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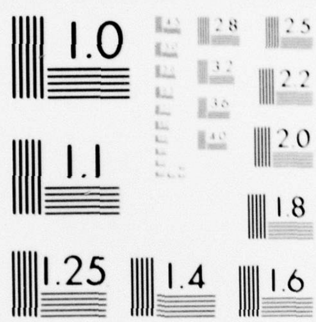

MICROCOPY RESOLUTION TEST CHART

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SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER	2. GOVT ACCESSION NO.	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle) Summary Questionnaire		5. TYPE OF REPORT & PERIOD COVERED Summary. Nov. 1,1977 - Oct. 31,1978
		6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s) E. W. McDaniel and I. R. Gatland		8. CONTRACT OR GRANT NUMBER(s) N00014-76-C-0015
9. PERFORMING ORGANIZATION NAME AND ADDRESS School of Physics, Georgia Institute of Technology, Atlanta, Ga. 30332		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS NR 394-002
11. CONTROLLING OFFICE NAME AND ADDRESS Office of Naval Research, Physics Program Office, Arlington, Va. 22217		12. REPORT DATE Nov. 1, 1978
		13. NUMBER OF PAGES 4
14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office)		15. SECURITY CLASS. (of this report) Unclassified
		15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

LEVEL II

(16) (11) (15) (11) 1 Nov 78 (12) 5 p.

AD A061886

DDC FILE COPY

16. DISTRIBUTION STATEMENT (of this Report)

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

(9) Summary rept. 1 Nov 77 - 31 Oct 78

DDC RECEIVED DEC 1 1978 F

18. SUPPLEMENTARY NOTES

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

Ionic Mobilities
Diffusion Coefficients
Interaction Potentials
Alkali ions
Halogen ions
Noble Gases

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

The Ga Tech program of research on ionic transport in gases is described. Experimental measurements of ionic mobilities and diffusion coefficients are discussed. The use of the mobility data to obtain ion-neutral interaction potentials is described. References to recent publications are given, and the program for the next year is outlined.

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O. N. R. SUMMARY QUESTIONNAIRE

Contract N00014-76-C-0015

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Atlanta, Georgia 30332

1. Contract Description

The experimental program consists 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 ^{o}K to about 10 eV. The data are of immediate practical value in applications involving ionized gases. They are also used to test theoretical ion-neutral interaction potentials, to determine directly such interaction potentials, and to test theories of ionic transport in gases.

During the coming year, we propose to make accurate measurements of the mobilities and longitudinal diffusion coefficients of F^-, Br^-, and I^- ions in Ne and Ar and of Li^+ and Na^+ ions in Kr and Xe over a wide range of E/N, and to continue the program of obtaining interaction potentials.

2. Scientific Problem

Our measurements of transport properties of ions in gases provide data of immediate practical use in the quantitative analysis of electrical discharges in the laboratory and in the explanation of various natural phenomena. However, the most important use of the drift velocity data will be 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 to be obtained for the (halogen and alkali) ion-rare gas combinations will have applications in excimer lasers.

We shall also calculate from our measured drift velocities the zero-field mobilities of these ions in various gases at temperatures ranging from 300°K to ∿ 10^4 °K by the techniques we have described. (See E. A. Mason, L. A. Viehland, H. W. Ellis, D. R. James, and E. W. McDaniel, "The Mobilities of K^+ Ions in Hot Gases", Phys. Fluids 18, 1070 (1975)). Finally we shall use our diffusion coefficients to test the theories of diffusion of gaseous ions in electric fields which have been developed during the last few years. (See L. A. Viehland and E. A. Mason, Annals of Physics 91, 499 (1975); 110, 287 (1978). S. L. Lin, L. A. Viehland and E. A. Mason, "Three-Temperature Theory of Gaseous Ion Transport", Chem. Phys., in press.)

3. 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 mobilities 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.

4. Progress

During the current O. N. R. contract period, we have measured the mobilities and longitudinal diffusion coefficients of F^-, Cl^-, Br^-, and I^- in Kr and Xe and

Cl^- in N_2. These measurements were made at 300°K and over a substantial range of the energy parameter E/N. Our data are the first to be obtained for the systems listed above. These studies of the negative halogen ions required considerably more time than anticipated, principally because of the difficulty in obtaining suitable amounts of F^- ions in suitably shaped pulses for insertion into the drift region. However, we regarded the F^- ion-noble gas combinations as important enough to warrant our spending the time required, although this decision prevented us from undertaking the additional studies of Tl^+ in various gases that we had proposed for this contract period.

The interaction potential for Cl^- - Xe has been determined directly from the data, and similar studies for Cl^- - Kr are underway.

5. Publications (During 1977-78 and to be published)

1. M. G. Thackston, F. L. Eisele, H. W. Ellis, and E. W. McDaniel, "Mobilities of Cs^+ Ions in Molecular Gases: H_2, N_2, O_2, CO, and CO_2", Jour. Chem. Phys. 67, 1276 (1977).

2. F. L. Eisele, M. G. Thackston, W. M. Pope, I. R. Gatland, H. W. Ellis, and E. W. McDaniel, "Experimental Test of the Generalized Einstein Relation for Cs^+ Ions in Molecular Gases: H_2, N_2, O_2, CO, and CO_2", Jour. Chem. Phys. 67, 1278 (1977).

3. M. G. Thackston, F. L. Eisele, W. M. Pope, H. W. Ellis, and E. W. McDaniel, "Further Tests of the Generalized Einstein Relation: Cs^+ Ions in Ar, Kr, and Xe", Jour. Chem. Phys. 68, 3950 (1978).

4. W. M. Pope, H. W. Ellis, F. L. Eisele, M. G. Thackston, E. W. McDaniel, and R. A. Langley, "Mobilities and Longitudinal Diffusion Coefficients for Cs^+ Ions in He and Ne Gas", Jour. Chem. Phys. 68, 4761 (1978).

5. W. M. Pope, F. L. Eisele, M. G. Thackston, and E. W. McDaniel, "Longitudinal Diffusion Coefficients and Test of the Generalized Einstein Relation for Rb^+ - Kr, Rb^+ - Xe, K^+ - Kr, and K^+ - Xe", Jour. Chem. Phys. (Oct. 15, 1978 issue).

6. M. G. Thackston, F. L. Eisele, W. M. Pope, H. W. Ellis, I. R. Gatland, and E. W. McDaniel, "Mobility of Cl^- Ions in Ne, Ar, and Kr", to be submitted to Jour. Chem. Phys.

7. F. L. Eisele, M. G. Thackston, W. M. Pope, H. W. Ellis, and E. W. McDaniel, "Calculated and Experimental Values of Longitudinal Diffusion Coefficients for Cl^- Ions in Ne, Ar, Kr, and Xe", submitted to Jour Chem. Phys.

8. F. L. Eisele, M. G. Thackston, W. M. Pope, H. W. Ellis, and E. W. McDaniel, "Mobilities and Diffusion Coefficients for F^- Ions in Kr, and Xe", submitted to Jour. Chem. Phys.

9. H. W. Ellis, E. W. McDaniel, D. L. Albritton, L. A. Viehland, S. L. Lin, and E. A. Mason, "Transport Properties of Gaseous Ions Over a Wide Energy Range - Part II", Atomic Data and Nuclear Data Tables, in press.

10. M. G. Thackston, F. L. Eisele, W. M. Pope, H. W. Ellis, E. W. McDaniel, and I. R. Gatland, "Mobility of Cl^- Ions in Xe, and The Cl^- - Xe Interaction Potential", to be submitted to Jour. Chem. Phys.

11. I. R. Gatland, W. F. Morrison, H. W. Ellis, M. G. Thackston, E. W. McDaniel, M. H. Alexander, L. A. Viehland, and E. A. Mason, "The Li^+ - He Interaction Potential", Jour. Chem. Phys. 66, 5121 (1977).

12. I. R. Gatland, M. G. Thackston, W. M. Pope, F. L. Eisele, H. W. Ellis, and E. W. McDaniel, "Mobilities and Interaction Potentials for Cs^+ - Ar, Cs^+ - Kr, and Cs^+ - Xe", Jour. Chem. Phys. 68, 2775 (1978).

13. I. R. Gatland, D. R. Lamm, M. G. Thackston, W. M. Pope, F. L. Eisele, H. W. Ellis, and E. W. McDaniel, "Mobilities and Interaction Potentials for Rb^+ - Ar, Rb^+ - Kr, and Rb^+ - Xe", Jour. Chem. Phys. (Dec. 1, 1978 issue).

14. I. R. Gatland, L. A. Viehland, and E. A. Mason, "Tests of Alkali Ion-Inert Gas Interaction Potentials by Gaseous Ion Mobility Experiments", Jour. Chem. Phys. 66, 537 (1977).

6. Extenuating Circumstances

None.

7. Personnel Involved in the Research

(A) E. W. McDaniel, Regents' Professor of Physics - Project Director.

(B) I. R. Gatland, Professor of Physics. (Co-Principal Investigator).

(C) H. W. Ellis, Research Scientist. Dr. Ellis obtained his Ph.D. degree in Physics from the Georgia Institute of Technology in March, 1974, and began work with us at that time. He terminated on Sept. 1, 1978.

(D) F. L. Eisele, Postdoctoral Fellow. Dr. Eisele obtained his Ph.D. degree in Atomic Collisions Physics at the University of Vermont and then spent a year at the University of Georgia. He joined us on July 1, 1976.

(E) W. M. Pope. Dr. Pope obtained his Ph.D. degree at Florida State University in Atomic Collisions Physics and then spent a year at the University of Texas (Austin). He joined us on November 1, 1976 and terminated on Sept. 1, 1978.

(F) Michael G. Thackston. Mr. Thackston joined us in the summer of 1975 and is doing a Ph.D. research problem with us.

8. Graduate Students Who Earned Advanced Degrees During Contract Period

None.