BB35	-3.05 BB40 1.83 BB36 -1.69 BB33						
NORMAL MODE 19	OBSERVED=	426.0 CM-1	CALCULATED=	427.8 CM-1	ERROR=	-1.8 CM-1	OR	-0.4 PERCENT	
INTERNAL COORDINATES-	87.45	OCC 6.99 CCH9	6.03 CCH8 6.03 CCH7						
FORCE CONSTANTS-	87.45	CCO 19.06 CC6H	5.17 CC3H						
OFF DIAGONAL-	-17.01	BB44 -3.76 BB45	-3.41 BB46 2.95 SB26 1.94 BB43 -1.65 BB37						
NORMAL MODE 20	OBSERVED=	0.0 CM-1	CALCULATED=	249.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	99.11	T-C							
FORCE CONSTANTS-	99.11	TC-C							
OFF DIAGONAL -	NONE								
NORMAL MODE 21	OBSERVED=	0.0 CM-1	CALCULATED=	154.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	98.98	T-C							
FORCE CONSTANTS-	98.98	TC-O							
OFF DIAGONAL -	NONE								

12. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 5.32

TABLE LIII (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 300				PAGE 1	
MOLECULE 7		-6 NG= 201 ETHANOL, CH3CD2OH (TRANS)			
NORMAL MODE 7	OBSERVED= 1456.0 CM-1	CALCULATED= 1455.4 CM-1	ERROR= 0.6 CM-1 OR 0.0 PERCENT		
INTERNAL COORDINATES-	50.13 H7H8 11.92 H7H9 11.90 H8H9 8.01 CCH9				
FORCE CONSTANTS-	73.94 HC6H 12.61 CC6H				
OFF DIAGONAL-	6.29 BB40 4.37 BB34				
NORMAL MODE 8	OBSERVED= 1448.0 CM-1	CALCULATED= 1451.6 CM-1	ERROR= -3.6 CM-1 OR -0.3 PERCENT		
INTERNAL COORDINATES-	38.70 H8H9 38.68 H7H9 5.44 CCH7 5.44 CCH8				
FORCE CONSTANTS-	77.37 HC6H 10.88 CC6H				
OFF DIAGONAL-	6.00 BB40 4.58 BB34				
NORMAL MODE 9	OBSERVED= 1385.0 CM-1	CALCULATED= 1392.9 CM-1	ERROR= -7.9 CM-1 OR -0.6 PERCENT		
INTERNAL COORDINATES-	85.64 HOC 8.26 C-C				
FORCE CONSTANTS-	85.64 COH 8.26 C-C				
OFF DIAGONAL-	3.25 SB21 -2.80 SB25 -1.86 BB31				
NORMAL MODE 10	OBSERVED= 1379.0 CM-1	CALCULATED= 1379.1 CM-1	ERROR= -0.1 CM-1 OR -0.0 PERCENT		
INTERNAL COORDINATES-	19.01 CCH7 19.01 CCH8 15.46 H8H9 15.46 H7H9 14.73 CCH9 10.97 H7H8 6.64 C-C				
FORCE CONSTANTS-	52.75 CC6H 41.89 HC6H 6.64 C-C				
OFF DIAGONAL-	19.29 BB40 -9.74 SB24 -8.57 BB35 -4.91 BB34				
NORMAL MODE 11	OBSERVED= 1161.0 CM-1	CALCULATED= 1168.7 CM-1	ERROR= -7.7 CM-1 OR -0.7 PERCENT		
INTERNAL COORDINATES-	46.58 C-O 15.62 CCH9 11.89 OCH5 11.89 OCH4 9.38 H7H8 9.08 HOC 6.41 H5CC 6.40 H4CC 6.30 C-C				
FORCE CONSTANTS-	46.58 C-O 23.79 OCH 17.58 CC6H 12.81 CC3H 10.23 HC6H 9.08 COH 6.30 C-C				
OFF DIAGONAL-	-20.30 SB22 -7.87 SB21 -5.69 SB23 -5.13 SB25 -3.80 BB40 2.15 BB33 1.72 BB46 -1.68 SB20 1.54 BB31				
NORMAL MODE 12	OBSERVED= 1128.0 CM-1	CALCULATED= 1097.8 CM-1	ERROR= 30.2 CM-1 OR 2.7 PERCENT		
INTERNAL COORDINATES-	51.72 CCH7 30.63 CCH8 7.83 H5CC 7.82 H4CC 6.26 HOC				
FORCE CONSTANTS-	51.72 HC3H 22.63 C-C 15.65 CC3H 6.26 COH				
OFF DIAGONAL-	-10.74 SB25 7.30 BB40 -2.67 SB26				
NORMAL MODE 13	OBSERVED= 1025.0 CM-1	CALCULATED= 1023.8 CM-1	ERROR= 1.2 CM-1 OR 0.1 PERCENT		
INTERNAL COORDINATES-	30.63 CCH7 30.63 CCH8 8.46 H4CC 8.45 H5CC 6.96 H8H9 6.96 H7H9				
FORCE CONSTANTS-	61.26 CC6H 16.91 CC3H 13.92 HC6H				
OFF DIAGONAL-	6.71 BB37 6.36 BB35 -6.04 BB40				
NORMAL MODE 14	OBSERVED= 0.0 CM-1	CALCULATED= 1013.0 CM-1	ERROR= 0.0 CM-1 OR 0.0 PERCENT		
INTERNAL COORDINATES-	23.87 C-C 20.50 HCH 17.04 CCH9 10.20 OCH4 10.20 OCH5				
FORCE CONSTANTS-	24.37 CC6H 23.87 C-C 20.50 HC3H 20.40 OCH 5.16 HC6H				
OFF DIAGONAL-	-3.46 BB38 -3.04 SB22 2.78 BB44 -2.62 SB26 1.95 BB35 1.84 BB33 1.69 SB25 -1.69 BB46 -1.55 BB40				
NORMAL MODE 15	OBSERVED= 966.0 CM-1	CALCULATED= 953.5 CM-1	ERROR= 12.5 CM-1 OR 1.3 PERCENT		
INTERNAL COORDINATES-	35.36 C-O 13.09 OCH4 13.09 OCH5 7.34 H4CC 7.34 H5CC				
FORCE CONSTANTS-	35.36 C-O 26.17 OCH 14.68 CC3H				
OFF DIAGONAL-	18.55 SB22 4.00 SB25 2.36 BB33 -1.63 SB21				
NORMAL MODE 16	OBSERVED= 912.0 CM-1	CALCULATED= 917.6 CM-1	ERROR= -5.6 CM-1 OR -0.6 PERCENT		
INTERNAL COORDINATES-	44.33 OCH4 44.33 OCH5 6.69 H4CC 6.69 H5CC				
FORCE CONSTANTS-	88.66 OCH 13.39 CC3H				
OFF DIAGONAL-	-8.00 BB33				
NORMAL MODE 17	OBSERVED= 849.0 CM-1	CALCULATED= 862.9 CM-1	ERROR= -13.9 CM-1 OR -1.6 PERCENT		
INTERNAL COORDINATES-	35.94 C-C 28.32 C-O 16.00 CCH9				
FORCE CONSTANTS-	35.94 C-C 28.32 C-O 22.56 CC6H				
OFF DIAGONAL-	7.53 SB25 -6.91 SB22 3.13 SB20 -1.85 SB23 -1.66 BB40				
NORMAL MODE 18	OBSERVED= 675.0 CM-1	CALCULATED= 672.3 CM-1	ERROR= 2.7 CM-1 OR 0.4 PERCENT		
INTERNAL COORDINATES-	30.33 H4CC 30.33 H5CC 9.45 OCH4 9.45 OCH5 8.65 CCH7 8.65 CCH8				
FORCE CONSTANTS-	60.65 CC3H 18.90 OCH 17.29 CC6H				
OFF DIAGONAL-	-6.75 BB37 6.32 BB35 -1.71 BB33 1.51 BB36				
NORMAL MODE 19	OBSERVED= 430.0 CM-1	CALCULATED= 430.5 CM-1	ERROR= -0.5 CM-1 OR -0.1 PERCENT		
INTERNAL COORDINATES-	87.99 UCC 7.05 CCH9 6.09 CCH8 6.09 CCH7				
FORCE CONSTANTS-	87.99 CCO 19.24 CC6H 6.11 CC3H				
OFF DIAGONAL-	-17.15 BB44 -3.79 BB45 -3.44 BB46 2.89 SB26 2.11 BB43 -1.80 BB37 -1.59 SB25				
NORMAL MODE 20	OBSERVED= 0.0 CM-1	CALCULATED= 242.2 CM-1	ERROR= 0.0 CM-1 OR 0.0 PERCENT		
INTERNAL COORDINATES-	97.95 T-CC				
FORCE CONSTANTS-	97.95 TC-C				
OFF DIAGONAL -	NONE				
NORMAL MODE 21	OBSERVED= 0.0 CM-1	CALCULATED= 207.7 CM-1	ERROR= 0.0 CM-1 OR 0.0 PERCENT		
INTERNAL COORDINATES-	98.90 T-CO				
FORCE CONSTANTS-	98.90 TC-O				
OFF DIAGONAL -	NONE				

12. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 7.21

TABLE LIII (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 300										PAGE 1
MOLECULE 8		-6 NG= 201		ETHANOL, CH3CD2OD (TRANS)						
NORMAL MODE 7	OBSERVED=	1460.0	CM-1	CALCULATED=	1455.3	CM-1	ERROR=	4.6	CM-1 OR 0.3 PERCENT	
INTERNAL COORDINATES-	50.20	H7H8	11.93	H7H9	11.91	H8H9	8.00	CCH9		
FORCE CONSTANTS-	74.03	HC6H	12.60	CC6H						
OFF DIAGONAL-	6.30	BB40	4.38	BB34						
NORMAL MODE 8	OBSERVED=	1450.0	CM-1	CALCULATED=	1451.6	CM-1	ERROR=	-1.6	CM-1 OR -0.1 PERCENT	
INTERNAL COORDINATES-	38.69	H8H9	38.68	H7H9	5.44	CCH7	5.44	CCH8		
FORCE CONSTANTS-	77.37	HC6H	10.88	CC6H						
OFF DIAGONAL-	6.00	BB40	4.58	BB34						
NORMAL MODE 9	OBSERVED=	1384.0	CM-1	CALCULATED=	1379.1	CM-1	ERROR=	4.9	CM-1 OR 0.3 PERCENT	
INTERNAL COORDINATES-	19.06	CCH7	19.06	CCH8	15.56	H8H9	15.56	H7H9	14.68	
FORCE CONSTANTS-	52.80	CC6H	41.95	HC6H	7.74	C-C				
OFF DIAGONAL-	19.30	BB40-10.52	SB24	-8.58	BB35	-4.91	BB34			
NORMAL MODE 10	OBSERVED=	1200.0	CM-1	CALCULATED=	1210.8	CM-1	ERROR=	-10.8	CM-1 OR -0.9 PERCENT	
INTERNAL COORDINATES-	31.77	C-C	22.87	C-O	12.41	HOC	12.30	OCH4	12.30	
FORCE CONSTANTS-	31.77	C-C	24.61	OCH	22.87	C-O	22.39	CC3H	12.41	
OFF DIAGONAL-	-15.23	SB25-14.47	SB22	6.45	SB21	-2.65	SS20	2.47	SB24	
								2.22	BB33 -1.83	
									BB31 -1.66	
									BB35	
NORMAL MODE 11	OBSERVED=	1157.0	CM-1	CALCULATED=	1140.7	CM-1	ERROR=	16.3	CM-1 OR 1.4 PERCENT	
INTERNAL COORDINATES-	28.35	HCH	20.00	C-O	15.72	CCH9	13.83	HOC	10.49	
FORCE CONSTANTS-	28.35	HC3H	20.00	C-O	19.12	CC6H	13.83	COH	10.49	
OFF DIAGONAL-	-6.53	SB23	-6.37	SB21	-6.24	SB22	3.13	BB44	-2.44	
								SB26	-2.06	
								BB38	1.95	
								BB45	-1.77	
								BB40		
NORMAL MODE 12	OBSERVED=	1057.0	CM-1	CALCULATED=	1040.0	CM-1	ERROR=	17.0	CM-1 OR 1.6 PERCENT	
INTERNAL COORDINATES-	45.84	HCH	15.84	HOC	6.93	OCH5	6.93	OCH4	6.16	
FORCE CONSTANTS-	45.84	HC3H	15.84	COH	13.86	OCH	8.18	CC6H	6.32	
OFF DIAGONAL-	-4.26	BB38	3.87	BB40	3.49	SB22	-2.34	SB21	1.99	
								SB25	-1.55	
								BB31		
NORMAL MODE 13	OBSERVED=	1025.0	CM-1	CALCULATED=	1023.8	CM-1	ERROR=	1.2	CM-1 OR 0.1 PERCENT	
INTERNAL COORDINATES-	30.63	CCH7	30.63	CCH8	8.45	H4CC	8.45	H5CC	6.96	
FORCE CONSTANTS-	61.26	CC6H	16.90	CC3H	13.92	HC6H				
OFF DIAGONAL-	6.71	BB37	6.36	BB35	-6.04	BB40				
NORMAL MODE 14	OBSERVED=	962.0	CM-1	CALCULATED=	968.3	CM-1	ERROR=	-6.3	CM-1 OR -0.7 PERCENT	
INTERNAL COORDINATES-	40.32	C-O	25.29	HOC	17.32	C-C	8.65	CCH9		
FORCE CONSTANTS-	40.32	C-O	25.29	COH	17.32	C-C	13.14	CC6H		
OFF DIAGONAL-	-12.22	SB21	5.10	SB22	4.16	SB25	-2.60	SS20		
NORMAL MODE 15	OBSERVED=	0.0	CM-1	CALCULATED=	924.5	CM-1	ERROR=	0.0	CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	29.91	HOC	16.06	OCH4	16.06	OCH5	9.03	H4CC	9.03	
FORCE CONSTANTS-	32.12	OCH	29.91	COH	18.06	CC3H	9.39	CC6H		
OFF DIAGONAL-	3.24	BB31	2.90	BB33	2.51	SB22	-1.58	BB37	1.52	
								SB21		
NORMAL MODE 16	OBSERVED=	913.0	CM-1	CALCULATED=	917.6	CM-1	ERROR=	-4.6	CM-1 OR -0.5 PERCENT	
INTERNAL COORDINATES-	44.33	OCH4	44.32	OCH5	6.70	H4CC	6.69	H5CC		
FORCE CONSTANTS-	88.66	OCH	13.39	CC3H						
OFF DIAGONAL-	-8.00	BB33								
NORMAL MODE 17	OBSERVED=	847.0	CM-1	CALCULATED=	849.2	CM-1	ERROR=	-2.2	CM-1 OR -0.3 PERCENT	
INTERNAL COORDINATES-	40.88	C-C	26.29	C-O	10.98	CCH9	6.41	HOC		
FORCE CONSTANTS-	40.88	C-C	26.29	C-O	15.11	CC6H	6.41	COH		
OFF DIAGONAL-	4.97	SB21	4.28	SB25	3.22	SS20	-2.89	SB22	-1.92	
								SB23		
NORMAL MODE 18	OBSERVED=	674.0	CM-1	CALCULATED=	672.2	CM-1	ERROR=	1.8	CM-1 OR 0.3 PERCENT	
INTERNAL COORDINATES-	30.35	H4CC	30.35	H5CC	9.46	OCH4	9.46	OCH5	8.65	
FORCE CONSTANTS-	60.71	CC3H	18.92	OCH	17.30	CC6H				
OFF DIAGONAL-	-6.76	BB37	6.33	BB35	-1.71	BB33	1.51	BB36		
NORMAL MODE 19	OBSERVED=	425.0	CM-1	CALCULATED=	423.1	CM-1	ERROR=	1.9	CM-1 OR 0.4 PERCENT	
INTERNAL COORDINATES-	87.93	UCC	6.92	CCH9	5.99	CCH8	5.99	CCH7		
FORCE CONSTANTS-	87.93	CCD	18.90	CC6H	5.84	CC3H				
OFF DIAGONAL-	-17.00	BB44	-3.75	BB45	-3.54	BB46	2.66	SB26	2.07	
								BB43	-1.74	
								BB37		
NORMAL MODE 20	OBSERVED=	0.0	CM-1	CALCULATED=	242.2	CM-1	ERROR=	0.0	CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	98.11	T-CC								
FORCE CONSTANTS-	98.11	TC-C								
OFF DIAGONAL -	NONE									
NORMAL MODE 21	OBSERVED=	0.0	CM-1	CALCULATED=	153.4	CM-1	ERROR=	0.0	CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	99.09	T-CO								
FORCE CONSTANTS-	99.09	TC-O								
OFF DIAGONAL -	NONE									

12. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 6.11

TABLE LIII (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 300
 MOLECULE 9 -6 NG= 201 ETHANOL, CD3CH2OH (TRANS)

PAGE 1

NORMAL MODE 7	OBSERVED=	1482.0 CM-1	CALCULATED=	1490.7 CM-1	ERROR=	-8.7 CM-1 OR	-0.6 PERCENT
INTERNAL COORDINATES-	68.72	HCH 7.74 H4CC 7.74 H5CC 6.63 HOC					
FORCE CONSTANTS-	68.72	HC3H 15.47 CC3H 6.63 COH					
OFF DIAGONAL-	8.91	BB40 -3.40 SB25 -2.98 BB38					
NORMAL MODE 8	OBSERVED=	1422.0 CM-1	CALCULATED=	1418.9 CM-1	ERROR=	3.1 CM-1 OR	0.2 PERCENT
INTERNAL COORDINATES-	38.39	HOC 23.80 OCH4 23.80 OCH5 6.68 C-C 6.51 HCH 6.42 H4CC 6.42 H5CC					
FORCE CONSTANTS-	47.60	UCH 38.39 COH 12.85 CC3H 6.68 C-C 6.51 HC3H					
OFF DIAGONAL-	-7.29	SB22 -5.29 SB25 -4.47 BB31 4.30 BB33 4.11 SB21 -2.98 BB38 -2.47 BB40					
NORMAL MODE 9	OBSERVED=	1323.0 CM-1	CALCULATED=	1326.6 CM-1	ERROR=	-3.6 CM-1 OR	-0.3 PERCENT
INTERNAL COORDINATES-	50.91	HOC 11.83 OCH4 11.83 OCH5 11.74 H4CC 11.74 H5CC					
FORCE CONSTANTS-	50.91	COH 23.67 UCH 23.48 CC3H					
OFF DIAGONAL-	-4.48	SB22 -4.13 SB21 3.63 BB31 2.14 BB33 -1.86 BB35					
NORMAL MODE 10	OBSERVED=	1292.0 CM-1	CALCULATED=	1276.9 CM-1	ERROR=	15.1 CM-1 OR	1.2 PERCENT
INTERNAL COORDINATES-	34.88	UCH4 34.88 OCH5 16.16 H4CC 16.16 H5CC					
FORCE CONSTANTS-	69.76	UCH 32.32 CC3H					
OFF DIAGONAL-	-6.30	BB33 2.62 BB35					
NORMAL MODE 11	OBSERVED=	1136.0 CM-1	CALCULATED=	1128.2 CM-1	ERROR=	7.8 CM-1 OR	0.7 PERCENT
INTERNAL COORDINATES-	34.19	C-C 33.39 C-O 11.34 CCH7 11.33 CCH8 10.82 H7H8					
FORCE CONSTANTS-	34.19	C-C 33.39 C-O 23.78 CC6H 17.45 HC6H					
OFF DIAGONAL-	-13.71	SB24 7.92 BB40 -4.46 SB21 -3.32 SS20 -3.01 BB35 -2.27 SB23 2.17 BB44 1.95 SB22 -1.81 BB34					
NORMAL MODE 12	OBSERVED=	1064.0 CM-1	CALCULATED=	1075.4 CM-1	ERROR=	-11.4 CM-1 OR	-1.1 PERCENT
INTERNAL COORDINATES-	29.07	C-O 24.65 CCH9 14.80 H8H9 14.80 H7H9 11.59 C-C					
FORCE CONSTANTS-	32.12	HC6H 29.07 C-O 26.46 CC6H 11.59 C-C					
OFF DIAGONAL-	8.77	BB40 -7.04 SB24 -3.98 SB23 1.80 SS20 -1.69 BB35 -1.52 SB26					
NORMAL MODE 13	OBSERVED=	1041.0 CM-1	CALCULATED=	1040.0 CM-1	ERROR=	1.0 CM-1 OR	0.1 PERCENT
INTERNAL COORDINATES-	36.31	H8H9 36.30 H7H9 6.18 CCH7 6.18 CCH8					
FORCE CONSTANTS-	72.60	HC6H 12.36 CC6H					
OFF DIAGONAL-	6.19	BB40 4.29 BB34					
NORMAL MODE 14	OBSERVED=	0.0 CM-1	CALCULATED=	1011.1 CM-1	ERROR=	0.0 CM-1 OR	0.0 PERCENT
INTERNAL COORDINATES-	56.39	H7H8 27.56 C-O					
FORCE CONSTANTS-	66.30	HC6H 27.56 C-O					
OFF DIAGONAL-	-4.07	SB23 3.37 BB34 1.98 BB40 -1.65 SB21 -1.65 BB44					
NORMAL MODE 15	OBSERVED=	0.0 CM-1	CALCULATED=	971.7 CM-1	ERROR=	0.0 CM-1 OR	0.0 PERCENT
INTERNAL COORDINATES-	18.90	H4CC 18.90 H5CC 15.92 OCH4 15.92 OCH5 6.66 CCH7 6.65 CCH8 5.88 H8H9 5.88 H7H9					
FORCE CONSTANTS-	37.79	CC3H 31.83 OCH 13.31 CC6H 11.77 HC6H					
OFF DIAGONAL-	4.68	BB37 4.15 BB35 -2.87 BB33 -2.59 BB40					
NORMAL MODE 16	OBSERVED=	940.0 CM-1	CALCULATED=	946.3 CM-1	ERROR=	-6.3 CM-1 OR	-0.7 PERCENT
INTERNAL COORDINATES-	37.89	C-C 12.00 OCC 9.09 CCH8 9.08 CCH7					
FORCE CONSTANTS-	37.89	C-C 18.53 CC6H 12.00 CCO 10.04 HC6H					
OFF DIAGONAL-	10.05	SB24 7.73 BB44 -5.83 SB26 2.67 BB40 1.62 SB23					
NORMAL MODE 17	OBSERVED=	755.0 CM-1	CALCULATED=	748.1 CM-1	ERROR=	6.8 CM-1 OR	0.9 PERCENT
INTERNAL COORDINATES-	41.82	CCH9 18.24 C-O 13.37 C-C 7.13 H7H8					
FORCE CONSTANTS-	47.74	CC6H 18.24 C-O 13.37 C-C 7.13 HC6H					
OFF DIAGONAL-	-3.58	SB22 3.33 SB24 3.14 BB35 2.46 SB23 -1.90 BB40 1.63 BB44 1.53 SS20					
NORMAL MODE 18	OBSERVED=	667.0 CM-1	CALCULATED=	667.4 CM-1	ERROR=	-0.4 CM-1 OR	-0.1 PERCENT
INTERNAL COORDINATES-	33.60	CCH7 33.60 CCH8 9.72 H4CC 9.72 H5CC					
FORCE CONSTANTS-	67.19	CC6H 19.45 CC3H 9.79 HC6H 6.70 OCH					
OFF DIAGONAL-	-7.54	BB37 7.05 BB35 -5.30 BB40 1.68 BB36					
NORMAL MODE 19	OBSERVED=	0.0 CM-1	CALCULATED=	385.4 CM-1	ERROR=	0.0 CM-1 OR	0.0 PERCENT
INTERNAL COORDINATES-	80.11	OCC 11.64 CCH9 9.59 CCH8 9.59 CCH7					
FORCE CONSTANTS-	80.11	CCO 30.83 CC6H 5.24 HC6H 5.24 CC3H					
OFF DIAGONAL-	-20.53	BB44 -4.65 BB45 2.89 SB26 -2.83 BB46 -2.09 BB37 1.87 BB43 -1.63 BB40 -1.54 SB25					
NORMAL MODE 20	OBSERVED=	0.0 CM-1	CALCULATED=	207.5 CM-1	ERROR=	0.0 CM-1 OR	0.0 PERCENT
INTERNAL COORDINATES-	97.41	T-CO					
FORCE CONSTANTS-	97.41	TC-CO					
OFF DIAGONAL-	NONE						
NORMAL MODE 21	OBSERVED=	0.0 CM-1	CALCULATED=	190.7 CM-1	ERROR=	0.0 CM-1 OR	0.0 PERCENT
INTERNAL COORDINATES-	98.01	T-CC					
FORCE CONSTANTS-	98.01	TC-C					
OFF DIAGONAL-	NONE						

10. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 6.43

TABLE LIII (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 300									
MOLECULE 10		-6 .NG= 201		ETHANOL, CD3CH2OD (TRANS)					
PAGE 1									
NORMAL MODE 7	OBSERVED=	1482.0 CM-1	CALCULATED=	1485.4 CM-1	ERROR=	-3.4 CM-1	OR	-0.2 PERCENT	
INTERNAL COORDINATES-	74.86	HCH 6.53 H4CC 6.53 H5CC							
FORCE CONSTANTS-	74.86	HC3H 13.06 CC3H 8.50 OCH							
OFF DIAGONAL-	8.55	BB40 -4.27 BB38 -2.26 SB25							
NORMAL MODE 8	OBSERVED=	1384.0 CM-1	CALCULATED=	1385.7 CM-1	ERROR=	-1.7 CM-1	OR	-0.1 PERCENT	
INTERNAL COORDINATES-	33.40	UCH4 33.40 OCH5 18.15 H4CC 18.15 H5CC 6.72 C-C							
FORCE CONSTANTS-	66.80	UCH 36.29 CC3H 6.72 C-C							
OFF DIAGONAL-	-11.08	SB22 -8.92 SB25 6.03 BB33 -2.88 BB35							
NORMAL MODE 9	OBSERVED=	1292.0 CM-1	CALCULATED=	1276.9 CM-1	ERROR=	15.1 CM-1	OR	1.2 PERCENT	
INTERNAL COORDINATES-	34.88	UCH4 34.88 OCH5 16.16 H4CC 16.16 H5CC							
FORCE CONSTANTS-	69.76	UCH 32.32 CC3H							
OFF DIAGONAL-	-6.30	BB33 2.62 BB35							
NORMAL MODE 10	OBSERVED=	1141.0 CM-1	CALCULATED=	1137.5 CM-1	ERROR=	3.5 CM-1	OR	0.3 PERCENT	
INTERNAL COORDINATES-	49.36	C-C 17.15 C-O 8.41 CCH7 8.41 CCH8 8.19 H7H8							
FORCE CONSTANTS-	49.36	C-C 19.92 CC6H 17.15 C-O 15.67 HC6H							
OFF DIAGONAL-	-15.99	SB24 7.22 BB40 3.80 SB25 -3.11 BB35 3.05 SB21 -2.86 SS20 1.97 SB22 -1.75 BB34							
NORMAL MODE 11	OBSERVED=	1082.0 CM-1	CALCULATED=	1092.8 CM-1	ERROR=	-10.8 CM-1	OR	-1.0 PERCENT	
INTERNAL COORDINATES-	42.62	C-O 30.24 HOC 12.05 CCH9 8.56 OCC 6.45 C-C							
FORCE CONSTANTS-	42.62	C-O 30.24 COH 14.27 CC6H 10.18 HC6H 8.56 CCO 6.45 C-C							
OFF DIAGONAL-	-13.74	SB21 -8.61 SB23 2.55 BB40 2.29 BB44 -2.03 SB26 1.63 SS20 1.55 SB25 1.54 BB45							
NORMAL MODE 12	OBSERVED=	1050.0 CM-1	CALCULATED=	1046.1 CM-1	ERROR=	3.9 CM-1	OR	0.4 PERCENT	
INTERNAL COORDINATES-	28.78	HOC 16.61 H8H9 16.59 H7H9 9.67 CCH9 5.11 CCH8 5.11 CCH7							
FORCE CONSTANTS-	35.04	HC6H 28.78 COH 19.90 CC6H							
OFF DIAGONAL-	7.82	BB40 -3.19 BB35 2.70 SB21 2.56 BB44							
NORMAL MODE 13	OBSERVED=	1042.0 CM-1	CALCULATED=	1040.0 CM-1	ERROR=	2.0 CM-1	OR	0.2 PERCENT	
INTERNAL COORDINATES-	36.32	H7H9 36.29 H8H9 6.18 CCH7 6.18 CCH8							
FORCE CONSTANTS-	72.61	HC6H 12.36 CC6H							
OFF DIAGONAL-	6.19	BB40 4.29 BB34							
NORMAL MODE 14	OBSERVED=	1020.0 CM-1	CALCULATED=	1009.6 CM-1	ERROR=	10.4 CM-1	OR	1.0 PERCENT	
INTERNAL COORDINATES-	55.45	H7H8 28.86 C-O 7.76 CC6H							
FORCE CONSTANTS-	60.66	HC6H 28.86 C-O 7.76 CC6H							
OFF DIAGONAL-	3.52	BB40 -2.96 SB23 2.53 BB34 -1.62 BB44							
NORMAL MODE 15	OBSERVED=	979.0 CM-1	CALCULATED=	971.7 CM-1	ERROR=	7.3 CM-1	OR	0.8 PERCENT	
INTERNAL COORDINATES-	18.90	H4CC 18.90 H5CC 15.92 OCH4 15.92 OCH5 6.66 CCH7 6.66 CCH8 5.88 H8H9 5.88 H7H9							
FORCE CONSTANTS-	37.80	CC3H 31.83 OCH 13.32 CC6H 11.76 HC6H							
OFF DIAGONAL-	4.68	BB37 4.15 BB35 -2.87 BB33 -2.59 BB40							
NORMAL MODE 16	OBSERVED=	900.0 CM-1	CALCULATED=	889.1 CM-1	ERROR=	10.9 CM-1	OR	1.2 PERCENT	
INTERNAL COORDINATES-	38.31	HOC 27.09 C-C 6.78 OCC 5.69 CCH7 5.69 CCH8							
FORCE CONSTANTS-	38.31	COH 27.09 C-C 14.48 CC6H 6.78 CCO							
OFF DIAGONAL-	4.72	SB24 4.60 BB44 -3.71 SB26 -2.53 SB21							
NORMAL MODE 17	OBSERVED=	752.0 CM-1	CALCULATED=	743.3 CM-1	ERROR=	8.7 CM-1	OR	1.2 PERCENT	
INTERNAL COORDINATES-	39.77	CCH9 17.96 C-O 15.64 C-C 6.82 H7H8							
FORCE CONSTANTS-	44.95	CC6H 17.96 C-O 15.64 C-C 6.83 HC6H							
OFF DIAGONAL-	3.68	SB24 -3.28 SB22 2.89 BB35 2.21 SB23 1.65 SS20 -1.62 BB40							
NORMAL MODE 18	OBSERVED=	666.0 CM-1	CALCULATED=	667.3 CM-1	ERROR=	-1.3 CM-1	OR	-0.2 PERCENT	
INTERNAL COORDINATES-	33.60	CCH7 33.60 CCH8 9.75 H4CC 9.75 H5CC							
FORCE CONSTANTS-	67.20	CC6H 19.49 CC3H 9.79 HC6H 6.71 OCH							
OFF DIAGONAL-	-7.55	BB37 7.06 BB35 -5.31 BB40 1.69 BB36							
NORMAL MODE 19	OBSERVED=	386.0 CM-1	CALCULATED=	378.8 CM-1	ERROR=	7.2 CM-1	OR	1.8 PERCENT	
INTERNAL COORDINATES-	80.39	OCC 11.45 CCH9 9.40 CCH8 9.40 CCH7							
FORCE CONSTANTS-	80.39	CCO 30.26 CC6H 5.13 HC6H 5.13 CC3H							
OFF DIAGONAL-	-20.36	BB44 -4.62 BB45 -2.89 BB46 2.70 SB26 -2.05 BB37 1.85 BB43 -1.61 BB40							
NORMAL MODE 20	OBSERVED=	0.0 CM-1	CALCULATED=	191.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	98.75	T-CC							
FORCE CONSTANTS-	98.75	TC-C							
OFF DIAGONAL -	NONE								
NORMAL MODE 21	OBSERVED=	0.0 CM-1	CALCULATED=	152.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	98.48	T-CO							
FORCE CONSTANTS-	98.48	TC-O							
OFF DIAGONAL -	NONE								

13. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 6.63

TABLE LIII (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 300										PAGE	1
MOLECULE 11 -6 NG= 201 ETHANOL, CD3CD2OH (TRANS)											
NORMAL MODE 7	OBSERVED=	1385.0 CM-1	CALCULATED=	1392.3 CM-1	ERROR=	-7.3 CM-1	OR	-0.5 PERCENT			
INTERNAL COORDINATES-	85.94	HOC 7.83 C-C									
FORCE CONSTANTS-	85.94	COH 7.83 C-C									
OFF DIAGONAL-	3.35	SB21 -2.72 SB25 -1.87 BB31									
NORMAL MODE 8	OBSERVED=	1177.0 CM-1	CALCULATED=	1169.6 CM-1	ERROR=	7.4 CM-1	OR	0.6 PERCENT			
INTERNAL COORDINATES-	44.89	C-O 27.52 C-C 12.70 HOC 11.02 OCH4 11.02 OCH5 6.43 CCH7 6.43 CCH8 6.04 H4CC 6.04 H5CC									
FORCE CONSTANTS-	44.89	C-O 27.52 C-C 22.03 OCH 13.08 CC6H 12.70 COH 12.08 CC3H 6.26 HC6H									
OFF DIAGONAL-	-19.18	SB22-10.41 SB25 -9.14 SB21 -7.29 SB24 -3.45 SS20 -3.28 SB23 2.60 BB37 2.04 BB44 1.99 BB33									
NORMAL MODE 9	OBSERVED=	1120.0 CM-1	CALCULATED=	1101.9 CM-1	ERROR=	18.1 CM-1	OR	1.6 PERCENT			
INTERNAL COORDINATES-	47.49	HCH 18.41 C-C 11.04 CCH9 6.08 C-O 5.23 H7H9 5.22 H8H9									
FORCE CONSTANTS-	47.49	HC3H 18.41 C-C 11.91 CC6H 10.65 HC6H 6.12 OCH 6.08 C-O									
OFF DIAGONAL-	7.71	BB40 -5.99 SB24 -5.29 SB25 -3.72 SB22 -2.88 BB38 -2.18 SB26 -2.06 SB23									
NORMAL MODE 10	OBSERVED=	1065.0 CM-1	CALCULATED=	1064.9 CM-1	ERROR=	0.1 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	17.39	HCH 14.89 CCH9 10.78 H8H9 10.78 H7H9 7.69 H5CC 7.69 H4CC 7.20 C-O 7.00 CCH8 6.99 CCH7									
FORCE CONSTANTS-	28.89	CC6H 24.05 HC6H 17.39 HC3H 15.37 CC3H 7.20 C-O									
OFF DIAGONAL-	15.02	BB40 -5.72 BB35 -4.56 SB24 3.71 SB25 -3.06 BB37 -2.50 BB34 -1.95 SB22 -1.68 BB36									
NORMAL MODE 11	OBSERVED=	1053.0 CM-1	CALCULATED=	1038.8 CM-1	ERROR=	14.2 CM-1	OR	1.3 PERCENT			
INTERNAL COORDINATES-	39.63	H8H9 39.62 H7H9									
FORCE CONSTANTS-	79.25	HC6H 8.41 CC6H									
OFF DIAGONAL-	5.34	BB40 4.69 BB34									
NORMAL MODE 12	OBSERVED=	0.0 CM-1	CALCULATED=	1027.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	58.07	H7H8 7.00 H7H9 6.99 H8H9 5.64 OCH5 5.64 OCH4									
FORCE CONSTANTS-	72.06	HC6H 11.28 OCH									
OFF DIAGONAL-	3.94	BB34 2.65 BB40 -2.20 SB22									
NORMAL MODE 13	OBSERVED=	974.0 CM-1	CALCULATED=	957.1 CM-1	ERROR=	16.9 CM-1	OR	1.7 PERCENT			
INTERNAL COORDINATES-	33.68	C-O 15.30 OCH4 15.30 OCH5 5.26 OCC									
FORCE CONSTANTS-	33.68	C-O 30.61 OCH 7.98 HC6H 5.56 CC3H 5.26 CCO									
OFF DIAGONAL-	19.58	SB22 -6.00 SB23 2.76 BB33 -2.53 SB25 -2.42 BB46 -1.62 BB40									
NORMAL MODE 14	OBSERVED=	901.0 CM-1	CALCULATED=	926.4 CM-1	ERROR=	-25.4 CM-1	OR	-2.8 PERCENT			
INTERNAL COORDINATES-	30.46	UCH4 30.46 OCH5 16.97 H4CC 16.96 H5CC									
FORCE CONSTANTS-	60.92	UCH 33.93 CC3H									
OFF DIAGONAL-	-5.50	BB33 3.12 BB35 2.58 BB37									
NORMAL MODE 15	OBSERVED=	0.0 CM-1	CALCULATED=	907.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	29.77	C-C 7.52 OCC 7.33 CCH7 7.33 CCH8									
FORCE CONSTANTS-	29.77	C-C 17.07 CC6H 7.58 CC3H 7.52 CCO									
OFF DIAGONAL-	8.57	SB25 6.34 SB24 5.50 BB44 -4.09 SB26 2.73 SB23 2.31 BB40 2.20 BB37									
NORMAL MODE 16	OBSERVED=	875.0 CM-1	CALCULATED=	864.8 CM-1	ERROR=	10.2 CM-1	OR	1.2 PERCENT			
INTERNAL COORDINATES-	17.69	CCH7 17.69 CCH8 17.27 OCH4 17.27 OCH5 7.95 H4CC 7.95 H5CC									
FORCE CONSTANTS-	35.37	CC6H 34.54 OCH 15.89 CC3H 8.90 HC6H									
OFF DIAGONAL-	4.94	BB37 4.17 BB35 -3.67 BB40 -3.12 BB33									
NORMAL MODE 17	OBSERVED=	737.0 CM-1	CALCULATED=	740.0 CM-1	ERROR=	-3.0 CM-1	OR	-0.4 PERCENT			
INTERNAL COORDINATES-	39.67	CCH9 15.98 C-C 15.11 C-O 7.15 H7H8									
FORCE CONSTANTS-	44.59	CC6H 15.98 C-C 15.11 C-O 7.16 HC6H									
OFF DIAGONAL-	-5.21	SB22 3.80 SB24 2.74 BB35 2.28 SB25 2.18 SB23 -1.67 BB40 1.53 SS20									
NORMAL MODE 18	OBSERVED=	587.0 CM-1	CALCULATED=	595.1 CM-1	ERROR=	-8.1 CM-1	OR	-1.4 PERCENT			
INTERNAL COORDINATES-	22.25	CCH7 22.25 CCH8 20.38 H4CC 20.38 H5CC 5.51 OCH4 5.51 OCH5									
FORCE CONSTANTS-	44.49	CC6H 40.77 CC3H 11.01 OCH 6.25 HC6H									
OFF DIAGONAL-	-8.88	BB37 6.93 BB35 -3.45 BB40 1.98 BB36									
NORMAL MODE 19	OBSERVED=	382.0 CM-1	CALCULATED=	381.9 CM-1	ERROR=	0.1 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	80.66	OCC 11.63 CCH9 9.46 CCH8 9.46 CCH7									
FORCE CONSTANTS-	80.66	CCO 30.55 CC6H 5.96 CC3H 5.18 HC6H									
OFF DIAGONAL-	-20.46	BB44 -4.66 BB45 -2.86 BB46 2.64 SB26 -2.21 BB37 2.00 BB43 -1.66 SB23 -1.56 BB40									
NORMAL MODE 20	OBSERVED=	0.0 CM-1	CALCULATED=	207.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	97.69	T-CO									
FORCE CONSTANTS-	97.69	TC-O									
OFF DIAGONAL -	NONE										
NORMAL MODE 21	OBSERVED=	0.0 CM-1	CALCULATED=	182.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT			
INTERNAL COORDINATES-	97.53	T-CC									
FORCE CONSTANTS-	97.53	TC-C									
OFF DIAGONAL -	NONE										

11. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR =10.07

TABLE LIII (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 300												PAGE 1
MOLECULE 12		-6 NG= 201		ETHANOL, CD3CD2OD (TRANS)								
NORMAL MODE 7	OBSERVED=	1222.0 CM-1		CALCULATED=	1217.1 CM-1		ERROR=	4.9 CM-1	OR	0.4 PERCENT		
INTERNAL COORDINATES-	44.70	C-C 22.01	C-O	11.33	OCH4	11.33	OCH5	10.87	HOC	9.82 H4CC	9.82 H5CC	
FORCE CONSTANTS-	44.70	C-C 22.65	OCH	22.01	C-O	19.64	CC3H	10.87	COH	5.74	CC6H	
OFF DIAGONAL-	-16.91	S825-13.62	S822	-6.85	S824	5.92	S821	-3.08	SS20	2.81	BB40 2.21 BB37 -2.07 BB35 2.05 BB33	
NORMAL MODE 8	OBSERVED=	1124.0 CM-1		CALCULATED=	1123.3 CM-1		ERROR=	0.6 CM-1	OR	0.1 PERCENT		
INTERNAL COORDINATES-	42.03	HCH 26.63	C-O	13.80	HOC	7.28	OCC					
FORCE CONSTANTS-	42.03	HC3H 26.63	C-O	13.80	COH	9.01	CC6H	8.55	OCH	7.28	CCO	
OFF DIAGONAL-	-9.20	S822 -7.34	S821	-6.28	S823	-3.21	BB38	3.18	BB40	2.95	BB44	
NORMAL MODE 9	OBSERVED=	1065.0 CM-1		CALCULATED=	1073.7 CM-1		ERROR=	-8.7 CM-1	OR	-0.8 PERCENT		
INTERNAL COORDINATES-	20.41	CCH9 15.65	H8H9	15.64	H7H9	10.80	C-C	10.33	CCH8	10.33	CCH7	
FORCE CONSTANTS-	41.07	CC6H 34.64	HC6H	10.80	C-C	5.63	OCH					
OFF DIAGONAL-	15.35	BB40-10.83	S824	-6.81	BB35	4.11	S825	-3.56	BB34	-2.48	S822 -2.08 BB37	
NORMAL MODE 10	OBSERVED=	1041.0 CM-1		CALCULATED=	1038.8 CM-1		ERROR=	2.2 CM-1	OR	0.2 PERCENT		
INTERNAL COORDINATES-	39.63	H8H9 39.63	H7H9									
FORCE CONSTANTS-	79.25	HC6H 8.41	CC6H									
OFF DIAGONAL-	5.34	BB40	4.69	BB34								
NORMAL MODE 11	OBSERVED=	0.0 CM-1		CALCULATED=	1033.9 CM-1		ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	27.73	H7H8 25.21	HCH	12.69	HOC	6.73	OCH4	6.73	OCH5			
FORCE CONSTANTS-	36.23	HC6H 25.21	HC3H	13.46	OCH	12.69	COH					
OFF DIAGONAL-	4.05	S822	3.63	BB40	-3.11	BB38	-2.47	S821	2.07	BB34		
NORMAL MODE 12	OBSERVED=	0.0 CM-1		CALCULATED=	1015.8 CM-1		ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	31.66	H7H8 28.18	HOC	20.72	C-O	6.12	HCH					
FORCE CONSTANTS-	41.28	HC6H 28.18	COH	20.72	C-O	7.01	CC3H	6.12	HC3H			
OFF DIAGONAL-	-9.25	S821 -4.04	S823	2.35	BB34	1.80	BB40					
NORMAL MODE 13	OBSERVED=	924.0 CM-1		CALCULATED=	928.5 CM-1		ERROR=	-4.5 CM-1	OR	-0.5 PERCENT		
INTERNAL COORDINATES-	22.64	C-O 9.73	OCH5	9.60	OCH4	8.89	H5CC	8.79	H4CC			
FORCE CONSTANTS-	22.64	C-O 19.34	OCH	17.68	CC3H							
OFF DIAGONAL-	12.76	S822	4.14	S825	3.87	S821	1.75	BB33	-1.63	BB35	1.61 BB40	
NORMAL MODE 14	OBSERVED=	904.0 CM-1		CALCULATED=	926.4 CM-1		ERROR=	-22.4 CM-1	OR	-2.5 PERCENT		
INTERNAL COORDINATES-	30.53	OCH4 30.40	OCH5	17.01	H4CC	16.92	H5CC					
FORCE CONSTANTS-	60.93	OCH 33.93	CC3H									
OFF DIAGONAL-	-5.50	BB33	3.12	BB35	2.58	BB37						
NORMAL MODE 15	OBSERVED=	0.0 CM-1		CALCULATED=	875.6 CM-1		ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	30.00	HOC 27.01	C-C	7.15	OCC	5.97	CCH7	5.97	CCH8			
FORCE CONSTANTS-	30.00	COH 27.01	C-C	16.32	CC6H	7.15	CCO	6.13	OCH			
OFF DIAGONAL-	4.84	BB44	4.37	S824	-3.80	S826						
NORMAL MODE 16	OBSERVED=	875.0 CM-1		CALCULATED=	864.8 CM-1		ERROR=	10.2 CM-1	OR	1.2 PERCENT		
INTERNAL COORDINATES-	17.70	CCH8 17.69	CCH7	17.27	OCH4	17.27	OCH5	7.95	H4CC	7.95	H5CC	
FORCE CONSTANTS-	35.39	CC6H 34.54	OCH	15.89	CC3H	8.90	HC6H					
OFF DIAGONAL-	4.94	BB37	4.17	BB35	-3.67	BB40	-3.12	BB33				
NORMAL MODE 17	OBSERVED=	736.0 CM-1		CALCULATED=	736.5 CM-1		ERROR=	-0.5 CM-1	OR	-0.1 PERCENT		
INTERNAL COORDINATES-	38.32	CCH9 17.70	C-C	15.43	C-O	6.90	H7H8					
FORCE CONSTANTS-	42.81	CC6H 17.70	C-C	15.43	C-O	6.92	HC6H					
OFF DIAGONAL-	-4.83	S822	4.04	S824	2.60	BB35	2.13	S825	2.03	S823	1.62 SS20	
NORMAL MODE 18	OBSERVED=	587.0 CM-1		CALCULATED=	595.0 CM-1		ERROR=	-8.0 CM-1	OR	-1.4 PERCENT		
INTERNAL COORDINATES-	22.25	CCH7 22.25	CCH8	20.42	H4CC	20.42	H5CC	5.52	OCH4	5.52	OCH5	
FORCE CONSTANTS-	44.51	CC6H 40.85	CC3H	11.04	OCH	6.26	HC6H					
OFF DIAGONAL-	-8.89	BB37	6.94	BB35	-3.45	BB40	1.99	BB36				
NORMAL MODE 19	OBSERVED=	380.0 CM-1		CALCULATED=	375.3 CM-1		ERROR=	4.7 CM-1	OR	1.2 PERCENT		
INTERNAL COORDINATES-	80.95	OCC 11.41	CCH9	9.27	CCH8	9.27	CCH7					
FORCE CONSTANTS-	80.95	CCO 29.94	CC6H	5.76	CC3H	5.07	HC6H					
OFF DIAGONAL-	-20.28	BB44	-4.62	BB45	-2.96	BB46	2.46	S826	-2.15	BB37	1.97 BB43 -1.54 BB40 -1.52 S823	
NORMAL MODE 20	OBSERVED=	0.0 CM-1		CALCULATED=	183.3 CM-1		ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	97.26	T-CC										
FORCE CONSTANTS-	97.26	TC-C										
OFF DIAGONAL -	NONE											
NORMAL MODE 21	OBSERVED=	0.0 CM-1		CALCULATED=	152.2 CM-1		ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	98.00	T-CO										
FORCE CONSTANTS-	98.00	TC-O										
OFF DIAGONAL -	NONE											

10. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 6.66

TABLE LIV

POTENTIAL ENERGY DISTRIBUTIONS FOR GASEOUS ETHANOL (GAUCHE)

Explanation of the table:

This table is presented in the same format as Table XXXIV except that the force constant and internal coordinate description codes are found in Tables XLIII and XLIV, respectively.

TABLE LIV

POTENTIAL ENERGY DISTRIBUTIONS FOR GASEOUS ETHANOL (GAUCHE)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 301										PAGE 1	
MOLECULE 1		-6 NG= 209		ETHANOL, CH3CH2OH, GAUCHE							
NORMAL MODE 7	OBSERVED=	0.0 CM-1		CALCULATED=		1496.7 CM-1		ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	68.92	HCH	8.52 OCH5	7.85		UCH4					
FORCE CONSTANTS-	68.92	HC3H	16.38 OCH	6.35		CC3H					
OFF DIAGONAL-	5.72	BB40	-3.84 BB38	-2.18		SB22					
NORMAL MODE 8	OBSERVED=	0.0 CM-1		CALCULATED=		1456.3 CM-1		ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	44.70	H7H8	20.30 H8H9	6.48		CCH9		5.02	HCH		
FORCE CONSTANTS-	68.99	HC6H	10.70 CC6H	5.02		HC3H					
OFF DIAGONAL-	6.08	BB40	4.48 BB34								
NORMAL MODE 9	OBSERVED=	0.0 CM-1		CALCULATED=		1456.0 CM-1		ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	44.76	H7H9	29.80 H8H9	6.44		CCH8					
FORCE CONSTANTS-	76.22	HC6H	10.61 CC6H								
OFF DIAGONAL-	5.47	BB40	4.95 BB34								
NORMAL MODE 10	OBSERVED=	0.0 CM-1		CALCULATED=		1411.8 CM-1		ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	32.11	UCH5	17.32 H5CC	15.11		UCH4		15.00	H4CC	11.22	HOC 8.44 C-C
FORCE CONSTANTS-	47.23	UCH	32.32 CC3H	11.22		COH		8.44	C-C	5.27	HC6H
OFF DIAGONAL-	-8.89	SB25	-7.16 SB22	4.53		BB32		3.97	BB33	-2.33	SB21 -2.17 BB35 -1.98 SB24
NORMAL MODE 11	OBSERVED=	0.0 CM-1		CALCULATED=		1380.7 CM-1		ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	17.82	CCH7	17.78 CCH8	15.32		CCH9		15.13	H8H9	12.83	H7H9 12.58 H7H8
FORCE CONSTANTS-	50.92	CC6H	40.54 HC6H								
OFF DIAGONAL-	17.08	BB40	-7.75 SB24	-6.27		BB35		-5.25	BB34		
NORMAL MODE 12	OBSERVED=	0.0 CM-1		CALCULATED=		1304.6 CM-1		ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	46.79	UCH4	21.95 HOC	18.60		H4CC		10.21	UCH5		
FORCE CONSTANTS-	57.00	UCH	21.95 COH	19.81		CC3H					
OFF DIAGONAL-	-3.94	BB33	3.57 BB32	-3.52		BB31		1.89	SB21	-1.58	SB22
NORMAL MODE 13	OBSERVED=	0.0 CM-1		CALCULATED=		1224.0 CM-1		ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	41.15	HOC	23.01 H5CC	13.55		UCH5		5.10	H4CC		
FORCE CONSTANTS-	41.15	COH	28.11 CC3H	14.96		UCH		6.83	CC6H		
OFF DIAGONAL-	-5.64	BB32	4.72 SB21	2.16		BB37		-1.98	SB22	1.68	BB35
NORMAL MODE 14	OBSERVED=	0.0 CM-1		CALCULATED=		1103.4 CM-1		ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	58.53	C-O	12.61 CCH9	8.65		C-C		7.67	HOC	5.28	H7H8 5.27 CCH8
FORCE CONSTANTS-	58.53	C-O	17.90 CC6H	8.65		C-C		7.67	COH	6.75	HC6H
OFF DIAGONAL-	-8.71	SB21	-6.12 SB23	5.09		SB22		-1.81	BB40	1.52	SB26
NORMAL MODE 15	OBSERVED=	0.0 CM-1		CALCULATED=		1053.9 CM-1		ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	38.76	C-C	18.80 CCH8	7.45		CCH9		6.64	UCH4		
FORCE CONSTANTS-	38.76	C-C	28.46 CC6H	9.92		UCH		6.20	HC6H	5.02	CC3H
OFF DIAGONAL-	-4.32	SB26	-2.51 BB40	2.11		SB23		2.03	BB37	2.00	BB35 1.98 SB25 1.75 BB44
NORMAL MODE 16	OBSERVED=	0.0 CM-1		CALCULATED=		1020.7 CM-1		ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	26.45	CCH7	16.88 C-C	16.19		HOC		12.73	UCH5	8.64	CCH9 5.48 H8H9
FORCE CONSTANTS-	39.77	CC6H	16.88 C-C	16.21		UCH		16.19	COH	8.19	HC6H
OFF DIAGONAL-	-3.43	BB32	-3.39 BB40	2.61		BB35		-2.14	SB26	1.67	BB37
NORMAL MODE 17	OBSERVED=	0.0 CM-1		CALCULATED=		872.9 CM-1		ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	44.65	C-O	28.41 C-C	19.76		CCH9					
FORCE CONSTANTS-	44.65	C-O	28.41 C-C	27.86		CC6H					
OFF DIAGONAL-	-4.90	SB22	-3.20 SB21	-3.16		SB23		2.75	SB25	-1.93	BB40 1.89 SS20 1.64 BB35 -1.62 SB26
NORMAL MODE 18	OBSERVED=	0.0 CM-1		CALCULATED=		788.7 CM-1		ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	23.08	H4CC	21.72 H5CC	18.14		CCH8		16.60	CCH7	10.42	UCH5 9.50 UCH4
FORCE CONSTANTS-	44.81	CC3H	34.77 CC6H	19.92		UCH		5.03	HC6H		
OFF DIAGONAL-	-7.94	BB37	4.85 BB35	-2.49		BB40		-1.80	BB33		
NORMAL MODE 19	OBSERVED=	0.0 CM-1		CALCULATED=		433.7 CM-1		ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	86.51	OCC	6.70 CCH9								
FORCE CONSTANTS-	86.51	CCO	16.04 CC6H	7.75		CC3H					
OFF DIAGONAL-	-11.15	BB44	-3.85 BB45	3.61		SB26		-1.92	SB23	-1.85	SB25 -1.71 BB37
NORMAL MODE 20	OBSERVED=	0.0 CM-1		CALCULATED=		251.4 CM-1		ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	90.62	T-CC	8.62 T-CO								
FORCE CONSTANTS-	90.62	TC-C	8.62 TC-O								
OFF DIAGONAL -	NONE										
NORMAL MODE 21	OBSERVED=	0.0 CM-1		CALCULATED=		205.8 CM-1		ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	89.66	T-CO	8.53 T-CC								
FORCE CONSTANTS-	89.66	TC-O	8.53 TC-C								
OFF DIAGONAL -	NONE										

0. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 0.0

TABLE LIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 301									
MOLECULE 2 -6 NG= 209 ETHANOL, CH3CH2OD, GAUCHE									
PAGE 1									
NORMAL MODE 7	OBSERVED=	0.0 CM-1	CALCULATED=	1496.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	69.10	HCH 7.76 OCH5	7.71	UCH4					
FORCE CONSTANTS-	69.10	HC3H 15.47 OCH	6.79	CC3H					
OFF DIAGONAL-	5.92	BB40 -3.73 BB38	-2.10	SB22					
NORMAL MODE 8	OBSERVED=	0.0 CM-1	CALCULATED=	1456.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	46.06	H7H8 12.96 H7H9	8.98	H8H9 6.68 CCH9	5.46	HCH			
FORCE CONSTANTS-	67.99	HC6H 10.63 CC6H	5.46	HC3H					
OFF DIAGONAL-	6.17	BB40 4.42 BB34							
NORMAL MODE 9	OBSERVED=	0.0 CM-1	CALCULATED=	1455.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	41.13	H8H9 36.61 H7H9	5.61	CCH7					
FORCE CONSTANTS-	77.87	HC6H 10.62 CC6H							
OFF DIAGONAL-	5.41	BB40 5.06 BB34							
NORMAL MODE 10	OBSERVED=	0.0 CM-1	CALCULATED=	1397.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	24.95	UCH5 20.57 UCH4	15.91	H4CC 15.81 H5CC 11.73	C-C 6.90	H7H9 5.16	H8H9		
FORCE CONSTANTS-	45.52	UCH 31.71 CC3H	12.06	HC6H 11.73	C-C 10.44	CC6H			
OFF DIAGONAL-	-10.39	SB25 -8.20 SB22	-5.54	SB24 4.09	BB33 3.56	BB40 3.26	BB37 -3.16	BB35	
NORMAL MODE 11	OBSERVED=	0.0 CM-1	CALCULATED=	1377.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	14.71	H7H8 14.45 CCH7	14.31	CCH9 14.29 CCH8 10.52	H8H9 9.36	H7H9 7.19	UCH5 5.42	UCH4	
FORCE CONSTANTS-	43.06	CC6H 34.59 HC6H	12.61	UCH 7.62	CC3H				
OFF DIAGONAL-	14.47	BB40 -5.74 BB35	-4.43	BB34 -4.03	SB24 -2.98	BB37 1.81	SB25		
NORMAL MODE 12	OBSERVED=	0.0 CM-1	CALCULATED=	1280.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	37.24	UCH4 31.23 UCH5	17.74	H4CC 13.37	H5CC				
FORCE CONSTANTS-	68.47	UCH 31.12 CC3H							
OFF DIAGONAL-	-6.15	BB33 1.92 BB35	1.59	BB32					
NORMAL MODE 13	OBSERVED=	0.0 CM-1	CALCULATED=	1117.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	39.59	C-O 19.24 CCH9	9.56	CCH7 7.69	H7H8 6.96	OCC			
FORCE CONSTANTS-	39.59	C-O 28.81 CC6H	10.43	HC6H 6.96	CCO				
OFF DIAGONAL-	-8.08	SB23 4.67 SB21	-3.09	BB40 2.33	BB44 1.89	BB35 1.85	BB45 1.77	SB22	
NORMAL MODE 14	OBSERVED=	0.0 CM-1	CALCULATED=	1090.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	20.84	C-O 14.49 HOC	13.10	C-C 11.71	CCH8 9.96	CCH7 9.60	H5CC 6.88	UCH4	
FORCE CONSTANTS-	22.23	CC6H 20.84 C-O	14.49	COH 13.67	CC3H 13.10	C-C 9.56	UCH 5.94	HC6H	
OFF DIAGONAL-	-7.14	SB21 3.36 BB37	2.11	BB35 -2.09	BB40 1.99	SB22			
NORMAL MODE 15	OBSERVED=	0.0 CM-1	CALCULATED=	1053.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	46.85	C-C 15.21 CCH8	9.35	CCH9 6.02	OCC				
FORCE CONSTANTS-	46.85	C-C 25.08 CC6H	6.51	UCH 6.02	CCO 5.36	HC6H			
OFF DIAGONAL-	-5.27	SB26 2.48 SB23	2.33	SB25 -2.19	BB40 2.17	BB44 1.68	BB35		
NORMAL MODE 16	OBSERVED=	0.0 CM-1	CALCULATED=	888.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	63.95	HOC 15.74 CCH7	8.04	C-C 7.92	CCH8				
FORCE CONSTANTS-	63.95	COH 24.32 CC6H	8.04	C-C					
OFF DIAGONAL-	-5.06	SB21 -2.48 BB32	-2.08	BB37 -1.81	BB40 1.71	BB35			
NORMAL MODE 17	OBSERVED=	0.0 CM-1	CALCULATED=	871.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	42.84	C-O 24.08 C-C	21.53	CCH9 7.23	CCH7				
FORCE CONSTANTS-	42.84	C-O 31.27 CC6H	24.08	C-C					
OFF DIAGONAL-	-5.49	SB22 -3.17 SB23	2.90	SB25 -2.20	BB40 1.84	BB35 1.70	SS20 -1.53	SB26	
NORMAL MODE 18	OBSERVED=	0.0 CM-1	CALCULATED=	771.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	22.51	H4CC 16.83 HOC	16.62	H5CC 14.80	CCH8 13.36	UCH5 9.58	UCH4 9.02	CCH7	
FORCE CONSTANTS-	39.14	CC3H 24.26 CC6H	22.94	UCH 16.83	COH				
OFF DIAGONAL-	-6.14	BB37 3.83 BB35	-3.58	BB32 -2.04	BB33 -1.73	BB40			
NORMAL MODE 19	OBSERVED=	0.0 CM-1	CALCULATED=	425.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	85.74	OCC 6.36 CCH9							
FORCE CONSTANTS-	85.74	CCO 15.31 CC6H	7.44	CC3H					
OFF DIAGONAL-	-10.88	BB44 -3.73 BB45	3.39	SB26 -1.98	SB23 -1.71	SB25 -1.64	BB37		
NORMAL MODE 20	OBSERVED=	0.0 CM-1	CALCULATED=	248.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	96.89	T-CC							
FORCE CONSTANTS-	96.89	TC-C							
OFF DIAGONAL -	NONE								
NORMAL MODE 21	OBSERVED=	0.0 CM-1	CALCULATED=	154.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	96.23	T-CO							
FORCE CONSTANTS-	96.23	TC-O							
OFF DIAGONAL -	NONE								

O. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 0.0

TABLE LIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 301					PAGE 1	
MOLECULE	3	-6	NG= 209	ETHANOL, CH ₃ CD ₂ OH, GAUCHE		
NORMAL MODE 7	OBSERVED=	0.0	CM-1	CALCULATED=	1457.5	CM-1
INTERNAL COORDINATES-	50.98	H7H8	14.69	H8H9	10.22	H7H9
FORCE CONSTANTS-	75.89	HC6H	11.49	CC6H	7.41	CC6H
OFF DIAGONAL-	5.54	BB40	4.93	BB34		
ERROR=	0.0	CM-1	OR	0.0	PERCENT	
NORMAL MODE 8	OBSERVED=	0.0	CM-1	CALCULATED=	1454.5	CM-1
INTERNAL COORDINATES-	41.49	H7H9	36.71	H8H9	5.38	CC6H
FORCE CONSTANTS-	78.34	HC6H	10.20	CC6H		
OFF DIAGONAL-	5.32	BB40	5.09	BB34		
ERROR=	0.0	CM-1	OR	0.0	PERCENT	
NORMAL MODE 9	OBSERVED=	0.0	CM-1	CALCULATED=	1381.9	CM-1
INTERNAL COORDINATES-	18.80	CCH7	18.76	CC6H	15.48	CCH9
FORCE CONSTANTS-	53.03	CC6H	42.24	HC6H	8.03	C-C
OFF DIAGONAL-	17.74	BB40-10.42	SB24	-6.48	BB35	-5.46
ERROR=	0.0	CM-1	OR	0.0	PERCENT	
NORMAL MODE 10	OBSERVED=	0.0	CM-1	CALCULATED=	1274.9	CM-1
INTERNAL COORDINATES-	79.49	HOC	7.51	OCH5	6.17	C-C
FORCE CONSTANTS-	79.49	COH	7.62	OCH	6.17	C-C
OFF DIAGONAL-	5.83	BB32	-4.77	SB21	-2.34	SB25
ERROR=	0.0	CM-1	OR	0.0	PERCENT	
NORMAL MODE 11	OBSERVED=	0.0	CM-1	CALCULATED=	1184.7	CM-1
INTERNAL COORDINATES-	41.76	C-O	18.71	C-C	16.23	OCH4
FORCE CONSTANTS-	41.76	C-O	26.14	OCH	18.71	C-C
OFF DIAGONAL-	-20.54	SB22	-9.84	SB25	4.71	SB21
ERROR=	0.0	CM-1	OR	0.0	PERCENT	
NORMAL MODE 12	OBSERVED=	0.0	CM-1	CALCULATED=	1106.3	CM-1
INTERNAL COORDINATES-	58.63	HCH	14.17	C-C	5.08	H5CC
FORCE CONSTANTS-	58.63	HC3H	14.17	C-C	8.89	CC3H
OFF DIAGONAL-	-6.03	SB25	4.95	BB40	-2.64	SB26
ERROR=	0.0	CM-1	OR	0.0	PERCENT	
NORMAL MODE 13	OBSERVED=	0.0	CM-1	CALCULATED=	1023.1	CM-1
INTERNAL COORDINATES-	35.73	CC6H	19.47	CC6H	8.99	H4CC
FORCE CONSTANTS-	57.96	CC6H	14.97	CC3H	6.98	H7H9
OFF DIAGONAL-	5.78	BB37	-4.67	BB40	5.97	H5CC
ERROR=	0.0	CM-1	OR	0.0	PERCENT	
NORMAL MODE 14	OBSERVED=	0.0	CM-1	CALCULATED=	1011.5	CM-1
INTERNAL COORDINATES-	19.07	CCH9	15.74	CCH7	15.69	C-C
FORCE CONSTANTS-	34.89	CC6H	15.91	OCH	13.58	OCH4
OFF DIAGONAL-	-2.54	SB26	2.41	BB44	12.41	HC3H
ERROR=	0.0	CM-1	OR	0.0	PERCENT	
NORMAL MODE 15	OBSERVED=	0.0	CM-1	CALCULATED=	954.3	CM-1
INTERNAL COORDINATES-	37.18	C-O	17.82	OCH4	8.89	H4CC
FORCE CONSTANTS-	37.18	C-O	22.45	OCH	5.22	H5CC
OFF DIAGONAL-	17.21	SB22	-4.78	SB21	14.11	CC3H
ERROR=	0.0	CM-1	OR	0.0	PERCENT	
NORMAL MODE 16	OBSERVED=	0.0	CM-1	CALCULATED=	895.5	CM-1
INTERNAL COORDINATES-	49.89	OCH5	30.54	OCH4	9.92	H5CC
FORCE CONSTANTS-	80.43	OCH	14.35	CC3H	7.49	HOC
OFF DIAGONAL-	-7.04	BB33	-4.61	BB32	6.24	CC6H
ERROR=	0.0	CM-1	OR	0.0	PERCENT	
NORMAL MODE 17	OBSERVED=	0.0	CM-1	CALCULATED=	852.5	CM-1
INTERNAL COORDINATES-	37.27	C-C	29.86	C-O	14.67	CCH9
FORCE CONSTANTS-	37.27	C-C	29.86	C-O	20.23	CC6H
OFF DIAGONAL-	8.46	SB25	-8.08	SB22	6.61	CC3H
ERROR=	0.0	CM-1	OR	0.0	PERCENT	
NORMAL MODE 18	OBSERVED=	0.0	CM-1	CALCULATED=	658.7	CM-1
INTERNAL COORDINATES-	31.83	H4CC	29.35	H5CC	10.54	OCH5
FORCE CONSTANTS-	61.18	CC3H	20.42	OCH	9.88	OCH4
OFF DIAGONAL-	-6.57	BB37	4.78	BB35	9.40	CC6H
ERROR=	0.0	CM-1	OR	0.0	PERCENT	
NORMAL MODE 19	OBSERVED=	0.0	CM-1	CALCULATED=	428.4	CM-1
INTERNAL COORDINATES-	86.93	OCC	6.70	CCH9		
FORCE CONSTANTS-	86.93	CCO	15.99	CC6H	9.08	CC3H
OFF DIAGONAL-	-11.15	BB44	-3.86	BB45	3.17	SB26
ERROR=	0.0	CM-1	OR	0.0	PERCENT	
NORMAL MODE 20	OBSERVED=	0.0	CM-1	CALCULATED=	244.0	CM-1
INTERNAL COORDINATES-	91.15	T-CC	7.36	T-CO		
FORCE CONSTANTS-	91.15	TC-C	7.36	TC-O		
OFF DIAGONAL-	NONE					
ERROR=	0.0	CM-1	OR	0.0	PERCENT	
NORMAL MODE 21	OBSERVED=	0.0	CM-1	CALCULATED=	205.5	CM-1
INTERNAL COORDINATES-	91.13	T-CO	7.16	T-CC		
FORCE CONSTANTS-	91.13	TC-O	7.16	TC-C		
OFF DIAGONAL-	NONE					
ERROR=	0.0	CM-1	OR	0.0	PERCENT	

0. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 0.0

TABLE LIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 301									
MOLECULE 4 -6 NG= 209 ETHANOL, CH3CD2OD, GAUCHE									
PAGE 1									
NORMAL MODE 7	OBSERVED=	0.0 CM-1	CALCULATED=	1457.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	51.13	H7H8 13.21 H8H9	11.67	H7H9 7.43 CCH9					
FORCE CONSTANTS-	76.00	HC6H 11.46 CC6H							
OFF DIAGONAL-	5.54	BB40 4.94 BB34							
NORMAL MODE 8	OBSERVED=	0.0 CM-1	CALCULATED=	1454.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	40.05	H7H9 38.42 H8H9	5.18	CCH8					
FORCE CONSTANTS-	78.49	HC6H 10.17 CC6H							
OFF DIAGONAL-	5.32	BB40 5.10 BB34							
NORMAL MODE 9	OBSERVED=	0.0 CM-1	CALCULATED=	1381.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	18.78	CCH7 18.78 CCH8	15.51	CCH9 15.14 H8H9 15.08					
FORCE CONSTANTS-	53.07	CC6H 42.26 HC6H	8.17	C-C					
OFF DIAGONAL-	17.75	BB40-10.51 SB24	-6.49	BB35 -5.47 BB34					
NORMAL MODE 10	OBSERVED=	0.0 CM-1	CALCULATED=	1120.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	45.63	HCH 11.40 C-C	10.51	CCH9 8.72 OCC	7.03	C-O			
FORCE CONSTANTS-	37.94	C-O 30.61 OCH	28.87	C-C 22.89 CC3H	6.16	CC6H			
OFF DIAGONAL-	-21.30	SB22-13.85 SB25	2.73	BB33 2.29 SB24	1.99	BB32 -1.76 SS20			
NORMAL MODE 11	OBSERVED=	0.0 CM-1	CALCULATED=	1195.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	37.94	C-O 28.87 C-C	17.43	OCCH5 13.19 OCCH4 11.92					
FORCE CONSTANTS-	45.63	HC3H 14.22 CC6H	11.40	C-C 8.72 CCO	7.03	C-O 5.46 HC6H			
OFF DIAGONAL-	-3.81	SB23 -3.78 SB25	-3.13	SB26 -2.95 SB22	2.16	BB44 2.11 SB21	1.90	BB40 1.53 BB45	
NORMAL MODE 12	OBSERVED=	0.0 CM-1	CALCULATED=	1048.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	20.67	HCH 16.75 CCH7	13.74	HOC 13.01 OCCH5 6.77					
FORCE CONSTANTS-	26.94	CC6H 20.67 HC3H	13.74	COH 13.43 OCH	5.99	HC6H 5.87 CC3H			
OFF DIAGONAL-	3.19	BB32 2.07 BB37	1.71	BB35 -1.56 BB38					
NORMAL MODE 13	OBSERVED=	0.0 CM-1	CALCULATED=	1022.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	33.41	CCH8 10.23 CCH7	7.78	H4CC 7.63 HCH	7.47	CCH9 6.46 H7H9			
FORCE CONSTANTS-	51.11	CC6H 11.37 CC3H	10.06	HC6H 7.63 HC3H	6.45	UCH			
OFF DIAGONAL-	4.46	BB37 -3.83 BB40	3.77	BB35					
NORMAL MODE 14	OBSERVED=	0.0 CM-1	CALCULATED=	968.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	26.53	OCCH4 22.29 HOC	16.37	OCCH5 11.16 C-C	5.19	CCH9			
FORCE CONSTANTS-	42.90	UCH 22.29 COH	11.16	C-C 10.00 CC6H	7.48	CC3H			
OFF DIAGONAL-	4.56	BB32 -3.76 BB33	-2.67	BB31 1.67 SB21					
NORMAL MODE 15	OBSERVED=	0.0 CM-1	CALCULATED=	953.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	35.98	C-O 23.30 OCCH4	9.99	H4CC					
FORCE CONSTANTS-	35.98	C-O 25.75 OCH	14.14	CC3H					
OFF DIAGONAL-	16.98	SB22 -5.34 SB21	3.79	SB25					
NORMAL MODE 16	OBSERVED=	0.0 CM-1	CALCULATED=	853.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	37.21	C-C 30.02 C-O	10.60	CCH9 8.26 OCCH4 7.24					
FORCE CONSTANTS-	37.21	C-C 30.02 C-O	15.43	CC6H 8.46 OCH	7.24	COH 5.94 CC3H			
OFF DIAGONAL-	6.64	SB25 -6.06 SB21	-5.90	SB22 -1.93 SB23	1.77	SS20			
NORMAL MODE 17	OBSERVED=	0.0 CM-1	CALCULATED=	836.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	39.39	HOC 25.52 OCCH5	15.36	H5CC 10.88 CCH7	5.34	CCH9			
FORCE CONSTANTS-	39.39	COH 30.23 OCH	17.08	CC6H 16.75 CC3H					
OFF DIAGONAL-	-7.57	BB32 2.92 SB21	-2.82	BB37 -1.98 BB33	1.61	BB35			
NORMAL MODE 18	OBSERVED=	0.0 CM-1	CALCULATED=	647.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	31.39	H4CC 24.72 H5CC	12.64	OCCH5 10.89 OCCH4	9.16	CCH8 6.44 HOC 5.82 CCH7			
FORCE CONSTANTS-	56.11	CC3H 23.53 OCH	15.18	CC6H 6.44 COH					
OFF DIAGONAL-	-5.83	BB37 4.31 BB35	-2.15	BB32 -2.12 BB33					
NORMAL MODE 19	OBSERVED=	0.0 CM-1	CALCULATED=	420.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	86.00	OCC 6.34 CCH9	5.29	H5CC					
FORCE CONSTANTS-	86.00	CCO 15.23 CC6H	8.73	CC3H					
OFF DIAGONAL-	-10.85	BB44 -3.73 BB45	2.97	SB26 -2.29 SB23	-1.77	BB37 -1.61 SB25			
NORMAL MODE 20	OBSERVED=	0.0 CM-1	CALCULATED=	241.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	96.85	T-CC							
FORCE CONSTANTS-	96.85	TC-C							
OFF DIAGONAL -	NONE								
NORMAL MODE 21	OBSERVED=	0.0 CM-1	CALCULATED=	152.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	97.15	T-CO							
FORCE CONSTANTS-	97.15	TC-O							
OFF DIAGONAL -	NONE								

0. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 0.0

TABLE LIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 301										PAGE 1	
MOLECULE 5		-6 NG= 209		ETHANOL, CD3CH2OH, GAUCHE							
NORMAL MODE 7	OBSERVED=	0.0 CM-1		CALCULATED=		1494.0 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT		
INTERNAL COORDINATES-	74.14	HCH	8.31	OCH5	7.58	OCH4					
FORCE CONSTANTS-	74.14	HC3H	15.89	OCH	7.81	CC3H					
OFF DIAGONAL-	6.00	BB40	-3.92	BB38	-1.59	SB22					
NORMAL MODE 8	OBSERVED=	0.0 CM-1		CALCULATED=		1411.1 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT		
INTERNAL COORDINATES-	34.62	OCH5	18.73	H5CC	15.87	H4CC	15.22	OCH4	12.84	HOC 6.74 C-C	
FORCE CONSTANTS-	49.84	OCH	34.61	CC3H	12.84	COH	6.74	C-C			
OFF DIAGONAL-	-8.22	SB25	-7.70	SB22	5.03	BB32	4.14	BB33	-2.61	SB21 -2.08 BB35 1.54 BB31	
NORMAL MODE 9	OBSERVED=	0.0 CM-1		CALCULATED=		1304.0 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT		
INTERNAL COORDINATES-	48.52	OCH4	23.59	HOC	18.10	H4CC	9.79	OCH5			
FORCE CONSTANTS-	58.30	OCH	23.59	COH	18.91	CC3H					
OFF DIAGONAL-	-3.93	BB33	-3.72	BB31	3.63	BB32	2.22	SB21	-1.89	SB22	
NORMAL MODE 10	OBSERVED=	0.0 CM-1		CALCULATED=		1212.6 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT		
INTERNAL COORDINATES-	45.02	HOC	22.89	H5CC	17.02	OCH5					
FORCE CONSTANTS-	45.02	COH	27.79	CC3H	19.20	OCH					
OFF DIAGONAL-	-6.61	BB32	5.63	SB21	-2.39	SB22					
NORMAL MODE 11	OBSERVED=	0.0 CM-1		CALCULATED=		1136.6 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT		
INTERNAL COORDINATES-	43.76	C-C	22.51	C-O	10.91	CCH8	9.59	H7H8	8.89	CCH7	
FORCE CONSTANTS-	43.76	C-C	23.12	CC6H	22.51	C-O	18.14	HC6H			
OFF DIAGONAL-	-15.65	SB24	7.55	BB40	-3.72	SB21	-2.61	BB35	2.54	SB25 2.37 SB22 -2.22 BB34 -1.67 SS20	
NORMAL MODE 12	OBSERVED=	0.0 CM-1		CALCULATED=		1068.6 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT		
INTERNAL COORDINATES-	31.63	C-O	20.83	CCH9	17.35	H7H9	13.67	H8H9	6.40	H7H8	
FORCE CONSTANTS-	37.43	HC6H	31.63	C-O	22.16	CC6H					
OFF DIAGONAL-	7.15	BB40	-4.88	SB21	-3.86	SB24	-3.26	SB23			
NORMAL MODE 13	OBSERVED=	0.0 CM-1		CALCULATED=		1040.7 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT		
INTERNAL COORDINATES-	43.50	H8H9	35.14	H7H9							
FORCE CONSTANTS-	78.78	HC6H	9.01	CC6H							
OFF DIAGONAL-	5.11	BB34	5.01	BB40							
NORMAL MODE 14	OBSERVED=	0.0 CM-1		CALCULATED=		1014.0 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT		
INTERNAL COORDINATES-	53.87	H7H8	32.26	C-O							
FORCE CONSTANTS-	60.34	HC6H	32.26	C-O	6.14	CC6H					
OFF DIAGONAL-	-4.11	SB23	-3.10	SB21	2.99	BB34	2.30	BB40			
NORMAL MODE 15	OBSERVED=	0.0 CM-1		CALCULATED=		958.5 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT		
INTERNAL COORDINATES-	17.24	CCH8	16.46	H4CC	13.24	OCH4	11.33	OCH5	9.63	H5CC 8.28 C-C 8.26 H7H9	
FORCE CONSTANTS-	26.09	CC3H	24.57	OCH	17.77	CC6H	8.53	HC6H	8.28	C-C	
OFF DIAGONAL-	3.82	BB37	2.71	SB24	-2.21	BB33	1.98	BB35	1.88	BB44 -1.77 SB26	
NORMAL MODE 16	OBSERVED=	0.0 CM-1		CALCULATED=		923.3 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT		
INTERNAL COORDINATES-	27.91	C-C	17.31	CCH7	9.64	OCC	9.44	HOC	7.51	OCH5 7.20 H8H9	
FORCE CONSTANTS-	27.91	C-C	19.50	CC6H	9.68	OCH	9.64	CCO	9.44	COH 8.63 HC6H 6.80 CC3H	
OFF DIAGONAL-	6.99	SB24	-5.15	SB26	4.63	BB44	-2.01	BB32	-1.86	SB23 1.68 SB25 -1.56 SB21 1.52 BB37	
NORMAL MODE 17	OBSERVED=	0.0 CM-1		CALCULATED=		743.2 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT		
INTERNAL COORDINATES-	43.09	CCH9	18.43	C-O	12.66	C-C	6.03	H7H8			
FORCE CONSTANTS-	50.50	CC6H	18.43	C-O	12.66	C-C	6.04	HC6H			
OFF DIAGONAL-	-3.73	SB22	2.82	SB24	2.68	SB23	2.64	BB35	-1.83	BB40	
NORMAL MODE 18	OBSERVED=	0.0 CM-1		CALCULATED=		660.3 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT		
INTERNAL COORDINATES-	34.70	CCH8	33.45	CCH7	10.92	H4CC	10.71	H5CC			
FORCE CONSTANTS-	68.16	CC6H	21.62	CC3H	8.44	HC6H	7.08	OCH			
OFF DIAGONAL-	-7.72	BB37	5.49	BB35	-4.51	BB40					
NORMAL MODE 19	OBSERVED=	0.0 CM-1		CALCULATED=		387.7 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT		
INTERNAL COORDINATES-	78.83	OCC	11.26	CCH9	8.08	CCH8	7.51	CCH7			
FORCE CONSTANTS-	78.83	CCO	26.85	CC6H	7.48	CC3H					
OFF DIAGONAL-	-13.76	BB44	-4.76	BB45	3.29	SB26	-3.06	SB23	-2.17	BB37 -1.74 SB25 -1.73 BB40	
NORMAL MODE 20	OBSERVED=	0.0 CM-1		CALCULATED=		215.6 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT		
INTERNAL COORDINATES-	76.84	T-CO	21.19	T-CC							
FORCE CONSTANTS-	76.84	TC-O	21.19	TC-C							
OFF DIAGONAL -	NONE										
NORMAL MODE 21	OBSERVED=	0.0 CM-1		CALCULATED=		181.5 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT		
INTERNAL COORDINATES-	78.01	T-CC	20.73	T-CO							
FORCE CONSTANTS-	78.01	TC-C	20.73	TC-O							
OFF DIAGONAL -	NONE										

0. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 0.0

TABLE LIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 301										PAGE 1	
MOLECULE 6		-6 NG= 209		ETHANOL, CD3CH2OD, GAUCHE							
NORMAL MODE 7	OBSERVED=	0.0 CM-1		CALCULATED=		1493.6 CM-1		ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	74.49	HCH	7.45 OCH5	7.40		UCH4					
FORCE CONSTANTS-	74.49	HC3H	14.85 OCH	8.42		CC3H					
OFF DIAGONAL-	6.25	BB40	-3.80 BB38								
NORMAL MODE 8	OBSERVED=	0.0 CM-1		CALCULATED=		1393.8 CM-1		ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	32.99	UCH5	26.39 UCH4	20.63		H5CC 20.47 H4CC 7.50		C-C			
FORCE CONSTANTS-	59.38	UCH	41.10 CC3H	7.50		C-C					
OFF DIAGONAL-	-10.39	SB22	-9.46 SB25	5.32		BB33 -2.47 BB35					
NORMAL MODE 9	OBSERVED=	0.0 CM-1		CALCULATED=		1277.3 CM-1		ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	39.72	UCH4	32.42 UCH5	16.80		H4CC 12.07 H5CC					
FORCE CONSTANTS-	72.15	UCH	28.86 CC3H								
OFF DIAGONAL-	-6.47	BB33	1.78 BB32	1.73		BB35					
NORMAL MODE 10	OBSERVED=	0.0 CM-1		CALCULATED=		1137.5 CM-1		ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	41.95	C-C	26.13 C-O	10.95		CC7H 10.21 CC8H 10.05		H7H8			
FORCE CONSTANTS-	41.95	C-C	26.13 C-O	23.51		CC6H 18.04 HC6H					
OFF DIAGONAL-	-15.18	SB24	7.50 BB40	-2.53		BB35 -2.17 BB34 -1.76		SS20 1.76	SB22		
NORMAL MODE 11	OBSERVED=	0.0 CM-1		CALCULATED=		1077.3 CM-1		ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	28.80	C-O	21.75 CC9H	14.71		H8H9 8.61 H7H9 8.11		C-C			
FORCE CONSTANTS-	28.80	C-O	27.00 HC6H	23.29		CC6H 8.11 C-C					
OFF DIAGONAL-	6.20	BB40	-5.13 SB23	-4.52		SB24 3.71 SB21 -1.75		SB26			
NORMAL MODE 12	OBSERVED=	0.0 CM-1		CALCULATED=		1049.1 CM-1		ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	34.66	H7H9	11.34 HOC	10.47		CC7H 8.00 H5CC 7.22		H8H9			
FORCE CONSTANTS-	43.54	HC6H	16.45 CC6H	12.26		CC3H 11.34 COH					
OFF DIAGONAL-	5.08	BB40	2.75 BB37	2.59		BB34 -2.08 SB21					
NORMAL MODE 13	OBSERVED=	0.0 CM-1		CALCULATED=		1027.9 CM-1		ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	40.65	H8H9	16.77 HOC	10.32		H5CC 9.32 H7H9					
FORCE CONSTANTS-	53.96	HC6H	16.77 COH	14.37		CC3H 5.18 OCH					
OFF DIAGONAL-	3.39	BB34									
NORMAL MODE 14	OBSERVED=	0.0 CM-1		CALCULATED=		1013.3 CM-1		ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	50.83	H7H8	32.77 C-O	5.21		H7H9					
FORCE CONSTANTS-	56.81	HC6H	32.77 C-O	6.92		CC6H					
OFF DIAGONAL-	-4.14	SB21	-3.68 SB23	2.67		BB34 2.47 BB40					
NORMAL MODE 15	OBSERVED=	0.0 CM-1		CALCULATED=		950.7 CM-1		ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	23.95	C-C	18.32 CC8H	11.00		OCC 8.80 H7H9 7.85		H4CC 5.92	UCH4		
FORCE CONSTANTS-	23.95	C-C	20.54 CC6H	11.00		CCO 10.28 HC6H 9.68		CC3H 9.05	UCH		
OFF DIAGONAL-	7.17	SB24	5.19 BB44	-5.09		SB26 2.71 SB25 2.04		BB37 1.51	BB40		
NORMAL MODE 16	OBSERVED=	0.0 CM-1		CALCULATED=		834.4 CM-1		ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	60.07	HOC	13.69 C-C	8.99		CC7H 8.25 UCH5					
FORCE CONSTANTS-	60.07	COH	13.69 C-C	11.78		UCH 10.01 CC6H					
OFF DIAGONAL-	-6.39	SB21	-5.32 BB32	2.87		SB24 1.60 BB31					
NORMAL MODE 17	OBSERVED=	0.0 CM-1		CALCULATED=		737.3 CM-1		ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	43.09	CC9H	16.43 C-O	9.32		C-C 7.17 CC7H 5.69		H7H8			
FORCE CONSTANTS-	52.60	CC6H	16.43 C-O	9.32		C-C 5.80 HC6H					
OFF DIAGONAL-	-3.85	SB22	2.87 BB35	2.64		SB21 2.35 SB23 -2.20		BB40 2.10	SB24		
NORMAL MODE 18	OBSERVED=	0.0 CM-1		CALCULATED=		658.8 CM-1		ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	35.22	CC8H	30.95 CC7H	11.58		H4CC 10.67 H5CC					
FORCE CONSTANTS-	66.28	CC6H	22.25 CC3H	8.24		HC6H 7.96 OCH					
OFF DIAGONAL-	-7.72	BB37	5.41 BB35	-4.40		BB40					
NORMAL MODE 19	OBSERVED=	0.0 CM-1		CALCULATED=		381.7 CM-1		ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	79.06	OCC	10.74 CC9H	7.78		CC8H 7.26 CC7H					
FORCE CONSTANTS-	79.06	CCO	25.79 CC6H	7.29		CC3H					
OFF DIAGONAL-	-13.53	BB44	-4.66 BB45	3.18		SB26 -3.07 SB23 -2.11		BB37 -1.67	BB40 -1.66	SB25	
NORMAL MODE 20	OBSERVED=	0.0 CM-1		CALCULATED=		193.3 CM-1		ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	85.63	T-CC	13.27 T-CO								
FORCE CONSTANTS-	85.63	TC-C	13.27 TC-O								
OFF DIAGONAL -	NONE										
NORMAL MODE 21	OBSERVED=	0.0 CM-1		CALCULATED=		148.3 CM-1		ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	84.64	T-CO	13.46 T-CC								
FORCE CONSTANTS-	84.64	TC-O	13.46 TC-C								
OFF DIAGONAL -	NONE										

0. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 0.0

TABLE LIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 301
MOLECULE 7 -6 NC= 209 ETHANOL, CD3CD2OH, GAUCHE

PAGE 1

NORMAL MODE 7	OBSERVED=	0.0 CM-1	CALCULATED=	1274.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	79.39	HOC 7.86 OCH5	6.88	C-C				
FORCE CONSTANTS-	79.39	COH 8.00 OCH	6.88	C-C				
OFF DIAGONAL-	5.97	BB32 -5.15 SB21	-2.57	SR25 -1.98 SB22				
NORMAL MODE 8	OBSERVED=	0.0 CM-1	CALCULATED=	1191.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	36.77	C-C 36.05 C-O	14.21 OCH4	7.33 OCH5 7.33	H5CC 6.80 H4CC	5.95 CCH7	5.45	HOC
FORCE CONSTANTS-	36.77	C-C 36.05 C-O	21.55 OCH	14.13 CC3H	10.42 CC6H	5.45 COH	5.38	HC6H
OFF DIAGONAL-	-17.23	SB22-12.28 SB25	-7.66 SB24	5.76 SB21	2.43 BB37	2.01 BB40	-1.93	SS20 1.84 BB33 -1.51 BB32
NORMAL MODE 9	OBSERVED=	0.0 CM-1	CALCULATED=	1105.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	56.27	HCH 10.50 C-C	9.26 C-O	7.66 CCH9	6.92 OCH5			
FORCE CONSTANTS-	56.27	HC6H 10.88 OCH	12.82 CC3H	10.87 HC3H	5.71 C-O			
OFF DIAGONAL-	-6.23	SB22 5.69 BB40	-3.48 SB25	-3.00 SB24	-2.80 BB38	-2.65 SB23	-1.81	SB26 -1.60 SB21
NORMAL MODE 10	OBSERVED=	0.0 CM-1	CALCULATED=	1070.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	17.35	CC9H 13.89 H8H9	11.55 H7H9	10.87 HCH	8.98 CCH8	7.61 CCH7	6.45	H5CC 6.38 H4CC 5.71 C-O
FORCE CONSTANTS-	33.94	CC6H 28.41 HC6H	12.82 CC3H	10.87 HC3H	5.71 C-O			
OFF DIAGONAL-	14.26	BB40 -5.84 SB24	-4.73 BB35	3.89 SB25	-3.24 BB34	-2.93 BB37	-2.28	SB22
NORMAL MODE 11	OBSERVED=	0.0 CM-1	CALCULATED=	1040.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	44.14	H7H9 36.29 H8H9						
FORCE CONSTANTS-	80.94	HC6H 7.09 CC6H						
OFF DIAGONAL-	5.26	BB34 4.51 BB40						
NORMAL MODE 12	OBSERVED=	0.0 CM-1	CALCULATED=	1032.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	57.79	H7H8 11.64 H8H9	5.86	UCH4				
FORCE CONSTANTS-	73.37	HC6H 9.78 OCH						
OFF DIAGONAL-	4.45	BB34 2.63 BB40						
NORMAL MODE 13	OBSERVED=	0.0 CM-1	CALCULATED=	961.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	42.40	C-O 24.10 OCH4	6.99 HOC	5.04 OCC	5.01 H7H8			
FORCE CONSTANTS-	42.40	C-O 27.38 OCH	7.39 HC6H	6.99 COH	5.04 CCO			
OFF DIAGONAL-	19.39	SB22 -7.12 SB23	-7.07 SB21	-1.61 SB25	1.61 BB33			
NORMAL MODE 14	OBSERVED=	0.0 CM-1	CALCULATED=	916.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	28.64	UCH5 25.54 H5CC	15.42 H4CC	14.90 OCH4				
FORCE CONSTANTS-	43.54	UCH 40.96 CC3H	8.94 CC6H					
OFF DIAGONAL-	3.84	BB37 -3.73 BB33	2.95 BB35	-2.03 BB32				
NORMAL MODE 15	OBSERVED=	0.0 CM-1	CALCULATED=	888.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	26.52	C-C 14.07 CCH8	9.23 H4CC	8.10 OCC				
FORCE CONSTANTS-	26.52	C-C 21.42 CC6H	11.20 CC3H	8.10 CCO	5.72 HC6H			
OFF DIAGONAL-	8.71	SB25 5.87 SB24	-4.60 SR26	4.54 BB44	2.86 BB37	1.80 BB40		
NORMAL MODE 16	OBSERVED=	0.0 CM-1	CALCULATED=	846.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	24.31	UCH5 21.33 CCH7	19.71 OCH4	11.59 CCH8	6.39 HOC			
FORCE CONSTANTS-	44.02	UCH 32.98 CC6H	7.36 CC3H	6.60 HC6H	6.39 COH			
OFF DIAGONAL-	-3.95	BB33 3.12 BB37	-2.98 BB32	-2.60 BB40	2.41 BB35			
NORMAL MODE 17	OBSERVED=	0.0 CM-1	CALCULATED=	734.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	40.17	CCH9 16.09 C-C	15.49 C-O	6.04 H7H8				
FORCE CONSTANTS-	45.99	CC6H 16.09 C-C	15.49 C-O	6.07 HC6H				
OFF DIAGONAL-	-5.39	SB22 3.46 SB24	2.38 SB25	2.32 SB23	2.21 BB35	1.52 SB26		
NORMAL MODE 18	OBSERVED=	0.0 CM-1	CALCULATED=	585.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	23.30	CCH8 22.12 H4CC	21.26 CCH7	21.09 H5CC	6.13 OCH5	5.76 OCH4		
FORCE CONSTANTS-	44.58	CC6H 43.21 CC3H	11.90 OCH	5.39 HC6H				
OFF DIAGONAL-	-8.83	BB37 5.35 BB35	-2.92 BB40					
NORMAL MODE 19	OBSERVED=	0.0 CM-1	CALCULATED=	383.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	79.37	OCC 11.32 CCH9	7.70 CCH8	7.61 CCH7				
FORCE CONSTANTS-	79.37	CCO 26.63 CC6H	8.64 CC3H					
OFF DIAGONAL-	-13.68	BB44 -4.79 BB45	-3.29 SB23	2.93 SB26	-2.31 BB37	-1.67 BB40	-1.66	SB25
NORMAL MODE 20	OBSERVED=	0.0 CM-1	CALCULATED=	211.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	85.86	T-CO 12.27 T-CC						
FORCE CONSTANTS-	85.86	TC-O 12.27 TC-C						
OFF DIAGONAL-	NONE							
NORMAL MODE 21	OBSERVED=	0.0 CM-1	CALCULATED=	177.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	86.22	T-CC 12.01 T-CO						
FORCE CONSTANTS-	86.22	TC-C 12.01 TC-O						
OFF DIAGONAL-	NONE							

0. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 0.0

TABLE LIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 301
MOLECULE 8 -6 NG= 209 ETHANOL, CD3CD2OD, GAUCHE

PAGE 1

NORMAL MODE 7	OBSERVED=	0.0 CM-1	CALCULATED=	1204.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	45.28	C-C 33.48 C-O 15.06 OCH5 11.38 OCH4 9.78 H4CC 9.23 H5CC						
FORCE CONSTANTS-	45.28	C-C 33.48 C-O 26.44 OCH 19.01 CC3H 7.77 CC6H						
OFF DIAGONAL-	-18.59	S822-15.81 SB25 -7.85 SB24 -4.52 SB21 2.44 BB37 2.36 BB33 2.32 BB40 -2.07 SS20 1.76 BB32						
NORMAL MODE 8	OBSERVED=	0.0 CM-1	CALCULATED=	1111.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	56.71	HCH 12.33 C-O 6.24 C-C 5.90 OCH4 5.89 CCH9						
FORCE CONSTANTS-	56.71	HC3H 12.33 C-O 8.86 OCH 6.67 CC6H 6.24 C-C						
OFF DIAGONAL-	-6.45	SB22 5.03 BB40 -3.81 SB23 -2.77 SB25 -2.52 BB38 -1.74 SB26 1.73 SB21						
NORMAL MODE 9	OBSERVED=	0.0 CM-1	CALCULATED=	1076.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	17.02	CCH9 16.35 H7H9 12.34 CCH7 10.75 H8H9 8.52 CCH8 6.96 C-C 5.39 OCH5						
FORCE CONSTANTS-	37.89	HC6H 31.49 HC6H 8.49 CC3H 6.96 C-C 6.62 OCH						
OFF DIAGONAL-	13.80	BB40 -8.12 SB24 -5.02 BB35 4.14 SB25 -3.72 BB34 -3.13 SB22 -2.66 BB37 -1.68 SB21						
NORMAL MODE 10	OBSERVED=	0.0 CM-1	CALCULATED=	1044.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	43.40	H8H9 19.22 H7H9						
FORCE CONSTANTS-	65.47	HC6H 8.59 CC6H 5.34 OCH						
OFF DIAGONAL-	4.77	BB40 4.24 BB34						
NORMAL MODE 11	OBSERVED=	0.0 CM-1	CALCULATED=	1036.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	40.77	H7H8 25.90 H7H9 7.71 HCH 5.95 OCH5						
FORCE CONSTANTS-	66.67	HC6H 9.87 OCH 7.71 HC3H 5.14 CC6H						
OFF DIAGONAL-	4.21	BB34 3.06 BB40						
NORMAL MODE 12	OBSERVED=	0.0 CM-1	CALCULATED=	1005.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	23.86	HOC 15.48 H7H8 12.83 C-O 10.77 OCH5 10.55 H8H9						
FORCE CONSTANTS-	26.43	HC6H 23.86 COH 14.56 OCH 12.83 C-O						
OFF DIAGONAL-	7.19	SB21 3.83 BB32 -3.65 SB23 2.12 SB22 1.60 BB34						
NORMAL MODE 13	OBSERVED=	0.0 CM-1	CALCULATED=	954.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	41.81	OC4 30.24 C-O 14.82 HOC 7.06 H4CC						
FORCE CONSTANTS-	42.11	OC4 30.24 C-O 14.82 COH 7.40 CC3H						
OFF DIAGONAL-	14.41	SB22 -8.70 SB21 -3.87 SB23 -2.73 BB31						
NORMAL MODE 14	OBSERVED=	0.0 CM-1	CALCULATED=	909.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	33.40	H5CC 15.77 OCH5 11.62 CCH7 11.10 H4CC 6.76 HOC						
FORCE CONSTANTS-	44.51	CC3H 19.15 OCH 15.90 CC6H 6.76 COH						
OFF DIAGONAL-	5.32	BB37 3.25 BB35 -2.47 BB32 -2.02 SB21 1.79 SB22						
NORMAL MODE 15	OBSERVED=	0.0 CM-1	CALCULATED=	886.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	23.53	C-C 20.37 CCH8 13.24 H4CC 6.69 OCC 5.60 H7H9						
FORCE CONSTANTS-	23.60	CC6H 23.53 C-C 13.30 CC3H 6.69 CCO 6.11 HC6H						
OFF DIAGONAL-	7.20	SB25 5.19 SB24 -3.93 SB26 3.80 BB44 3.34 BB37						
NORMAL MODE 16	OBSERVED=	0.0 CM-1	CALCULATED=	794.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	36.34	HOC 15.97 OCH5 14.68 CCH7 13.91 OCH4 9.18 C-C 7.03 CCH8						
FORCE CONSTANTS-	36.34	COH 29.88 OCH 22.58 CC6H 9.18 C-C						
OFF DIAGONAL-	-5.75	BB32 -4.51 SB21 -2.69 BB33 2.47 BB31 1.87 SB24						
NORMAL MODE 17	OBSERVED=	0.0 CM-1	CALCULATED=	728.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	39.58	CCH9 13.26 C-O 11.53 C-C 7.94 CCH7 5.75 OCH5 5.56 H7H8						
FORCE CONSTANTS-	48.44	CC6H 13.26 C-O 11.53 C-C 6.41 OCH 5.79 HC6H						
OFF DIAGONAL-	-5.18	SB22 2.93 SB21 2.49 SB24 2.49 BB35 2.22 SB25 1.93 SB23 -1.93 BB40						
NORMAL MODE 18	OBSERVED=	0.0 CM-1	CALCULATED=	581.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	23.41	CCH8 22.94 H4CC 20.03 H5CC 18.42 CCH7 7.30 OCH5 6.32 OCH4						
FORCE CONSTANTS-	42.97	CC3H 42.01 CC6H 13.63 OCH 5.09 HC6H						
OFF DIAGONAL-	-8.53	BB37 5.17 BB35 -2.75 BB40						
NORMAL MODE 19	OBSERVED=	0.0 CM-1	CALCULATED=	377.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	79.53	OCC 10.78 CCH9 7.52 CCH7 7.24 CCH8						
FORCE CONSTANTS-	79.53	CCO 25.55 CC6H 8.43 CC3H						
OFF DIAGONAL-	-13.45	BB44 -4.68 BB45 -3.29 SB23 2.82 SB26 -2.24 BB37 -1.61 BB40 -1.57 SB25						
NORMAL MODE 20	OBSERVED=	0.0 CM-1	CALCULATED=	185.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	86.12	T-CC 12.48 T-CO						
FORCE CONSTANTS-	86.12	TC-C 12.48 TC-O						
OFF DIAGONAL-	NONE							
NORMAL MODE 21	OBSERVED=	0.0 CM-1	CALCULATED=	148.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	85.75	T-CO 12.40 T-CC						
FORCE CONSTANTS-	85.75	TC-O 12.40 TC-C						
OFF DIAGONAL-	NONE							

0. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 0.0

TABLE LIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 301										PAGE 1
MOLECULE 9		-6 NG= 209		ETHANOL, CH3CHDOH, GAUCHE, D4						
NORMAL MODE 7	OBSERVED=	0.0 CM-1		CALCULATED=		1458.9 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	49.87	H7H8	16.87	H8H9	7.71	H7H9	7.46	CCH9		
FORCE CONSTANTS-	74.45	HC6H	11.90	CC6H						
OFF DIAGONAL-	5.55	BB40	4.84	BB34						
NORMAL MODE 8	OBSERVED=	0.0 CM-1		CALCULATED=		1455.4 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	42.96	H7H9	33.90	H8H9	5.77	CCH8				
FORCE CONSTANTS-	77.40	HC6H	10.37	CC6H						
OFF DIAGONAL-	5.32	BB40	5.03	BB34						
NORMAL MODE 9	OBSERVED=	0.0 CM-1		CALCULATED=		1389.4 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	43.16	OC H5	14.60	HOC	12.83	H5CC	9.53	C-C	7.22 H7H9 5.19 CCH7	
FORCE CONSTANTS-	44.23	OC H	14.60	COH	14.05	CC3H	12.16	CC6H	11.17 HC6H 9.53 C-C	
OFF DIAGONAL-	5.99	BB32	-5.51	SB25	-5.42	SB22	-5.41	SB24	2.92 BB40 -2.53 SB21 2.08 BB37 -1.94 BB35	
NORMAL MODE 10	OBSERVED=	0.0 CM-1		CALCULATED=		1379.7 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	14.52	CCH8	13.77	CCH7	12.60	H8H9	12.57	CCH9	12.14 OC H5 11.41 H7H8 8.66 H7H9 6.92 HOC	
FORCE CONSTANTS-	40.85	CC6H	32.67	HC6H	12.21	OC H	6.92	COH		
OFF DIAGONAL-	13.48	BB40	-5.08	BB35	-4.62	SB24	-4.21	BB34	2.19 BB32 -1.54 BB37	
NORMAL MODE 11	OBSERVED=	0.0 CM-1		CALCULATED=		1325.9 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	65.61	HCH	20.83	H5CC						
FORCE CONSTANTS-	65.61	HC3H	23.20	CC3H						
OFF DIAGONAL-	8.67	BB40	-4.09	SB25						
NORMAL MODE 12	OBSERVED=	0.0 CM-1		CALCULATED=		1234.9 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	53.65	HOC	12.12	H5CC	9.06	OC H5	8.13	C-O	5.58 OC H4 5.10 CCH9	
FORCE CONSTANTS-	53.65	COH	14.63	OC H	12.29	CC3H	8.13	C-O	6.90 CC6H 5.17 HC6H	
OFF DIAGONAL-	8.58	SB21	-6.78	SB22	-5.26	BB32	-2.16	SB23	-1.90 BB31 -1.87 BB40	
NORMAL MODE 13	OBSERVED=	0.0 CM-1		CALCULATED=		1125.2 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	43.13	C-O	21.48	C-C	10.41	H4CC	10.10	OC H4	8.15 HOC 5.56 CCH9	
FORCE CONSTANTS-	43.13	C-O	21.48	C-C	13.88	CC3H	13.21	OC H	10.03 CC6H 8.15 COH	
OFF DIAGONAL-	-7.71	SB21	-4.11	SB22	-2.41	SB25	-1.62	SS20	1.55 BB37 -1.51 SB23	
NORMAL MODE 14	OBSERVED=	0.0 CM-1		CALCULATED=		1037.2 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	30.83	C-C	22.26	CCH9	11.91	HOC	9.67	CCH7	8.65 OCC 5.61 OC H4 5.07 H7H8	
FORCE CONSTANTS-	34.01	CC6H	30.83	C-C	11.91	COH	8.65	CCO	7.85 OC H 7.53 HC6H	
OFF DIAGONAL-	-5.12	SB26	3.71	BB44	-3.03	BB40	2.54	SB22	2.22 BB45 2.14 BB35 -2.13 SB23 -2.11 SB21 -1.94 SB25	
NORMAL MODE 15	OBSERVED=	0.0 CM-1		CALCULATED=		1011.3 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	32.48	CCH8	20.54	CCH7	8.51	H4CC	6.51	C-O	6.23 H7H9 5.03 HOC	
FORCE CONSTANTS-	54.16	CC6H	10.59	HC6H	8.82	CC3H	6.51	C-O	5.03 COH	
OFF DIAGONAL-	-4.00	BB40	3.85	BB37	3.51	BB35	-2.35	SB21	1.99 SB25	
NORMAL MODE 16	OBSERVED=	0.0 CM-1		CALCULATED=		935.8 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	50.90	OC H4	16.31	C-O	10.46	H4CC	6.35	OC H5		
FORCE CONSTANTS-	57.25	OC H	16.31	C-O	10.49	CC3H	7.12	CC6H		
OFF DIAGONAL-	8.25	SB22	-3.24	BB33						
NORMAL MODE 17	OBSERVED=	0.0 CM-1		CALCULATED=		864.2 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	35.31	C-O	32.72	C-C	16.96	CCH9	8.59	OC H4	5.05 CCH7	
FORCE CONSTANTS-	35.31	C-O	32.72	C-C	23.98	CC6H	8.59	OC H		
OFF DIAGONAL-	-7.76	SB22	5.10	SB25	-3.25	SB21	-2.55	SB23	1.80 SS20 -1.80 BB40 -1.58 SB26	
NORMAL MODE 18	OBSERVED=	0.0 CM-1		CALCULATED=		701.3 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	35.35	H4CC	19.78	H5CC	10.59	CCH8	10.54	OC H5	9.99 OC H4 9.79 CCH7	
FORCE CONSTANTS-	55.13	CC3H	20.53	OC H	20.42	CC6H				
OFF DIAGONAL-	-6.69	BB37	4.46	BB35	-1.85	BB33				
NORMAL MODE 19	OBSERVED=	0.0 CM-1		CALCULATED=		431.4 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	86.73	OCC	6.73	CCH9	5.01	H4CC				
FORCE CONSTANTS-	86.73	CCO	16.06	CC6H	8.47	CC3H				
OFF DIAGONAL-	-11.16	BB44	-3.86	BB45	3.38	SB26	-2.06	SB23	-1.81 SB25 -1.79 BB37	
NORMAL MODE 20	OBSERVED=	0.0 CM-1		CALCULATED=		247.0 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	91.23	T-CC	7.54	T-CO						
FORCE CONSTANTS-	91.23	TC-C	7.54	TC-O						
OFF DIAGONAL -	NONE									
NORMAL MODE 21	OBSERVED=	0.0 CM-1		CALCULATED=		205.6 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	90.85	T-CO	7.41	T-CC						
FORCE CONSTANTS-	90.85	TC-O	7.41	TC-C						
OFF DIAGONAL -	NONE									

0. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 0.0

TABLE LIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 301									
MOLECULE 10		-6 NG= 209		ETHANOL, CH3CH000, GAUCHE, D4				PAGE 1	
NORMAL MODE 7	OBSERVED=	0.0 CM-1		CALCULATED=	1458.9 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	50.05	H7H8	15.60	H8H9	8.69	H7H9	7.48	CCH9	
FORCE CONSTANTS-	74.35	HC6H	11.88	CC6H					
OFF DIAGONAL-	5.53	BB40	4.83	BB34					
NORMAL MODE 8	OBSERVED=	0.0 CM-1		CALCULATED=	1455.0 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	42.34	H7H9	35.42	H8H9	5.62	CCH8			
FORCE CONSTANTS-	78.07	HC6H	10.36	CC6H					
OFF DIAGONAL-	5.35	BB40	5.07	BB34					
NORMAL MODE 9	OBSERVED=	0.0 CM-1		CALCULATED=	1383.5 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	18.14	CCH7	17.12	CCH8	15.38	H7H9	15.10	H8H9	13.75
FORCE CONSTANTS-	49.01	CC6H	39.42	HC6H	10.12	C-C			
OFF DIAGONAL-	16.18	BB40	-11.24	SB24	-6.06	BB35	-5.01	BB34	-2.28
							SB25	1.60	BB37
NORMAL MODE 10	OBSERVED=	0.0 CM-1		CALCULATED=	1354.7 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	64.12	OCH5	21.33	H5CC					
FORCE CONSTANTS-	66.36	OCH	22.63	CC3H	5.36	HC6H			
OFF DIAGONAL-	-8.25	SB22	-2.95	SB25	2.73	BB32	2.16	BB33	
NORMAL MODE 11	OBSERVED=	0.0 CM-1		CALCULATED=	1325.9 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	65.30	HCH	21.28	H5CC					
FORCE CONSTANTS-	65.30	HC3H	23.68	CC3H					
OFF DIAGONAL-	8.74	BB40	-4.15	SB25					
NORMAL MODE 12	OBSERVED=	0.0 CM-1		CALCULATED=	1134.1 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	49.17	C-O	14.42	CCH9	13.70	OCH4	8.89	C-C	6.63
FORCE CONSTANTS-	49.17	C-O	17.45	CC6H	16.48	OCH	8.89	C-C	7.56
OFF DIAGONAL-	-6.33	SB22	-5.99	SB23	-2.40	SB25	-2.14	BB40	1.87
							SB21	1.64	SB26
NORMAL MODE 13	OBSERVED=	0.0 CM-1		CALCULATED=	1092.9 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	28.10	C-C	16.50	CCH7	14.02	HOC	7.69	H4CC	7.17
FORCE CONSTANTS-	28.10	C-C	25.71	CC6H	14.86	CC3H	14.02	COH	6.45
OFF DIAGONAL-	-4.15	SB26	3.09	BB37	2.47	BB35	-2.41	BB40	1.70
							BB44		
NORMAL MODE 14	OBSERVED=	0.0 CM-1		CALCULATED=	1017.6 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	32.95	CCH8	18.79	C-C	9.54	CCH9	6.81	CCH7	6.60
FORCE CONSTANTS-	49.30	CC6H	18.79	C-C	9.81	HC6H	6.58	OCH	
OFF DIAGONAL-	-3.86	BB40	3.16	BB35	2.47	BB37	-2.21	SB26	1.99
							SB25		
NORMAL MODE 15	OBSERVED=	0.0 CM-1		CALCULATED=	958.4 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	45.20	OCH4	21.89	HOC	19.55	C-O	11.95	H4CC	
FORCE CONSTANTS-	45.84	OCH	21.89	COH	19.55	C-O	12.24	CC3H	
OFF DIAGONAL-	11.60	SB22	-8.51	SB21	-3.46	BB31			
NORMAL MODE 16	OBSERVED=	0.0 CM-1		CALCULATED=	876.6 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	33.17	HOC	20.33	CCH7	14.30	C-O	12.70	CCH9	
FORCE CONSTANTS-	33.84	CC6H	33.17	COH	14.30	C-O	5.59	CC3H	
OFF DIAGONAL-	8.95	SB21	-2.64	BB32	-2.42	BB40	2.38	BB35	-2.03
							BB37		
NORMAL MODE 17	OBSERVED=	0.0 CM-1		CALCULATED=	860.0 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	34.82	C-C	24.24	C-O	20.20	HOC	12.31	OCH4	8.07
FORCE CONSTANTS-	34.82	C-C	24.24	C-O	20.20	COH	12.93	OCH	12.28
OFF DIAGONAL-	-9.10	SB21	-5.93	SB22	4.82	SB25	1.73	BB31	1.54
							SS20		
NORMAL MODE 18	OBSERVED=	0.0 CM-1		CALCULATED=	686.3 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	33.85	H4CC	16.63	H5CC	12.12	OCH5	11.27	OCH4	9.73
FORCE CONSTANTS-	50.48	CC3H	23.39	OCH	16.58	CC6H	9.23	COH	
OFF DIAGONAL-	-5.76	BB37	3.89	BB35	-2.53	BB32	-2.11	BB33	
NORMAL MODE 19	OBSERVED=	0.0 CM-1		CALCULATED=	423.7 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	86.05	OCC	6.39	CCH9					
FORCE CONSTANTS-	86.05	CCO	15.37	CC6H	8.01	CC3H			
OFF DIAGONAL-	-10.91	BB44	-3.75	BB45	3.19	SB26	-2.09	SB23	-1.71
							BB37	-1.67	SB25
NORMAL MODE 20	OBSERVED=	0.0 CM-1		CALCULATED=	244.5 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	96.92	T-CC							
FORCE CONSTANTS-	96.92	TC-C							
OFF DIAGONAL-	NONE								
NORMAL MODE 21	OBSERVED=	0.0 CM-1		CALCULATED=	153.1 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	96.83	T-CO							
FORCE CONSTANTS-	96.83	TC-O							
OFF DIAGONAL-	NONE								

O. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 0.0

TABLE LIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 301										PAGE 1						
MOLECULE 11		-6 NG= 209		ETHANOL, CD3CHDOH, GAUCHE, D4												
NORMAL MODE 7	OBSERVED=	0.0 CM-1		CALCULATED=		1387.8 CM-1		ERROR=	0.0 CM-1	OR	0.0 PERCENT					
INTERNAL COORDINATES-	56.80	OCH5	21.64	HOC	14.78	H5CC										
FORCE CONSTANTS-	57.92	OCH	21.64	COH	16.09	CC3H										
OFF DIAGONAL-	8.37	BB32	-6.19	SB22	-3.98	SB25	-3.11	SB21								
NORMAL MODE 8	OBSERVED=	0.0 CM-1		CALCULATED=		1325.6 CM-1		ERROR=	0.0 CM-1	OR	0.0 PERCENT					
INTERNAL COORDINATES-	66.46	HCH	20.30	H5CC												
FORCE CONSTANTS-	66.46	HC3H	22.89	CC3H												
OFF DIAGONAL-	8.79	BB40	-4.28	SB25												
NORMAL MODE 9	OBSERVED=	0.0 CM-1		CALCULATED=		1228.8 CM-1		ERROR=	0.0 CM-1	OR	0.0 PERCENT					
INTERNAL COORDINATES-	56.49	HOC	12.58	H5CC	10.65	C-O	9.96	OCH5	6.89	OCH4						
FORCE CONSTANTS-	56.49	COH	16.85	OCH	13.05	CC3H	10.65	C-O								
OFF DIAGONAL-	10.08	SB21	-8.36	SB22	-5.66	BB32	-2.55	SB25	-2.17	BB31	-2.01	SB23				
NORMAL MODE 10	OBSERVED=	0.0 CM-1		CALCULATED=		1146.7 CM-1		ERROR=	0.0 CM-1	OR	0.0 PERCENT					
INTERNAL COORDINATES-	42.22	C-C	21.71	C-O	9.24	CC8H	7.57	HOC	6.96	H7H8	5.65	CCH7				
FORCE CONSTANTS-	42.22	C-C	21.71	C-O	17.13	CC6H	13.29	HC6H	8.33	OCH	7.69	CC3H	7.57	COH		
OFF DIAGONAL-	-13.10	SB24	5.45	BB40	-5.27	SB21	-1.61	BB34	-1.61	SS20						
NORMAL MODE 11	OBSERVED=	0.0 CM-1		CALCULATED=		1067.7 CM-1		ERROR=	0.0 CM-1	OR	0.0 PERCENT					
INTERNAL COORDINATES-	25.14	C-O	21.97	CCH9	21.38	H8H9	13.72	H7H9	5.71	HOC						
FORCE CONSTANTS-	37.77	HC6H	25.93	CC6H	25.14	C-O	5.71	COH								
OFF DIAGONAL-	8.67	BB40	-4.92	SB21	-4.73	SB24	-1.80	BB35	-1.71	SB23	-1.68	SB22				
NORMAL MODE 12	OBSERVED=	0.0 CM-1		CALCULATED=		1040.9 CM-1		ERROR=	0.0 CM-1	OR	0.0 PERCENT					
INTERNAL COORDINATES-	45.04	H7H9	33.72	H8H9	5.01	CC8H										
FORCE CONSTANTS-	80.62	HC6H	7.32	CC6H												
OFF DIAGONAL-	5.22	BB34	4.56	BB40												
NORMAL MODE 13	OBSERVED=	0.0 CM-1		CALCULATED=		1023.7 CM-1		ERRDR=	0.0 CM-1	OR	0.0 PERCENT					
INTERNAL COORDINATES-	55.60	H7H8	11.59	C-O	8.95	OCH4	7.43	CCH7	6.27	H8H9	5.76	H4CC				
FORCE CONSTANTS-	62.11	HC6H	11.59	C-O	10.18	CC6H	9.12	OCH	5.95	CC3H						
OFF DIAGONAL-	4.25	BB40	-3.88	SB22	2.75	BB34										
NORMAL MODE 14	OBSERVED=	0.0 CM-1		CALCULATED=		964.3 CM-1		ERROR=	0.0 CM-1	OR	0.0 PERCENT					
INTERNAL COORDINATES-	26.08	OCH4	25.46	C-O	13.13	H4CC	7.97	C-C	7.92	OCC	5.78	HOC				
FORCE CONSTANTS-	26.10	OCH	25.46	C-O	14.75	CC3H	7.97	C-C	7.96	HC6H	7.92	CCO	5.78	COH	5.60	CC6H
OFF DIAGONAL-	11.15	SB22	-6.91	SB23	-4.99	SB21	-2.53	SB25	-2.49	SB26	2.03	BB44				
NORMAL MODE 15	OBSERVED=	0.0 CM-1		CALCULATED=		900.8 CM-1		ERRDR=	0.0 CM-1	OR	0.0 PERCENT					
INTERNAL COORDINATES-	25.26	C-C	14.51	OCH4	8.47	CC8H	7.50	H4CC	7.01	OCC	6.09	CCH7				
FORCE CONSTANTS-	25.26	C-C	18.03	OCH	16.21	CC6H	7.75	CC3H	7.01	CCO	5.61	HC6H				
OFF DIAGONAL-	6.20	SB25	6.00	SB24	-4.17	SB26	3.95	BB44	1.85	BB37						
NORMAL MODE 16	OBSERVED=	0.0 CM-1		CALCULATED=		873.8 CM-1		ERROR=	0.0 CM-1	OR	0.0 PERCENT					
INTERNAL COORDINATES-	20.09	CC8H	18.62	OCH4	13.23	H4CC	12.24	CCH7	10.13	OCH5	6.16	H5CC				
FORCE CONSTANTS-	32.75	CC6H	28.75	OCH	19.39	CC3H	6.51	HC6H								
OFF DIAGONAL-	5.03	BB37	3.09	BB35	-2.48	BB33	-2.40	BB40								
NORMAL MODE 17	OBSERVED=	0.0 CM-1		CALCULATED=		739.3 CM-1		ERROR=	0.0 CM-1	OR	0.0 PERCENT					
INTERNAL COORDINATES-	41.48	CCH9	17.01	C-O	14.26	C-C	6.01	H7H8	5.66	CCH7						
FORCE CONSTANTS-	48.66	CC6H	17.01	C-O	14.26	C-C	6.07	HC6H								
OFF DIAGONAL-	-4.62	SB22	3.12	SB24	2.50	SB23	2.47	BB35	-1.68	BB40						
NORMAL MODE 18	OBSERVED=	0.0 CM-1		CALCULATED=		614.8 CM-1		ERROR=	0.0 CM-1	OR	0.0 PERCENT					
INTERNAL COORDINATES-	26.44	CCH7	25.33	CC8H	21.56	H4CC	13.38	H5CC	5.47	OCH5	5.13	OCH4				
FORCE CONSTANTS-	51.81	CC6H	34.94	CC3H	10.60	OCH	6.30	HC6H								
OFF DIAGONAL-	-8.49	BB37	5.23	BB35	-3.21	BB40										
NORMAL MODE 19	OBSERVED=	0.0 CM-1		CALCULATED=		385.8 CM-1		ERROR=	0.0 CM-1	OR	0.0 PERCENT					
INTERNAL COORDINATES-	79.04	OCC	11.32	CCH9	8.41	CC8H	7.09	CCH7								
FORCE CONSTANTS-	79.04	CCO	26.82	CC6H	8.14	CC3H										
OFF DIAGONAL-	-13.72	BB44	-4.78	BB45	-3.16	SB23	3.10	SB26	-2.26	BB37	-1.73	BB40	-1.70	SB25		
NORMAL MODE 20	OBSERVED=	0.0 CM-1		CALCULATED=		212.7 CM-1		ERROR=	0.0 CM-1	OR	0.0 PERCENT					
INTERNAL COORDINATES-	82.42	T-CO	15.58	T-CC												
FORCE CONSTANTS-	82.42	TC-O	15.58	TC-C												
OFF DIAGONAL -	NONE															
NORMAL MODE 21	OBSERVED=	0.0 CM-1		CALCULATED=		179.5 CM-1		ERROR=	0.0 CM-1	OR	0.0 PERCENT					
INTERNAL COORDINATES-	83.22	T-CC	15.29	T-CO												
FORCE CONSTANTS-	83.22	TC-C	15.29	TC-O												
OFF DIAGONAL -	NONE															

0. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 0.0

TABLE LIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 301										PAGE 1
MOLECULE 12		-6 NG= 209		ETHANOL, CD3CHDOO, GAUCHE, D4						
NORMAL MODE 7	OBSERVED=	0.0 CM-1		CALCULATED=		1356.9 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	71.46	OCH5	20.50 H5CC	5.81 HCH	5.26 C-O	5.24 C-C				
FORCE CONSTANTS-	74.27	OCH	21.89 CC3H	5.81 HC3H	5.26 C-O	5.24 C-C				
OFF DIAGONAL-	-10.29	SB22	-4.98 SB25	2.99 BB32	2.56 BB33	-2.39 BB40	-1.97 BB38			
NORMAL MODE 8	OBSERVED=	0.0 CM-1		CALCULATED=		1325.4 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	64.15	HCH	23.28 H5CC							
FORCE CONSTANTS-	64.15	HC3H	26.11 CC3H							
OFF DIAGONAL-	9.19	BB40	-4.91 SB25							
NORMAL MODE 9	OBSERVED=	0.0 CM-1		CALCULATED=		1151.4 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	39.15	C-C	30.81 C-O	9.02 OCH4	8.54 CCH8	8.31 CCH7	7.46 H7H8			
FORCE CONSTANTS-	39.15	C-C	30.81 C-O	17.56 CC6H	12.75 HC6H	11.11 OCH				
OFF DIAGONAL-	-12.13	SB24	5.13 BB40	-3.82 SB22	-2.41 SB25	-1.84 SS20				
NORMAL MODE 10	OBSERVED=	0.0 CM-1		CALCULATED=		1080.3 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	24.01	CCH9	22.40 C-O	18.76 H8H9	10.99 C-C	7.90 H7H9	5.51 OCH4			
FORCE CONSTANTS-	27.50	HC6H	27.32 CC6H	22.40 C-O	10.99 C-C	5.83 OCH				
OFF DIAGONAL-	7.60	BB40	-6.74 SB24	-4.02 SB23	-3.74 SB22	3.57 SB21	2.58 SB25 -1.81 SB26			
NORMAL MODE 11	OBSERVED=	0.0 CM-1		CALCULATED=		1042.4 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	51.83	H7H9	19.82 H8H9							
FORCE CONSTANTS-	75.04	HC6H	9.52 CC6H							
OFF DIAGONAL-	4.97	BB40	4.82 BB34							
NORMAL MODE 12	OBSERVED=	0.0 CM-1		CALCULATED=		1023.4 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	55.47	H7H8	11.71 C-O	9.17 OCH4	7.17 CCH7	6.72 H8H9	5.66 H4CC			
FORCE CONSTANTS-	62.39	HC6H	11.71 C-O	9.87 CC6H	9.36 OCH	5.81 CC3H				
OFF DIAGONAL-	4.12	BB40	-3.94 SB22	2.79 BB34						
NORMAL MODE 13	OBSERVED=	0.0 CM-1		CALCULATED=		1016.3 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	29.93	HOC	21.66 H8H9	9.87 H5CC	8.72 CCH7	7.06 H4CC	6.33 OCC			
FORCE CONSTANTS-	29.93	COH	22.72 HC6H	16.93 CC3H	9.65 CC6H	6.33 CCO				
OFF DIAGONAL-	2.68	SB24	2.66 BB44	-1.70 SB26						
NORMAL MODE 14	OBSERVED=	0.0 CM-1		CALCULATED=		954.4 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	43.64	OCH4	26.93 C-O	14.00 HOC	9.13 H4CC					
FORCE CONSTANTS-	44.75	OCH	26.93 C-O	14.00 COH	9.14 CC3H					
OFF DIAGONAL-	12.77	SB22	-7.98 SB21	-3.89 SB23	-2.72 BB31	-1.51 SB25				
NORMAL MODE 15	OBSERVED=	0.0 CM-1		CALCULATED=		888.9 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	24.75	CCH8	20.32 C-C	18.20 H4CC	6.16 H7H9	5.82 OCC				
FORCE CONSTANTS-	26.69	CC6H	20.32 C-C	20.08 CC3H	6.33 HC6H	5.82 CCO				
OFF DIAGONAL-	4.97	SB25	4.46 SB24	4.33 BB37	-3.41 SB26	3.19 BB44	1.64 BB35			
NORMAL MODE 16	OBSERVED=	0.0 CM-1		CALCULATED=		812.3 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	44.62	HOC	14.80 OCH4	13.20 CCH7	8.77 OCH5	8.62 C-C	5.05 CCH8			
FORCE CONSTANTS-	44.62	COH	23.57 OCH	18.80 CC6H	8.62 C-C					
OFF DIAGONAL-	-4.72	BB32	-3.28 SB21	2.82 BB31	-2.06 BB33	1.82 SB24				
NORMAL MODE 17	OBSERVED=	0.0 CM-1		CALCULATED=		734.6 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	41.38	CCH9	15.65 C-O	10.74 C-C	9.72 CCH7	5.65 H7H8				
FORCE CONSTANTS-	51.80	CC6H	15.65 C-O	10.74 C-C	5.95 HC6H					
OFF DIAGONAL-	-4.36	SB22	2.77 BB35	2.37 SB24	2.30 SB21	2.23 SB23	-2.11 BB40			
NORMAL MODE 18	OBSERVED=	0.0 CM-1		CALCULATED=		610.6 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	25.33	CCH8	23.00 CCH7	22.57 H4CC	13.01 H5CC	6.46 OCH5	5.74 OCH4			
FORCE CONSTANTS-	48.55	CC6H	35.58 CC3H	12.20 OCH	5.92 HC6H					
OFF DIAGONAL-	-8.29	BB37	5.05 BB35	-2.98 BB40						
NORMAL MODE 19	OBSERVED=	0.0 CM-1		CALCULATED=		379.9 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	79.33	OCC	10.83 CCH9	8.00 CCH8	6.98 CCH7					
FORCE CONSTANTS-	79.33	CCO	25.81 CC6H	7.84 CC3H						
OFF DIAGONAL-	-13.52	BB44	-4.68 BB45	-3.16 SB23	3.00 SB26	-2.18 BB37	-1.69 BB40 -1.62 SB25			
NORMAL MODE 20	OBSERVED=	0.0 CM-1		CALCULATED=		188.5 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	86.29	T-CC	12.39 T-CO							
FORCE CONSTANTS-	86.29	TC-C	12.39 TC-O							
OFF DIAGONAL-	NONE									
NORMAL MODE 21	OBSERVED=	0.0 CM-1		CALCULATED=		148.2 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	85.69	T-CO	12.46 T-CC							
FORCE CONSTANTS-	85.69	TC-O	12.46 TC-C							
OFF DIAGONAL-	NONE									

0. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 0.0

TABLE LIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 301										PAGE 1
MOLECULE 13		-6 NG= 209		ETHANOL, CH3CHDOH, GAUCHE, D5						
NORMAL MODE 7	OBSERVED=	0.0 CM-1	CALCULATED=	1458.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	50.24	H7H8 14.05 H7H9	9.97	H8H9 7.52 CCH9						
FORCE CONSTANTS-	74.27	HC6H 11.89 CC6H								
OFF DIAGONAL-	5.53	BB40 4.82 BB34								
NORMAL MODE 8	OBSERVED=	0.0 CM-1	CALCULATED=	1455.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	40.97	H8H9 36.90 H7H9	5.48	CCH7						
FORCE CONSTANTS-	77.98	HC6H 10.42 CC6H								
OFF DIAGONAL-	5.37	BB40 5.07 BB34								
NORMAL MODE 9	OBSERVED=	0.0 CM-1	CALCULATED=	1383.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	18.48	CCH8 17.44 CCH7	15.63	H7H9 15.15 H8H9 14.07 CCH9 9.72 C-C 9.36 H7H8						
FORCE CONSTANTS-	49.99	CC6H 40.14 HC6H 9.72 C-C								
OFF DIAGONAL-	16.55	BB40-11.12 SB24 -6.16 BB35 -5.12 BB34 -2.02 SB25								
NORMAL MODE 10	OBSERVED=	0.0 CM-1	CALCULATED=	1350.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	54.32	UCH4 30.32 H4CC								
FORCE CONSTANTS-	58.16	UCH 31.91 CC3H								
OFF DIAGONAL-	-8.04	SB22 -4.48 SB25 2.60 BB33 1.73 BB31 -1.71 SB21 1.58 SB24								
NORMAL MODE 11	OBSERVED=	0.0 CM-1	CALCULATED=	1329.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	64.03	HCH 11.36 OCH4 10.55 H4CC 5.79 HOC								
FORCE CONSTANTS-	64.03	HC3H 12.23 CC3H 11.52 OCH 5.79 COH								
OFF DIAGONAL-	6.35	BB40 -2.80 SB25 -2.44 BB38								
NORMAL MODE 12	OBSERVED=	0.0 CM-1	CALCULATED=	1257.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	75.18	HOC 5.31 HCH								
FORCE CONSTANTS-	75.18	COH 7.65 OCH 5.31 HC3H 5.02 CC3H								
OFF DIAGONAL-	4.44	BB32 -1.67 BB31								
NORMAL MODE 13	OBSERVED=	0.0 CM-1	CALCULATED=	1134.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	52.13	C-O 13.35 C-C 11.47 CCH9 11.13 OCH5 7.94 H5CC 5.49 H7H8								
FORCE CONSTANTS-	52.13	C-O 14.72 CC6H 13.44 OCH 13.35 C-C 8.76 CC3H 6.37 HC6H								
OFF DIAGONAL-	-5.80	SB22 -4.84 SB23 -2.66 SB25 -1.70 BB40 1.58 SB26								
NORMAL MODE 14	OBSERVED=	0.0 CM-1	CALCULATED=	1058.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	27.43	C-C 24.35 CCH8 13.16 CCH9 7.28 OCC 6.57 H5CC 5.51 H7H9								
FORCE CONSTANTS-	39.63	CC6H 27.43 C-C 9.46 CC3H 9.23 HC6H 7.28 CCO								
OFF DIAGONAL-	-4.43	SB26 -3.47 BB40 2.95 BB35 2.60 BB44 2.44 BB37 -1.72 SB25 1.56 BB45								
NORMAL MODE 15	OBSERVED=	0.0 CM-1	CALCULATED=	1004.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	32.41	CCH7 18.46 C-C 7.87 CCH8 7.51 CCH9 6.11 H8H9 5.89 H5CC 5.09 C-O								
FORCE CONSTANTS-	47.79	CC6H 18.46 C-C 8.87 HC6H 6.10 CC3H 5.09 C-O								
OFF DIAGONAL-	-3.53	BB40 3.22 SB25 3.06 BB35 3.04 BB37 -1.64 SB26								
NORMAL MODE 16	OBSERVED=	0.0 CM-1	CALCULATED=	916.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	51.85	UCH5 18.52 C-O 12.81 HOC 12.46 H5CC								
FORCE CONSTANTS-	55.95	UCH 18.52 C-O 12.81 COH 12.49 CC3H 5.71 CC6H								
OFF DIAGONAL-	9.87	SB22 -6.33 SB21 -6.15 BB32 -2.63 BB33								
NORMAL MODE 17	OBSERVED=	0.0 CM-1	CALCULATED=	865.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	32.85	C-O 30.45 C-C 18.56 CCH9 9.78 OCH5 5.59 CCH8								
FORCE CONSTANTS-	32.85	C-O 30.45 C-C 26.42 CC6H 9.79 OCH								
OFF DIAGONAL-	-8.27	SB22 5.36 SB25 -2.49 SB23 -2.02 BB40 1.68 SS20 -1.54 SB26								
NORMAL MODE 18	OBSERVED=	0.0 CM-1	CALCULATED=	703.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	32.93	H5CC 21.21 H4CC 11.33 CCH8 10.70 OCH5 9.72 OCH4 9.37 CCH7								
FORCE CONSTANTS-	54.14	CC3H 20.72 CC6H 20.41 OCH								
OFF DIAGONAL-	-6.65	BB37 4.47 BB35 -1.84 BB33								
NORMAL MODE 19	OBSERVED=	0.0 CM-1	CALCULATED=	430.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	86.55	OCC 6.67 CCH9 5.57 H5CC								
FORCE CONSTANTS-	86.55	CCO 15.95 CC6H 8.63 CC3H								
OFF DIAGONAL-	-11.12	BB44 -3.84 BB45 3.35 SB26 -2.13 SB23 -1.80 SB25 -1.79 BB37								
NORMAL MODE 20	OBSERVED=	0.0 CM-1	CALCULATED=	247.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	90.62	T-CC 8.31 T-CO								
FORCE CONSTANTS-	90.62	TC-C 8.31 TC-O								
OFF DIAGONAL -	NONE									
NORMAL MODE 21	OBSERVED=	0.0 CM-1	CALCULATED=	205.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	90.14	T-CO 8.09 T-CC								
FORCE CONSTANTS-	90.14	TC-O 8.09 TC-C								
OFF DIAGONAL -	NONE									

0. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 0.0

TABLE LIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 301									
MOLECULE 14		-6 NG= 209		ETHANOL, CH3CHDOO, GAUCHE, D5				PAGE 1	
NORMAL MODE 7	OBSERVED=	0.0 CM-1		CALCULATED=	1458.9 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	50.13	H7H8	15.02	H7H9	9.18	H8H9	7.50	CCH9	
FORCE CONSTANTS-	74.32	HC6H	11.87	CC6H					
OFF DIAGONAL-	5.53	BB40	4.83	BB34					
NORMAL MODE 8	OBSERVED=	0.0 CM-1		CALCULATED=	1454.9 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	41.96	H8H9	35.98	H7H9	5.56	CCH7			
FORCE CONSTANTS-	78.17	HC6H	10.37	CC6H					
OFF DIAGONAL-	5.36	BB40	5.08	BB34					
NORMAL MODE 9	OBSERVED=	0.0 CM-1		CALCULATED=	1383.3 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	18.49	CCH8	17.48	CCH7	15.62	H7H9	15.18	H8H9	14.09
FORCE CONSTANTS-	50.06	CC6H	40.19	HC6H	9.67	C-C			
OFF DIAGONAL-	16.57	BB40	-11.10	SB24	-6.17	BB35	-5.13	BB34	-1.99
								SB25	
NORMAL MODE 10	OBSERVED=	0.0 CM-1		CALCULATED=	1347.1 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	64.14	OCH4	25.91	H4CC					
FORCE CONSTANTS-	67.26	OCH	27.08	CC3H					
OFF DIAGONAL-	-8.51	SB22	-3.32	SB25	2.55	BB33			
NORMAL MODE 11	OBSERVED=	0.0 CM-1		CALCULATED=	1325.6 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	65.63	HCH	19.49	H4CC					
FORCE CONSTANTS-	65.63	HC3H	21.93	CC3H					
OFF DIAGONAL-	8.48	BB40	-4.13	SB25					
NORMAL MODE 12	OBSERVED=	0.0 CM-1		CALCULATED=	1136.3 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	49.78	C-O	16.94	C-C	16.36	OCH5	8.33	CCH9	7.80
FORCE CONSTANTS-	49.78	C-O	19.45	OCH	16.94	C-C	10.42	CC6H	8.96
OFF DIAGONAL-	-7.16	SB22	-6.04	SB21	-3.24	SB23	-2.69	SB25	2.01
								BB32	-1.54
								SS20	
NORMAL MODE 13	OBSERVED=	0.0 CM-1		CALCULATED=	1075.1 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	24.28	C-C	20.83	CCH9	11.03	OCC	10.64	HOC	6.51
FORCE CONSTANTS-	29.61	CC6H	24.28	C-C	11.03	CCO	10.64	COH	7.57
OFF DIAGONAL-	-5.13	SB26	3.77	BB44	-2.76	BB40	2.42	BB45	-2.27
								SB23	1.99
								BB32	1.92
								BB35	1.88
								SB21	1.87
								SB22	
NORMAL MODE 14	OBSERVED=	0.0 CM-1		CALCULATED=	1043.1 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	25.20	CCH8	22.18	CCH7	12.57	HOC	8.32	H5CC	5.77
FORCE CONSTANTS-	47.42	CC6H	12.57	COH	10.56	HC6H	10.47	OCH	10.21
OFF DIAGONAL-	4.12	BB37	-3.79	BB40	3.39	BB35	1.89	BB32	
NORMAL MODE 15	OBSERVED=	0.0 CM-1		CALCULATED=	967.8 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	21.48	OCH5	16.14	C-C	12.81	C-O	9.31	HOC	7.88
FORCE CONSTANTS-	23.41	OCH	16.14	C-C	12.81	C-O	11.11	CC6H	9.31
OFF DIAGONAL-	5.15	SB22	4.49	SB21	4.31	SB25	3.38	BB32	1.56
								BB37	
NORMAL MODE 16	OBSERVED=	0.0 CM-1		CALCULATED=	875.0 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	40.19	C-O	26.11	C-C	20.95	HOC	9.94	CC8	9.00
FORCE CONSTANTS-	40.19	C-O	26.11	C-C	20.95	COH	19.30	CC6H	
OFF DIAGONAL-	-11.93	SB21	-2.51	SB23	1.72	SS20			
NORMAL MODE 17	OBSERVED=	0.0 CM-1		CALCULATED=	842.7 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	35.17	HOC	24.18	OCH5	13.78	H5CC	10.66	CCH7	10.35
FORCE CONSTANTS-	35.17	COH	24.27	OCH	21.02	CC6H	13.78	CC3H	5.20
OFF DIAGONAL-	-6.96	BB32	4.87	SB21	-4.08	SB22	3.29	SB25	-2.44
								BB37	-1.76
								BB40	
NORMAL MODE 18	OBSERVED=	0.0 CM-1		CALCULATED=	693.6 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	27.25	H5CC	21.46	H4CC	13.63	OCH5	10.84	CCH8	10.01
FORCE CONSTANTS-	48.71	CC3H	23.63	OCH	17.63	CC6H	7.76	COH	
OFF DIAGONAL-	-5.76	BB37	4.01	BB35	-2.45	BB32	-2.11	BB33	
NORMAL MODE 19	OBSERVED=	0.0 CM-1		CALCULATED=	421.9 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	85.55	OCC	6.29	CCH9	5.83	H5CC			
FORCE CONSTANTS-	85.55	CCO	15.16	CC6H	8.41	CC3H			
OFF DIAGONAL-	-10.80	BB44	-3.71	BB45	3.13	SB26	-2.19	SB23	-1.72
								BB37	-1.65
								SB25	
NORMAL MODE 20	OBSERVED=	0.0 CM-1		CALCULATED=	244.6 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	96.86	T-CC							
FORCE CONSTANTS-	96.86	TC-C							
OFF DIAGONAL -	NONE								
NORMAL MODE 21	OBSERVED=	0.0 CM-1		CALCULATED=	153.5 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	96.70	T-CO							
FORCE CONSTANTS-	96.70	TC-O							
OFF DIAGONAL -	NONE								

O. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 0.0

TABLE LIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 301
 MOLECULE 15 -6 NG= 209 ETHANOL, CD3CHDOH, GAUCHE, 05

PAGE 1

NORMAL MODE 7	OBSERVED=	0.0 CM-1	CALCULATED=	1351.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	63.65	0CH4 27.86 H4CC	6.34	C-C 5.12 C-O				
FORCE CONSTANTS-	68.19	0CH 29.46 CC3H	6.34	C-C 5.12 C-O				
OFF DIAGONAL-	-10.13	SB22 -6.28 SB25	3.07	BB33 -1.76 SB21 -1.76	BB40	1.66	BB31	
NORMAL MODE 8	OBSERVED=	0.0 CM-1	CALCULATED=	1329.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	63.07	HCH 13.92 H4CC	7.10	HOC 7.04 0CH4				
FORCE CONSTANTS-	63.07	HC3H 16.08 CC3H	7.10	COH 7.09 0CH				
OFF DIAGONAL-	7.29	BB40 -3.43 SB25	-1.84	BB38				
NORMAL MODE 9	OBSERVED=	0.0 CM-1	CALCULATED=	1256.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	76.07	HOC 5.38 HCH						
FORCE CONSTANTS-	76.07	COH 8.35 0CH	5.38	HC3H 5.18 CC3H				
OFF DIAGONAL-	4.54	BB32 -1.82 BB31						
NORMAL MODE 10	OBSERVED=	0.0 CM-1	CALCULATED=	1151.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	38.70	C-C 32.37 C-O	9.55	CCH7 7.48 H7H8 7.39	CCH8	6.20	0CH5	
FORCE CONSTANTS-	38.70	C-C 32.37 C-O	17.61	CC6H 12.62 HC6H 7.72	0CH	5.04	CC3H	
OFF DIAGONAL-	-12.03	SB24 5.13 BB40	-3.17	SB22 -2.26 SB25 -1.88	SS20			
NORMAL MODE 11	OBSERVED=	0.0 CM-1	CALCULATED=	1074.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	25.88	C-O 24.86 CCH9	21.20	H7H9 12.10 H8H9 8.59	C-C			
FORCE CONSTANTS-	34.52	HC6H 29.04 CC6H	25.88	C-O 8.59 C-C				
OFF DIAGONAL-	9.12	BB40 -6.69 SB24	-2.99	SB23 -2.91 SB22 -2.03	BB35	1.75	SB25	
NORMAL MODE 12	OBSERVED=	0.0 CM-1	CALCULATED=	1040.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	47.96	H8H9 31.93 H7H9						
FORCE CONSTANTS-	80.92	HC6H 7.59 CC6H						
OFF DIAGONAL-	5.25	BB34 4.65 BB40						
NORMAL MODE 13	OBSERVED=	0.0 CM-1	CALCULATED=	1022.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	59.39	H7H8 13.24 C-O	5.97	H7H9 5.83 0CH5 5.65	CCH8			
FORCE CONSTANTS-	66.85	HC6H 13.24 C-O	8.13	CC6H 5.87 0CH				
OFF DIAGONAL-	-3.56	SB22 3.52 BB40	3.28	BB34 -1.59 SB23				
NORMAL MODE 14	OBSERVED=	0.0 CM-1	CALCULATED=	959.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	17.53	H5CC 14.71 C-C	14.47	CCH8 12.19 C-O 9.81	0CC	7.51	H7H9 6.69 H4CC 5.80 0CH5	
FORCE CONSTANTS-	24.23	CC3H 14.92 CC6H	14.71	C-C 12.19 C-O 9.81	CCO	9.57	HC6H 7.00 0CH	
OFF DIAGONAL-	5.42	SB22 -5.33 SB23	-3.77	SB26 3.72 SB24 3.45	BB44	-3.18	SB21 -2.34 SB25 1.84 BB37 1.55 BB35	
NORMAL MODE 15	OBSERVED=	0.0 CM-1	CALCULATED=	909.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	33.35	0CH5 12.36 C-C	10.96	H5CC 8.05 C-O				
FORCE CONSTANTS-	37.31	0CH 12.36 C-C	11.37	CC3H 9.13 CC6H 8.05	C-O			
OFF DIAGONAL-	5.29	SB25 4.76 SB22	3.33	SB24 -2.48 BB32 2.46	SB23	-2.10	SB21 -2.07 BB33 2.02 BB44 -1.96 SB26	
NORMAL MODE 16	OBSERVED=	0.0 CM-1	CALCULATED=	861.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	24.88	CCH7 19.31 0CH5	8.53	H5CC 7.66 HOC 7.42	C-C	6.24	0CH4 5.79 H8H9 5.74 CCH8	
FORCE CONSTANTS-	31.26	CC6H 25.54 0CH	12.98	CC3H 7.66 COH 7.42	C-C	6.43	HC6H	
OFF DIAGONAL-	3.95	BB37 -2.90 BB32	2.47	BB35 -1.98 BB33 -1.90	BB40	-1.53	SB21	
NORMAL MODE 17	OBSERVED=	0.0 CM-1	CALCULATED=	738.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	41.91	CCH9 16.35 C-O	13.88	C-C 6.04 H7H8				
FORCE CONSTANTS-	48.75	CC6H 16.35 C-O	13.88	C-C 6.04 HC6H				
OFF DIAGONAL-	-4.82	SB22 3.04 SB24	2.48	BB35 2.46 SB23 -1.73	BB40			
NORMAL MODE 18	OBSERVED=	0.0 CM-1	CALCULATED=	615.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	28.58	CCH8 23.72 CCH7	20.69	H5CC 13.82 H4CC 5.38	0CH5	5.05	0CH4	
FORCE CONSTANTS-	52.31	CC6H 34.51 CC3H	10.43	0CH 6.36 HC6H				
OFF DIAGONAL-	-8.46	BB37 5.25 BB35	-3.26	BB40				
NORMAL MODE 19	OBSERVED=	0.0 CM-1	CALCULATED=	385.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	79.06	0CC 11.24 CCH9	8.07	CCH7 7.33 CCH8 5.00	H5CC			
FORCE CONSTANTS-	79.06	CCO 26.64 CC6H	8.20	CC3H				
OFF DIAGONAL-	-13.69	BB44 -4.76 BB45	-3.20	SB23 3.09 SB26 -2.25	BB37	-1.70	SB25 -1.68 BB40	
NORMAL MODE 20	OBSERVED=	0.0 CM-1	CALCULATED=	213.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	82.04	T-CO 16.13 T-CC						
FORCE CONSTANTS-	82.04	TC-O 16.13 TC-C						
OFF DIAGONAL -	NONE							
NORMAL MODE 21	OBSERVED=	0.0 CM-1	CALCULATED=	179.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	82.70	T-CC 15.73 T-CO						
FORCE CONSTANTS-	82.70	TC-C 15.73 TC-O						
OFF DIAGONAL -	NONE							

0. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 0.0

TABLE LIV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 301
MOLECULE 16 -6 NG= 209 ETHANOL, CD3CHDOD, GAUCHE, D5

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NORMAL MODE 7	OBSERVED=	0.0 CM-1	CALCULATED=	1348.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	71.49	OCH4 23.04 H4CC	6.74	HCH 5.14 C-O				
FORCE CONSTANTS-	75.27	OCH 24.17 CC3H	6.74	HC3H 5.14 C-O				
OFF DIAGONAL-	-10.45	SB22 -4.94 SB25	2.97	BB33 -2.65 BB40 -2.18	BB38			
NORMAL MODE 8	OBSERVED=	0.0 CM-1	CALCULATED=	1325.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	63.16	HCH 23.34 H4CC						
FORCE CONSTANTS-	63.16	HC3H 26.33 CC3H						
OFF DIAGONAL-	9.19	BB40 -5.19 SB25						
NORMAL MODE 9	OBSERVED=	0.0 CM-1	CALCULATED=	1155.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	39.35	C-C 30.76 C-O	10.77	OCH5 7.41 CCH7 7.02	CCH8 6.61 H7H8			
FORCE CONSTANTS-	39.35	C-C 30.76 C-O	15.25	CC6H 13.32 OCH 11.38	HC6H 5.43 CC3H			
OFF DIAGONAL-	-11.48	SB24 4.54 BB40	-4.21	SB21 -4.14 SB22 -1.85	SS20 -1.78 SB25			
NORMAL MODE 10	OBSERVED=	0.0 CM-1	CALCULATED=	1074.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	23.82	CCH9 23.23 C-O	23.06	H7H9 10.65 H8H9 8.58	C-C 6.52 OCH5			
FORCE CONSTANTS-	34.27	HC6H 29.68 CC6H	23.23	C-O 8.58 C-C 7.31	OCH			
OFF DIAGONAL-	9.45	BB40 -7.01 SB24	-3.56	SB22 -3.07 SB21 -2.36	BB35 -2.29 SB23 1.76	SB25		
NORMAL MODE 11	OBSERVED=	0.0 CM-1	CALCULATED=	1049.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	27.85	H8H9 12.78 H7H8	11.07	H7H9 11.06 HOC 10.02	OCH5 9.06 CCH7			
FORCE CONSTANTS-	51.70	HC6H 11.06 COH	10.51	OCH 10.04 CC6H				
OFF DIAGONAL-	4.27	BB40 3.19 BB34	2.51	BB32				
NORMAL MODE 12	OBSERVED=	0.0 CM-1	CALCULATED=	1032.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	24.84	H7H9 20.74 H7H8	14.76	H8H9 9.77 CCH8 9.21	OCH5 7.66 HOC			
FORCE CONSTANTS-	60.34	HC6H 10.09 CC6H	9.59	OCH 7.66 COH				
OFF DIAGONAL-	4.76	BB40 3.16 BB34	2.01	BB32				
NORMAL MODE 13	OBSERVED=	0.0 CM-1	CALCULATED=	1006.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	29.47	H7H8 23.85 C-O	12.60	HOC 10.77 H8H9 7.52	OCC			
FORCE CONSTANTS-	41.09	HC6H 23.85 C-O	12.60	COH 7.52 CCO				
OFF DIAGONAL-	7.13	SB21 -6.52 SB23	2.57	BB34 2.38 SB22				
NORMAL MODE 14	OBSERVED=	0.0 CM-1	CALCULATED=	946.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	18.69	CCH8 18.51 H5CC	12.50	C-C 12.24 HOC 8.99	H7H9 8.96 H4CC			
FORCE CONSTANTS-	27.47	CC3H 19.38 CC6H	12.50	C-C 12.24 COH 8.99	HC6H 5.26 OCH			
OFF DIAGONAL-	3.48	SB24 3.32 BB37	-2.43	SB21 -2.42 SB26 2.12	BB44 2.05 BB35 -1.79	SB23 -1.76	SB25	
NORMAL MODE 15	OBSERVED=	0.0 CM-1	CALCULATED=	906.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	21.39	OCH5 19.28 H5CC	12.54	C-C 9.85 CCH7 7.19	C-O			
FORCE CONSTANTS-	22.77	OCH 19.30 CC3H	12.54	C-C 12.15 CC6H 7.19	C-O			
OFF DIAGONAL-	5.75	SB25 4.10 SB22	3.22	SB24 2.75 BB37 2.50	SB23 -2.46 BB32 -2.45	SB21 2.24	BB44 -2.13	SB26
NORMAL MODE 16	OBSERVED=	0.0 CM-1	CALCULATED=	807.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	41.16	HOC 15.00 CCH7	14.56	OCH5 11.00 C-C 6.01	CCH8 5.95 C-O			
FORCE CONSTANTS-	41.16	COH 21.76 CC6H	18.86	OCH 11.00 C-C 5.95	C-O			
OFF DIAGONAL-	-6.44	SB21 -5.84 BB32	2.22	SB24 1.88 SB22				
NORMAL MODE 17	OBSERVED=	0.0 CM-1	CALCULATED=	730.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	41.16	CCH9 13.40 C-O	9.65	C-C 6.99 OCH5 6.46	CCH7 5.54 H7H8			
FORCE CONSTANTS-	49.93	CC6H 13.40 C-O	9.65	C-C 7.17 OCH 5.66	HC6H			
OFF DIAGONAL-	-4.97	SB22 3.22 SB21	2.67	BB35 -2.14 BB40 2.13	SB24 2.00 SB23			
NORMAL MODE 18	OBSERVED=	0.0 CM-1	CALCULATED=	613.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	28.82	CCH8 21.16 CCH7	19.97	H5CC 14.52 H4CC 6.48	OCH5 5.33 OCH4			
FORCE CONSTANTS-	50.10	CC6H 34.49 CC3H	11.82	OCH 6.11 HC6H				
OFF DIAGONAL-	-8.25	BB37 5.12 BB35	-3.14	BB40				
NORMAL MODE 19	OBSERVED=	0.0 CM-1	CALCULATED=	378.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	79.19	OCC 10.69 CCH9	7.85	CCH7 6.97 CCH8 5.25	H5CC			
FORCE CONSTANTS-	79.19	CCO 25.50 CC6H	8.08	CC3H				
OFF DIAGONAL-	-13.44	BB44 -4.65 BB45	-3.21	SB23 2.97	SB26 -2.18 BB37 -1.61	SB25 -1.60	BB40	
NORMAL MODE 20	OBSERVED=	0.0 CM-1	CALCULATED=	189.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	85.45	T-CC 13.38 T-CO						
FORCE CONSTANTS-	85.45	TC-C 13.38 TC-O						
OFF DIAGONAL-	NONE							
NORMAL MODE 21	OBSERVED=	0.0 CM-1	CALCULATED=	148.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	84.74	T-CO 13.37 T-CC						
FORCE CONSTANTS-	84.74	TC-O 13.37 TC-C						
OFF DIAGONAL-	NONE							

0. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 0.0

TABLE LV

POTENTIAL ENERGY DISTRIBUTIONS FOR LIQUID ETHANOL (GAUCHE)

Explanation of the table:

This table is presented in the same format as Table XXXIV except that the force constant and internal coordinate description codes are found in Tables XLIII and XLIV, respectively.

TABLE LV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 301										PAGE 1	
MOLECULE 2		-6 NG= 209		ETHANOL, CH3CH2OD, GAUCHE							
NORMAL MODE 7		OBSERVED= 0.0 CM-1		CALCULATED= 1488.0 CM-1		ERROR= 0.0 CM-1		OR 0.0 PERCENT			
INTERNAL COORDINATES-		66.70	HCH 5.83 OCH4	5.59	H7H8 5.45	OCH5					
FORCE CONSTANTS-		66.70	HC3H 11.28 OCH	8.52	CC3H 8.24	HC6H					
OFF DIAGONAL-		7.44	BB40 -4.64 BB38	-1.76	SB22						
NORMAL MODE 8		OBSERVED= 0.0 CM-1		CALCULATED= 1453.5 CM-1		ERROR= 0.0 CM-1		OR 0.0 PERCENT			
INTERNAL COORDINATES-		40.38	H7H8 20.67 H7H9	7.93	HCH 5.91	CCH9					
FORCE CONSTANTS-		62.70	HC6H 11.27 CC6H	7.93	HC3H 5.32	CC3H					
OFF DIAGONAL-		7.28	BB40 3.69 BB34								
NORMAL MODE 9		OBSERVED= 0.0 CM-1		CALCULATED= 1453.2 CM-1		ERROR= 0.0 CM-1		OR 0.0 PERCENT			
INTERNAL COORDINATES-		45.93	H8H9 26.57 H7H9	7.35	CCH7						
FORCE CONSTANTS-		75.58	HC6H 11.38 CC6H								
OFF DIAGONAL-		6.18	BB40 4.47 BB34								
NORMAL MODE 10		OBSERVED= 0.0 CM-1		CALCULATED= 1396.2 CM-1		ERROR= 0.0 CM-1		OR 0.0 PERCENT			
INTERNAL COORDINATES-		20.16	OCH5 16.44 OCH4	11.25	H7H9 10.75	H5CC 10.71	H4CC 10.19	C-C 9.17	H8H9 7.94		
FORCE CONSTANTS-		36.60	OCH 21.46 CC3H	20.70	HC6H 20.38	CC6H 10.19	C-C				
OFF DIAGONAL-		-8.44	SB25 -7.46 SB24	-7.04	SB22 6.38	BB40 -4.99	BB35 3.84	BB37 3.29	BB33 -1.60		
									BB36 1.51		
NORMAL MODE 11		OBSERVED= 0.0 CM-1		CALCULATED= 1366.7 CM-1		ERROR= 0.0 CM-1		OR 0.0 PERCENT			
INTERNAL COORDINATES-		16.14	OCH5 13.08 H7H8	11.76	CCH9 10.62	CCH7 10.47	CCCH8 10.32	OCH4 7.64	H8H9 7.58		
FORCE CONSTANTS-		32.84	CC6H 26.72 HC6H	26.45	OCH 14.38	CC3H					
OFF DIAGONAL-		11.73	BB40 -6.51 BB35	-3.63	BB37 -3.39	SB22 -3.03	BB34 2.33	BB33 -1.67	BB36		
NORMAL MODE 12		OBSERVED= 0.0 CM-1		CALCULATED= 1290.0 CM-1		ERROR= 0.0 CM-1		OR 0.0 PERCENT			
INTERNAL COORDINATES-		38.44	OCH4 29.20 OCH5	17.63	H4CC 10.98	H5CC					
FORCE CONSTANTS-		67.64	OCH 28.60 CC3H								
OFF DIAGONAL-		-6.05	BB33 2.30 BB35	2.16	BB32						
NORMAL MODE 13		OBSERVED= 0.0 CM-1		CALCULATED= 1143.2 CM-1		ERROR= 0.0 CM-1		OR 0.0 PERCENT			
INTERNAL COORDINATES-		22.73	HOC 13.37 CCH9	9.59	CCH7 8.73	H5CC 7.85	C-O 7.73	OCC 6.56	H7H8		
FORCE CONSTANTS-		23.64	CC6H 22.73 COH	11.85	CC3H 10.23	HC6H 7.85	C-O 7.73	CCO			
OFF DIAGONAL-		5.11	SB21 -3.51 SB23	-2.92	BB40 2.62	BB35 2.34	BB44 2.21	BB37 -1.67	SB26 1.55		
									BB45		
NORMAL MODE 14		OBSERVED= 0.0 CM-1		CALCULATED= 1101.8 CM-1		ERROR= 0.0 CM-1		OR 0.0 PERCENT			
INTERNAL COORDINATES-		45.59	C-O 13.28 HOC	9.73	CCH8 9.10	CCH9 5.48	C-C 5.01	H5CC			
FORCE CONSTANTS-		45.59	C-O 19.81 CC6H	13.28	COH 7.77	HC6H 7.19	CC3H 5.48	C-C			
OFF DIAGONAL-		-9.42	SB21 5.08 SB22	-4.26	SB23 -2.37	BB40 2.09	BB35 -1.55	SS20			
NORMAL MODE 15		OBSERVED= 0.0 CM-1		CALCULATED= 1057.3 CM-1		ERROR= 0.0 CM-1		OR 0.0 PERCENT			
INTERNAL COORDINATES-		50.59	C-C 12.34 CCH8	11.55	C-O 6.51	OCH4					
FORCE CONSTANTS-		50.59	C-C 18.61 CC6H	11.55	C-O 8.32	OCH					
OFF DIAGONAL-		-3.69	SB26 2.91 SB23	-2.37	SS20 -1.92	BB40 1.85	BB35 -1.76	SB22 1.62	BB37		
NORMAL MODE 16		OBSERVED= 0.0 CM-1		CALCULATED= 946.2 CM-1		ERROR= 0.0 CM-1		OR 0.0 PERCENT			
INTERNAL COORDINATES-		52.19	HOC 17.88 CCH7	13.97	C-C 7.92	CCH8 5.82	OCH5				
FORCE CONSTANTS-		52.19	COH 27.00 CC6H	13.97	C-C 6.85	OCH 5.41	HC6H				
OFF DIAGONAL-		-3.76	BB32 -2.47 BB40	2.18	BB35 -1.94	SB21					
NORMAL MODE 17		OBSERVED= 0.0 CM-1		CALCULATED= 882.5 CM-1		ERROR= 0.0 CM-1		OR 0.0 PERCENT			
INTERNAL COORDINATES-		41.99	C-O 22.87 CCH9	20.78	C-C 7.25	CCH7					
FORCE CONSTANTS-		41.99	C-O 33.28 CC6H	20.78	C-C						
OFF DIAGONAL-		-4.72	SB22 2.90 SS20	-2.72	BB40 2.65	BB35 -2.45	SB23 2.29	SB25			
NORMAL MODE 18		OBSERVED= 0.0 CM-1		CALCULATED= 784.1 CM-1		ERROR= 0.0 CM-1		OR 0.0 PERCENT			
INTERNAL COORDINATES-		22.57	H4CC 18.74 H5CC	16.01	CCH8 13.14	OCH5 10.92	OCH4 10.88	CCH7 7.79	HOC		
FORCE CONSTANTS-		41.32	CC3H 27.17 CC6H	24.06	OCH 7.79	COH					
OFF DIAGONAL-		-6.94	BB37 5.54 BB35	-2.29	BB40 -2.18	BB32 -2.16	BB33 1.55	BB36			
NORMAL MODE 19		OBSERVED= 0.0 CM-1		CALCULATED= 429.5 CM-1		ERROR= 0.0 CM-1		OR 0.0 PERCENT			
INTERNAL COORDINATES-		86.12	OCC 6.57 CCH9	5.86	CCH8 5.76	CCH7					
FORCE CONSTANTS-		86.12	CCO 18.19 CC6H								
OFF DIAGONAL-		-16.57	BB44 -3.62 BB45	-3.44	BB46 3.11	SB26 1.89	BB43 -1.58	BB37 -1.56	SB25		
NORMAL MODE 20		OBSERVED= 0.0 CM-1		CALCULATED= 248.3 CM-1		ERROR= 0.0 CM-1		OR 0.0 PERCENT			
INTERNAL COORDINATES-		96.91	T-CC								
FORCE CONSTANTS-		96.91	TC-C								
OFF DIAGONAL -		NONE									
NORMAL MODE 21		OBSERVED= 0.0 CM-1		CALCULATED= 154.0 CM-1		ERROR= 0.0 CM-1		OR 0.0 PERCENT			
INTERNAL COORDINATES-		96.26	T-CO								
FORCE CONSTANTS-		96.26	TC-O								
OFF DIAGONAL -		NONE									

0. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 0.0

TABLE IV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 301										PAGE 1	
MOLECULE 3		-6		NG= 209		ETHANOL, CH3CD2OH, GAUCHE					
NORMAL MODE 7		OBSERVED=		0.0 CM-1		CALCULATED=		1456.1 CM-1		ERROR= 0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-		47.77		H7H8 20.00 H8H9		7.62		CCH9			
FORCE CONSTANTS-		72.49		HC6H 12.73 CC6H							
OFF DIAGONAL-		6.27		BB40 4.28 BB34							
NORMAL MODE 8		OBSERVED=		0.0 CM-1		CALCULATED=		1452.4 CM-1		ERROR= 0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-		45.85		H7H9 28.27 H8H9		6.54		CCH8			
FORCE CONSTANTS-		76.12		HC6H 11.02 CC6H							
OFF DIAGONAL-		5.99		BB40 4.50 BB34							
NORMAL MODE 9		OBSERVED=		0.0 CM-1		CALCULATED=		1393.8 CM-1		ERROR= 0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-		76.13		HOC 7.52 H8H9							
FORCE CONSTANTS-		76.13		COH 8.49 HC6H		6.82		CC6H			
OFF DIAGONAL-		2.73		BB32 2.51 BB40							
NORMAL MODE 10		OBSERVED=		0.0 CM-1		CALCULATED=		1376.9 CM-1		ERROR= 0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-		16.70		CCH8 16.11 CCH7		14.77 H7H9		13.11 CCH9 12.48		HOC 11.20 H7H8 10.50 H8H9 9.39 C-C	
FORCE CONSTANTS-		45.93		CC6H 36.48 HC6H		12.48 COH		9.39 C-C			
OFF DIAGONAL-		16.85		BB40-10.81 SB24		-7.50 BB35		-4.28 BB34			
NORMAL MODE 11		OBSERVED=		0.0 CM-1		CALCULATED=		1182.3 CM-1		ERROR= 0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-		44.71		C-O 15.02 C-C		14.97 OCH4		13.06 OCH5 12.49		CCH9 9.34 H5CC 9.23 H4CC 8.07 H7H8	
FORCE CONSTANTS-		44.71		C-O 28.03 OCH		18.57 CC3H		15.02 C-C 13.69		CC6H 8.64 HC6H	
OFF DIAGONAL-		-21.57		SB22 -9.53 SB25		-3.56 SB23		-2.55 SS20 2.52		BB33 -2.50 BB40 2.32 SB24	
NORMAL MODE 12		OBSERVED=		0.0 CM-1		CALCULATED=		1110.4 CM-1		ERROR= 0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-		50.18		HCH 24.53 C-C		6.58 OCC		6.48 H5CC 5.41		H4CC	
FORCE CONSTANTS-		50.18		HC3H 24.53 C-C		11.89 CC3H		6.77 CC6H 6.58		CCO	
OFF DIAGONAL-		-9.74		SB25 5.74 BB40		-3.47 SB26		1.79 BB44			
NORMAL MODE 13		OBSERVED=		0.0 CM-1		CALCULATED=		1022.5 CM-1		ERROR= 0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-		33.42		CCH8 20.54 CCH7		9.59 H4CC		7.37 H7H9 5.48		H5CC	
FORCE CONSTANTS-		55.93		CC6H 15.07 CC3H		12.59 HC6H					
OFF DIAGONAL-		5.95		BB37 5.73 BB35		-5.19 BB40					
NORMAL MODE 14		OBSERVED=		0.0 CM-1		CALCULATED=		1015.9 CM-1		ERROR= 0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-		20.65		HCH 18.43 C-C		14.27 CCH9		13.33 OCH4 12.97		CCH7	
FORCE CONSTANTS-		27.25		CC6H 20.65 HC3H		18.43 C-C		17.98 OCH 5.87		HC6H	
OFF DIAGONAL-		-3.15		BB38 2.37 BB35		2.34 BB44		2.16 SB25 -2.14		SB26	
NORMAL MODE 15		OBSERVED=		0.0 CM-1		CALCULATED=		951.1 CM-1		ERROR= 0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-		38.17		C-O 17.50 OCH4		7.85 H4CC		7.41 OCH5 5.36		H5CC	
FORCE CONSTANTS-		38.17		C-O 24.91 OCH		13.21 CC3H					
OFF DIAGONAL-		18.39		SB22 4.10 SB25		-3.49 SB21		2.06 BB33			
NORMAL MODE 16		OBSERVED=		0.0 CM-1		CALCULATED=		902.5 CM-1		ERROR= 0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-		48.48		OCH5 33.35 OCH4		9.35 H5CC		5.30 H4CC			
FORCE CONSTANTS-		81.83		OCH 14.65 CC3H		5.93 CC6H					
OFF DIAGONAL-		-7.26		BB33 -3.21 BB32		-1.93 BB37		1.62 BB35			
NORMAL MODE 17		OBSERVED=		0.0 CM-1		CALCULATED=		866.6 CM-1		ERROR= 0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-		33.47		C-C 27.10 C-O		17.00 CCH9					
FORCE CONSTANTS-		33.47		C-C 27.10 C-O		24.05 CC6H		5.89 CC3H 5.55		OCH	
OFF DIAGONAL-		8.01		SB25 -7.48 SB22		2.96 SS20		-1.73 BB40 -1.67		SB23	
NORMAL MODE 18		OBSERVED=		0.0 CM-1		CALCULATED=		663.8 CM-1		ERROR= 0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-		30.50		H4CC 28.67 H5CC		11.15 OCH5		10.96 OCH4 8.71		CCH8 7.32 CCH7	
FORCE CONSTANTS-		59.17		CC3H 22.11 OCH		16.06 CC6H					
OFF DIAGONAL-		-6.42		BB37 6.10 BB35		-2.00 BB33					
NORMAL MODE 19		OBSERVED=		0.0 CM-1		CALCULATED=		432.5 CM-1		ERROR= 0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-		87.06		OCC 6.86 CCH9		6.05 CCH7		5.92 CCH8			
FORCE CONSTANTS-		87.06		CCO 18.82 CC6H		6.05 CC3H					
OFF DIAGONAL-		-16.90		BB44 -3.72 BB45		-3.40 BB46		2.96 SB26 2.09		BB43 -1.77 BB37 -1.62 SB25	
NORMAL MODE 20		OBSERVED=		0.0 CM-1		CALCULATED=		244.0 CM-1		ERROR= 0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-		91.18		T-CC 7.34 T-CO							
FORCE CONSTANTS-		91.18		TC-C 7.34 TC-O							
OFF DIAGONAL -		NONE									
NORMAL MODE 21		OBSERVED=		0.0 CM-1		CALCULATED=		205.5 CM-1		ERROR= 0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-		91.19		T-CO 7.13 T-CC							
FORCE CONSTANTS-		91.19		TC-O 7.13 TC-C							
OFF DIAGONAL -		NONE									

0. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 0.0

TABLE LV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 301										PAGE 1
MOLECULE 4 -6 NG= 209 ETHANOL, CH3CD2OD, GAUCHE										
NORMAL MODE 7	OBSERVED=	0.0 CM-1	CALCULATED=	1455.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	50.13	H7H8 13.08 H8H9	10.71	H7H9 8.00 CCH9						
FORCE CONSTANTS-	73.92	HC6H 12.64 CC6H								
OFF DIAGONAL-	6.30	BB40 4.37 BB34								
NORMAL MODE 8	OBSERVED=	0.0 CM-1	CALCULATED=	1451.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	39.90	H7H9 37.30 H8H9	5.62	CCH8 5.29 CCH7						
FORCE CONSTANTS-	77.25	HC6H 10.92 CC6H								
OFF DIAGONAL-	6.01	BB40 4.57 BB34								
NORMAL MODE 9	OBSERVED=	0.0 CM-1	CALCULATED=	1379.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	19.07	CCH7 19.05 CCH8	15.72	H8H9 15.48 H7H9 14.66	CCH9 10.75 H7H8 7.48	C-C				
FORCE CONSTANTS-	52.78	CC6H 41.95 HC6H	7.48	C-C						
OFF DIAGONAL-	19.29	BB40-10.34 SB24	-8.58	BB35 -4.91 BB34						
NORMAL MODE 10	OBSERVED=	0.0 CM-1	CALCULATED=	1189.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	39.52	C-O 24.62 C-C	18.40	OCH5 11.74 H4CC 10.63	OCH4 10.26 H5CC 9.36	HOC 6.47 CCH9				
FORCE CONSTANTS-	39.52	C-O 29.03 OCH	24.62	C-C 22.00 CC3H 9.36	COH 7.06 CC6H					
OFF DIAGONAL-	-20.47	SB22-13.28 SB25	-7.36	SB21 -3.06 SS20 2.83	BB32 2.53 BB33 2.34	SB24				
NORMAL MODE 11	OBSERVED=	0.0 CM-1	CALCULATED=	1143.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	25.17	HCH 17.08 HOC	13.00	CCH9 10.75 C-C 9.97	OCC 6.76 H7H8 6.14	C-O				
FORCE CONSTANTS-	25.17	HC3H 17.08 COH	16.45	CC6H 10.75 C-C 9.97	CCO 8.18 HC6H 6.14	C-O				
OFF DIAGONAL-	3.92	SB21 -3.53 SB23	-2.83	SB26 2.75 BB44 -2.10	SB25 -1.93 SB22 1.73	BB45				
NORMAL MODE 12	OBSERVED=	0.0 CM-1	CALCULATED=	1067.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	34.35	HCH 27.05 HOC	9.96	OCH5 8.14 H5CC 5.27	CCH7					
FORCE CONSTANTS-	34.35	HC3H 27.05 COH	10.44	OCH 9.61 CC6H 9.56	CC3H					
OFF DIAGONAL-	3.55	BB40 3.54 BB32	-2.72	SB25 -1.72 BB38						
NORMAL MODE 13	OBSERVED=	0.0 CM-1	CALCULATED=	1021.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	30.13	CCH8 11.40 CCH7	10.91	HCH 8.62 H4CC 6.53	H7H9 5.80 C-C 5.61	CCH9				
FORCE CONSTANTS-	47.14	CC6H 11.58 CC3H	10.91	HC3H 10.54 HC6H 6.81	OCH 5.80 C-C					
OFF DIAGONAL-	4.66	BB35 4.57 BB37	-3.82	BB40						
NORMAL MODE 14	OBSERVED=	0.0 CM-1	CALCULATED=	996.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	27.17	OCH4 18.07 HOC	16.74	C-C 12.27 CCH7 7.23	CCH9 5.38 HCH					
FORCE CONSTANTS-	27.87	OCH 20.20 CC6H	18.07	COH 16.74 C-C 7.62	CC3H 5.38 HC3H					
OFF DIAGONAL-	2.26	BB35 -1.98 BB40	1.68	BB37 -1.64 BB31						
NORMAL MODE 15	OBSERVED=	0.0 CM-1	CALCULATED=	949.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	37.66	C-O 12.78 OCH4	10.49	OCH5 6.59 H4CC 6.36	H5CC 5.34 C-C					
FORCE CONSTANTS-	37.66	C-O 23.27 OCH	12.95	CC3H 5.34 C-C						
OFF DIAGONAL-	18.03	SB22 4.74 SB25	-2.28	SB21 2.09 BB33						
NORMAL MODE 16	OBSERVED=	0.0 CM-1	CALCULATED=	874.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	23.68	OCH4 17.81 HOC	17.55	OCH5 16.96 C-C 10.38	C-O 8.15 H4CC 5.68	CCH8				
FORCE CONSTANTS-	41.23	OCH 17.81 COH	16.96	C-C 11.62 CC3H 10.38	C-O 9.55 CC6H					
OFF DIAGONAL-	-5.20	SB21 -3.81 BB32	-3.68	BB33 -1.89 BB37 1.65	SB25 1.63 BB35 1.52	BB31				
NORMAL MODE 17	OBSERVED=	0.0 CM-1	CALCULATED=	861.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	18.44	OCH5 17.99 C-O	16.60	C-C 15.66 CCH9 10.44	H5CC 9.92 CCH7 6.58	HOC				
FORCE CONSTANTS-	26.00	CC6H 19.19 OCH	17.99	C-O 16.60 C-C 10.47	CC3H 6.58 COH					
OFF DIAGONAL-	-6.26	SB22 5.63 SB25	4.16	SB21 -2.37 BB32 -2.15	BB37 2.02 BB35 -2.01	BB40 1.70 SS20				
NORMAL MODE 18	OBSERVED=	0.0 CM-1	CALCULATED=	654.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	30.17	H4CC 25.51 H5CC	12.68	OCH5 12.23 OCH4 8.73	CCH8 5.57 CCH7					
FORCE CONSTANTS-	55.67	CC3H 24.91 OCH	14.46	CC6H						
OFF DIAGONAL-	-5.87	BB37 5.67 BB35	-2.25	BB33 -1.57 BB32						
NORMAL MODE 19	OBSERVED=	0.0 CM-1	CALCULATED=	424.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	86.39	OCC 6.52 CCH9	5.97	CCH7 5.57 CCH8						
FORCE CONSTANTS-	86.39	CCO 18.07 CC6H	5.87	CC3H						
OFF DIAGONAL-	-16.54	BB44 -3.61 BB45	-3.45	BB46 2.79 SB26 2.04	BB43 -1.71 BB37 -1.51	SB25				
NORMAL MODE 20	OBSERVED=	0.0 CM-1	CALCULATED=	241.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	96.87	T-CC								
FORCE CONSTANTS-	96.87	TC-C								
OFF DIAGONAL -	NONE									
NORMAL MODE 21	OBSERVED=	0.0 CM-1	CALCULATED=	152.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT		
INTERNAL COORDINATES-	97.18	T-CO								
FORCE CONSTANTS-	97.18	TC-O								
OFF DIAGONAL -	NONE									

O. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 0.0

TABLE LV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 301									
MOLECULE 5 -6 NG= 209 ETHANOL, CD3CH2OH, GAUCHE									
PAGE 1									
NORMAL MODE 7	OBSERVED=	0.0 CM-1	CALCULATED=	1484.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	75.36	HCH 6.31 H5CC	5.80 H4CC	5.33 OCH4					
FORCE CONSTANTS-	75.36	HC3H 12.11 CC3H	9.79 OCH						
OFF DIAGONAL-	8.26	BB40 -4.59 BB38	-1.90 SB25						
NORMAL MODE 8	OBSERVED=	0.0 CM-1	CALCULATED=	1443.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	56.47	HOC 27.57 OCH5	6.39 H5CC						
FORCE CONSTANTS-	56.47	COH 29.54 OCH	9.84 CC3H						
OFF DIAGONAL-	8.51	BB32 -3.49 SB21	-3.48 SB22 -2.97 SB25						
NORMAL MODE 9	OBSERVED=	0.0 CM-1	CALCULATED=	1353.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	47.82	UCH4 22.08 H4CC	19.68 HOC	8.34 H5CC 5.22 OCH5					
FORCE CONSTANTS-	53.05	UCH 30.43 CC3H	19.68 COH						
OFF DIAGONAL-	-8.21	SB22 -5.20 SB25	3.52 SB21 2.85 BB33 -2.27 BB31 -2.19 BB32 -2.11 BB35						
NORMAL MODE 10	OBSERVED=	0.0 CM-1	CALCULATED=	1253.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	32.89	UCH5 24.31 H5CC	17.41 UCH4 14.11 HOC 11.46 H4CC						
FORCE CONSTANTS-	50.30	UCH 35.77 CC3H	14.11 COH						
OFF DIAGONAL-	-4.64	BB32 -4.32 BB33	2.77 BB35						
NORMAL MODE 11	OBSERVED=	0.0 CM-1	CALCULATED=	1129.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	40.60	C-C 27.68 C-O	11.30 CCH8 10.47 H7H8 10.43 CCH7						
FORCE CONSTANTS-	40.60	C-C 27.68 C-O	23.73 CC6H 18.04 HC6H						
OFF DIAGONAL-	-15.36	SB24 8.22 BB40 -3.30 BB35 -3.29 SS20 -2.57 SB21 2.41 SB22 -1.94 BB34 1.76 SB25							
NORMAL MODE 12	OBSERVED=	0.0 CM-1	CALCULATED=	1075.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	32.98	C-O 23.02 CCH9	14.28 H7H9 12.70 H8H9 10.41 C-C						
FORCE CONSTANTS-	32.98	C-O 30.25 HC6H	24.16 CC6H 18.04 HC6H						
OFF DIAGONAL-	7.82	BB40 -6.04 SB24 -4.44 SB23 -3.78 SB21 1.82 SS20 1.75 SB22 -1.51 SB26							
NORMAL MODE 13	OBSERVED=	0.0 CM-1	CALCULATED=	1038.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	40.99	H8H9 34.82 H7H9	5.89 CCH8						
FORCE CONSTANTS-	75.85	HC6H 10.81 CC6H							
OFF DIAGONAL-	5.92	BB40 4.48 BB34							
NORMAL MODE 14	OBSERVED=	0.0 CM-1	CALCULATED=	1011.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	55.46	H7H8 27.70 C-O	6.34 H7H9						
FORCE CONSTANTS-	66.10	HC6H 27.70 C-O							
OFF DIAGONAL-	-4.17	SB23 3.43 BB34 -2.20 SB21 1.77 BB40 -1.58 BB44							
NORMAL MODE 15	OBSERVED=	0.0 CM-1	CALCULATED=	966.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	18.64	C-C 17.06 CCH8	11.39 UCH4 10.86 H7H9 9.98 H4CC 6.89 H5CC 6.63 OCC						
FORCE CONSTANTS-	18.64	C-C 17.38 CC6H	16.87 CC3H 15.73 UCH 11.34 HC6H 6.63 CCO						
OFF DIAGONAL-	6.06	SB24 4.47 BB44 -3.04 SB26 2.41 BB37							
NORMAL MODE 16	OBSERVED=	0.0 CM-1	CALCULATED=	940.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	18.05	C-C 17.02 CCH7	14.85 UCH5 8.99 H5CC 8.59 H8H9 7.88 H4CC 6.60 HOC 5.76 UCH4 5.15 OCC						
FORCE CONSTANTS-	20.61	UCH 18.05 C-C	17.08 CC6H 16.87 CC3H 8.72 HC6H 6.60 COH 5.15 CCO						
OFF DIAGONAL-	4.88	SB24 3.42 BB44 -2.64 SB26 2.62 BB37 -2.13 BB32 -1.67 BB33 1.57 BB35							
NORMAL MODE 17	OBSERVED=	0.0 CM-1	CALCULATED=	749.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	42.97	CCH9 17.76 C-O	11.56 C-C 7.21 H7H8						
FORCE CONSTANTS-	49.61	CC6H 17.76 C-O	11.56 C-C 7.22 HC6H						
OFF DIAGONAL-	-3.66	SB22 3.35 BB35 2.98 SB24 2.54 SB23 -2.14 BB40 1.81 BB44							
NORMAL MODE 18	OBSERVED=	0.0 CM-1	CALCULATED=	666.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	33.72	CCH8 32.52 CCH7	10.13 H4CC 9.98 H5CC						
FORCE CONSTANTS-	66.25	CC6H 20.10 CC3H	9.68 HC6H 7.41 UCH						
OFF DIAGONAL-	-7.61	BB37 7.03 BB35 -5.24 BB40 1.70 BB36							
NORMAL MODE 19	OBSERVED=	0.0 CM-1	CALCULATED=	388.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	78.92	OCC 11.26 CCH9	9.72 CCH8 9.13 CCH7						
FORCE CONSTANTS-	78.92	CCO 30.12 CC6H	5.17 HC6H 5.09 CC3H						
OFF DIAGONAL-	-20.20	BB44 -4.54 BB45 2.97 SB26 -2.83 BB46 -2.04 BB37 1.83 BB43 -1.63 SB23 -1.57 SB25 -1.55 BB40							
NORMAL MODE 20	OBSERVED=	0.0 CM-1	CALCULATED=	215.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	76.79	T-CO 21.28 T-CC							
FORCE CONSTANTS-	76.79	TC-O 21.28 TC-C							
OFF DIAGONAL -	NONE								
NORMAL MODE 21	OBSERVED=	0.0 CM-1	CALCULATED=	181.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	77.87	T-CC 20.87 T-CO							
FORCE CONSTANTS-	77.87	TC-C 20.87 TC-O							
OFF DIAGONAL -	NONE								

0. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 0.0

TABLE LV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 301									
MOLECULE 6 -6 NG= 209 ETHANOL, CD3CH2OD, GAUCHE									
PAGE 1									
NORMAL MODE 7	OBSERVED=	0.0 CM-1	CALCULATED=	1483.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	75.56	HCH 6.02 H5CC	5.59 H4CC	5.43 OCH4	5.06 OCH5				
FORCE CONSTANTS-	75.56	HC3H 11.61 CC3H	10.49 OCH						
OFF DIAGONAL-	8.10	BB40 -4.76 BB38	-1.77 SB25						
NORMAL MODE 8	OBSERVED=	0.0 CM-1	CALCULATED=	1384.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	37.24	UCH5 27.47 OCH4	19.51 H5CC	18.61 H4CC	6.19 C-C	5.72 C-O			
FORCE CONSTANTS-	64.71	UCH 38.12 CC3H	6.19 C-C	5.72 C-O					
OFF DIAGONAL-	-11.70	SB22 -8.77 SB25	5.77 BB33	-3.04 BB35	1.69 BB32				
NORMAL MODE 9	OBSERVED=	0.0 CM-1	CALCULATED=	1287.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	40.54	UCH4 29.97 OCH5	16.73 H4CC	9.80 H5CC					
FORCE CONSTANTS-	70.51	UCH 26.53 CC3H							
OFF DIAGONAL-	-6.29	BB33 2.37 BB32	2.08 BB35						
NORMAL MODE 10	OBSERVED=	0.0 CM-1	CALCULATED=	1128.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	37.44	C-C 28.85 C-O	12.28 CCH7	10.83 H7H8	10.68 CCH8				
FORCE CONSTANTS-	37.44	C-C 28.85 C-O	24.40 CC6H	18.06 HC6H					
OFF DIAGONAL-	-14.68	SB24 8.23 BB40	-3.23 SS20	-3.20 BB35	2.18 SB22	-1.91 BB34	1.80 BB44	-1.74 SB23	
NORMAL MODE 11	OBSERVED=	0.0 CM-1	CALCULATED=	1107.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	36.61	HOC 13.94 H5CC	10.34 C-C	7.86 CCH9	5.62 OCC				
FORCE CONSTANTS-	36.61	COH 17.73 CC3H	12.18 CC6H	10.34 C-C	5.62 CCO				
OFF DIAGONAL-	4.79	SB21 2.32 SB25	-2.27 SB24	-2.21 SB23	-2.08 SB26	1.81 BB37	1.72 BB35		
NORMAL MODE 12	OBSERVED=	0.0 CM-1	CALCULATED=	1069.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	26.82	C-O 18.35 H7H9	16.22 CCH9	14.11 HOC	7.73 H8H9				
FORCE CONSTANTS-	29.24	HC6H 26.82 C-O	20.81 CC6H	14.11 COH	6.43 CC3H				
OFF DIAGONAL-	-7.44	SB21 6.95 BB40	-3.80 SB24	-1.86 SB23	1.68 SB22				
NORMAL MODE 13	OBSERVED=	0.0 CM-1	CALCULATED=	1035.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	48.18	H8H9 30.32 H7H9	5.05 CCH8						
FORCE CONSTANTS-	78.64	HC6H 6.93 CC6H							
OFF DIAGONAL-	4.77	BB40 4.58 BB34							
NORMAL MODE 14	OBSERVED=	0.0 CM-1	CALCULATED=	1010.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	54.97	H7H8 28.36 C-O	6.34 H7H9						
FORCE CONSTANTS-	65.45	HC6H 28.36 C-O							
OFF DIAGONAL-	-4.26	SB23 3.39 BB34	-2.19 SB21	1.69 BB40	-1.57 BB44				
NORMAL MODE 15	OBSERVED=	0.0 CM-1	CALCULATED=	966.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	22.43	C-C 16.99 CCH8	10.61 H7H9	9.56 OCH4	7.99 OCC	7.88 H4CC			
FORCE CONSTANTS-	22.43	C-C 18.01 CC6H	12.83 CC3H	12.35 OCH	11.43 HC6H	7.99 CCO			
OFF DIAGONAL-	7.25	SB24 5.37 BB44	-3.66 SB26	1.95 BB37	1.86 BB40	1.53 SB23			
NORMAL MODE 16	OBSERVED=	0.0 CM-1	CALCULATED=	877.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	39.66	HOC 14.73 C-C	12.83 OCH5	12.36 CCH7	5.78 OCH4	5.58 H4CC			
FORCE CONSTANTS-	39.66	COH 18.61 OCH	14.73 C-C	13.19 CC6H	9.31 CC3H				
OFF DIAGONAL-	-4.86	BB32 3.52 SB24	-2.18 SB21	1.83 BB37	-1.56 BB33				
NORMAL MODE 17	OBSERVED=	0.0 CM-1	CALCULATED=	744.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	43.10	CCH9 17.20 C-O	9.30 C-C	6.91 H7H8	5.81 CCH7				
FORCE CONSTANTS-	51.20	CC6H 17.20 C-O	9.30 C-C	7.00 HC6H					
OFF DIAGONAL-	-3.78	SB22 3.60 BB35	-2.46 BB40	2.42 SB24	2.37 SB23	1.84 BB44	1.61 SB21		
NORMAL MODE 18	OBSERVED=	0.0 CM-1	CALCULATED=	664.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	34.22	CCH8 30.61 CCH7	10.62 H4CC	10.02 H5CC	5.01 H7H9				
FORCE CONSTANTS-	64.91	CC6H 20.64 CC3H	9.50 HC6H	8.12 OCH					
OFF DIAGONAL-	-7.63	BB37 6.96 BB35	-5.14 BB40	1.70 BB36					
NORMAL MODE 19	OBSERVED=	0.0 CM-1	CALCULATED=	382.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	79.28	OCC 10.80 CCH9	9.43 CCH8	8.88 CCH7					
FORCE CONSTANTS-	79.28	CCO 29.12 CC6H	5.05 HC6H						
OFF DIAGONAL-	-19.95	BB44 -4.45 BB45	-2.91 BB46	2.87 SB26	-1.99 BB37	1.81 BB43	-1.56 SB23		
NORMAL MODE 20	OBSERVED=	0.0 CM-1	CALCULATED=	193.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	85.63	T-CC 13.30 T-CO							
FORCE CONSTANTS-	85.63	TC-C 13.30 TC-O							
OFF DIAGONAL-	NONE								
NORMAL MODE 21	OBSERVED=	0.0 CM-1	CALCULATED=	148.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	84.65	F-CO 13.48 T-CC							
FORCE CONSTANTS-	84.65	TC-O 13.48 TC-C							
OFF DIAGONAL-	NONE								

0. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 0.0

TABLE IV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 301										PAGE 1		
MOLECULE 7		-6 NG= 209		ETHANOL, CD3CD2OH, GAUCHE								
NORMAL MODE 7	OBSERVED=	0.0 CM-1		CALCULATED=		1392.5 CM-1		ERROR=		0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	91.02	HOC										
FORCE CONSTANTS-	91.02	COH										
OFF DIAGONAL-	3.50	BB32 -2.28 SB21										
NORMAL MODE 8	OBSERVED=	0.0 CM-1		CALCULATED=		1187.4 CM-1		ERROR=		0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	40.61	C-O 37.86	C-C	14.05	OCH4	11.44	OCH5	8.55	H5CC	8.45	H4CC	5.86 CCH7 5.32 CCH8
FORCE CONSTANTS-	40.61	C-O 37.86	C-C	25.49	OCH	17.00	CC3H	11.31	CC6H	5.41	HC6H	
OFF DIAGONAL-	-19.59	SB22-14.48	SB25	-8.09	SB24	-3.85	SS20	2.87	BB37	2.29	BB33	2.18 BB40 -2.01 BB35 -1.59 SB23
NORMAL MODE 9	OBSERVED=	0.0 CM-1		CALCULATED=		1108.2 CM-1		ERROR=		0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	50.85	HCH 15.90	C-C	10.10	C-O	9.44	CCH9					
FORCE CONSTANTS-	50.85	HC3H 15.90	C-C	10.10	C-O	9.56	CC6H	7.93	HC6H	6.72	OCH	
OFF DIAGONAL-	6.76	BB40 -4.96	SB22	-4.91	SB25	-4.22	SB24	-3.08	BB38	-3.03	SB23	-2.31 SB26
NORMAL MODE 10	OBSERVED=	0.0 CM-1		CALCULATED=		1066.7 CM-1		ERROR=		0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	16.25	CCH9 13.46	HCH	12.99	H8H9	11.02	H7H9	8.82	CCH8	7.68	CCH7	6.81 H5CC 6.75 H4CC 5.51 C-O
FORCE CONSTANTS-	32.74	CC6H 27.15	HC6H	13.55	CC3H	13.46	HC3H	5.51	C-O			
OFF DIAGONAL-	15.68	BB40 -6.21	BB35	-5.80	SB24	4.15	SB25	-3.12	BB37	-2.87	BB34	-1.96 SB22 -1.67 BB36
NORMAL MODE 11	OBSERVED=	0.0 CM-1		CALCULATED=		1038.2 CM-1		ERROR=		0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	41.49	H7H9 38.22	H8H9									
FORCE CONSTANTS-	79.77	HC6H 8.07	CC6H									
OFF DIAGONAL-	5.26	BB40 4.72	BB34									
NORMAL MODE 12	OBSERVED=	0.0 CM-1		CALCULATED=		1028.0 CM-1		ERROR=		0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	58.00	H7H8 8.83	H8H9	5.90	OCH4	5.59	H7H9	5.08	HCH			
FORCE CONSTANTS-	72.41	HC6H 10.63	OCH	5.08	HC3H							
OFF DIAGONAL-	3.97	BB34 2.82	BB40	-1.73	SB22							
NORMAL MODE 13	OBSERVED=	0.0 CM-1		CALCULATED=		960.8 CM-1		ERROR=		0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	33.30	C-O 24.96	OCH4	6.36	OCC	5.89	OCH5					
FORCE CONSTANTS-	33.30	C-O 30.86	OCH	8.65	HC6H	6.36	CCO					
OFF DIAGONAL-	18.47	SB22 -6.56	SB23	-4.41	SB21	-2.52	BB46	2.19	BB33	-2.09	SB25	-1.73 BB38 -1.64 BB40 1.58 BB44
NORMAL MODE 14	OBSERVED=	0.0 CM-1		CALCULATED=		920.8 CM-1		ERROR=		0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	31.27	OCH5 24.94	H5CC	15.98	OCH4	13.87	H4CC					
FORCE CONSTANTS-	47.25	OCH 38.80	CC3H	7.21	CC6H							
OFF DIAGONAL-	-4.04	BB33 3.59	BB35	3.48	BB37	-1.64	BB32					
NORMAL MODE 15	OBSERVED=	0.0 CM-1		CALCULATED=		908.4 CM-1		ERROR=		0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	26.37	C-C 10.61	CCH8	9.79	H4CC	6.17	OCC	6.01	C-O			
FORCE CONSTANTS-	26.37	C-C 15.90	CC6H	11.27	CC3H	6.17	CCO	6.01	C-O			
OFF DIAGONAL-	9.00	SB25 5.86	SB24	4.72	BB44	-3.49	SB26	2.74	SB23	2.60	BB37	2.44 BB40
NORMAL MODE 16	OBSERVED=	0.0 CM-1		CALCULATED=		848.5 CM-1		ERROR=		0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	22.83	OCH5 20.09	CCH7	19.99	OCH4	13.89	CCH8	5.20	H8H9			
FORCE CONSTANTS-	42.82	OCH 33.97	CC6H	9.01	CC3H	8.22	HC6H					
OFF DIAGONAL-	-3.86	BB33 3.64	BB37	3.46	BB35	-3.35	BB40	-2.00	BB32			
NORMAL MODE 17	OBSERVED=	0.0 CM-1		CALCULATED=		740.5 CM-1		ERROR=		0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	40.65	CCH9 14.38	C-O	14.32	C-C	7.24	H7H8					
FORCE CONSTANTS-	46.20	CC6H 14.38	C-O	14.32	C-C	7.25	HC6H	5.22	OCH			
OFF DIAGONAL-	-5.25	SB22 3.50	SB24	2.91	BB35	2.29	SB25	2.21	SB23	-1.87	BB40	1.59 BB44
NORMAL MODE 18	OBSERVED=	0.0 CM-1		CALCULATED=		590.8 CM-1		ERROR=		0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	22.38	CCH8 21.10	H4CC	20.34	H5CC	20.33	CCH7	6.53	OCH5	6.31	OCH4	
FORCE CONSTANTS-	42.74	CC6H 41.44	CC3H	12.84	OCH	6.02	HC6H					
OFF DIAGONAL-	-8.77	BB37 6.84	BB35	-3.32	BB40	1.96	BB36					
NORMAL MODE 19	OBSERVED=	0.0 CM-1		CALCULATED=		385.1 CM-1		ERROR=		0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	79.43	OCC 11.29	CCH9	9.35	CCH8	9.26	CCH7					
FORCE CONSTANTS-	79.43	CCO 29.90	CC6H	5.87	CC3H	5.12	HC6H					
OFF DIAGONAL-	-20.13	BB44 -4.55	BB45	-2.80	BB46	2.70	SB26	-2.18	BB37	1.97	BB43	-1.81 SB23 -1.53 SB25
NORMAL MODE 20	OBSERVED=	0.0 CM-1		CALCULATED=		211.3 CM-1		ERROR=		0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	85.92	T-CO 12.25	T-CC									
FORCE CONSTANTS-	85.92	TC-O 12.25	TC-C									
OFF DIAGONAL -	NONE											
NORMAL MODE 21	OBSERVED=	0.0 CM-1		CALCULATED=		177.5 CM-1		ERROR=		0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	86.25	T-CC 11.98	T-CO									
FORCE CONSTANTS-	86.25	TC-C 11.98	TC-O									
OFF DIAGONAL -	NONE											

0. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 0.0

TABLE IV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 301
MOLECULE 8 -6 NG= 209 ETHANOL, CD3CD2OD, GAUCHE

PAGE 1

NORMAL MODE 7	OBSERVED=	0.0 CM-1	CALCULATED=	1196.6 CM-1	ERROR=	0.0 CM-1 OR	0.0 PERCENT
INTERNAL COORDINATES-	41.98	C-C 35.16 C-O	16.31	OCH5 9.94 H4CC 9.38	OCH4 9.11 H5CC 8.58	HOC	
FORCE CONSTANTS-	41.98	C-C 35.16 C-O	25.69	OCH 19.05 CC3H 8.58	COH 7.78 CC6H		
OFF DIAGONAL-	-18.15	SB22-16.14 SB25	-7.57	SB24 -6.65 SB21 -3.77	SS20 2.55 BB32 2.53 BB37	2.52 BB40 2.23 BB33	
NORMAL MODE 8	OBSERVED=	0.0 CM-1	CALCULATED=	1126.4 CM-1	ERROR=	0.0 CM-1 OR	0.0 PERCENT
INTERNAL COORDINATES-	37.67	HCH 15.58 HOC	12.62	C-O 7.39 OCH4 7.33	OCC		
FORCE CONSTANTS-	37.67	HC3H 15.58 COH	12.62	C-O 8.48 CC6H 7.63	OCH 7.33 CCO		
OFF DIAGONAL-	5.37	SB21 -4.91 SB22	-4.34	SB23 3.36 BB40 2.68	BB44 -2.35 BB38		
NORMAL MODE 9	OBSERVED=	0.0 CM-1	CALCULATED=	1084.5 CM-1	ERROR=	0.0 CM-1 OR	0.0 PERCENT
INTERNAL COORDINATES-	21.93	HOC 16.50 H7H9	13.16	CCH9 12.99 C-C 10.95	OCH5 10.90 CCH7 6.44	H8H9 5.51 C-O	
FORCE CONSTANTS-	27.73	CC6H 24.56 HC6H	21.93	COH 12.99 C-C 10.98	OCH 5.51 C-O		
OFF DIAGONAL-	9.85	BB40 -9.59 SB24	-4.21	SB21 -4.13 BB35 -3.53	SB22 3.34 BB32 -2.21	BB34	
NORMAL MODE 10	OBSERVED=	0.0 CM-1	CALCULATED=	1055.0 CM-1	ERROR=	0.0 CM-1 OR	0.0 PERCENT
INTERNAL COORDINATES-	21.84	HCH 20.13 H8H9	12.81	HOC 6.39 CCH9 6.49	CCH8 6.18 H4CC 6.01	H5CC	
FORCE CONSTANTS-	21.84	HC3H 20.40 HC6H	14.82	CC6H 12.81 COH 12.18	CC3H 6.23 OCH		
OFF DIAGONAL-	9.77	BB40 -2.34 BB35	2.23	SB21			
NORMAL MODE 11	OBSERVED=	0.0 CM-1	CALCULATED=	1034.2 CM-1	ERROR=	0.0 CM-1 OR	0.0 PERCENT
INTERNAL COORDINATES-	45.49	H7H9 18.53 H8H9	6.32	H7H8 6.03 HCH			
FORCE CONSTANTS-	70.24	HC6H 6.03 HC3H	5.80	CC6H			
OFF DIAGONAL-	4.54	BB40 4.15 BB34					
NORMAL MODE 12	OBSERVED=	0.0 CM-1	CALCULATED=	1025.8 CM-1	ERROR=	0.0 CM-1 OR	0.0 PERCENT
INTERNAL COORDINATES-	52.71	H7H8 19.27 H8H9	7.27	OCH4			
FORCE CONSTANTS-	72.11	HC6H 8.40 OCH					
OFF DIAGONAL-	3.89	BB34 2.47 BB40	-2.01	SB22			
NORMAL MODE 13	OBSERVED=	0.0 CM-1	CALCULATED=	958.6 CM-1	ERROR=	0.0 CM-1 OR	0.0 PERCENT
INTERNAL COORDINATES-	32.30	C-O 31.94 OCH4	5.66	HOC 5.23 OCC			
FORCE CONSTANTS-	34.49	OCH 32.30 C-O	7.64	HC6H 5.66 COH 5.23	CCO		
OFF DIAGONAL-	17.76	SB22 -5.86 SB23	-5.18	SB21 -2.23 BB46 -2.10	SB25 1.63 BB33		
NORMAL MODE 14	OBSERVED=	0.0 CM-1	CALCULATED=	917.2 CM-1	ERROR=	0.0 CM-1 OR	0.0 PERCENT
INTERNAL COORDINATES-	29.82	H5CC 24.88 OCH5	8.10	CCH7 7.81 OCH4 7.71	H4CC 5.68 C-O		
FORCE CONSTANTS-	37.52	CC3H 32.69 OCH	9.53	CC6H 5.68 C-O			
OFF DIAGONAL-	3.88	BB37 3.10 BB35	-2.52	BB33 2.25 SB22 -1.91	BB32 1.71 SB25 -1.62	SB21	
NORMAL MODE 15	OBSERVED=	0.0 CM-1	CALCULATED=	902.8 CM-1	ERROR=	0.0 CM-1 OR	0.0 PERCENT
INTERNAL COORDINATES-	23.05	C-C 17.83 CCH8	17.22	H4CC			
FORCE CONSTANTS-	23.05	C-C 19.14 CC6H	17.78	CC3H 5.37 HC6H			
OFF DIAGONAL-	6.59	SB25 5.12 SB24	3.73	BB44 3.59 BB37 -2.86	SB26 1.74 SB23		
NORMAL MODE 16	OBSERVED=	0.0 CM-1	CALCULATED=	816.2 CM-1	ERROR=	0.0 CM-1 OR	0.0 PERCENT
INTERNAL COORDINATES-	20.33	HOC 19.81 OCH5	18.92	OCH4 18.29 CCH7 9.69	CCH8 5.90 C-C		
FORCE CONSTANTS-	38.72	OCH 28.41 CC6H	20.33	COH 6.58 HC6H 5.90	C-C		
OFF DIAGONAL-	-4.33	BB32 -3.50 BB33	2.24	BB35 -2.18 BB40 1.70	BB37 -1.56 SB21		
NORMAL MODE 17	OBSERVED=	0.0 CM-1	CALCULATED=	735.6 CM-1	ERROR=	0.0 CM-1 OR	0.0 PERCENT
INTERNAL COORDINATES-	40.55	CCH9 13.84 C-O	11.45	C-C 6.86 H7H8 6.45	CCH7 5.02 OCH5		
FORCE CONSTANTS-	48.15	CC6H 13.84 C-O	11.45	C-C 7.04 HC6H 6.01	OCH		
OFF DIAGONAL-	-5.19	SB22 3.21 BB35	2.81	SB24 -2.27 BB40 2.15	SB25 2.02 SB23 1.79	SB21 1.61 BB44	
NORMAL MODE 18	OBSERVED=	0.0 CM-1	CALCULATED=	587.1 CM-1	ERROR=	0.0 CM-1 OR	0.0 PERCENT
INTERNAL COORDINATES-	22.60	CC6H 21.75 H4CC	19.64	H5CC 17.91 CCH7 7.49	OCH5 6.95 OCH4		
FORCE CONSTANTS-	41.39	CC3H 40.66 CC6H	14.44	OCH 5.74 HC6H			
OFF DIAGONAL-	-8.53	BB37 6.66 BB35	-3.15	BB40 1.91 BB36			
NORMAL MODE 19	OBSERVED=	0.0 CM-1	CALCULATED=	379.1 CM-1	ERROR=	0.0 CM-1 OR	0.0 PERCENT
INTERNAL COORDINATES-	79.73	OCC 10.81 CCH9	9.16	CCH7 8.89 CCH8			
FORCE CONSTANTS-	79.73	CCO 28.86 CC6H	5.75	CC3H			
OFF DIAGONAL-	-19.87	BB44 -4.47 BB45	-2.88	BB46 2.61 SB26 -2.12	BB37 1.95 BB43 -1.74	SB23	
NORMAL MODE 20	OBSERVED=	0.0 CM-1	CALCULATED=	185.3 CM-1	ERROR=	0.0 CM-1 OR	0.0 PERCENT
INTERNAL COORDINATES-	86.12	T-CC 12.50 T-CO					
FORCE CONSTANTS-	86.12	TC-C 12.50 TC-O					
OFF DIAGONAL-	NONE						
NORMAL MODE 21	OBSERVED=	0.0 CM-1	CALCULATED=	148.2 CM-1	ERROR=	0.0 CM-1 OR	0.0 PERCENT
INTERNAL COORDINATES-	85.76	T-CO 12.41 T-CC					
FORCE CONSTANTS-	85.76	TC-O 12.41 TC-C					
OFF DIAGONAL-	NONE						

O. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 0.0

TABLE IV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 301									
MOLECULE 9 -6 NG= 209 ETHANOL, CH3CHDOH, GAUCHE, D4									
PAGE 1									
NORMAL MODE 7	OBSERVED=	0.0 CM-1	CALCULATED=	1459.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	33.40 H8H9 30.85 H7H8	8.55 HOC	7.00 CCH7	5.06 CCH9					
FORCE CONSTANTS-	64.57 HC6H 12.05 CC6H	8.55 COH							
OFF DIAGONAL-	5.83 BB40 3.81 BB34								
NORMAL MODE 8	OBSERVED=	0.0 CM-1	CALCULATED=	1455.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	43.71 H7H9 18.28 H7H8	7.24 CCH8	5.96 H8H9	5.10 HOC					
FORCE CONSTANTS-	67.95 HC6H 10.92 CC6H	5.10 COH							
OFF DIAGONAL-	5.50 BB40 4.02 BB34								
NORMAL MODE 9	OBSERVED=	0.0 CM-1	CALCULATED=	1434.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	49.26 HOC 21.14 OCH5	9.64 H8H9	6.39 H7H9	5.11 H5CC					
FORCE CONSTANTS-	49.26 COH 21.18 OCH	16.31 HC6H	5.81 CC3H						
OFF DIAGONAL-	6.96 BB32 -2.65 SB21	-2.05 SB22	-1.77 SB25						
NORMAL MODE 10	OBSERVED=	0.0 CM-1	CALCULATED=	1381.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	18.99 CCH7 17.87 CCH8	17.27 H8H9	14.96 H7H9	13.40 CCH9	8.27 H7H8	7.80 C-C			
FORCE CONSTANTS-	50.27 CC6H 40.50 HC6H	7.80 C-C							
OFF DIAGONAL-	16.27 BB40 -10.30 SB24	-8.21 BB35	-4.63 BB34	-1.81 SB25	1.52 BB44				
NORMAL MODE 11	OBSERVED=	0.0 CM-1	CALCULATED=	1320.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	65.69 HCH 20.95 H5CC								
FORCE CONSTANTS-	65.69 HC3H 23.14 CC3H								
OFF DIAGONAL-	9.47 BB40 -3.71 SB25	-2.19 BB38							
NORMAL MODE 12	OBSERVED=	0.0 CM-1	CALCULATED=	1296.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	38.53 OCH5 24.28 HOC	21.22 H5CC	6.81 H7H8	5.35 C-O	5.11 CCH9				
FORCE CONSTANTS-	42.80 OCH 24.28 COH	21.65 CC3H	7.23 HC6H	6.05 CC6H	5.35 C-O				
OFF DIAGONAL-	-8.25 SB22 -6.59 BB32	4.36 SB21	2.32 BB33	-2.15 BB38	-1.74 BB40				
NORMAL MODE 13	OBSERVED=	0.0 CM-1	CALCULATED=	1126.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	48.84 C-O 12.34 C-C	10.71 CCH9	10.12 OCH4	9.22 H4CC	5.61 HOC	5.52 H7H8			
FORCE CONSTANTS-	48.84 C-O 14.62 CC6H	13.94 OCH	12.34 C-C	10.91 CC3H	6.69 HC6H	5.61 COH			
OFF DIAGONAL-	-6.33 SB21 -3.89 SB23	-3.69 SB22	-2.46 SB25	-2.41 SS20	-1.79 BB40	1.71 BB35			
NORMAL MODE 14	OBSERVED=	0.0 CM-1	CALCULATED=	1054.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	45.54 C-C 15.48 CCH9	9.68 CCH7	8.75 OCC	6.56 OCH4	5.55 HOC				
FORCE CONSTANTS-	45.54 C-C 25.34 CC6H	10.00 OCH	8.75 CCO	6.83 HC6H	5.55 COH				
OFF DIAGONAL-	-5.46 SB26 3.88 BB44	-3.80 SB25	-2.74 BB40	2.24 BB35	1.77 BB45	-1.76 BB46			
NORMAL MODE 15	OBSERVED=	0.0 CM-1	CALCULATED=	1014.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	31.69 CCH8 20.85 CCH7	7.83 H4CC	6.91 H7H9	6.50 C-C	6.43 C-O	5.09 H8H9			
FORCE CONSTANTS-	53.81 CC6H 12.18 HC6H	8.45 CC3H	6.50 C-C	6.43 C-O					
OFF DIAGONAL-	-4.79 BB40 4.74 BB35	4.03 BB37	2.07 SB25						
NORMAL MODE 16	OBSERVED=	0.0 CM-1	CALCULATED=	934.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	50.85 OCH4 18.06 C-O	11.12 H4CC							
FORCE CONSTANTS-	55.69 OCH 18.06 C-O	11.14 CC3H	6.05 CC6H						
OFF DIAGONAL-	9.03 SB22 -2.83 BB33								
NORMAL MODE 17	OBSERVED=	0.0 CM-1	CALCULATED=	877.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	32.12 C-O 28.73 C-C	19.28 CCH9	8.74 OCH4	5.72 CCH7					
FORCE CONSTANTS-	32.12 C-O 28.73 C-C	27.63 CC6H	8.74 OCH						
OFF DIAGONAL-	-7.29 SB22 4.73 SB25	2.98 SS20	-2.44 BB40	-2.33 SB21	2.06 BB35	-1.88 SB23			
NORMAL MODE 18	OBSERVED=	0.0 CM-1	CALCULATED=	706.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	33.88 H4CC 19.34 H5CC	11.42 OCH4	10.85 OCH5	9.88 CCH8	9.03 CCH7				
FORCE CONSTANTS-	53.22 CC3H 22.27 OCH	18.94 CC6H							
OFF DIAGONAL-	-6.57 BB37 5.69 BB35	-2.01 BB33							
NORMAL MODE 19	OBSERVED=	0.0 CM-1	CALCULATED=	435.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	86.85 OCC 6.90 CCH9	6.33 CCH8	5.70 CCH7						
FORCE CONSTANTS-	86.85 CCO 18.93 CC6H	5.64 CC3H							
OFF DIAGONAL-	-16.92 BB44 -3.72 BB45	-3.31 BB46	3.12 SB26	2.01 BB43	-1.71 BB37	-1.65 SB25			
NORMAL MODE 20	OBSERVED=	0.0 CM-1	CALCULATED=	247.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	91.25 T-CC 7.53 T-CO								
FORCE CONSTANTS-	91.25 TC-C 7.53 TC-O								
OFF DIAGONAL-	NONE								
NORMAL MODE 21	OBSERVED=	0.0 CM-1	CALCULATED=	205.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	90.91 T-CO 7.39 T-CC								
FORCE CONSTANTS-	90.91 TC-O 7.39 TC-C								
OFF DIAGONAL-	NONE								

0. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 0.0

TABLE LV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 301									
MOLECULE 10 -6 NG= 209 ETHANOL, CH3CHODD, GAUCHE, D4									
PAGE 1									
NORMAL MODE 7	OBSERVED=	0.0 CM-1	CALCULATED=	1457.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	48.93	H7H8 15.93 H8H9	7.99	CCH9 7.24 H7H9					
FORCE CONSTANTS-	72.10	HC6H 13.20 CC6H							
OFF DIAGONAL-	6.31	BB40 4.26 BB34							
NORMAL MODE 8	OBSERVED=	0.0 CM-1	CALCULATED=	1452.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	42.62	H7H9 33.61 H8H9	6.18	CCH8					
FORCE CONSTANTS-	46.15	CC6H 37.37 HC6H	9.65	C-C 7.12 OCH					
OFF DIAGONAL-	6.04	BB40 4.54 BB34							
NORMAL MODE 9	OBSERVED=	0.0 CM-1	CALCULATED=	1383.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	17.88	CCH7 16.26 CCH8	15.24	H7H9 15.19 H8H9 12.00	CCH9 9.65	C-C 6.94	H7H8 6.71	DOH5	
FORCE CONSTANTS-	57.17	CC6H 37.37 HC6H	9.65	C-C 7.12 OCH					
OFF DIAGONAL-	16.64	BB40-10.96 SB24	-7.66	BB35 -4.23 BB34 -3.34	SB25 2.32	BB37 -1.66	SB22		
NORMAL MODE 10	OBSERVED=	0.0 CM-1	CALCULATED=	1348.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	55.92	DOH5 26.49 H5CC	5.08	H7H8					
FORCE CONSTANTS-	57.17	DOH 28.07 CC3H	7.40	CC6H 6.81 HC6H					
OFF DIAGONAL-	-7.07	SB22 3.10 BB32	-3.03	SB25 -2.16 BB35 1.95	BB40 1.62	SB24 -1.58	BB37 1.51	BB33	
NORMAL MODE 11	OBSERVED=	0.0 CM-1	CALCULATED=	1319.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	69.55	HCH 13.70 H5CC	8.85	DOH5					
FORCE CONSTANTS-	69.55	HC3H 15.41 CC3H	9.48	DOH					
OFF DIAGONAL-	8.00	BB40 -3.76 BB38	-2.77	SB25					
NORMAL MODE 12	OBSERVED=	0.0 CM-1	CALCULATED=	1150.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	22.84	C-C 18.62 CCH9	15.35	HOC 9.81 H7H8 8.76	DOH4 8.01	OCC			
FORCE CONSTANTS-	23.49	CC6H 22.84 C-C	15.35	COH 11.86 HC6H 10.72	DOH 8.01	CCO			
OFF DIAGONAL-	7.17	SB21 -6.09 SB23	-3.26	BB40 -3.22 SB22 2.65	BB44 1.86	BB45			
NORMAL MODE 13	OBSERVED=	0.0 CM-1	CALCULATED=	1112.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	31.95	C-C 26.19 C-C	18.23	HOC 11.79 H4CC 5.63	H5CC				
FORCE CONSTANTS-	31.95	C-C 26.19 C-C	18.23	COH 17.42 CC3H 9.32	CC6H 5.38	DOH			
OFF DIAGONAL-	-8.36	SB21 -3.29 SB22	-2.84	SS20 2.59	BB37 -2.42	SB25 2.07	BB35 1.92	SB23	
NORMAL MODE 14	OBSERVED=	0.0 CM-1	CALCULATED=	1023.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	28.38	C-C 24.41 CCH8	11.17	DOH4 8.90 CCH9 5.72	H7H9 5.03	HOC			
FORCE CONSTANTS-	37.72	CC6H 28.38 C-C	11.26	DOH 8.94 HC6H 5.03	COH				
OFF DIAGONAL-	-3.75	BB40 3.22 BB35	-2.64	SB26 1.91	BB44				
NORMAL MODE 15	OBSERVED=	0.0 CM-1	CALCULATED=	987.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	32.74	HOC 18.61 DOH4	15.33	C-C 12.18 CCH7 11.74	H4CC 5.52	CCH8			
FORCE CONSTANTS-	32.74	COH 19.50 DOH	18.85	CC6H 15.33 C-C 11.85	CC3H				
OFF DIAGONAL-	8.87	SB22 -8.58 SB21	-1.83	BB31 -1.78	BB40 -1.61	SB25			
NORMAL MODE 16	OBSERVED=	0.0 CM-1	CALCULATED=	904.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	25.62	DOH4 18.87 HOC	12.71	CCH7 10.42 C-C 7.66	H4CC 5.60	DOH5			
FORCE CONSTANTS-	31.22	DOH 18.87 COH	18.46	CC6H 10.42 C-C 8.77	CC3H				
OFF DIAGONAL-	5.37	SB21 3.75 SB22	-2.22	BB32 -2.16	BB33 1.98	BB35 -1.70	BB37 -1.70	BB40 1.63	BB31
NORMAL MODE 17	OBSERVED=	0.0 CM-1	CALCULATED=	876.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	31.42	C-C 29.62 C-C	18.40	CCH9 9.66 DOH4					
FORCE CONSTANTS-	31.42	C-C 29.62 C-C	26.12	CC6H 9.67 DOH					
OFF DIAGONAL-	-7.34	SB22 4.88 SB25	3.00	SS20 -2.93	SB21 -2.32	BB40 1.94	BB35 -1.79	SB23	
NORMAL MODE 18	OBSERVED=	0.0 CM-1	CALCULATED=	695.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	32.90	H4CC 17.38 H5CC	13.04	DOH4 12.06 DOH5 9.49	CCH8 6.62	CCH7 5.63	HOC		
FORCE CONSTANTS-	50.28	CC3H 25.09 DOH	16.29	CC6H 5.63 COH					
OFF DIAGONAL-	-5.92	BB37 5.20 BB35	-2.26	BB33 -1.78	BB32				
NORMAL MODE 19	OBSERVED=	0.0 CM-1	CALCULATED=	427.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	86.42	OCC 6.60 CCH9	6.03	CCH8 5.62 CCH7					
FORCE CONSTANTS-	86.42	CCO 18.25 CC6H	5.36	CC3H					
OFF DIAGONAL-	-16.61	BB44 -3.63 BB45	-3.33	BB46 2.96	SB26 1.96	BB43 -1.65	BB37 -1.54	SB25	
NORMAL MODE 20	OBSERVED=	0.0 CM-1	CALCULATED=	244.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	96.94	T-CC							
FORCE CONSTANTS-	96.94	TC-C							
OFF DIAGONAL -	NONE								
NORMAL MODE 21	OBSERVED=	0.0 CM-1	CALCULATED=	153.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	96.85	T-CO							
FORCE CONSTANTS-	96.85	TC-O							
OFF DIAGONAL -	NONE								

0. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 0.0

TABLE LV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 301									
MOLECULE 11 -6 NG= 209 ETHANOL, CD3CHDOH, GAUCHE, D4									
PAGE 1									
NORMAL MODE 7	OBSERVED=	0.0 CM-1	CALCULATED=	1438.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	62.84	HOC 25.40 OCH5	5.70	H5CC					
FORCE CONSTANTS-	62.84	COH 25.41 OCH	6.49	CC3H					
OFF DIAGONAL-	8.61	BB32 -2.84 SB21	-2.06	SB22 -2.04	SB25				
NORMAL MODE 8	OBSERVED=	0.0 CM-1	CALCULATED=	1320.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	69.21	HCH 16.95 H5CC	5.39	UCH5					
FORCE CONSTANTS-	69.21	HC3H 19.13 CC3H	5.89	UCH					
OFF DIAGONAL-	9.00	BB40 -3.57 SB25	-3.01	BB38					
NORMAL MODE 9	OBSERVED=	0.0 CM-1	CALCULATED=	1296.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	40.13	UCH5 26.66 HOC	26.37	H5CC	7.25	C-0			
FORCE CONSTANTS-	45.11	UCH 27.31 CC3H	26.66	COH	7.25	C-0			
OFF DIAGONAL-	-9.95	SB22 -7.05 BB32	5.32	SB21 -4.04	SB25 2.55	BB33 -1.67	BB40 -1.52	BB38	
NORMAL MODE 10	OBSERVED=	0.0 CM-1	CALCULATED=	1142.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	40.16	C-C 30.10 C-0	9.39	CCH8	7.44	H7H8	7.27	UCH4 7.26	CCH7
FORCE CONSTANTS-	40.16	C-C 30.10 C-0	17.53	CC6H	12.82	HC6H	10.05	UCH	6.36 CC3H
OFF DIAGONAL-	-12.78	SB24 5.74 BB40	-3.73	SB21 -3.42	SS20 -2.43	SB22 -2.00	SB25 -1.76	BB35	
NORMAL MODE 11	OBSERVED=	0.0 CM-1	CALCULATED=	1073.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	26.37	C-0 24.20 CCH9	19.24	H8H9	12.59	H7H9	9.85	C-C	
FORCE CONSTANTS-	33.09	HC6H 27.96 CC6H	26.37	C-0	9.85	C-C			
OFF DIAGONAL-	9.69	BB40 -7.23 SB24	-3.67	SB21 -2.77	SB23 -2.51	BB35 1.58	SS20 1.54	SB25	
NORMAL MODE 12	OBSERVED=	0.0 CM-1	CALCULATED=	1038.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	44.26	H7H9 33.18 H8H9	5.60	CCH8					
FORCE CONSTANTS-	79.16	HC6H 8.42 CC6H							
OFF DIAGONAL-	5.32	BB40 4.67 BB34							
NORMAL MODE 13	OBSERVED=	0.0 CM-1	CALCULATED=	1019.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	56.13	H7H8 11.47 C-0	9.11	UCH4	6.96	CCH7	6.80	H8H9 5.80	H4CC
FORCE CONSTANTS-	63.44	HC6H 11.47 C-0	9.31	CC6H	9.21	UCH	5.92	CC3H	
OFF DIAGONAL-	4.41	BB40 -3.95 SB22	2.72	BB34					
NORMAL MODE 14	OBSERVED=	0.0 CM-1	CALCULATED=	973.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	19.80	UCH4 15.52 C-C	14.05	C-0	11.05	H4CC	10.88	UCH 7.27	CCH7 5.22
FORCE CONSTANTS-	20.30	UCH 15.52 C-C	14.05	C-0	12.84	HC6H	12.52	CC3H 10.88	CC0 8.43
OFF DIAGONAL-	8.33	SB22 -5.57 SB23	4.49	BB44	3.83	SB24 -3.55	SB26 -3.36	SB25 -2.83	SB21 -2.29
NORMAL MODE 15	OBSERVED=	0.0 CM-1	CALCULATED=	916.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	19.72	C-C 17.81 UCH4	12.31	H4CC	8.13	CCH8	7.40	C-0	
FORCE CONSTANTS-	20.75	UCH 19.72 C-C	12.33	CC3H	11.23	CC6H	7.40	C-0	
OFF DIAGONAL-	6.05	SB25 4.78 SB24	3.24	BB44	2.94	SB22 2.43	SB23 -2.41	SB26 2.04	BB37
NORMAL MODE 16	OBSERVED=	0.0 CM-1	CALCULATED=	874.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	22.88	UCH4 17.68 CCH8	13.05	CCH7	11.16	H4CC	9.99	UCH5 6.80	H5CC
FORCE CONSTANTS-	32.86	UCH 31.03 CC6H	17.97	CC3H	7.96	HC6H			
OFF DIAGONAL-	4.89	BB37 3.94 BB35	-3.01	BB40 -2.73	BB33				
NORMAL MODE 17	OBSERVED=	0.0 CM-1	CALCULATED=	745.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	41.63	CCH9 16.07 C-0	12.89	C-C	7.19	H7H8	5.14	CCH7	
FORCE CONSTANTS-	48.19	CC6H 16.07 C-0	12.89	C-C	7.26	HC6H			
OFF DIAGONAL-	-4.53	SB22 3.23 SB24	3.18	BB35	2.38	SB23 -2.04	BB40 1.69	BB44	
NORMAL MODE 18	OBSERVED=	0.0 CM-1	CALCULATED=	620.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	25.40	CCH7 24.58 CCH8	20.51	H4CC	12.76	H5CC	5.69	UCH4 5.66	UCH5
FORCE CONSTANTS-	50.02	CC6H 33.27 CC3H	11.35	UCH	7.11	HC6H			
OFF DIAGONAL-	-8.44	BB37 6.69 BB35	-3.69	BB40 1.90	BB36				
NORMAL MODE 19	OBSERVED=	0.0 CM-1	CALCULATED=	387.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	79.11	UCH 11.31 CCH9	10.04	CCH8	8.74	CCH7			
FORCE CONSTANTS-	79.11	CC0 30.09 CC6H	5.53	CC3H	5.16	HC6H			
OFF DIAGONAL-	-20.18	BB44 -4.55 BB45	2.83	SB26 -2.75	BB46 -2.12	BB37 1.90	BB43 -1.71	SB23 -1.56	BB40 -1.55
NORMAL MODE 20	OBSERVED=	0.0 CM-1	CALCULATED=	212.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	82.45	T-CO 15.59 T-C							
FORCE CONSTANTS-	82.45	TC-0 15.59 TC-C							
OFF DIAGONAL -	NONE								
NORMAL MODE 21	OBSERVED=	0.0 CM-1	CALCULATED=	179.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	83.20	T-CC 15.31 T-CO							
FORCE CONSTANTS-	83.20	TC-C 15.31 TC-0							
OFF DIAGONAL -	NONE								

0. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 0.0

TABLE LV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 301									
MOLECULE 12 -6 NG= 209 ETHANOL, CD3CHDOO, GAUCHE, D4									
PAGE 1									
NORMAL MODE 7	OBSERVED=	0.0 CM-1	CALCULATED=	1351.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	66.38	OCH5 28.05 H5CC	5.68	C-C 5.56 C-O					
FORCE CONSTANTS-	68.19	OCH 29.96 CC3H	5.68	C-C 5.56 C-O					
OFF DIAGONAL-	-9.65	SB22 -6.42 SB25	3.49	BB32 1.98 BB33 -1.79	SB21				
NORMAL MODE 8	OBSERVED=	0.0 CM-1	CALCULATED=	1320.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	70.00	HCH 15.36 H5CC	6.71	OCH5					
FORCE CONSTANTS-	70.00	HC3H 17.40 CC3H	7.32	OCH					
OFF DIAGONAL-	8.66	BB40 -3.37 BB38	-3.24	SB25					
NORMAL MODE 9	OBSERVED=	0.0 CM-1	CALCULATED=	1146.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	35.25	C-O 28.53 C-C	11.97	OCH4 10.21 CCH7 7.52	CCH8 7.09 H7H8				
FORCE CONSTANTS-	35.25	C-O 28.53 C-C	17.74	CC6H 13.82 OCH 10.99	HC6H				
OFF DIAGONAL-	-9.68	SB24 -5.37 SB22	4.78	BB40 -3.99 SB25 -3.11	SS20 -3.03 SB23 2.97 SB21 2.49 BB44 1.65 SB26				
NORMAL MODE 10	OBSERVED=	0.0 CM-1	CALCULATED=	1107.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	32.67	HOC 23.42 C-C	12.64	CCH9 8.18 H5CC 5.83	H8H9 5.43 OCC				
FORCE CONSTANTS-	32.67	COH 23.42 C-C	16.30	CC6H 8.66 CC3H 8.38	HC6H 5.43 CCO				
OFF DIAGONAL-	-7.24	SB24 4.24 SB25	3.50	BB40 3.12 SB21 -3.08	SB26				
NORMAL MODE 11	OBSERVED=	0.0 CM-1	CALCULATED=	1059.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	22.79	HOC 20.34 H7H9	19.80	C-O 13.07 CCH9 9.65	H8H9 6.71 CCH7				
FORCE CONSTANTS-	32.38	HC6H 22.79 COH	20.15	CC6H 19.80 C-O 5.07	CC3H				
OFF DIAGONAL-	-8.13	SB21 7.50 BB40	-1.83	SB24 -1.74 BB35					
NORMAL MODE 12	OBSERVED=	0.0 CM-1	CALCULATED=	1036.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	41.48	H8H9 34.94 H7H9	6.30	CCH8					
FORCE CONSTANTS-	77.68	HC6H 6.99 CC6H							
OFF DIAGONAL-	4.75	BB40 4.43 BB34							
NORMAL MODE 13	OBSERVED=	0.0 CM-1	CALCULATED=	1019.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	56.07	H7H8 11.44 C-O	9.36	OCH4 7.81 H8H9 6.45	CCH7 5.55 H4CC				
FORCE CONSTANTS-	64.31	HC6H 11.44 C-O	9.49	OCH 8.63 CC6H 5.62	CC3H				
OFF DIAGONAL-	4.13	BB40 -3.93 SB22	2.84	BB34					
NORMAL MODE 14	OBSERVED=	0.0 CM-1	CALCULATED=	964.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	34.13	OCH4 20.63 C-O	10.74	H4CC 9.79 HOC 8.43	C-C 6.39 OCC				
FORCE CONSTANTS-	34.13	OCH 20.63 C-O	10.94	CC3H 9.79 COH 8.63	HC6H 8.43 C-C 6.39 CCO				
OFF DIAGONAL-	11.41	SB22 -5.44 SB21	-5.17	SB23 -3.32 SB25 2.27	BB44 -2.01 SB26 -1.98 BB46 1.78 SB24				
NORMAL MODE 15	OBSERVED=	0.0 CM-1	CALCULATED=	903.9 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	21.60	C-C 18.55 H4CC	18.51	CCH8					
FORCE CONSTANTS-	21.60	C-C 20.56 CC3H	19.39	CC6H 5.33 HC6H					
OFF DIAGONAL-	5.42	SB25 4.86 SB24	3.83	BB37 3.39 BB44 -2.64	SB26 1.59 BB35				
NORMAL MODE 16	OBSERVED=	0.0 CM-1	CALCULATED=	837.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	23.53	OCH4 23.49 HOC	15.65	CCH7 10.99 OCH5 8.38	CCH8				
FORCE CONSTANTS-	34.52	OCH 24.51 CC6H	23.49	COH 5.91 HC6H 5.74	CC3H				
OFF DIAGONAL-	-3.46	BB37 -2.90 BB33	2.41	BB37 2.21 BB35 -1.87	BB40 1.74 BB31				
NORMAL MODE 17	OBSERVED=	0.0 CM-1	CALCULATED=	741.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	41.66	CCH9 15.98 C-O	10.59	C-C 7.95 CCH7 6.88	H7H8				
FORCE CONSTANTS-	50.42	CC6H 15.98 C-O	10.59	C-C 7.13 HC6H					
OFF DIAGONAL-	-4.38	SB22 3.48 BB35	2.68	SB24 -2.39 BB40 2.24	SB23 1.72 BB44				
NORMAL MODE 18	OBSERVED=	0.0 CM-1	CALCULATED=	616.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	24.70	CCH8 22.58 CCH7	21.31	H4CC 12.60 H5CC 6.46	OCH5 6.36 OCH4				
FORCE CONSTANTS-	47.46	CC6H 33.90 CC3H	12.81	OCH 6.76 HC6H					
OFF DIAGONAL-	-8.30	BB37 6.52 BB35	-3.48	BB40 1.86 BB36					
NORMAL MODE 19	OBSERVED=	0.0 CM-1	CALCULATED=	381.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	79.52	UCC 10.87 CCH9	9.64	CCH8 8.63 CCH7					
FORCE CONSTANTS-	79.52	CCO 29.14 CC6H	5.33	CC3H 5.04 HC6H					
OFF DIAGONAL-	-19.95	BB44 -4.47 BB45	-2.81	BB46 2.74 SB26 -2.06	BB37 1.88 BB43 -1.63 SB23 -1.52 BB40				
NORMAL MODE 20	OBSERVED=	0.0 CM-1	CALCULATED=	188.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	86.30	T-CC 12.41 T-CO							
FORCE CONSTANTS-	86.30	TC-C 12.41 TC-O							
OFF DIAGONAL-	NONE								
NORMAL MODE 21	OBSERVED=	0.0 CM-1	CALCULATED=	148.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	85.70	T-CO 12.47 T-CC							
FORCE CONSTANTS-	85.70	TC-O 12.47 TC-C							
OFF DIAGONAL-	NONE								

0. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 0.0

TABLE LV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 301
MOLECULE 13 -6 NG= 209 ETHANOL, CH3CDOOH, GAUCHE, 05

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NORMAL MODE 7	OBSERVED=	0.0 CM-1	CALCULATED=	1457.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	48.50	H7H8 14.16 H8H9	8.01	H7H9 7.92 CCH9				
FORCE CONSTANTS-	70.67	HC6H 13.20 CC6H						
OFF DIAGONAL-	6.26	BB40 4.17 BB34						
NORMAL MODE 8	OBSERVED=	0.0 CM-1	CALCULATED=	1453.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	41.50	H7H9 33.25 H8H9	6.18	CCH8 5.03 CCH7				
FORCE CONSTANTS-	75.18	HC6H 11.28 CC6H						
OFF DIAGONAL-	6.03	BB40 4.45 BB34						
NORMAL MODE 9	OBSERVED=	0.0 CM-1	CALCULATED=	1397.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	77.05	HOC 6.05 H8H9						
FORCE CONSTANTS-	77.05	COH 6.18 HC6H						
OFF DIAGONAL-	2.75	BB32 -2.05 SB21 1.71 BB40						
NORMAL MODE 10	OBSERVED=	0.0 CM-1	CALCULATED=	1382.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	17.41	CCH8 15.89 H7H9	15.33	CCH7 12.19 H8H9 11.50	CCH9 10.78	C-C 7.50	H7H8 5.56	H4CC 5.33 OCH4
FORCE CONSTANTS-	44.24	CC6H 35.58 HC6H	10.78	C-C 6.26 OCH 6.06	CC3H			
OFF DIAGONAL-	16.22	BB40-11.34 SB24 -7.41 BB35 -4.07 BB34 -4.06	SB25 2.63	BB37 -1.77	SB22			
NORMAL MODE 11	OBSERVED=	0.0 CM-1	CALCULATED=	1336.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	61.92	UCH4 24.73 H4CC	6.50	H7H8				
FORCE CONSTANTS-	63.41	UCH 25.59 CC3H	7.38	HC6H 7.06 CC6H				
OFF DIAGONAL-	-6.97	SB22 -1.82 BB38 1.73 BB33 -1.71 BB35 -1.59	SB25					
NORMAL MODE 12	OBSERVED=	0.0 CM-1	CALCULATED=	1310.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	64.54	HCH 15.26 H4CC	7.64	HOC				
FORCE CONSTANTS-	64.54	HC3H 17.14 CC3H	7.64	COH 5.63 OCH				
OFF DIAGONAL-	8.23	BB40 -3.16 BB38 -2.20	SB25					
NORMAL MODE 13	OBSERVED=	0.0 CM-1	CALCULATED=	1135.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	50.39	C-O 15.51 CCH9	10.26	UCH5 8.09 H7H8 6.93	H5CC 5.97	C-C		
FORCE CONSTANTS-	50.39	C-O 18.92 CC6H	13.77	UCH 9.27 HC6H 7.30	CC3H 5.97	C-C		
OFF DIAGONAL-	-6.12	SB23 -4.07 SB22 -2.44 BB40 -2.00 SB25 1.71	BB44 -1.70	SS20 -1.68	SB21 1.61	BB35		
NORMAL MODE 14	OBSERVED=	0.0 CM-1	CALCULATED=	1066.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	43.99	C-C 16.71 CCH8	9.57	CCH9 7.71 H5CC 7.16	OCC			
FORCE CONSTANTS-	43.99	C-C 28.00 CC6H	9.90	CC3H 7.58 HC6H 7.16	CCO 5.45	UCH		
OFF DIAGONAL-	-4.85	SB26 -3.47 SB25 2.94 BB35 -2.88 BB40 2.75	BB44 2.02	BB37				
NORMAL MODE 15	OBSERVED=	0.0 CM-1	CALCULATED=	1008.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	31.10	CCH7 16.83 C-C	13.38	CCH8 6.67 H8H9 6.31	C-O 5.77	H5CC		
FORCE CONSTANTS-	48.27	CC6H 16.83 C-C	10.54	HC6H 6.31 C-O 6.26	CC3H			
OFF DIAGONAL-	-4.30	BB40 4.21 BB35 3.33 BB37 2.81	SB25					
NORMAL MODE 16	OBSERVED=	0.0 CM-1	CALCULATED=	922.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	52.47	UCH5 20.29 C-O	12.67	H5CC 7.51 HOC				
FORCE CONSTANTS-	56.13	UCH 20.29 C-O	12.69	CC3H 7.51 COH				
OFF DIAGONAL-	10.35	SB22 -4.73 SB21 -4.28	BB32 -2.50	BB33				
NORMAL MODE 17	OBSERVED=	0.0 CM-1	CALCULATED=	877.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	29.92	C-O 26.61 C-C	20.54	CCH9 10.12 UCH5 5.79	CCH8			
FORCE CONSTANTS-	29.92	C-O 29.52 CC6H	26.61	C-C 10.13 OCH				
OFF DIAGONAL-	-7.73	SB22 4.96 SB25 2.77	SS20 -2.64	BB40 2.18	BB35 -1.82	SB23		
NORMAL MODE 18	OBSERVED=	0.0 CM-1	CALCULATED=	709.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	32.16	H5CC 20.42 H4CC	11.64	UCH5 10.59 CCH8 10.33	UCH4 8.65	CCH7		
FORCE CONSTANTS-	52.58	CC3H 21.97 OCH	19.26	CC6H				
OFF DIAGONAL-	-6.54	BB37 5.72 BB35 -1.98	BB33					
NORMAL MODE 19	OBSERVED=	0.0 CM-1	CALCULATED=	434.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	86.70	OCC 6.84 CCH9	6.30	CCH7 5.65 CCH8				
FORCE CONSTANTS-	86.70	CCO 18.79 CC6H	5.79	CC3H				
OFF DIAGONAL	-16.85	BB44 -3.70 BB45 -3.43	BB46 3.09	SB26 2.02	BB43 -1.72	BB37 -1.64	SB25	
NORMAL MODE 20	OBSERVED=	0.0 CM-1	CALCULATED=	247.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	90.61	T-CC 8.33 T-CO						
FORCE CONSTANTS-	90.61	TC-C 8.33 TC-O						
OFF DIAGONAL -	NONE							
NORMAL MODE 21	OBSERVED=	0.0 CM-1	CALCULATED=	205.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT
INTERNAL COORDINATES-	90.16	T-CO 8.10 T-CC						
FORCE CONSTANTS-	90.16	TC-O 8.10 TC-C						
OFF DIAGONAL -	NONE							

O. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 0.0

TABLE IV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 301									
MOLECULE 14 -6 NG= 209 ETHANOL, CH3CHODD, GAUCHE, D5									
PAGE 1									
NORMAL MODE 7	OBSERVED=	0.0 CM-1	CALCULATED=	1457.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	49.25	H7H8 13.91 H7H9	8.84	H8H9 8.04 CCH9					
FORCE CONSTANTS-	72.00	HC6H 13.18 CC6H							
OFF DIAGONAL-	6.30	BB40 4.25 BB34							
NORMAL MODE 8	OBSERVED=	0.0 CM-1	CALCULATED=	1452.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	40.97	H8H9 35.75 H7H9	5.94	CCH7 5.17 CCH8					
FORCE CONSTANTS-	76.89	HC6H 11.13 CC6H							
OFF DIAGONAL-	6.05	BB40 4.55 BB34							
NORMAL MODE 9	OBSERVED=	0.0 CM-1	CALCULATED=	1338.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	53.72	OCH4 34.12 H4CC	5.24	H7H8					
FORCE CONSTANTS-	47.39	CC6H 38.34 HC6H	9.06	C-C 5.66 OCH					
OFF DIAGONAL-	17.10	BB40-10.77 SB24	-7.82	BB35 -4.35 BB34 -2.94	SB25 2.14	BB37			
NORMAL MODE 10	OBSERVED=	0.0 CM-1	CALCULATED=	1382.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	18.29	CCH8 16.73 CCH7	15.92	H7H9 15.19 H8H9 12.37	CCH9 9.06	C-C 7.23	H7H8 5.27	OCH4	
FORCE CONSTANTS-	55.75	OCH 35.67 CC3H	6.76	CC6H 6.39	HC6H				
OFF DIAGONAL-	-7.07	SB22 -3.43 SB25	-2.09	BB35 1.91	BB40 1.89	BB33 1.53	SB24		
NORMAL MODE 11	OBSERVED=	0.0 CM-1	CALCULATED=	1320.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	68.49	HCH 12.33 OCH4	10.36	H4CC					
FORCE CONSTANTS-	68.49	HC3H 12.76 OCH	12.04	CC3H					
OFF DIAGONAL-	7.14	BB40 -4.12 BB38	-2.73	SB25					
NORMAL MODE 12	OBSERVED=	0.0 CM-1	CALCULATED=	1142.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	44.87	C-O 21.43 OCH5	18.40	HOC 14.30 C-C 5.97	CCH9 5.68	H5CC			
FORCE CONSTANTS-	44.87	C-O 24.53 OCH	18.40	COH 14.30 C-C 7.01	CC6H 6.33	CC3H			
OFF DIAGONAL-	-11.00	SB21 -8.28 SB22	-4.28	BB32 -2.49	SS20 -2.40	SB25 -2.13	SB23		
NORMAL MODE 13	OBSERVED=	0.0 CM-1	CALCULATED=	1110.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	25.29	HOC 18.32 CCH9	9.51	C-C 9.48 OCC 7.26	H7H8 5.17	C-O			
FORCE CONSTANTS-	25.29	COH 23.81 CC6H	9.51	C-C 9.48 CCO 8.85	HC6H 5.17	C-O			
OFF DIAGONAL-	4.38	SB21 3.45 BB44	-3.15	SB23 2.75	SB22 -2.60	SB26 -2.50	BB40 2.02	BB32 2.01	BB45 1.78
NORMAL MODE 14	OBSERVED=	0.0 CM-1	CALCULATED=	1055.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	23.78	CCH8 20.45 C-C	11.53	CCH7 10.82 H5CC 9.23	HOC 6.28	H7H9			
FORCE CONSTANTS-	37.47	CC6H 20.45 C-C	13.40	CC3H 9.82	HC6H 9.23	COH 5.08	OCH		
OFF DIAGONAL-	3.96	BB37 3.91 BB35	-3.56	BB40 -3.07	SB25 -1.83	SB26			
NORMAL MODE 15	OBSERVED=	0.0 CM-1	CALCULATED=	979.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	24.38	C-C 14.99 CCH7	11.41	HOC 11.12 C-O 6.09	OCH5 5.65	H5CC			
FORCE CONSTANTS-	24.38	C-C 22.00 CC6H	11.41	COH 11.12 C-O 6.27	OCH 5.68	CC3H			
OFF DIAGONAL-	4.43	SB25 4.31 SB21	2.93	SB22 1.99	BB37 -1.86	BB40 1.85	BB35 1.80	BB32 -1.62	SS20
NORMAL MODE 16	OBSERVED=	0.0 CM-1	CALCULATED=	901.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	29.02	C-O 23.28 OCH5	23.00	HOC 9.38 C-C 8.27	CCH8 8.26	H5CC			
FORCE CONSTANTS-	29.02	C-O 25.58 OCH	23.00	COH 13.44 CC6H 9.38	C-C 8.71	CC3H			
OFF DIAGONAL-	-9.89	SB21 7.69 SB22	-4.99	BB32 -2.72	SB25 1.62	SS20			
NORMAL MODE 17	OBSERVED=	0.0 CM-1	CALCULATED=	867.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	21.38	OCH5 18.85 CCH9	17.40	C-O 15.45 C-C 8.31	CCH7 7.68	HOC 7.54	H5CC		
FORCE CONSTANTS-	28.85	CC6H 21.44 OCH	17.40	C-O 15.45 C-C 7.86	CC3H 7.68	COH			
OFF DIAGONAL-	-7.89	SB22 5.26 SB25	4.42	SB21 -2.76	BB32 -2.76	BB40 2.10	BB35 -1.80	BB37 1.61	SS20
NORMAL MODE 18	OBSERVED=	0.0 CM-1	CALCULATED=	701.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	28.59	H5CC 20.74 H4CC	13.73	OCH5 10.85 OCH4 10.51	CCH8 6.59	CCH7			
FORCE CONSTANTS-	49.33	CC3H 24.58 OCH	17.27	CC6H					
OFF DIAGONAL-	-5.94	BB37 5.35 BB35	-2.20	BB33 -1.71	BB32				
NORMAL MODE 19	OBSERVED=	0.0 CM-1	CALCULATED=	426.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	85.97	OCC 6.44 CCH9	6.14	CCH7 5.37	CCH8				
FORCE CONSTANTS-	85.97	CCO 18.00 CC6H	5.70	CC3H					
OFF DIAGONAL-	-16.46	BB44 -3.59 BB45	-3.53	BB46 2.91	SB26 1.97	BB43 -1.66	BB37 -1.52	SB25	
NORMAL MODE 20	OBSERVED=	0.0 CM-1	CALCULATED=	244.7 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	96.88	T-CC							
FORCE CONSTANTS-	96.88	TC-C							
OFF DIAGONAL-	NONE								
NORMAL MODE 21	OBSERVED=	0.0 CM-1	CALCULATED=	153.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	96.72	T-CO							
FORCE CONSTANTS-	96.72	TC-O							
OFF DIAGONAL-	NONE								

0. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 0.0

TABLE LV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 301									
MOLECULE 15 -6 NG= 209 ETHANOL, CD3CHDOH, GAUCHE, D5									
PAGE 1									
NORMAL MODE 7	OBSERVED=	0.0 CM-1	CALCULATED=	1397.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	83.77 HOC								
FORCE CONSTANTS-	83.77 COH								
OFF DIAGONAL-	3.13 BB32 -2.43 SB21								
NORMAL MODE 8	OBSERVED=	0.0 CM-1	CALCULATED=	1340.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	71.07 OCH4 27.16 H4CC 5.12 C-O								
FORCE CONSTANTS-	73.40 OCH 28.35 CC3H 5.12 C-O								
OFF DIAGONAL-	-9.71 SB22 -5.02 SB25 -2.37 BB40 -2.35 BB38 2.32 BB33								
NORMAL MODE 9	OBSERVED=	0.0 CM-1	CALCULATED=	1310.6 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	63.98 HCH 16.86 H4CC 7.82 HOC								
FORCE CONSTANTS-	63.98 HC3H 19.02 CC3H 7.82 COH								
OFF DIAGONAL-	8.62 BB40 -2.95 SB25 -2.75 BB38								
NORMAL MODE 10	OBSERVED=	0.0 CM-1	CALCULATED=	1145.8 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	35.91 C-O 35.19 C-C 9.47 CCH7 8.04 CCH8 7.71 OCH5 7.48 H7H8								
FORCE CONSTANTS-	35.91 C-O 35.19 C-C 17.75 CC6H 12.01 HC6H 9.67 OCH 5.32 CC3H								
OFF DIAGONAL-	-11.43 SB24 5.36 BB40 -3.55 SB22 -3.49 SS20 -3.06 SB25 -2.05 SB23 1.66 BB44 -1.60 BB35								
NORMAL MODE 11	OBSERVED=	0.0 CM-1	CALCULATED=	1078.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	25.65 CCH9 24.02 C-O 18.69 H7H9 14.77 C-C 11.37 H8H9								
FORCE CONSTANTS-	30.53 HC6H 29.82 CC6H 24.02 C-O 14.77 C-C								
OFF DIAGONAL-	9.90 BB40 -9.11 SB24 -3.43 SB23 -2.72 BB35 2.35 SB25 1.85 SS20 -1.71 SB22 -1.63 SB26 -1.61 BB44								
NORMAL MODE 12	OBSERVED=	0.0 CM-1	CALCULATED=	1038.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	46.99 H8H9 31.21 H7H9								
FORCE CONSTANTS-	79.26 HC6H 8.71 CC6H								
OFF DIAGONAL-	5.41 BB40 4.68 BB34								
NORMAL MODE 13	OBSERVED=	0.0 CM-1	CALCULATED=	1019.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	59.41 H7H8 12.32 C-O 6.99 H7H9 6.23 OCH5 5.28 CCH8								
FORCE CONSTANTS-	68.23 HC6H 12.32 C-O 7.26 CC6H 6.28 OCH								
OFF DIAGONAL-	3.66 BB40 -3.42 SB22 3.22 BB34 -1.53 SB23								
NORMAL MODE 14	OBSERVED=	0.0 CM-1	CALCULATED=	972.1 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	21.59 C-C 13.99 CCH8 12.95 H5CC 11.60 OCC 10.23 H7H9 5.67 OCH5								
FORCE CONSTANTS-	21.59 C-C 17.37 CC3H 14.96 CC6H 13.29 HC6H 11.60 CCO 7.93 OCH								
OFF DIAGONAL-	6.24 SB24 5.93 BB44 -4.33 SB26 3.41 SB22 -3.12 SB23 -2.81 SB25 -1.78 BB46								
NORMAL MODE 15	OBSERVED=	0.0 CM-1	CALCULATED=	920.0 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	32.28 OCH5 15.28 H5CC 15.10 C-O 9.21 C-C								
FORCE CONSTANTS-	35.14 OCH 15.28 CC3H 15.10 C-O 9.21 C-C 6.00 CC6H								
OFF DIAGONAL-	6.69 SB22 4.74 SB25 2.40 SB24 -2.26 SB21 2.08 SB23 -1.86 BB32 -1.73 BB33 1.73 BB37								
NORMAL MODE 16	OBSERVED=	0.0 CM-1	CALCULATED=	866.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	22.62 OCH5 22.30 CCH7 8.83 H5CC 7.95 CCH8 7.04 OCH4 6.16 H8H9 5.92 H4CC								
FORCE CONSTANTS-	30.50 CC6H 24.65 OCH 14.75 CC3H 7.72 HC6H								
OFF DIAGONAL-	4.36 BB37 3.50 BB35 -2.63 BB40 -2.28 BB33 -2.25 BB32								
NORMAL MODE 17	OBSERVED=	0.0 CM-1	CALCULATED=	744.4 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	42.00 CCH9 15.48 C-O 12.53 C-C 7.22 H7H8								
FORCE CONSTANTS-	48.26 CC6H 15.48 C-O 12.53 C-C 7.22 HC6H								
OFF DIAGONAL-	-4.72 SB22 3.19 BB35 3.15 SB24 2.34 SB23 -2.09 BB40 1.72 BB44								
NORMAL MODE 18	OBSERVED=	0.0 CM-1	CALCULATED=	621.3 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	27.50 CCH8 22.97 CCH7 19.85 H5CC 13.06 H4CC 5.83 OCH5 5.34 OCH4								
FORCE CONSTANTS-	50.48 CC6H 32.92 CC3H 11.16 OCH 7.18 HC6H								
OFF DIAGONAL-	-8.41 BB37 6.71 BB35 -3.74 BB40 1.89 BB36								
NORMAL MODE 19	OBSERVED=	0.0 CM-1	CALCULATED=	386.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	79.15 OCC 11.23 CCH9 9.68 CCH7 9.00 CCH8								
FORCE CONSTANTS-	79.15 CCO 29.91 CC6H 5.58 CC3H 5.13 HC6H								
OFF DIAGONAL-	-20.13 BB44 -4.54 BB45 -2.86 BB46 2.82 SB26 -2.12 BB37 1.90 BB43 -1.74 SB23 -1.55 SB25								
NORMAL MODE 20	OBSERVED=	0.0 CM-1	CALCULATED=	213.5 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	82.07 T-CO 16.15 T-CC								
FORCE CONSTANTS-	82.07 TC-O 16.15 TC-C								
OFF DIAGONAL -	NONE								
NORMAL MODE 21	OBSERVED=	0.0 CM-1	CALCULATED=	179.2 CM-1	ERROR=	0.0 CM-1	OR	0.0 PERCENT	
INTERNAL COORDINATES-	82.66 T-CC 15.77 T-CO								
FORCE CONSTANTS-	82.66 TC-C 15.77 TC-O								
OFF DIAGONAL -	NONE								

0. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 0.0

TABLE LV (Continued)

CONDENSED POTENTIAL ENERGY DISTRIBUTIONS FOR PROBLEM 301										PAGE 1
MOLECULE 16		-6 NG= 209		ETHANOL, CD3CHDOO, GAUCHE, D5						
NORMAL MODE 7	OBSERVED=	0.0 CM-1		CALCULATED=		1340.8 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	66.16	OCH4	33.02 H4CC	5.32	C-O	5.22	C-C			
FORCE CONSTANTS-	68.96	OCH	34.69 CC3H	5.32	C-O	5.22	C-C			
OFF DIAGONAL-	-9.75	SB22	-6.49 SB25	2.46	BB33					
NORMAL MODE 8	OBSERVED=	0.0 CM-1		CALCULATED=		1321.5 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	68.67	HCH	14.32 H4CC	7.50	OCH4					
FORCE CONSTANTS-	68.67	HC3H	16.50 CC3H	7.78	OCH					
OFF DIAGONAL-	8.44	BB40	-3.47 SB25	-3.24	BB38					
NORMAL MODE 9	OBSERVED=	0.0 CM-1		CALCULATED=		1155.8 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	33.21	C-O	33.13 C-C	16.03	OCH5	13.58	HOC	6.33	CCH8	
FORCE CONSTANTS-	33.21	C-O	33.13 C-C	18.40	OCH	13.58	COH	11.42	CC6H	
OFF DIAGONAL-	-9.05	SB24	-8.13 SB21	-6.12	SB22	3.44	BB40	-3.26	SS20	
								3.18	BB32 -2.26 SB25	
NORMAL MODE 10	OBSERVED=	0.0 CM-1		CALCULATED=		1089.5 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	39.98	HOC	13.61 CCH7	10.69	OCH5	10.05	H7H9	6.40	C-C	
FORCE CONSTANTS-	39.98	COH	20.24 CC6H	15.98	HC6H	10.88	OCH	6.40	C-C	
OFF DIAGONAL-	6.86	BB40	-5.58 SB24	4.46	BB32	-2.73	BB35	2.00	BB44 -1.57 BB34	
NORMAL MODE 11	OBSERVED=	0.0 CM-1		CALCULATED=		1075.9 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	25.29	C-O	22.49 CCH9	11.40	H8H9	10.73	C-C	10.18	H7H9	
FORCE CONSTANTS-	25.29	C-O	25.04 HC6H	22.68	CC6H	10.73	C-C			
OFF DIAGONAL-	6.70	BB40	-5.21 SB24	-4.91	SB23	4.05	SB21	-1.94	SB26	
								1.85	SB25 1.62 SS20 1.56 BB45	
NORMAL MODE 12	OBSERVED=	0.0 CM-1		CALCULATED=		1036.0 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	43.90	H8H9	32.98 H7H9	6.80	CCH8					
FORCE CONSTANTS-	77.03	HC6H	8.75 CC6H							
OFF DIAGONAL-	5.35	BB40	4.46 BB34							
NORMAL MODE 13	OBSERVED=	0.0 CM-1		CALCULATED=		1014.5 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	56.28	H7H8	16.34 C-O	6.72	H8H9					
FORCE CONSTANTS-	67.86	HC6H	16.34 C-O							
OFF DIAGONAL-	3.58	BB34	-3.46 SB23	2.19	SB21	-1.86	SB22	-1.54	BB44	
NORMAL MODE 14	OBSERVED=	0.0 CM-1		CALCULATED=		962.5 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	19.33	C-C	17.00 H5CC	16.70	CCH8	11.14	H7H9	8.98	HOC	
FORCE CONSTANTS-	23.14	CC3H	19.33 C-C	16.79	CC6H	11.52	HC6H	8.98	COH	
OFF DIAGONAL-	5.92	SB24	4.30 BB44	-3.21	SB26	-2.92	SB25	1.89	BB37	
NORMAL MODE 15	OBSERVED=	0.0 CM-1		CALCULATED=		918.1 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	28.30	OCH5	18.81 H5CC	15.04	C-O	8.78	C-C	5.91	CCH7	
FORCE CONSTANTS-	30.26	OCH	18.93 CC3H	15.04	C-O	8.78	C-C	6.79	CC6H	
OFF DIAGONAL-	6.55	SB22	4.78 SB25	-2.52	SB21	2.23	SB24	2.15	BB37	
								2.07	SB23 -1.94 BB32	
NORMAL MODE 16	OBSERVED=	0.0 CM-1		CALCULATED=		832.9 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	23.42	HOC	19.85 OCH5	19.32	CCH7	8.90	C-C	7.30	CCH8	
FORCE CONSTANTS-	26.84	CC6H	25.85 OCH	23.42	COH	8.90	C-C	6.71	CC3H	
OFF DIAGONAL-	-4.65	BB32	-2.96 SB21	2.68	BB37	2.35	BB35	-1.97	BB33	
								1.93	SB24 -1.81 BB40	
NORMAL MODE 17	OBSERVED=	0.0 CM-1		CALCULATED=		738.4 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	41.87	CCH9	14.41 C-O	9.77	C-C	6.83	H7H8	6.25	OCH5	
FORCE CONSTANTS-	49.51	CC6H	14.41 C-O	9.77	C-C	6.92	HC6H	6.51	OCH	
OFF DIAGONAL-	-4.93	SB22	3.43 BB35	2.47	SB24	-2.46	BB40	2.10	SB23	
								2.03	SB21 1.75 BB44	
NORMAL MODE 18	OBSERVED=	0.0 CM-1		CALCULATED=		619.0 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	27.82	CCH8	20.82 CCH7	19.42	H5CC	13.63	H4CC	6.74	OCH5	
FORCE CONSTANTS-	48.73	CC6H	33.05 CC3H	12.38	OCH	6.94	HC6H			
OFF DIAGONAL-	-8.25	BB37	6.59 BB35	-3.62	BB40	1.86	BB36			
NORMAL MODE 19	OBSERVED=	0.0 CM-1		CALCULATED=		380.3 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	79.43	OCC	10.73 CCH9	9.46	CCH7	8.63	CCH8			
FORCE CONSTANTS-	79.43	CCO	28.82 CC6H	5.53	CC3H					
OFF DIAGONAL-	-19.84	BB44	-4.44 BB45	-2.97	BB46	2.72	SB26	-2.06	BB37	
								1.88	BB43 -1.68 SB23	
NORMAL MODE 20	OBSERVED=	0.0 CM-1		CALCULATED=		189.0 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	85.45	T-CC	13.41 T-CO							
FORCE CONSTANTS-	85.45	TC-C	13.41 TC-O							
OFF DIAGONAL -	NONE									
NORMAL MODE 21	OBSERVED=	0.0 CM-1		CALCULATED=		148.3 CM-1		ERROR=	0.0 CM-1 OR 0.0 PERCENT	
INTERNAL COORDINATES-	84.75	T-CO	13.38 T-CC							
FORCE CONSTANTS-	84.75	TC-O	13.38 TC-C							
OFF DIAGONAL -	NONE									

0. EXPERIMENTAL FREQUENCIES

AVERAGE ERROR = 0.0

APPENDIX VI

INTRODUCTION TO THE THEORY AND NOTATION OF THE CALCULATIONS

INTRODUCTION

This appendix will very briefly describe some of the formalism and notation associated with the normal coordinate analysis calculations discussed in the main text. The underlying theory may be found in most texts on mechanics (105), and the classic discussion of its application to molecular vibrations has been given by Wilson, et al. (27). The transformation of Wilson, et al. methods into the computer programs used in this investigation was done primarily by Schachtschneider (32) and Pitzner (6).

FORMATION OF THE SECULAR EQUATION

The standard treatment of small vibrations in polyatomic molecules yields a series of simultaneous differential equations. Equation (1) is typical of such expressions, where the q 's are mass weighted Cartesian displacement coordinates,

$$\ddot{q}_i + \sum_{j=1}^{3N} f_{ij} q_j = 0, \quad j = 1 \rightarrow 3N \quad (1)$$

N is the number of atoms, and the f_{ij} 's or force constants are mixed partial derivatives of the potential with respect to coordinates i and j . The cosine function is well known as a general solution to such equations, but only few specific frequencies correspond to solutions where the atoms move in phase with nonzero amplitude. These frequencies are obtained from a determinantal equation known as the secular equation. As expressed in Equation (2), f is a matrix of the

$$\det (f - \lambda) = 0 \quad (2)$$

f_{ij} 's from Equation (1) and λ is a diagonal matrix of the frequencies corresponding to nontrivial solutions. This is readily recognized as a matrix eigenvalue problem.

The Wilson formalism sets up the same problem in a coordinate system utilizing internal measures such as the changes in bond lengths or angles. This system of internal coordinates associates the force constants with particular chemical bonds or groups and thus allows their approximate transfer from known to unknown systems with the same chemical groupings. One form of the secular equation, expressed in the Wilson notation, is shown in Equation (3).

$\underset{mn}{F}$ is analogous to $\underset{mn}{f}$ in Equation (2), being a matrix of partial derivatives of the

$$\det (\underset{mn}{G}\underset{mn}{F} - \lambda) = 0 \quad (3)$$

potential with respect to the internal coordinates. The $\underset{mn}{F}$ matrix is usually constructed from a small set of general force constants, ϕ , by means of a constraint matrix, $\underset{mn}{Z}$, as expressed in Equation (4). The $\underset{mn}{G}$ matrix, containing

$$F_{ij} = \sum_k Z_{ijk} \phi_k \quad (4)$$

the kinetic energy information, is constructed from known or assumed atomic positions and masses by the Wilson S vector method.

If the molecule has symmetry, it is possible to reduce the secular equation to a number of independent equations of lower order by transformation to a set of coordinates reflecting the molecular symmetry. The transformation is designated $\underset{mn}{U}$, and the product $\underset{mn}{U}(\underset{mn}{G}\underset{mn}{F} - \lambda)\underset{mn}{U}'$ is in block diagonal form. The various blocks may then be treated independently. In practice, the reduced equations are formed by first factoring the $\underset{mn}{G}$ and $\underset{mn}{Z}$ matrices with $\underset{mn}{U}$ and then proceeding with the factored blocks to form the appropriate products.

SOLUTION OF THE SECULAR EQUATION

Examination of Equation (4) reveals that the problem of finding the λ 's, or normal vibrational frequencies, is equivalent to finding a transformation, $\underset{mn}{L}$,

to a set of coordinates, Q , called normal coordinates, in which the GF product is in diagonal form. For purposes of machine computation, this diagonalization is done somewhat indirectly, involving successive Schmidt orthogonalization of the G and F matrices followed by Jacobi diagonalization.

The L matrix is of considerable importance in analysis of the results, since the k^{th} column of L gives the eigenvector of the k^{th} normal frequency. The elements of L are usually processed further to give potential energy distributions. These distributions can provide considerable insight into the form of the various normal modes. These distributions are most commonly evaluated in terms of the internal coordinates or force constants. The expressions are given in Equations (5) and (6), where J is the Jacobian matrix between the F matrix

$$P.E._{q_i} = L_{ik}^2 / \lambda_k \quad (5)$$

$$P.E._{\phi_i} = JZ_{ijk} \phi_i / \lambda_k \quad (6)$$

elements and the force constants. In simple terms, Equation (5) describes the relative contribution of the i^{th} internal coordinate to the k^{th} normal mode, while Equation (6) gives the sensitivity of the k^{th} calculated frequency to the i^{th} force constant. Further insight into the form of the normal modes may be gained by successive applications of L and B , the transformation from internal to Cartesian coordinates. Expression of the vibrations in Cartesian coordinates facilitates drawing of the normal mode diagrams which have been included in the text.

OPTIMIZATION OF THE FORCE CONSTANTS

Since the number of F matrix elements far exceeds the number of experimental frequencies even for molecules of modest size, they cannot be evaluated directly from the experimental data. Various indirect methods have been developed to estimate them from the data and other available information. The methods which

concern us use a $\underline{Z}$ matrix to express the $\underline{F}$ elements in terms of a small number of ϕ 's, which are initially transferred from similar systems. Corrections, $\Delta\phi$, are then sought to the ϕ 's, which will decrease the differences between the observed and calculated frequencies, $\Delta\lambda$. We have used two such procedures. In the linear least squares (LLS) algorithm, the corrections are given by Equation (7). Unfortunately, the internal coordinates used in Wilson's formalism are

$$\Delta\phi = [(\underline{JZ})'(\underline{JZ})]^{-1}(\underline{JZ})'\Delta\lambda \quad (7)$$

frequently redundant and in ring compounds they are unavoidably so. In such cases, the $\underline{JZ}$ matrix will be singular and the LLS algorithm may be very unstable. An alternative correction procedure, known as the Fletcher-Powell method (FPM), while slower computationally, does not employ the inverse $\underline{JZ}$ matrix and thus tends to be more stable computationally. The corrections are given by Equation (8), where

$$\Delta\phi = 2(\underline{D})(\underline{JZ})'\Delta\lambda \quad (8)$$

$\underline{D}$ is a Hessian matrix having elements [Equation (9)]

$$D_{ij} = \partial^2 Q / \partial\phi_i \partial\phi_j \quad (9)$$

In either case, the correction procedure is repeated until all the corrections fall below some preset level or the rate of error reduction falls below some pre-selected value. The resulting field, while not unique, provides the best description of the vibration available from the data and initial assumptions.