PHYSICAL REVIEW A VOLUME 25, NUMBER 3 MARCH 1982

Measurements of total cross sections for electron scattering by Li_2 (0.5 – 10 eV)

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(Received 24 September 1981)

Measurements have been made of total cross sections for the scattering of electrons by lithium-diatomic molecules over the electron energy range 0.5 – 10 eV, with the use of the molecular-beam recoil technique. The total cross sections in units of 10^{-16} cm^2 are 541 (0.5 eV), 307 (1 eV), 199 (2 eV), 160 (3 eV), 135 (6 eV), and 100 (10 eV). The uncertainty in these results is $\pm 16\%$.

The alkali-metal dimers are distinguished by their loosely bound nature (~ 1 eV), with large internuclear spacings ($\sim 3 - 4$ Å), and low ionization energies ($\sim 4 - 5$ eV).[1] Their very large electric-dipole polarizabilities[2,3] result in a dominating influence of the long-range polarizability interaction ($\sim \alpha r^{-4}$, where α is the polarizability) in quasielastic scattering, particularly in the total cross section in small-angle differential cross sections for scattering by low-energy electrons and ions.

We have previously reported total cross sections for electron scattering by Na_2 and K_2, and present here our results for Li_2. These cross sections represent the sum of all processes which may occur at a particular electron energy: elastic scattering; electronic, vibrational, and rotational excitation; and ionization. (There will be no electronic excitation below 1.74-eV electron energy, and no ionization below 5.0-eV electron energy.[1] Furthermore, the ionization cross section should be relatively small in our electron energy range.[4]) The distribution of internal energies for the target ensemble of Li_2 molecules may be assumed to follow a Boltzmann distribution characteristic of our oven temperature (~ 1000 K). At this temperature the average vibrational quantum number is 1.5 and the most probable rotational quantum number is 22.

Our crossed-beam apparatus has been previously described.[5] The beam source is a conventional effusive oven. Lithium atoms are removed from the beam with an inhomogenous magnetic field. The beam is detected via surface ionization followed by mass analysis. We obtain measurements of the attenuation ($\sim 0.1\%$) in the forward Li_2 beam intensity I_m when the electron beam is switched on. The effective total cross section is given by[5]

$$\sigma = h\bar{v}\Delta I_m/(I_m I_e) , \quad (1)$$

where h is the Li_2 beam height in the interaction region, $\bar{v}$ is the average Li_2 velocity, I_e is the electron particle current, and $\Delta I_m/I_m$ is the relative attenuation of the forward Li_2 beam intensity due to scattering. By using Eq. (1) we are assuming that the angular resolving power of the experiment is such that only a small fraction of the total scattering at small angles is unobservable. This is indeed the case for Li_2 (see below).

For the scattering of electrons by Li_2 we find the following total cross sections, in units of 10^{-16} cm^2: 541 (0.5 eV), 307 (1 eV), 199 (2 eV), 160 (3 eV), 135 (6 eV), and 100 (10 eV). The cross-section data are plotted in Fig. 1 along with atomic-lithium total cross sections. The molecular cross sections are larger ($\sim 60\%$) than the atomic ones at all energies studied, which is reasonable in view of the larger molecular polarizability,[2,3] averaged over all orientations of the molecule (34×10^{-24} cm^3 for Li_2 vs 24.3×10^{-24} cm^3 for Li). There have been no theoretical calculations of the electron-Li_2 scattering cross sections, to our knowledge. We parenthetically note that the total cross section for Li_2 at low energies is the largest cross section yet observed for any neutral diatomic molecule not possessing a permanent dipole moment.

The uncertainty in these results is $\pm 16\%$. The individual contributions include the uncertainty in h ($< 1\%$), I_e ($< 1\%$), and $\bar{v}$ (7%); and angular resolution error ($< 2\%$); and statistical variations of $\pm 5\%$. The angular resolution error was estimated

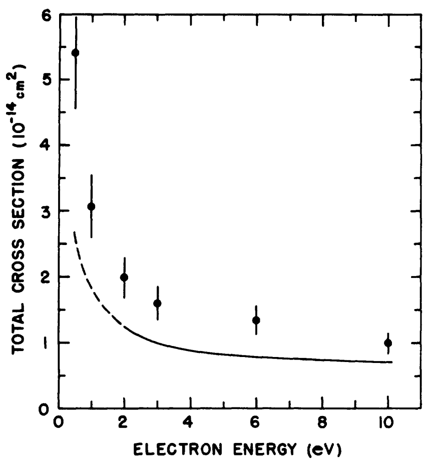

FIG. 1. A comparison of electron-scattering cross sections for Li_2 and Li. Points, with error bars: present total cross sections for electron scattering by Li_2 molecules. Solid line: smooth fit to the atomic-lithium cross sections of Ref. 6. Dashed line: atomic-lithium cross sections below 2 eV, determined in the present work but normalized to the absolute data of Ref. 6.

as described in Ref. 5 and was found to be a maximum of 1.6% around 1 eV. A number of consistency checks were made for this apparatus and have also been described in Ref. 5.

Recently, Jaduszliwer, Tino, Bederson, and Miller[6] used this same apparatus to measure electron-Li total cross sections with a velocity-selected Li beam. These absolute data, together with our present electron-Li and electron-Li_2 attenuation data using a non-velocity-selected (Maxwellian) beam, were used to infer the Li_2 velocity ($\bar{v}$), which otherwise can only be estimated from knowledge of the oven temperature, as the magnetic velocity selector[4] used with Li does not affect the spin-zero Li_2. In essence, then, our electron-Li_2 cross sections have been normalized against the absolute electron-Li results of Ref. 6. The uncertainty in the electron energies is 0.15 eV. The electron energy resolution is 250 meV full width at half maximum.

It would be interesting to conduct more detailed electron-scattering experiments and to carry out theoretical calculations for the alkali-metal dimers, to learn where effects of the unusually large spatial anisotropy of the molecules might show up, and to learn how the low-energy ($\sim$0.08 eV) shape resonance calculated for electron-Li scattering[7] is manifested in electron-Li_2 scattering.

This work was supported by the National Science Foundation.

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[3]R. W. Molof, H. L. Schwartz, T. M. Miller, and B. Bederson, Phys. Rev. A 10, 1131 (1974).

[4]I. S. Aleksahkin, I. P. Zapesochnyi, and O. B. Shpenik, *Proceedings of the Fifth International Conference on the Physics of Electronic and Atomic Collisions* (Nauka, Leningrad, 1967), p. 499. These electron-impact ionization measurements are for atomic lithium. However, one can guess that the ionization cross sections for Li_2 would rise nearly linearly from zero at 5 eV to 5 or 6×10^{-16} cm^2 at 10-eV electron energy.

[5]T. M. Miller and A. Kasdan, J. Chem. Phys. 59, 3913 (1973). In this paper a preliminary value of the polarizability of Na_2 was quoted; it should read $(30\pm3)\times10^{-24}$cm^3 as given in Ref. 2. Also, Ref. 2 contains a correction as to the vibrational state distributions for Na_2 and K_2.

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