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THE DRIFT, DIFFUSION, AND REACTIONS OF SLOW IONS IN GASES.(U)  
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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. 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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## The Drift, Diffusion, and Reactions of Slow Ions in Gases.

O. N. R. SUMMARY QUESTIONNAIRE

Contract No. / N00014-80-C-0243

Nov. 1, 1979 - Oct. 31, 1980

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

School of Physics, Georgia Institute of Technology

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  $300^{\circ}\text{K}$  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  $\text{Na}^+$ ,  $\text{Rb}^+$ , and  $\text{Cs}^+$  ions in molecular gases and of  $\text{Tl}^+$  ions in Ne, Ar, Kr, Xe,  $\text{N}_2$ , and  $\text{O}_2$  over a wide range of  $E/N$ , and to continue the program of obtaining interaction potentials.

The theoretical effort will involve a continuation and extension of the following studies now under way:

- (1) Determination of ion-neutral interaction potentials for sodium ions in rare gases.
- (2) Further investigation of the relation of the  $\text{Li}^+ - \text{H}_2$  interaction to mobility and diffusion.
- (3) Interaction potentials for  $\text{Br}^-$  and  $\text{F}^-$  in Ne, Ar, Kr, and Xe.
- (4) Mobilities and potentials for thallium ions in rare gases.

This case is of particular interest since it involves an ion which is not a closed shell structure.

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 obtain information on ion-neutral interaction potentials, covering a very wide range

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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.

In addition, the experimental transport data may be used in the calculation of ion-ion recombination coefficients (see, for example, M. R. Flannery, "Ionic Recombination", in Atomic Processes and Applications (P. G. Burke and B. L. Moiseiwitsch, Eds.) North-Holland, Amsterdam (1976) pp. 407-466.)

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  $\sim 10^4$  °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. 37, 411 (1979).]

### 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

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\*This instrument (abbreviated here as DTMS) is designed to operate at low pressures (usually well below 1 Torr). We also have a high pressure DTMS, which we occasionally use on the ONR research, although it is utilized mainly on research supported by NSF (see Section 10).

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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 a 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, or expect to measure, the mobility and longitudinal diffusion coefficient of  $\text{Br}^-$  in Ne, Ar, and Kr (at 300°K and over the widest possible range of  $E/N$ ). Our study of  $\text{Li}^+$  in Xe has been brought to completion. Extensive repairs and modifications that result in improved performance of the apparatus were made, and a  $\text{Tl}^+$  ion source was constructed and installed. It may be possible to make some studies with  $\text{Tl}^+$  ions in the time remaining, although the repairs and modifications consumed a significant fraction of the present contract period and threw us well behind schedule in our experimental program.

On the theoretical side, mobility calculations have been used to test the electron gas - Drude model potentials of Gordon and Waldman for  $\text{Li}^+$ ,  $\text{Na}^+$ ,  $\text{K}^+$ , and  $\text{Rb}^+$  in He, Ne, and Ar. The inversion procedure has been applied to  $\text{Cs}^+$ ,  $\text{Rb}^+$ , and  $\text{K}^+$  ions in Ar, Kr, and Xe, and is now being applied to  $\text{Na}^+$  in all of

the noble gases. Also three ab initio potentials calculated by full quantal means have been used to test the mobility theory. These are the  $\text{Li}^+$  - He potential of Hariharan and Staemmler, the  $\text{H}^+$  - He potential of Kolos and Peck, and the  $\text{Li}^+$  - Ar potential of Olsen and Liu.

The  $\text{H}^+$  - He case is particularly interesting. At high E/N the potential becomes Coulombic and the concept of mobility is not applicable. Rather the ions are subject to a continuously increasing acceleration if only elastic collisions are considered. The mobility theory responds to this situation by producing sensible results at low E/N (in good agreement with experiments) and giving unstable results at large values of the effective temperature. This runaway phenomenon has since been verified experimentally. The runaway effects appear to act like a depleting reaction with a time scale which, we conjecture, is related to fluctuations in the ion velocities. We are presently formulating and testing a Monte-Carlo simulation of this system.

An especially interesting (and difficult) case is that of  $\text{Li}^+$  -  $\text{H}_2$ . Our calculations to date indicate that the symmetric part of the potential gives reasonable results but is not in full agreement with experiment. Further studies are underway.

##### 5. Publications (Asterisk denotes O. N. R. Research)

- \* 1. M. G. Thackston, F. L. Eisele, W. M. Pope, H. W. Ellis, and E. W. McDaniel, "Mobilities and Longitudinal Diffusion Coefficients for  $\text{F}^-$  Ions in Kr and Xe", Jour. Chem. Phys. 73, 1477 (1980).
- \* 2. M. G. Thackston, M. S. Sanchez, G. W. Neeley, W. M. Pope, F. L. Eisele, I. R. Gatland, and E. W. McDaniel, "Mobilities and Longitudinal Diffusion Coefficients for  $\text{Na}^+$  Ions in Kr and Xe", Jour. Chem. Phys. 73, 2012 (1980).
- \* 3. M. G. Thackston, F. L. Eisele, W. M. Pope, H. W. Ellis, E. W. McDaniel, and I. R. Gatland, "Mobility of  $\text{Cl}^-$  Ions in Xe Gas and the  $\text{Cl}^-$  - Xe Interaction Potential", Jour. Chem. Phys. 73, 3183 (1980).
- \* 4. S. L. Lin, I. R. Gatland, and E. A. Mason, "Mobility and Diffusion of Protons and Deuterons in Helium - A Runaway Effect", J. Phys. B 12, 4179 (1979).
- \* 5. D. R. Lamm, M. G. Thackston, F. L. Eisele, H. W. Ellis, J. R. Twist, W. M. Pope, I. R. Gatland, and E. W. McDaniel, "Mobilities and Interaction Potentials for  $\text{K}^+$  - Ar,  $\text{K}^+$  - Kr, and  $\text{K}^+$  - Xe", Jour. Chem. Phys., in press.
- \* 6. J. R. Twist, F. L. Eisele, M. G. Thackston, F. B. Holleman, R. Chelf, D. R. Lamm, I. R. Gatland, and E. W. McDaniel, "The Mobilities and Longitudinal Diffusion Coefficients of  $\text{Br}^-$  Ions in Ne, Ar, Kr, and Xe", to be submitted to Jour. Chem. Phys.

- \* 7. M. G. Thackston, M. S. Sanchez, G. W. Neeley, W. M. Pope, J. R. Twist, and E. W. McDaniel, "The Mobilities and Longitudinal Diffusion Coefficients of  $\text{Li}^+$  Ions in Kr and Xe", to be submitted to Jour. Chem. Phys.
- \* 8. I. R. Gatland and D. R. Lamm, "Tests of  $\text{Li}^+$  - Ar Interaction Potentials by Drift Tube Experiments", to be submitted to Jour. Chem. Phys.
- 9. F. L. Eisele, M. D. Perkins, and E. W. McDaniel, "Mobilities of  $\text{NO}_2^-$ ,  $\text{NO}_3^-$ , and  $\text{CO}_3^-$  in  $\text{N}_2$  Over the Temperature Range 217 - 675 K", Jour. Chem. Phys. 73, 2517 (1980).
- 10. M. D. Perkins, F. L. Eisele, and E. W. McDaniel, "Temperature Dependent Mobilities:  $\text{NO}_2^-$ ,  $\text{NO}_3^-$ ,  $\text{CO}_3^-$ ,  $\text{CO}_4^-$  and  $\text{O}_2^+$  in  $\text{O}_2$ ", Jour. Chem. Phys., in press.
- 11. E. W. McDaniel, et al., "Compilation of Atomic and Molecular Data Relevant to Gas Lasers", Redstone Arsenal, Alabama; U.S. Army MICOM Technical Report H-78-1. Vol. VI (1979); Vol. VII (1980).
- 12. H. S. W. Massey, B. Bederson, and E. W. McDaniel (Eds.), Applied Atomic Collision Physics, 4 vols., Academic, New York, in press.
- 13. H. W. Ellis, E. W. McDaniel, and E. A. Mason, "Transport Properties of Gaseous Ions - Part III", to be submitted to Atomic Data and Nuclear Data Tables.
- 14. E. W. McDaniel and E. A. Mason, The Mobility and Diffusion of Ions in Gases (2nd. Ed.), Wiley, New York, in preparation.
- 15. E. W. McDaniel, "Ionic Transport Phenomena and Their Applications", invited paper presented at Sixth Int. Conf. on Atmospheric Electricity, Manchester, England, July 28 - August 1, 1980. Conf. Proceedings to be published.
- 16. C. F. Barnett, - - - - -, E. W. McDaniel, et al., "1978 Bibliography of Atomic and Molecular Processes (372 pp.), DOE/ER-0044; "1979 Bibliography of Atomic and Molecular Processes" (337 pp.), DOE/ER-0074. U. S. Dept. of Energy (1980).

#### 6. Extenuating Circumstances

Our low-pressure DTMS has been in operation since 1967, with an average of only about 5% downtime due to equipment failure until the beginning of the present contract period (March 1, 1980). At about this time we began to encounter a series of electrical and mechanical problems which cost us months of running time. The Granville Phillips Servo Leak Controller developed intermittent instabilities, and satisfactory operation was restored only by overhauling the unit, and designing, testing, and constructing a Signal Conditioning Circuit. A commercial Freon Cooler was installed in the gas feed line to save

liquid nitrogen costs; this device broke down and had to be returned to the manufacturer, temporary measures being adopted until its repair and return. A power outage during a storm on a weekend, combined with an equipment failure in our laboratory, resulted in the loss of a forepump, but the diffusion pumps were reactivated when the power was restored. This accident caused the apparatus to be exposed to hot pump oil vapour and necessitated a cleanup, gold-plating, and reassembly that consumed three months.

However, we were able to take some advantage of the downtime and disassembly of the DTMS. The interior surfaces are now cleaner than at any time since the early days of operation. Several valves, manifolds, pressure gauges, and fittings have been replaced. Automatic quick cools have been installed on the diffusion pumps, and a new safety circuit for control of the electrical power is on line. We appear to be fully protected against power and forepump failure, and the DTMS is in much improved overall condition.

7. Unspent Funds Remaining at End of Current Contract Period

None.

8. 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) J. R. Twist, Postdoctoral Fellow. Dr. Twist obtained his Ph.D. degree in Atomic Physics from the University of Oklahoma in June, 1979 and began work with us at that time.
- (D) M. G. Thackston, Graduate Student. Mr. Thackston joined us in the summer of 1975 and is doing a Ph.D. research problem with us.
- (E) M. S. Sanchez, Graduate Student. Mr. Sanchez started to work with us on the experimental aspects of our program in the winter of 1979. Mr. Sanchez left Georgia Tech in June, 1980 to enter dental school.
- (F) D. R. Lamm, Graduate Student. Mr. Lamm began work with us in October, 1979 on the theoretical aspects of our program for his Ph.D. research.
- (G) F. B. Holleman, Graduate Research Assistant. Mr. Holleman joined our group in June, 1980, when he entered graduate school at Georgia Tech.
- (H) R. D. Chelf, Research Scientist. Mr. Chelf started to work with us in October, 1980, when he passed the Comprehensive Examinations in Physics. He intends to do his Ph.D. research with us.



9. Graduate Students Who Earned Advanced Degrees During Contract Period

Mr. Thackston will receive his Ph.D. degree in Physics in December, 1980.

10. Other Government-Sponsored Research

We have recently obtained from the National Science Foundation a two-year extension of their support, the extension providing \$136,699 for a program entitled "Measurement of Ion Transport Properties, Ion Reaction Rates, and Trace Neutral Concentrations of Atmospheric Interest". The Grant Number is ATM-8016881. The NSF grant is scheduled to end on August 31, 1982. The NSF research involves measurements of ionic mobilities and reaction rates that are of atmospheric interest. Practically all of the measurements will be made with our high-pressure DTMS. There is no overlap between the research proposed to ONR in this document and that performed with NSF support, although equipment and personnel (E. W. McDaniel) will be shared.

We have no proposals outstanding at this time.

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