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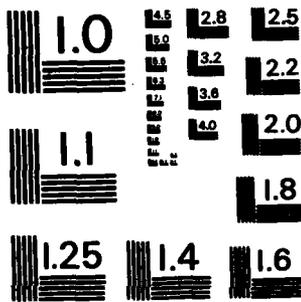   E W MCDANIEL ET AL. 30 MAR 83 N00014-80-C-0243

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REPORT DOCUMENTATION PAGE	READ INSTRUCTIONS BEFORE COMPLETING FORM

1. REPORT NUMBER	2. GOVT ACCESSION NO. AD-A126 604	3. RECIPIENT'S CATALOG NUMBER

4. TITLE (and Subtitle)	5. TYPE OF REPORT & PERIOD COVERED
Final Report	Final March 1, 1980 - Feb. 28, 1983
	6. PERFORMING ORG. REPORT NUMBER

7. AUTHOR(s)	8. CONTRACT OR GRANT NUMBER(s)
E. W. McDaniel and I. R. Gatland	N00014-80-C-0243

9. PERFORMING ORGANIZATION NAME AND ADDRESS	10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS
School of Physics Georgia Institute of Technology Atlanta, Ga. 30332	NR014-314

11. CONTROLLING OFFICE NAME AND ADDRESS	12. REPORT DATE
Office of Naval Research Physics Program Office Arlington, Va. 22217	March 30, 1983
	13. NUMBER OF PAGES 5

14. MONITORING AGENCY NAME & ADDRESS(If different from Controlling Office)	15. SECURITY CLASS. (of this report)
	Unclassified
	15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)

Approved for public release; distribution unlimited.

17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

DTIC
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APR 1 1 1983

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18. SUPPLEMENTARY NOTES

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

Ionic Mobilities	Halogen Ions
Diffusion Coefficients	Thallium Ions
Interaction Potentials	Noble Gases
Alkali Ions	Nitrogen Gas

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

The Georgia Tech program of research on ionic transport in gases is described. Measurements of ionic mobilities and diffusion coefficients are discussed. The use of the mobility data to obtain ion-neutral interaction potentials is described. References are given for publications covering this report period.

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The Drift, Diffusion, and Reactions of Slow Ions in Gases

O. N. R. FINAL REPORT

Contract N00014-80-C-0243

March 1, 1980 – February 28, 1983

E. W. McDaniel and I. R. Gatland, Co-Principal Investigators

School of Physics, Georgia Institute of Technology

Atlanta, Georgia · 30332

1. Scientific Problem

The experimental program consisted of measurements of the mobilities and longitudinal diffusion coefficients of ions in various gases at room temperature. By varying the energy parameter (E/N) of the ions, we may vary the average ionic energy from the thermal value at 300°K to about 10 eV. Our measured mobilities and diffusion coefficients are useful in calculations of properties of weakly ionized plasmas. In addition, the mobilities as a function of E/N can be inverted to obtain the interaction potential for the ion-neutral combination involved, and the mobilities are also useful in calculations of the rate of positive ion-negative ion recombination. Rate coefficients measured for ion-molecule reactions play a role in explaining plasma chemistry; ionic transport data are required for the accurate determination of these rate coefficients. Observations on ionic identity and abundances as functions of gas pressure and temperature are particularly important in atmospheric research.

The relevance of ionic transport phenomena to atmospheric problems arise partly from the concomitant transport of charge, mass, momentum, and energy through space. Further, the drift of ions in an electric field can significantly increase the kinetic energy of the ions, and can change their internal excitation energy by ion-molecule collisions. The changes in translational and internal energy can markedly affect the rates of ion-molecule reactions, and subsequently the rates of other kinds of collisions, notably ion-ion and electron-ion recombination, in the atmosphere.

The theoretical program involved the development of directly determined potentials for several ion-atom systems and the investigation of non-equilibrium situations in ion drift under special conditions. A Monte Carlo simulation of soft core potentials is underway, and extensions to potential "soft spots", where the regular theory does not converge well, is being studied.

From our standpoint the most important use of the mobility data is to generate ion-neutral interaction potentials covering a very wide range of ion-neutral separation distance by inverting the experimental data. The interaction potential for a two-particle system is one of the most fundamental properties of the system. It determines the mutual scattering behavior of the particles and hence the transport properties. The interaction potential also determines many properties of the system that is formed if the two particles can temporarily or permanently combine. In the case of radiative processes, for example, the interaction potentials for the upper and ground states of a neutral diatomic molecule or ion are required for the determination of the wave functions, transition probabilities and spectral features. The standard beam scattering technique used to obtain information about the interaction potential for an ion-neutral system covers a much smaller range of separation distance than does the new method described here. The interaction potentials obtained for the halogen ion-rare gas combinations may have applications in excimer lasers.

We also calculate from our measured drift velocities the zero-field mobilities of these ions in various gases at temperatures ranging from $300^{\circ}K$ to $\sim 10^4 \, ^{\circ}K$ by the techniques we have described in several publications.

2. Scientific and Technical Approach

The experiments are performed with a drift tube mass spectrometer, by techniques which permit accurate measurements to be made on individual ionic species even though several species may be simultaneously present and coupled by ion-molecule reactions. The drift tube gas is maintained at room temperature, but the average energy of a given species of ion can be varied from very close to thermal energy up to a maximum of about 10 eV in favorable cases. The average energy of the ions of a given type is determined by the parameter E/N, where E is the intensity of the electrostatic drift field and N is the number density of the neutral gas molecules contained in the drift tube. The measurements are made as a function of E/N.

The basic measurement made is of the arrival time spectra for each separate ionic species in the drift tube. The measurements are made as functions of drift distance, electric field strength (E) in the drift region, number density of gas molecules in the drift tube (N), and the energy parameter (E/N).

The theoretical calculations are concerned with the relation between the ion-neutral interaction potential and the measured values of the mobilities and diffusion coefficients. The calculation of the transport coefficients is based on a moment solution of the appropriate Boltzmann equation with basis functions which reflect the sometimes high random energy derived from the electric field and the non-symmetric character of the ionic velocity. This allows the mobility data to be used to test theoretical potentials and also to serve as an integral part of an iteration technique which determines the interaction potential directly from the data.

3. Results and Publications

The ion-gas combinations that we have studied during the period covered by this report are: $Li^+ + Xe$; $Tl^+ + He$, Ne, Ar, Kr, Xe; $Cl^- + N_2$; $Br^- + Ne$, Ar, Kr. The results that we obtained are indicated by the titles in the list of publications that follows. Also given in this list are the names of all of the scientific personnel who participated in the research. Of these personnel, the following have obtained their Ph.D. degrees in Physics at the Georgia Institute of Technology: M. G. Thackston, D. R. Lamm, and R. D. Chelf. It is anticipated that F. B. Holleman will obtain his Ph.D. degree in Physics here in 1984.

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