GEORGIA INSTITUTE OF TECHNOLOGY
OFFICE OF CONTRACT ADMINISTRATION
SPONSORED PROJECT INITIATION

Date: October 22, 1979

Project Title: Reactions and Transport Properties of Atmospheric Ions

Project No: A-2469 (Sub-project is G-41-686/McDaniel/Physics)

Project Director: Dr. Fred L. Eisele

Sponsor: National Science Foundation

Agreement Period: From 9/1/79 Until 1/31/81 (Grant Period)

Type Agreement: Grant No. ATM-7906109, dated August 24, 2979

Amount: $54,206 (A-2469) $4,430 (G-41-686) $58,636 NSF
        2,853 (E-240-814) 7,278 (G-41-326) 10,131 GIT
        $57,059 $11,708 $68,767

Reports Required:

Annual Progress Report (w/request for renewal); Final Project Report

Sponsor Contact Person(s):

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Washington, D.C. 20550
202/632-5892

Defense Priority Rating: N/A

Assigned to: EML/SSSD (Physics) (School/Laboratory)

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Reactions and Transport Properties of Atmospheric Ions

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Effective Termination Date: 1/31/81

Clearance of Accounting Charges: 1/31/81

Grant/Contract Closeout Actions Remaining:

- Final Invoice and Closing Documents
- Final Fiscal Report (FCTR)
- Final Report of Inventions (if positive)
- Govt. Property Inventory & Related Certificate
- Classified Material Certificate
- Other

Assigned to: EML/PSD (SEES Laboratory)

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Reactions and Transport Properties of Atmospheric Ions

The transport properties of several parent ions and ion clusters of atmospheric interest have been studied in both nitrogen and oxygen over a temperature range of 217-675 K.

A high-pressure drift tube mass spectrometer was modified so that it could be operated below as well as above 300 K while maintaining good temperature uniformity throughout the drift region. This apparatus was then used to measure the mobilities of NO\textsubscript{3}, NO\textsubscript{2}, CO\textsubscript{3}, NO\textsubscript{2}·H\textsubscript{2}O, NO\textsubscript{3}·H\textsubscript{2}O, CO\textsubscript{3}·H\textsubscript{2}O and CO\textsubscript{3}·H\textsubscript{2}O in N\textsubscript{2} and NO\textsubscript{2}, NO\textsubscript{3}, CO\textsubscript{3}, CO\textsubscript{3} and O\textsubscript{2} in O\textsubscript{2}. These measurements were made under approximately zero-field condition and in the pressure range 20-45 Torr.

These measurements are needed for atmospheric modeling both in the upper atmosphere where the ion mobilities and the diffusion coefficients calculated from them can be used directly and in the lower atmosphere where they are used to calculate ion-ion recombination rates. In addition, these mobility values make possible a better assessment of ion collection efficiencies in ion reaction rate measurements and provide an additional physical parameter by which ions may be identified.
The present grant period started in September 1979. Several modifications had to be made to the HPDTMS (high pressure drift tube mass spectrometer) before the measurements proposed for this period could be performed. A gas handling system had to be constructed in order to prepare, purify, and store gases such as NO$_2$, N$_2$O, CO$_2$, NO, and H$_2$O. These gases are added to the drift gas in the ion source region of the drift tube in order to produce specific ions such as NO$_2^-$, NO$_3^-$, CO$_3^-$, or ion clusters like NO$_2^-$(H$_2$O), etc. Typically, they are added in small amounts. In some cases, where amounts as large as a few tenths of a percent are added, the mobility is measured for several concentrations of these added gases, and a correction factor (which is usually quite small), is calculated.

The HPDTMS has recently been modified to operate at temperatures below 300 K. To permit the cooling of this instrument, eight cooling straps were constructed and installed around the drift tube and part of the analysis region. Cold methanol is circulated from a temperature controlled cooler through the eight cooling straps. The entire system is well insulated, and the temperature is monitored by four thermocouples inside and along the outside of the drift region. A temperature uniformity of ± 1% over most of the temperature range and ± 2% at the lowest measured temperature is presently obtainable.

The present grant made possible the addition of a capacitance manometer to the HPDTMS. This device permits the measurement of gas density with greater accuracy than previously attainable and also provides a pressure controlling device and safety circuits (also recently installed). These improvements, along with recently developed techniques for the production of specific ions, have resulted in measurements of the mobility of NO$_2^-$, NO$_3^-$, and CO$_3^-$ in N$_2$ over a temperature range of 217-650 K. These measurements have been published in J. Chem. Phys. and reprints are included with this report. To the best of our knowledge, none of these mobilities have previously been measured, either as a function of temperature or E/N.

Also measured during this grant period, were the temperature dependent mobilities of NO$_2^-$, NO$_3^-$, CO$_3^-$, CO$_4^-$ and O$_2^+$ in O$_2$. Preprints of this paper which has been accepted for publication in J. Chem. Phys. are also included with this report. We do not know of any previous measurements of NO$_2^-$ or NO$_3^-$.
in O\textsubscript{2} as either a function of temperature or E/N. CO\textsubscript{3}\textsuperscript{-} mobilities in O\textsubscript{2} have been measured previously on this same apparatus but over a smaller temperature range. The mobilities of CO\textsubscript{3}\textsuperscript{-}, CO\textsubscript{4}\textsuperscript{-} and O\textsubscript{2}\textsuperscript{+} in O\textsubscript{2} have, however, been measured previously as a function of E/N. Details of the relationship between these measurements and a comparison of the measured mobilities are included in the enclosed paper.

The remainder of this grant period was spent performing measurements of the mobilities of NO\textsubscript{2}\cdot\text{H\textsubscript{2}O}, NO\textsubscript{3}\cdot\text{H\textsubscript{2}O}, CO\textsubscript{3}\cdot\text{H\textsubscript{2}O}, and CO\textsubscript{4}\cdot\text{H\textsubscript{2}O} in N\textsubscript{2} as a function of temperature, none of which, to the best of our knowledge has been measured previously as either a function of temperature or E/N. These measurements have recently been submitted to J. Chem. Phys. and a preprint of this article has been enclosed as part of this report. In addition to the data described in the enclosed articles, observation and, in some cases, preliminary mobility measurements of NO\textsubscript{3}\cdot\text{HNO\textsubscript{3}}, NO\textsubscript{3}\cdot\text{(HNO\textsubscript{3})\textsubscript{2}}, NO\textsubscript{3}\cdot\text{(HNO\textsubscript{3})\textsubscript{3}}, NO\textsubscript{3}\cdot\text{(H\textsubscript{2}O)	extsubscript{2}}, CO\textsubscript{3}\cdot\text{(H\textsubscript{2}O)\textsubscript{2}}, CO\textsubscript{4}\cdot\text{(H\textsubscript{2}O)\textsubscript{2}}, NO\textsubscript{4}\textsuperscript{+}, NH\textsubscript{4} and O\textsubscript{4}\textsuperscript{-} ions in pure N\textsubscript{2} or O\textsubscript{2} have also been made.