9-1-1978

Mobility of α particles in helium

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(Received 15 May 1978)

The mobility of α particles in helium gas is calculated using the zeroth-order Viehland-Mason theory with interaction potentials recently computed by Cohen and Bardsley. The results show a dependence on field strength similar to the measurements of Johnsen and Biondi but are lower in magnitude by about 5%.

I. INTRODUCTION

The mobilities of doubly charged rare-gas ions in their parent gases have been measured recently by Johnsen and Biondi.[1] The only calculation available for comparison is by Dickinson[2] on He^{2+} in He. Theory and experiment cannot be compared directly since Dickinson calculated the zero-field mobility for temperatures between 10 and 300 K whereas the measurement was made at a gas temperature of 303 K with field strength to number density ratio between 10 and 70 Td (1 Td = 10^{-17} V cm^2) which produces an effective interaction temperature between 350 and 2000 K. Nevertheless, theory and experiment appear to differ significantly concerning the value of the zero-field mobility at 303 K and the dependence of the mobility on effective temperature.

II. CALCULATION

Cohen and Bardsley[3] have recently computed the interaction potentials relevant to the collisions of α particles with helium atoms in the ground state. The *ab initio* calculations reported in that paper were extended to larger nuclear separations by assuming that the average of the ${}^2\Sigma_g^+$ and ${}^2\Sigma_u^+$ potentials is given in atomic units by

$$V_0(R) = -2\alpha/R^4 , \tag{1}$$

with $\alpha = 1.383$, and by using the difference formula

$$V_g(R) - V_u(R) = 95.0\, R^{-0.537} e^{-2.688R} - 35.4\, R^{0.962} e^{-3.344R} . \tag{2}$$

The phase shifts η_l^g, η_l^u were computed numerically by the Numerov technique for 27 values of relative energy between 2.5 meV and 0.5 eV. At each value of E the phase shifts were computed for all appropriate values of l up to those for which the Born approximation is accurate. The phase shifts for higher partial waves were then calculated by adding to the Born values a small correction term obtained by extrapolation from the Numerov results at smaller l.

The diffusion cross section $Q^{(1)}$ was then calculated from the standard expression

$$Q^{(1)} = \frac{4\pi}{k^2} \sum_{n=0}^{\infty} [(2n+1)\sin^2(\eta_{2n+1}^u - \eta_{2n}^g) + (2n+2)\sin^2(\eta_{2n+2}^g - \eta_{2n+1}^u)] . \tag{3}$$

In Fig. 1 the results are compared with the classical polarization limit[4]

$$Q_{\text{pol}}^{(1)} = 2.21\pi(2\alpha/E)^{1/2} . \tag{4}$$

The ionic mobility has been calculated using the zeroth-order Viehland-Mason theory,[5] in which the relative velocity between the ions and neutral atoms is assumed to obey a Maxwell-Boltzmann distribution with an effective temperature T_{eff} that is defined by the Wannier law

$$\tfrac{3}{2} kT_{\text{eff}} = \tfrac{3}{2} kT_0 + \tfrac{1}{2} m v_d^2 . \tag{5}$$

Here T_0 represents the kinetic temperature of the neutral atoms, m is the mass of the helium atom, and v_d is the drift velocity. The reduced mobility K_0, defined in terms of v_d and the field strength $\mathcal{E}$ by

$$v_d = K_0 \mathcal{E} , \tag{6}$$

is calculated from the equation

$$K_0 = \frac{3e}{4N_0}\left(\frac{\pi}{mkT_{\text{eff}}}\right)^{1/2} \frac{1}{\Omega^{1,1}(T_{\text{eff}})} , \tag{7}$$

in which N_0 is the standard atomic number density (2.69×10^{19} cm^{-3}) and

$$\Omega^{(1,1)}(T) = \frac{1}{2(kT)^3} \int_0^\infty E^2 Q^{(1)}(E) \exp\left(-\frac{E}{kT}\right) dE . \tag{8}$$

For a given value of T_{eff} the reduced mobility can be calculated from Eqs. (7) and (8) and the cor-

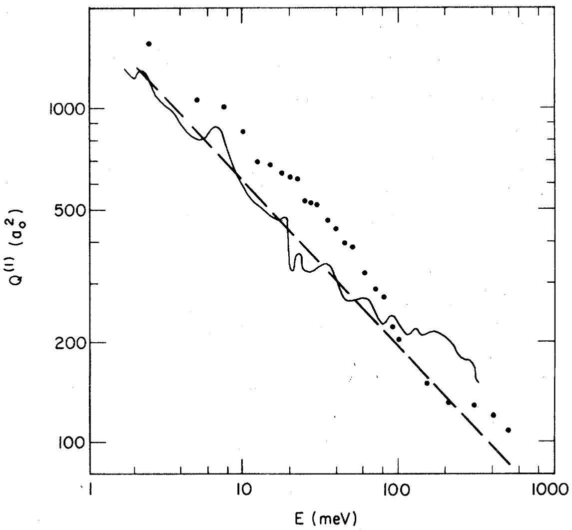

FIG. 1. Momentum transfer cross sections for He_2^+ in He as a function of relative energy, ··· this work, ——— Dickinson (Ref. 2), — — — polarization limit given by Eq. (4).

responding value of $\mathcal{E}/N$ can then be obtained from Eqs. (5)–(8). The results for gas temperatures of 77 and 303 K are shown in Fig. 2.

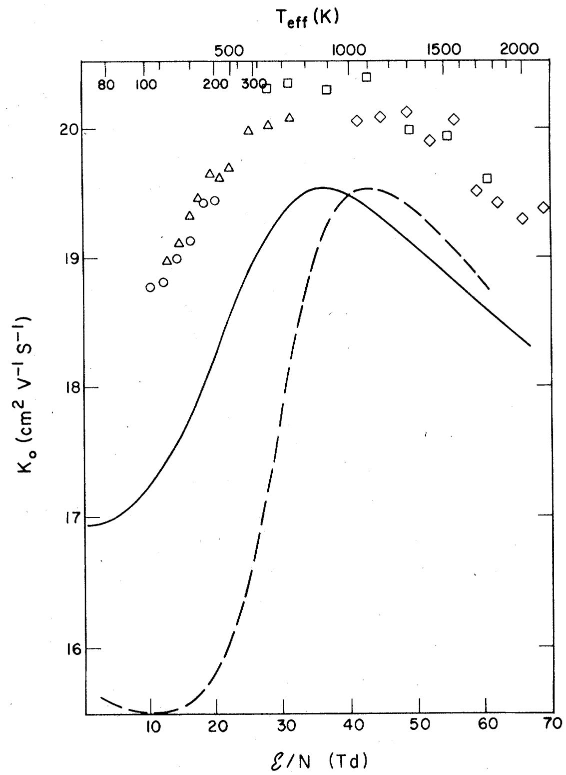

FIG. 2. Reduced mobility as a function of the ratio of field strength to number density; the points are the values measured at 303 K by Johnsen and Biondi (Ref. 1) at several pressures, ○ 0.887 Torr, △ 0.565 Torr, □ 0.287 Torr, ◇ 0.252 Torr; ——— this work for 303 K; — — — this work for 77 K. The calculated effective ion temperature is given at the top of the figure. The inner and outer scales refer to gas temperatures of 77 and 303 K, respectively.

III. DISCUSSION

For most of the energy range below 1 eV our calculated momentum transfer cross sections lie significantly above the polarization limit, whereas Dickinson's values oscillate about that limit for energies below 80 meV. Our results also show oscillations due to the discrete nature of the partial-wave sum and to the occurrence of resonances. However, these oscillations are not large and so have not been fully explored. The resonances may be more significant in radiative charge transfer and will be investigated further in that context.

Our computed mobility for a gas temperature of 303 K shows almost an identical dependence upon $\mathcal{E}/N$ as the measured values of Johnsen and Biondi, but is approximately 5% below those values. The experimental uncertainty is given as ±3%, and from an analysis of the pressure dependence of their results Johnsen and Biondi suggest that it is more likely that their values are too high rather than too low. In order to assess the reliability of our calculations we have checked the sensitivity of the results with respect to changes in the potential difference between the $^2\Sigma_g$ and $^2\Sigma_u$ curves. The difference potential given in Eq. (2) was reduced by 10% at all R, and the momentum-transfer cross sections at energies of 0.03, 0.04, and 0.05 eV were found to be smaller by approximately 12%. This extreme sensitivity is due to the importance of close encounters in which the phase shifts are large. Although we do not believe that Eq. (2) is wrong by so large an amount, it does seem possible that much of the discrepancy between theory and experiment could be due to errors in the assumed potentials and to the crude nature of the transport theory used in this work.

The zero-field mobility at 77 and 303 K is, in units of $cm^2\ V^{-1}\ sec^{-1}$, 15.6 and 16.9, respectively. The corresponding values calculated by Dickinson are 23.2 and 20.6. The large difference between the two results is further evidence of the extreme sensitivity of the mobility upon the short-range ion-atom interaction since both calculations assumed the same polarization interaction and used the same technique to obtain the scattering phase shifts.

ACKNOWLEDGMENT

Work performed under the auspices of the Department of Energy and supported by the Advanced Projects Research Agency through contract No. N000-1476-C-0098.

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