One may conclude from this work that the gross variation of the charge-transfer cross section is consistent with a model based on the formation of a complex N_2^+-O_2 due to the induced-dipole interaction.

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CROSS SECTION FOR THE PRODUCTION OF SINGLY IONIZED HELIUM BY ELECTRON IMPACT AT LOW ENERGIES*

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For an adequate understanding of electron-atom and electron-ion interactions, it is necessary that reliable experimental data from inelastic collision studies be available for comparison with theoretical results calculated using various models. This Letter reports the results of a direct experimental investigation of the energy dependence of the cross section for the formation of singly charged helium positive ions resulting from inelastic collisions between neutral helium atoms and electrons having a narrow energy bandwidth.

Because of the wide Maxwell-Boltzman energy distribution of thermionically emitted electrons, a detailed study of the exact form of ionization cross sections and threshold laws is impossible with conventional electron-impact sources. Clarke[1] has reviewed many of the problems involved in this type of work. The retarding potential difference (RPD) pseudo-monoenergetic electron source has been used by Fox and his co-workers[2] to study the ionization of helium in an attempt to determine the exact shape of the ionization efficiency curve. Fox reported a linear dependence for He^+ formation to within 0.2 V of the threshold. The RPD result, however, must be open to question in view of the possibility of space-charge-induced relaxation as pointed out by Marmet[3] and also because of the fact that the difference currents near threshold are subject to largest errors. On the other hand, any attempt to deconvolute[4] a conventional ionization efficiency curve would involve an exact knowledge of the electron energy spread. Because of the possibility of electron beam relaxation, surface charging, and electron optical effects, a simple knowledge of the cathode temperature is unlikely to provide the correct energy distribution function.[5]

A more direct approach having fewer objections is the use of an electron beam, energy selected by means of a monochromator. Using this technique, McGowan et al. have recently reported a study of the ionization of atomic hydrogen, finding a 1.127-power law in the region close to the threshold.[6] In the present work, we have used a 127° electrostatic energy selector[7] of the Marmet type[8] to produce an electron beam of about 3×10^{-8} A with an energy width at half-height of about 50 mV. Ions produced by electron impact are mass analyzed in a monopole mass filter and detected with an electron multiplier and vibrating-reed electrometer, the output of which is connected to a multichannel analyzer and data-processing system. Full details of the experimental arrangement will be published later.[9] The sample gas pressure is 8×10^{-6} mm mercury and the observed ion currents are a linear function of gas pressure. The ionizing electron current is found to be independent of electron energy in the range studied. Electron energy distributions are obtained by scanning an analyzing monochromator identical to the selector.

Figure 1 shows the observed ionization efficiency curve for He^+ formation. It can be seen that the curve is decidedly nonlinear over a region far in excess of what would be expected from the experimentally measured electron energy distribution ($\Delta E_{1/2} = 0.054$ V). The shape of the curve is found to be independent of the electron current over the range 10^{-8}-10^{-7} A. The large departure from linearity is not in agreement with the previously reported experiment.[2] Because of the random thermal motion of the molecules in the gas diffusion source used in this experiment, it is unlikely that the ion collection efficiency will vary significantly with electron energy. The effect of momentum transfer near threshold is likely to be a more serious problem where a molecular-beam gas source is used. In the development of the apparatus, minor variations of reaction chamber and ion gun geometry did not result in any observable change in the shape of the curve.

Using the quantum theory of inelastic scattering, Geltman[10] has predicted a linear threshold dependence for the ionization cross section as a function of electron energy. A similar result has been given more recently by Rudge and Seaton[11] and also by Peterkop.[12] These results have been questioned by Temkin.[13] Using an extension of the ideas of Wigner,[14] Wannier[15] has taken into account the three-body character of the ionization process and finds the result that the cross section depends on the excess energy raised to the power 1.127. In Fig. 1 the experimental curve is compared with the 1.127-power-law theory. An electron energy distribution of 54 mV half-width has been folded into the theoretical curve. The two curves have been arbitrarily normalized at 10 V above threshold. At higher energies the agreement is excellent, but below five volts there is some divergence. At these lower energies a somewhat higher power law may be operative. Omidvar[16] has suggested that the actual dependence may be a complicated function of energy. The thresholds of the theoretical and experimental curves can be matched to within 0.04 V (the width of one channel in the multichannel analyzer). The electron energy distribution may only be measured in the forward direction, and therefore any angular variation in this distribution or the presence of a significant number of higher energy stray electrons would affect the energy matching of theoretical and experimental curves. In this work, apart from the choice of threshold channel number, the whole process of data presentation and comparison has been automated. The output of the multichannel analyzer is read into an IBM 7044 computer by means of punched tape. It is then compared with theory and both results are displayed on the computer plotter. No smoothing programs are employed and the curves on Fig. 1 are a direct photograph of the computer output.

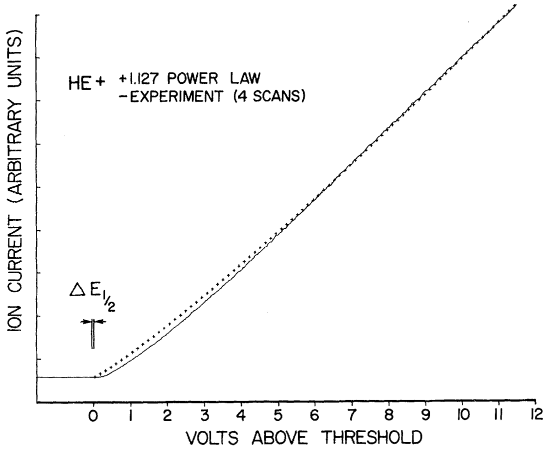

FIG. 1. The ionization of helium.

In conclusion, the present experiment using a direct monoenergetic electron technique indicates a nonlinear dependence for the helium ionization cross section as a function of electron energy. While the theory of Wannier fits closely at higher energies, a power in excess of 1.127 is indicated nearer to threshold.

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CONFIRMATION OF THE DISCREPANCY BETWEEN THE THEORETICAL AND EXPERIMENTAL GROUND-STATE ENERGIES OF H_2†

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A double-precision calculation of the dissociation energy of the hydrogen molecule has been carried out and the results confirm the existing discrepancy with the experimental value, the discrepancy being one order of magnitude larger than the experimental error.

A discrepancy exists between the experimental dissociation energy of the hydrogen molecule, $D_0 = 36\,113.6 \pm 0.3$ cm^{-1}, measured by Herzberg and Monfils,[1] and the theoretical value, $D_0 = 36\,117.3$ cm^{-1}, obtained by the present authors.[2-3] The larger theoretical value of the dissociation energy means that the theoretical total energy of the molecule is lower than the experimental one. However, since the discrepancy is in the sixth significant figure of the total energy which was calculated with an accuracy of eight significant figures, it was conceivable that part, if not all, of the discrepancy was caused by rounding errors in the numerical computation. To clarify the situation, a double-precision calculation with a more flexible wave function was carried out. The nonrelativistic four-particle Hamiltonian was used and the calculation was performed in the adiabatic approximation[1,4] which gives an upper bound to the exact eigenvalue. The relativistic and radiative corrections calculated as a perturbation were added to the final energy.

In the present work the electronic wave function was represented by an 80-term expansion in elliptic coordinates, identical with that used in the single-precision calculation,[2] and also by a more flexible 100-term expansion. Since the wave function depends explicitly on the interelectronic distance, and many of the integrals must be computed by numerical integration (Simpson's rule), it was proper to test the accuracy of the integration. The results of the fixed-nucleus calculation are shown in Table I where the first row represents the previous single-precision result. The next three rows represent, for the same wave function, the present results of the double-precision calculation with a varying number of integration points N. The next two rows show how a change of N affects the results obtained with

Table I. The fixed-nucleus total energy, E, and binding energy, D, for the electronic ground state of the hydrogen molecule calculated in double precision and varying the number of terms, n, in the electronic wave function, the number of integration points, N, and the internuclear distance R. Conversion factor for the energy: 1 a.u. = 219 474.62 cm^{-1}.

n	N	R (a.u.)	E (a.u.)	D (cm^{-1})
80	110	1.4011	-1.1744746	38292.8
80	150	1.4011	-1.174474657624	38292.75903
80	250	1.4011	-1.174474657935	38292.75910
80	350	1.4011	-1.174474657970	38292.75911
100	350	1.4011	-1.174474982924	38292.830427
100	500	1.4011	-1.174474982931	38292.830428
100	500	1.401075	-1.17447498301568	38292.83044693
100	500	1.401076	-1.17447498301674	38292.83044717
100	500	1.401077	-1.17447498301743	38292.83044732
100	500	1.401078	-1.17447498301776	38292.83044739
100	500	1.401079	-1.17447498301771	38292.83044738
100	500	1.401080	-1.17447498301730	38292.83044729