PROJECT ADMINISTRATION DATA SHEET

Project No. G33-616

Project Director: E. C. Ashley
School: Chemistry

Sponsor: The Petroleum Research Fund, American Chemical Society, 1155 Fifteenth St. N.W., Washington, D.C. 20036

Type Agreement: Grant No. 1402-AC4-TC

Award Period: From 9-1-82 To 8-31-85 (Performance) 8-31-85 (Reports)

Sponsor Amount: $45,000

Cost Sharing: None

Title: Single Electron Transfer in Organic Reactions

ADMINISTRATIVE DATA

OCA Contact: Don Harty

1) Sponsor Technical Contact:
Mr. Joseph C. Rogers, Jr.

2) Sponsor Admin/Contractual Matters:

Above address

Phone (202) 872-4481

Defense Priority Rating: N/A

Security Classification: N/A

RESTRICIONS

See Attached N/A Supplemental Information Sheet for Additional Requirements.

Travel: Foreign travel must have prior approval – Contact OCA in each case. Domestic travel requires sponsor approval where total will exceed greater of $500 or 125% of approved proposal budget category.

Equipment: Title vests with N/A - None Proposed

COMMENTS:

COPIES TO:

Research Security Services
Reports Coordinator (OCA)
Legal Services (OCA)
Library

EES Public Relations (2)
Computer Input
Project File
Other

Research Property Management
Accounting
Procurement/EES Supply Services

FORM OCC 4-77
SPONSORED PROJECT TERMINATION/CLOSEOUT SHEET

Date 9/19/86

Project No. G-33-616 School/Department Chemistry

Includes Subproject No.(s) N/A

Project Director(s) E. C. Ashby GTRC/Office

Sponsor The Petroleum Research Fund, American Chemical Society

Title Single Electron Transfer in Organic Reactions

Effective Completion Date: 8/31/85 (Performance) (Reports)

Grant/Contract Closeout Actions Remaining: No further reporting requirements per Ralph Grede.

☐ None
☐ Final Invoice or Final Fiscal Report
☐ Closing Documents
☐ Final Report of Inventions
☐ Govt. Property Inventory & Related Certificate
☐ Classified Material Certificate
☐ Other

Continues Project No. Continued by Project No.

COPIES TO:

Project Director Library
Research Administrative Network GTRC
Research Property Management Research Communications (2)
Accounting Project File
Procurement/GTRI Supply Services Other
Research Security Services I. Newton
Research Security Services A. Jones
Reports Coordinator (OCAP) R. Embry
Legal Services
May 15, 1986

Joseph E. Rodgers, Jr.
The Petroleum Research Fund
American Chemical Society
1155 Sixteenth Street, N.W.
Washington, D. C. 20036

Gentlemen:

Enclosed in duplicate is the Annual Financial Statement and Personnel Statement for PRF No. 14102-AC4-1C for the year ended August 31, 1985.

If you have questions or require any additional information, please contact this office at (404) 894-5523.

Sincerely,

Valeria D. Henderson, Accountant I
Grants & Contracts Accounting

Enclosures

cc: Dr. R. A. Pierotti/Chemistry
    Dr. E. C. Ashby/Chemistry
    Ms. Faith Gleason/OCA-PAD,
    File G-33-616 (R5532-IA0)
FINANCIAL STATEMENT
(Inert "ANNUAL" or "FINAL", as appropriate)

AMERICAN CHEMICAL SOCIETY - THE PETROLEUM RESEARCH FUND

For the Period: September 1, 1984 to August 31, 1985
(The preferred closing date for the reporting period is August 31.)

Balance Carried Over from Previous Reporting Period (from Same or Earlier Grant) $14,007.50
Received from PRF During Report Period (Include Supplements) -0-
Stipends to:
  a. Principal Investigator
     (Contribution Toward Summer Salary*)
  b. Undergraduate Students
  c. Graduate Students
     14,604.88
  d. Postdoctoral Fellows
  e. Summer Research Fellows (Only if funded by Summer Research Supplement)
     Faculty [ ] Student [ ] (check one)
  f. Other (Specify) Research Sci.
Tuition
Materials and Supplies (1,097.38)
Equipment
Computer Time Charges
Travel (Explain if in excess of budget)
Other Expenses (Attach itemized list)
Departmental Allocation* 500.00
*If provided in grant agreement
Total Expenditures During Reporting Period 14,007.50
Balance on Hand at End of Period -0-

Total of PRF Grant Payments Received to Date 45,000.00

Complete this section only for a FINANCIAL STATEMENT which shows a balance in the grant account at the termination date of the current grant agreement.

The balance in the grant account will be liquidated:

[ ] By refund of unspent and uncommitted funds. The check should be drawn to the order of American Chemical Society - The Petroleum Research Fund, and identified by the number of the grant.

[ ] By use in the completion of the grant project. We hereby request approval by the American Chemical Society of an extension of the grant agreement, without commitment of additional funds, until [ ] (Period up to one year, renewable).

We certify that the expenses reported herein were incurred for education and research in accord with the terms of the approved ACS-PRF grant-in-aid.

Georgia Institute of Technology
(Grantee Institution)
Valeria D. Henderson (404) 894-5523 5/15/86
Financial Officer (typed name) (Signature) (Telephone) (Date)
E. C. Ashby 14102-AC4-C
Name of Principal Investigator PRF Number

Please submit to The Petroleum Research Fund, American Chemical Society
1155 Sixteenth Street, N.W., Washington, D.C. 20036 Telephone (202) 872-4481

Rev. 11/82
PERSONNEL STATEMENT

PRF# 14102-AC4-1C REPORTING PERIOD September 1, 1984 TO August 31, 1985

GRANTEE INSTITUTION Georgia Institute of Technology DEPARTMENT Chemistry

PRINCIPAL INVESTIGATOR (S) E. C. Ashby

GRANT PROJECT TITLE Single Electron Transfer in Organic Reactions

List undergraduate, graduate, and postdoctoral co-workers receiving stipends under the above named grant:

<table>
<thead>
<tr>
<th>NAME</th>
<th>TITLE OR ACADEMIC APPOINTMENT</th>
<th>PREVIOUS EDUCATION &amp; DEGREES*</th>
<th>COUNTRY OF PERMANENT RESIDENCE</th>
<th>PERIOD OF SUPPORT (MONTHS)</th>
<th>PERCENT OF SUPPORT FROM PRF REPORTING PERIOD</th>
<th>DEGREES RECEIVED (IF ANY) DURING REPORTING PERIOD</th>
</tr>
</thead>
<tbody>
<tr>
<td>Argyropoulos, John</td>
<td>Research Asst</td>
<td>Yale, MS USA</td>
<td></td>
<td>1.5</td>
<td>100% (1.5 mo)</td>
<td>PHD Ga Tech, 1986</td>
</tr>
<tr>
<td>Baldwin, R. Keith</td>
<td>Graduate Teaching Asst</td>
<td>UGA, BS USA</td>
<td></td>
<td>1</td>
<td>100% 1 mo</td>
<td>None</td>
</tr>
<tr>
<td>Coleman, David</td>
<td>Graduate Teaching Asst</td>
<td>GA Tech, BS USA</td>
<td></td>
<td>4</td>
<td>100% (4 mo)</td>
<td>PHD GA Tech, 1986</td>
</tr>
<tr>
<td>Park, Bong-Jin</td>
<td>Graduate Research Asst</td>
<td>Portland Korea</td>
<td></td>
<td>8</td>
<td>50% (3 mos)</td>
<td>None</td>
</tr>
</tbody>
</table>

List other co-workers on grant project not directly supported with ACS-PRF funds:

<table>
<thead>
<tr>
<th>NAME</th>
<th>SOURCE OF SUPPORT</th>
<th>DATES ASSOCIATED WITH GRANT PROJECT</th>
</tr>
</thead>
</table>

For graduate students, indicate the College or University attended prior to graduate work. For postdoctoral fellows, give the name of the Ph. D. granting institution.
PRF# 14102-AC4-1C REPORTING PERIOD September 1, 1984 TO August 31, 1985

GRANTEE INSTITUTION Georgia Institute of Technology DEPARTMENT Chemistry

PRINCIPAL INVESTIGATOR (S) E. C. Ashby

GRANT PROJECT TITLE Single Electron Transfer in Organic Reactions

List undergraduate, graduate, and postdoctoral co-workers receiving stipends under the above named grant:

<table>
<thead>
<tr>
<th>NAME</th>
<th>TITLE OR ACADEMIC APPOINTMENT</th>
<th>PREVIOUS &amp; DEGREES*</th>
<th>COUNTRY OF PERMANENT RESIDENCE</th>
<th>PERIOD OF SUPPORT (MONTHS)</th>
<th>PERCENT OF SUPPORT FROM PRF</th>
<th>DEGREES RECEIVED (IF ANY) DURING REPORTING PERIOD</th>
</tr>
</thead>
<tbody>
<tr>
<td>Oswald, John</td>
<td>Graduate Teaching Asst</td>
<td>BS Chem</td>
<td>USA</td>
<td>1</td>
<td>100% (1 mo)</td>
<td>None</td>
</tr>
<tr>
<td>Pham, Tung-Ngoc</td>
<td>Graduate Research Asst</td>
<td>BS Chem</td>
<td>USA</td>
<td>7</td>
<td>100% (7 mos)</td>
<td>None</td>
</tr>
</tbody>
</table>

List other co-workers on grant project not directly supported with ACS - PRF funds:

<table>
<thead>
<tr>
<th>NAME</th>
<th>SOURCE OF SUPPORT</th>
<th>DATES ASSOCIATED WITH GRANT PROJECT</th>
</tr>
</thead>
</table>

For graduate students, indicate the College or University attended prior to graduate work. For postdoctoral fellows, give the name of the Ph. D. granting institution.
Single Electron Transfer in Organic Reactions

E. C. Ashby, Georgia Institute of Technology, Atlanta, Georgia 30332

Halogen-metal exchange has been studied by allowing t-Butyllithium to react with a series of alkyl halides containing a cyclizable radical probe in order to evaluate the occurrence of a radical intermediate in the reaction. It was found that radical intermediates, formed via a single electron transfer pathway, are involved in the reactions of t-BuLi with the radical probe, (endo)-5-(2'-bromoethyl)-2-norbornene in pentane: Et₂O at -78°C, since cyclized hydrocarbons were formed during the reaction. However, there was no evidence to support an electron transfer pathway in reactions of the corresponding iodide and chloride with t-BuLi under the same conditions since only the straight-chain organolithium compound was formed. However, evidence indicative of a radical intermediate was obtained from reactions of the iodo compound with t-BuLi in pentane:Et₂O at higher temperatures (-45° and -23°) and in pure pentane at -78°C and -23°C in which stable cyclized hydrocarbon product was obtained. Lithium complexing agents such as TMEDA, HMPA and 18-crown-6 were employed in these reactions in order to increase the carbanionic nature of the organolithium products. It was found that cyclization of the straight-chain organolithium compound to the corresponding cyclized organolithium compound in the presence of such complexing agents is relatively slow. On the other hand, the effectiveness of the complexing agents to increase carbanion character of the straight-chain organolithium compound was demonstrated by a significant lowering of the deuterium content of the straight-chain product due to ether cleavage by the straight-chain organolithium compound.