Integral elastic-scattering cross sections of $^2P_{3/2}$ and $^2P_{1/2}$ C^+ ions in collision with He atoms

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(Received 10 July 1981)

Integral elastic-scattering cross sections were measured for C^+ ions with kinetic energies in the range 0.5–3.0 keV scattered by stationary He atoms through effective laboratory angles greater than 5×10^{-3} rad. The cross sections are compared with two kinds of the weighted means of the cross sections for the $^2\Sigma$ and $^2\Pi$ potentials of HeC^+ obtained by *ab initio* calculation. Estimation of the population distribution of C^+ ions of $^2P_{3/2}$ and $^2P_{1/2}$ involved in the projectile ion beams may be achieved by the comparison.

A carbon ion (C^+) is a quasi-one-electron atom which has a $2p$ electron in the outermost shell. Interaction of the ground-state $C^+(^2P)$ ions with rare-gas atoms $R(^1S)$ provides two quasimolecular states $^2\Sigma$ and $^2\Pi$. In these open-shell systems experimental investigation of collision processes, particularly determination of elastic-scattering cross sections, is not simple, because discrimination of the scattering along the $^2\Sigma$ curve from that of the $^2\Pi$ is not possible, unless the experiment uses the C^+ ions with a selected spin-orbit level ($^2P_{3/2}$ or $^2P_{1/2}$). Experiments provide only scattering cross sections averaged over the population distribution of $C^+(^2P_{3/2})$ and $C^+(^2P_{1/2})$ involved in the projectile beams. The population distribution of the ions of $^2P_{3/2}$ and $^2P_{1/2}$ has been traditionally assumed as $\frac{2}{3}$ and $\frac{1}{3}$. Although in some cases this assumption has proved to be correct,[1,2] it is not always the case for the other ions and different methods of ion formation.[3-6] Therefore, establishment of the fraction of the ions with a selected spin-orbit energy level is essential to getting correct information out of such an experiment.

Recently a theoretical and experimental investigation was published on a few low-lying potential curves of ArC^+.[7] Those of HeC^+ were calculated by Tanaka and co-workers using a CI method with a basis having double-zeta plus polarization quality.[8] Since these calculations are thought to be accurate, they will be of help as the base to derive scattering cross sections along an individual potential curve.

This article presents the experimental results for integral elastic-scattering cross sections of C^+ ions in collision with He atoms, and suggests that the comparison of the results with the theoretically calculated cross sections may provide a method to determine the population distribution of $C^+(^2P_{3/2})$ and $C^+(^2P_{1/2})$ in the projectile beams.

Since the experimental apparatus for measuring integral scattering cross sections is the same as one used in a previously published work and the details of the apparatus and the procedures have been described there,[1] only a brief description is given here.

The C^+ ions are formed by discharge in CO gas introduced into a hot cathode ion source of Menzinger type.[9] Discharge voltage is about 50 V (20–30 mA) and the stagnation pressure of source gas is about 0.1 Torr.

The ions are extracted and accelerated to a specified energy in the range 0.5–3.0 keV. After being mass separated by a Wien filter, the selected ion beams are introduced into the collision chamber, where some of the projectile ions are scattered by room temperature He atoms in the range $(1.0-1.5)\times10^{-2}$ Torr that meets the single collision conditions. The pressure of the target gas is measured by a diaphragm manometer. The ions other than those scattered beyond the angle determined by the beam-detector geometry are caught by an electron multiplier.

It was experimentally confirmed that long-lived electronically excited ions that might be involved in the beams, energy spread (less than 1.5 eV) of the ion beams, and inelastic collisions between the projectile and the target did not affect the cross sections significantly.

Provided that I_0 is the beam flux before entering the collision chamber and I is that after leaving there, an integral scattering cross section Q is given by

$$Q=(1/nl)\ln(I_0/I)\,, \tag{1}$$

where n is the number density of the target atoms and l is the effective length of the collision chamber. Integral elastic-scattering cross sections obtained in this manner have proved to be very useful in deriving the repulsive potentials in the range 0.5–10 eV between closed-shell particles[10] and between some open-shell ions and He atoms.[1]

If the repulsive potentials between the colliding partners, which are most effective for the scattering in the collision energies used in the present work, are expressed by an exponential formula,

$$V(R)=A\exp(-\alpha R)\,, \tag{2}$$

where R is the interatomic distance, then the following relation holds between the integral elastic-scattering cross section Q and the potential parameters,[11]

$$\ln[(Q/\pi)^{1/4}E^{-1}]=\alpha(Q/\pi)^{1/2}-\ln[(\alpha\pi/2)^{1/2}(A/\theta_0)]\,, \tag{3}$$

where E is a projectile energy and θ_0 is the minimum scattering angle, both in the laboratory frame. When the potential (2) and the geometrical constant θ_0 are known, we can calculate Q using the relation (3) for a given value of E.

Several representative values of the cross sections experimentally determined are shown by open circles in Fig. 1. Each of the values is the mean of 10–15 runs. Experimental errors are within 15%. The value of θ_0 was determined to be 5.1×10^{-3} rad by numerical integration,[12] taking into consideration the beam-detector geometry as described previously.[10]

As stated earlier in this article, however, the cross sections determined experimentally are not for an individual potential $^2\Sigma$ or $^2\Pi$ of the quasimolecule, but for the weighted mean of the cross sections for the two lowest potentials,

$$\langle Q\rangle_{av}=\tfrac{1}{2}(1-f)Q_\Sigma+\tfrac{1}{2}(1+f)Q_\Pi\,, \tag{4}$$

where f is the fraction of the population of $C^+(^2P_{1/2})$ contained in the projectile beams. $C^+(^2P_{1/2})$, which is f of total C^+, is scattered along the $^2\Pi_{1/2}$ potential of HeC^+, while one half of $C^+(^2P_{3/2})$, i.e., $(1-f)/2$ of the total C^+ is

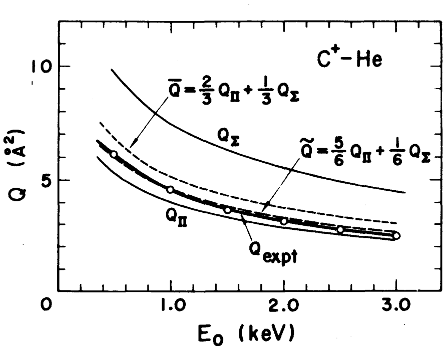

FIG. 1. Comparision between the cross sections experimentally obtained and those calculated from the theoretical potentials. Q_Π and Q_Σ are the cross sections derived from the two lowest potentials $^2\Pi$ and $^2\Sigma$, respectively, obtained by *ab initio* calculation (Ref. 8). $\bar{Q}$ and $\tilde{Q}$ are the weighted means of the cross sections Q_Π and Q_Σ as indicated in the figure.

scattered along the $^2\Pi_{3/2}$ and the other half along the $^2\Sigma$. The value of f must be determined before the physical meaning of the experimental scattering cross sections is established.

In Fig. 1 the cross sections experimentally determined (thick solid curve) and those derived from the theoretical potentials (thin solid curve) for the C^+-He system is exhibited for comparison. The cross sections Q_Π and Q_Σ for $^2\Pi$ and $^2\Sigma$, respectively, are obtained by Eq. (3), approximating the theoretical $^2\Pi$ and $^2\Sigma$ potentials[8] by the exponential formulas within the error limits of 5%, $V_\Pi=277\exp(-4.46R)$ and $V_\Sigma=407\exp(-3.54R)$, where V and R are in units of eV and Å, respectively, and assuming $\theta_0=5\times10^{-3}$ rad. In the Figure are also shown two kinds of the mean cross sections, $\bar{Q}$ and $\tilde{Q}$. The former mean cross section $\bar{Q}$ is obtained on the basis of the traditional hypothesis that $C^+(^2P_{3/2})$ and $C^+(^2P_{1/2})$ are formed in the ion source according to the statistical weight 2 to 1 ($f=1/3$). Agreement between the experimental cross sections and the mean cross section $\bar{Q}$ is poor.

If both of the experimental and theoretical values of the cross sections are correct enough, the remaining origin of the disagreement should be asked for in the estimation of the weight f in Eq. (4).

According to the works using ions formed by discharge,[3-6] the population of the ground-state ions formed in discharge involving high density of electrons, as is in the glow discharge plasma, is much greater than the statistical weight, because the ions in the metastable spin-orbit energy level are rapidly deexcited via superelastic electron-ion collisions. If a similar process occurs in our discharge-type ion source, the ground state $C^+(^2P_{1/2})$ may become much more than $f=\frac{1}{3}$. If one assumes $f=\frac{2}{3}$, the averaged cross section $\tilde{Q}$ is given by

$$\tilde{Q}=\tfrac{5}{6}Q_\Pi+\tfrac{1}{6}Q_\Sigma\,. \tag{5}$$

The cross sections $\tilde{Q}$ thus calculated are shown also in Fig. 1. It is very interesting that the agreement with the experimental values becomes complete.

Accurate determination of the population distribution of atoms or ions with different spin-orbit energies are essential to many fields of research. Particularly, difference of reaction rate constants for those particles has drawn special attention in recent chemical dynamics research. Since an exact value of f, however, is not very easy to determine, there always remains some ambiguity in the experimental results. The comparison described above seems to be a promising method for determining a value of f, if accurate potential values are obtained by theoretical computation, which becomes feasible at the present time.

We wish to thank Professor Kimio Ohno, Hokkaido University, for kindly sending us the unpublished results of *ab initio* calculation performed by his group. Stimulating discussion with Dr. S. Kita is much appreciated.

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