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Mobilities and interaction potentials for the O^+ -He and O^- -He systems

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Mobilities of O^+ and O^- ions in He gas have been measured as a function of electric field strength at temperatures from 93 to 568 K. The results are compared with previous work, and analyzed in terms of a temperature-field strength scaling rule and the O^+ -He and O^- -He potentials. Emphasis is placed on how much information on the potentials can be obtained from simple features of the mobility curve without extensive numerical computation.

I. INTRODUCTION

The differences between the mobilities of the positive and negative ions of the same atom through a neutral gas are sometimes quite striking. At first glance this may seem odd, because the long-range ion-neutral interactions are the same—usually the dominant r^{-4} potential between the ionic charge and the dipole it induces in the neutral molecule (the polarization potential), which depends only on the polarizability of the neutral. But at closer distances the interactions may be quite different because of the different electronic structures of the ions.

Kinetic theory furnishes an accurate description of the connection between the mobility and the interaction potential, and the behavior of the mobility as a function of temperature and electric field strength can be analyzed in some detail to furnish information on the interaction between an atomic ion and a neutral atom.¹

The mobilities of O^+ and O^- ions in He buffer gas have recently been determined in connection with measurements of some ion-molecule reaction rates.^{2,3} The purpose of this paper is to analyze these mobilities in terms of the O^+ -He and O^- -He potentials. There has been a substantial amount of theoretical work done on the HeO^+ system,^{4,5} which has a binding energy of about 50 meV or 1 kcal/mol, but very little on the HeO^- system, whose binding energy is an order of magnitude smaller.^{6,7}

An important feature of the present measurements is that both temperature and electric field were varied; all previous mobility measurements on these systems were performed only at about 300 K. This has two consequences. The first consequence is that a consistency check is possible via a theoretical scaling rule, in which a series of curves of mobility as a function of field strength, each at a different fixed temperature, are collapsed into a single curve of mobility as a function of an effective temperature.¹ That is, the two variables T and E/N (electric field strength divided by neutral gas number density) are reduced to a single variable, T_{eff} . This scaling rule also tests whether an ion-neutral interaction can be reasonably represented by a single effective potential when in fact two or more potentials are relevant.⁸ Such a situation arises with HeO^- , which has a $^2\Sigma$ and a $^2\Pi$ state, both of which dissociate to ground-state O (2P) and He(1S). The sec-

ond consequence is that the low-temperature measurements probe the potential to larger separations. Previous measurements on O^- -He probed only the repulsive part of the potential, for example, whereas the present measurements probe at least part of the attractive well.

In the following sections we first briefly describe the experiments, and then analyze the measurements for internal consistency and for agreement with previous measurements. All the experimental data are then analyzed for information on the ion-neutral potentials, with emphasis on how much information can be obtained from simple features of the mobility curves, without having to resort to full-scale numerical inversion to find the complete potential curve. Finally, comparison is made with other available information on the potential.

II. EXPERIMENT

The experimental measurements were performed using the variable-temperature-selected-ion flow-drift-tube apparatus at the Geophysics Directorate of Phillips Laboratory. The apparatus and technique have been described in detail elsewhere.⁹ Only details pertinent to the present study are given here. The O^+ ions were generated by electron impact on CO in a high pressure (0.1–1 torr) remote ion source. This source has been shown previously to produce 98% of the O^+ ions in the ground 4S state.¹⁰ Interference from the excited 2D and 2P states of O^+ is therefore negligible. The O^- ions were produced in the ion source from N_2O . The ion species of interest was then mass selected in a quadrupole mass spectrometer and injected into the flow tube through a Venturi inlet. Inside the flow tube the ions were entrained in a fast flow ($\sim 10^4$ cm/s at ~ 0.4 torr) of helium buffer gas. After being sampled through a 0.2 mm orifice in a sampling plate, the ions were mass analyzed in a second quadrupole mass spectrometer and detected by a channel particle multiplier. A heat exchanger in contact with the flow tube was used to vary the experimental temperature. Attached to the heat exchanger are liquid nitrogen cooling coils and electrical heaters.

Ion mobility measurements were made as a function of electric field strength at each of several temperatures by measuring ion flight times over known distances in the drift tube portion of the flow tube. The ion flight time was

determined by imposing a pulsed retarding potential on a drift tube guard ring and then measuring the arrival time of the perturbation in the ion swarm at the detector using a digital time-of-flight unit and a multichannel analyzer. This procedure was repeated at a second guard ring in order to subtract the contribution from end effects, and the flight times were converted to velocities using the known distances. The above method was also used at zero drift field in order to measure the flight time due to the He buffer gas (the zero-field ion velocity). The drift velocity v_d is equal to the ion velocity minus the zero-field ion velocity. The ion mobility K is calculated from the relation $K = v_d/E$ where E is electric field strength. The standard mobility K_0 is defined as $K_0 = K(p/760)$ (273.15/ T), where p is the buffer gas pressure in torr and T is the temperature in degrees kelvin.

III. RESULTS

We first briefly summarize the scaling rule, including its likely limitations, since it figures prominently in the analysis of the mobility data. The standard mobility K_0 , reduced to a value corresponding to a standard neutral gas number density at fixed T and E/N , is given by¹

$$K_0 = \frac{3q}{16N_0} \left(\frac{2\pi}{\mu k T_{\text{eff}}} \right)^{1/2} \frac{1+\alpha}{\bar{\Omega}^{(1,1)}(T_{\text{eff}})}, \quad (1)$$

$$\frac{3}{2}kT_{\text{eff}} = \frac{3}{2}kT + \frac{1}{2}Mv_d^2(1+\beta), \quad (2)$$

where q is the ionic charge, N_0 is the standard gas density (2.687×10^{19} molecules/cm³), $\mu = mM/(m+M)$ is the reduced mass for the collision of an ion (mass m) with a neutral (mass M), k is Boltzmann's constant, T_{eff} is the effective temperature for ion-neutral collisions at gas temperature T and field strength E/N , $\bar{\Omega}^{(1,1)}(T_{\text{eff}})$ is the temperature-averaged momentum-transfer cross section for ion-neutral collisions (normalized to be $\pi\sigma_{12}^2$ for collisions between hard spheres of mutual diameter σ_{12}), $v_d = K \cdot E = N_0 K_0 (E/N)$ is the ion drift velocity, and α and β are correction terms (functions of T and E/N) that include all the higher-order kinetic-theory contributions.

In first approximation, where both α and β are zero, it is clear that K_0 depends on the single variable T_{eff} , which in turn depends on both T and E/N through v_d . Thus all the isotherms of K_0 vs E/N can be collapsed to a single curve of K_0 vs T_{eff} . The structure of T_{eff} is surprisingly simple in first approximation. The effective average energy of collision, $(3/2)kT_{\text{eff}}$, consists of the thermal energy of the neutral gas, $(3/2)kT$, plus a term $(1/2)Mv_d^2$ that corresponds to the average energy which the ions have gained from the field and that has been randomized by collisions. The rest of the average ion energy is $(1/2)mv_d^2$, which is the drift energy in the field direction.

The main restriction on Eqs. (1) and (2) is that the ion-neutral collisions must be elastic. When this is the case, α and β are fairly small [usually less than about 10% (Ref. 1)], and moreover their effects tend to compensate or to be absorbed into $\bar{\Omega}^{(1,1)}(T_{\text{eff}})$.¹¹ The first-order scaling rule therefore holds to a very good approximation, al-

though very precise mobility data (e.g., electrons in noble gases) may show deviations of up to a few percent.¹¹

The case of multiple interaction potentials, which occurs for HeO^+ , is of more relevance here, since Eqs. (1) and (2) were originally derived for single potentials only. It was shown long ago¹² that the formulas for transport coefficients in general are not changed in form by multiple interactions, but that the cross sections must be calculated differently. A cross section is calculated for each potential curve and then an average cross section is calculated, weighted by the statistical probabilities (multiplicities) of the potential curves. That is, $\bar{\Omega}^{(1,1)}(T_{\text{eff}})$ in Eq. (1) is a weighted average over the multiple interactions. The new problem here is the meaning of T_{eff} . The solution is simple because the ions are present only in trace quantities. Each ion "sees" the neutral gas as a mixture of species, one for each interaction, and present in proportion to their statistical weights. The expression for T_{eff} for a general mixture has been worked out and is fairly complicated, with a different T_{eff} for each neutral species.¹³ But in the special case that the neutral species all have the same mass, the expression collapses back to Eq. (2), with v_d being the actual drift velocity in the mixture, and all the T_{eff} 's are equal.

The final result is that Eqs. (1) and (2) remain valid in the case of multiple interactions, and the scaling rule still holds as a good approximation. The only noticeable result of multiple interactions is that the final K_0 vs T_{eff} curve may have an unusual shape if the interactions are sufficiently different, so as to produce cross sections with very different dependences on energy (effective temperature). But if this does not happen, it may be reasonable to represent the multiple interactions by a single effective potential chosen so as to reproduce the experimental K_0 vs T_{eff} curve.

Finally, in the limit of very low energies (i.e., $E/N \rightarrow 0$, $T \rightarrow 0$), the interaction is dominated by the r^{-4} polarization potential and Eq. (1) becomes¹

$$K_{\text{pol}} = \frac{13.853}{(\mu\alpha_d)^{1/2}} \text{ cm}^2/\text{V s}, \quad (3)$$

where α_d is the dipole polarizability of the neutral in Å³ and μ is in amu. This leads to $K_{\text{pol}} = 17.1 \text{ cm}^2/\text{V s}$ for both O^+ and O^- in He.

A. HeO^+

The mobility of ground-state O^+ in He gas at about 300 K had been well determined by 1975 by a number of workers;¹⁴⁻¹⁷ these results have been summarized and smoothed by Ellis *et al.*¹⁸ Subsequent measurements,¹⁹⁻²² all at about 300 K, have served largely to verify and slightly extend the range of these.

There have been two *ab initio* calculations of the interaction potential for HeO^+ : Simpson, MacLagan, and Harland report the whole $V(r)$ curve, and Frenking *et al.*⁵ report only the depth and position of the potential well. There have been two determinations of $V(r)$ by fitting the mobility data at 300 K: a crude fit by Viehland and Mason⁶ using an (8,6,4) potential model, and a more elaborate fit by Lin and Bardsley⁷ using Monte Carlo simulation. Of all

TABLE I. Potential parameters for HeO^+ from various sources.

Source	ϵ (meV)	r_m (Å)
Simpson <i>et al.</i> ^a	38.8	2.42
Frenking <i>et al.</i> ^b	35	2.473
Viehland and Mason ^c	54	2.14
Lin and Bardsley ^d	52	2.13
Guest <i>et al.</i> ^e	< 56	...

^a*ab initio* calculation (Ref. 4).^b*ab initio* calculation (Ref. 5).^cMobility fit (Ref. 6).^dMobility fit (Ref. 7).^eRainbow scattering (Ref. 23).

these results, the most accurate is probably that of Lin and Bardsley, who fitted measurements, and the least accurate that of Frenking *et al.*, who used a less elaborate basis set than did Simpson, MacLagan, and Harland.

In addition, an upper bound for the potential well depth can be obtained from measurements of the differential cross section for scattering of O^+ ions in noble gases. Guest *et al.*²³ found rainbow structure in the differential cross sections for ArO^+ , KrO^+ , and XeO^+ , but not for HeO^+ and NeO^+ . The well depth ϵ is approximately proportional to the value of $E\theta$ at which the primary rainbow maximum occurs, where E is the energy (not the electric field strength) and θ is the scattering angle. The value of $(E\theta)_{\text{rbow}}$ for ArO^+ is about 60 eV deg, and the well depth is 0.67 eV.²³ For HeO^+ the smallest observed $E\theta$ value was about 5 eV deg, so that $(E\theta)_{\text{rbow}} < 5$ eV deg and the bound on the well depth is therefore $\epsilon < (5/60)(0.67) = 0.056$ eV.

The foregoing results are summarized in Table I.

The present mobility results are shown in Fig. 1 as K_0 vs T_{eff} together with a selection of the previous measurements. There is overall agreement of the present results with both the scaling rule and the previous measurements, but two discrepancies are apparent. First, the low-

temperature results (93 K) do not fit completely smoothly with the higher-temperature results, although they do agree within their estimated uncertainties of about 5%. Although the experiments were more difficult at 93 K, we do not feel that there is any compelling reason to justify adjusting the results for a smoother fit. Second, there is a systematic difference of about 4% between the present and the previous results. This is well within the respective uncertainties of 5% and 5%–7%, however.

The theoretical calculations of K_0 for the three complete determinations^{4,6,7} of $V(r)$ are also shown in Fig. 1. The agreement, although certainly not excellent, is within the uncertainty of the measurements. It does appear as if the calculated mobilities, if extrapolated to lower temperatures, would not agree with the present low-temperature measurements. This result suggests that the estimated long-range "tail" of $V(r)$ is somewhat in error.

It is worth pointing out that the binding energy and other major properties of a molecular ion such as HeO^+ can easily be estimated from a few of the salient features of a K_0 vs T_{eff} mobility curve, without the necessity of a full-scale numerical inversion^{24,25} to find the entire $V(r)$ curve, by means of just the first approximation of Eqs. (1) and (2). The two most obvious features of a mobility curve like that shown in Fig. 1 are the position and height of the mobility maximum, the height being measured by $K_{\text{max}}/K_{\text{pol}}$. The position $T_{\text{eff}}^{\text{max}}$ depends primarily on the potential well depth ϵ , and only secondarily on the potential shape.²⁶ The dimensionless ratio $K_{\text{max}}/K_{\text{pol}}$ gives a measure of the potential shape, or roughly speaking, the "width" of the potential well.²⁷ Given an estimate of the potential shape, the value of $T_{\text{eff}}^{\text{max}}$ determines ϵ , and then r_m follows from the known coefficient of the r^{-4} polarization energy.

Secondary features of a mobility curve can determine more subtle features of $V(r)$. For example, the slope of the high-field branch of K_0 determines the steepness of the repulsive branch of $V(r)$,¹ and the presence of a low-field minimum in K_0 indicates that $V(r)$ shows more attraction than the r^{-4} polarization as the particles approach each other.²⁸ However, we will not make use of these features here.

We first estimate the well depth for HeO^+ by analogy with that for ArO^+ , which is 0.67 eV.²³ From Fig. 1 we see $T_{\text{eff}}^{\text{max}} \approx 1000$ K for HeO^+ ; for ArO^+ the mobility maximum of $K_0 = 3.94$ cm²/V s occurs at $E/N = 3.0 \times 10^{-15}$ V cm² at 300 K,²⁸ corresponding to $T_{\text{eff}} \approx 16\,500$ K according to Eq. (2). Thus the well depth for HeO^+ is less than that for ArO^+ by a factor of $1000/16\,500$, or $\epsilon \approx 41$ meV. This is in reasonable accord with the more elaborate results in Table I, but is only a rough approximation because it involves the assumption that the potentials for HeO^+ and ArO^+ have the same shape. In fact, the shapes differ, as measured by the values of $K_{\text{max}}/K_{\text{pol}}$, which is about 1.50 for HeO^+ and 1.23 for ArO^+ . The fundamental reason that analogous ion-atom potentials do not have the same shape, whereas analogous atom-atom potentials often do, has been discussed by Koutselos, Mason, and Viehland.²⁹

A somewhat better estimate can be made by including the result for $K_{\text{max}}/K_{\text{pol}}$ from Fig. 1, which is about 25.6:

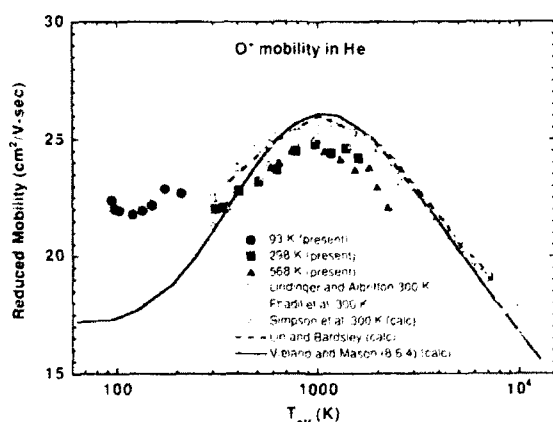


FIG. 1. Standard mobility of O^+ ions in He gas as a function of effective temperature. The solid symbols represent the present measurements: ●, 93 K; ■, 298 K; ▲, 568 K. The other symbols are □, Lindinger and Albritton, 300 K (Refs. 17,18); ○, Fhadil, Mathur, and Hasted, 293 K (Ref. 20); △, Simpson, MacLagan, and Harland (Ref. 4). Representative error bars are shown. The theoretical curves are ---, Lin and Bardsley (Ref. 7); —, Viehland and Mason (Ref. 6).

17.1 = 1.50. From calculations for $(n,6,4)$ potential models,³⁰ we can prepare graphs of $kT_{\text{eff}}^{\text{max}}/\epsilon$ vs $K_{\text{max}}/K_{\text{pol}}$,^{6,27} from which values of ϵ/k can be read. This yields a range of values for ϵ , depending on the particular $(n,6,4)$ potential selected, and the true value is likely to lie within this range. For HeO^+ we thereby obtain the estimate $51 \leq \epsilon \leq 65$ meV for $8 < n < 14$, with the corresponding range of the minimum position, or bond length, equal to $2.18 \geq r_m \geq 2.00$ Å. If we combined these estimates with the bound of $\epsilon < 56$ meV from the differential scattering measurements, we would obtain a final result for ϵ and r_m quite close to the best value of Lin and Bardsley, with n restricted to the range 8–10.

B. HeO^-

The mobility of O^- ions in He gas at about 300 K has been measured by McFarland *et al.*,¹⁶ whose results have been summarized and smoothed by Ellis *et al.*¹⁸ Both in these experiments and the present ones, it seems likely that the ion sources produced O^- ions that were a mixture of the $^2P_{3/2}$ ground state plus the $^2P_{1/2}$ first excited state, which lies only 0.028 eV above the ground state,³¹ probably in the 2:1 statistical ratio. At any rate, we shall assume this in the analysis. The resulting $^2\Pi_{3/2}$ and $^2\Pi_{1/2}$ molecular states should have nearly the same potential energy curves, differing only by (presumed small) spin-orbit interactions. The other molecular state formed from $O^- (^2P_{3/2})$ and $\text{He} (^1S_0)$ is $^2\Sigma_{1/2}$. We therefore make the assumption that the net interaction of O^- and He consists of $^2\Sigma$ and $^2\Pi$ molecular states, occurring with statistical weights of 1/3 and 2/3, respectively. By analogy with the isoelectronic system HeNe^+ , the $^2\Sigma$ state is probably the molecular ground state.³²

We know of no *ab initio* calculations of the potential for HeO^- , but there have been two determinations from fitting the mobility data at 300 K. Lin and Bardsley⁷ used a Monte Carlo simulation and imposed the constraint that the $^2\Sigma$ state lies above the $^2\Pi$ state. Although the potential curves they obtained were admittedly not unique, and the statistical weights used were probably wrong because of their assumption that the ground state was $^2\Pi$, the results are probably reasonable because the two curves are not very different. However, the mobility data did not extend to low enough energies to include the mobility maximum, and so did not probe the shallow potential wells. The potential wells obtained by Lin and Bardsley were the result of smoothly connecting the repulsive branches actually probed by the mobility measurements to the known r^{-4} attractive branch.

An average exponential repulsive potential was fitted to the mobility data by Bychkov,³³

$$V(r) = 640 \exp(-3.75r) \text{ eV}, \quad 1.8 < r < 2.2 \text{ Å} \quad (4)$$

This falls roughly midway between the two potentials of Lin and Bardsley.

The present mobility results are shown in Fig. 2 as K_0 vs T_{eff} , together with the previous measurements. There is excellent agreement, but again the 93 K results do not join

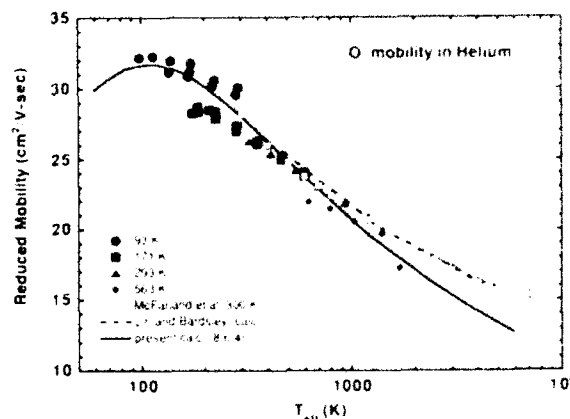


FIG. 2. Standard mobility of O^- ions in He gas as a function of effective temperature. The solid symbols represent the present measurements: ●, 93 K; ■, 171 K; ▲, 293 K; ◆, 563 K. The other symbol is □, McFarland *et al.*, 300 K (Refs. 16 and 18). Representative error bars are shown. The theoretical curves are — present fit, (8,6,4) model; --- Lin and Bardsley (Ref. 7).

smoothly with the higher-temperature results. A significant feature of the present results is that they extend to low enough temperatures to give an indication of the mobility maximum, which means that they probe the potential well to about r_m .¹

The theoretical calculation⁷ of K_0 for the Lin-Bardsley potentials is shown in Fig. 2, and accurately reproduces the data used to determine the potentials. Also shown is the calculated K_0 for an average (8,6,4) potential that we have obtained by a first-order fit around the mobility maximum. The disagreement with the measurements at the highest temperatures means that the inner repulsive wall of this model potential is too steep.

The estimates of the potential-well parameters obtained in the foregoing analyses are summarized in Table II. Given only the mobility data, it is impossible to determine both the $^2\Sigma$ and $^2\Pi$ potentials uniquely; additional information would be required. About all that can be said with assurance is that the potential wells are quite shallow, certainly less than 10 meV.

As a final point, it is interesting to make an easy estimate of the average well depth for HeO^- by analogy with that for HeAr^+ , which has a similar electronic structure. The mobility maximum for Ar^+ ions in He occurs at $T_{\text{eff}} \approx 500$ K, and the average HeAr^+ well depth is 27.3 meV.⁸

TABLE II. Estimated potential-well parameters for HeO^- from mobility data. (?) indicates state assignment is uncertain. See text.

	ϵ (meV)	r_m (Å)
Lin and Bardsley ^a		
$^2\Pi$ (?)	7.2	3.0
$^2\Sigma$ (?)	3.2	3.6
Present work ^b	5.12	3.53

^aReference 7.

^b(8,6,4) model with parameter $\gamma = 0.1$.

From Fig. 2 we estimate the mobility maximum for O^+ ions in He to occur at $T_{eff} \approx 110$ K, so that $\epsilon \approx (110/500)(27.3) = 6$ meV, which is in tolerable agreement with the values in Table II. This is only a rough estimate because the potentials for the two systems do not have the same shape, even in an average sense, as signaled by the values of K_{max}/K_{pol} (about 1.85 for HeO^+ and 1.40 for $HeAr^+$).

IV. CONCLUSION

The mobilities of O^+ and O^- ions in He gas are quite different, even though they approach a common value of $K_{pol} = 17.1$ cm²/V s at very low temperatures. The primary reason is the different binding energies of the molecular ions HeO^+ and HeO^- , which are approximately 50 and 5 meV, respectively. The average bond lengths are correspondingly different, about 2.1 Å for HeO^+ and 3.5 Å for HeO^- . The average potential well for HeO^- is also appreciably wider than that for HeO^+ , since $K_{max}/K_{pol} = 1.85$ for HeO^- , and 1.50 for HeO^+ . These numbers can be roughly translated into the relative potential well width at half the well depth, $\Delta r_{1/2}/r_m$, by assuming a potential model. For an (n,4) model the value of $\Delta r_{1/2}/r_m$ is about 0.47 for HeO^- and 0.39 for HeO^+ .

The potential curve for HeO^+ can now be claimed to be fairly well determined from mobility data and *ab initio* calculations. However, only an average potential for HeO^- can be determined from mobility data; additional information would be needed to resolve the individual $^2\Sigma$ and $^2\Pi$ potentials.

It is important to recognize that much information on ion-neutral potentials can be obtained from a few salient features of mobility curves, without the need for elaborate numerical computation.

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