Effect of exchange on the binary-encounter-electron double-differential cross section in C^{q+}-H_2 collisions at 0.75 MeV/amu

H.I. Hidmi, C.P. Bhalla, S.R. Grabbe, J.M. Sanders, P. Richard, and R. Shingal

J. R. Macdonald Laboratory, Department of Physics, Kansas State University, Manhattan, Kansas 66506

(Received 10 July 1992)

The production of binary-encounter electrons in collisions of C^{q+} ions with molecular hydrogen has been studied at an impact energy of 0.75 MeV/amu. The measured double-differential cross section (DDCS) at a forward angle ($\theta_{\rm lab}$=0), with respect to the beam direction, is in excellent agreement with the theoretical cross sections evaluated in the impulse approximation by using the elastic-electron–ion differential cross section with the Compton profile of the target electrons. The theoretically calculated DDCS is extremely sensitive to the impact energy. Hence a precise measurement of the projectile beam energy is required to compare predicted values with the data. The agreement between theory and experiment demonstrates the importance of exchange in the description of binary-encounter electrons and that the exchange increases with the number of electrons on the projectiles.

PACS number(s): 34.50.Fa

Hard collisions between an ion and an atom result in the production of energetic free electrons. These electrons, referred to as binary-encounter electrons (BEE's), have recently been extensively studied [1–7]. Richard *et al.* [3] have reported on the increase in the BEE double-differential cross section (DDCS) of F^{q+} colliding with H_2 and He as the number of electrons on the projectile is increased. Several theoretical calculations [8–10] using the static potential and impulse approximation (IA) gave qualitative agreement with the data. Taulbjerg [11] found that the agreement between theory and experiment for F^{8+} collisions is considerably improved if electron exchange is taken into account. Bhalla and Shingal [12] have calculated the enhancement ratio $R = \sigma(q)/\sigma(Z_p)$, where $\sigma(q)$ is the elastic-differential cross section for the collisions of electrons with ions of charge state q, and $\sigma(Z_p)$ is the corresponding Rutherford cross section for the collision of electrons with bare ions. The effect of electron exchange between the quasifree target electrons and the projectile electrons was also included in their calculations. They concluded that the effect of electron exchange on the elastic-differential cross section in collisions of electrons with carbon, fluorine, and magnesium ions was important at backward angles in the projectile frame and increasing with decreasing electron-impact energies. In addition, the contribution of exchange becomes larger with increasing number of electrons on the projectile.

It is the purpose of this paper to report on a direct comparison of theory with experimental DDCS for BEE's produced in the collisions of C^{q+} with H_2 and to ascertain the effects of electron exchange on the collision dynamics. The previous comparison with one-electron data and with F^{q+} ions suggested that calculations including both static potential and exchange were needed to explain the observation, however the calculated effects and the size of the relative errors in the data are comparable in magnitude. We have selected a collision system and bombarding energy where the electron exchange is expected to be significantly larger than the error in the data.

The measurements for 0.75-MeV/amu C^{q+} ions colliding with molecular hydrogen were carried out using a tandem 45° parallel-plate electron spectrometer in the J. R. Macdonald Laboratory at Kansas State University. The target gas pressure was maintained at 20 mTorr in a 10-cm-long differentially pumped gas cell. The background electron count was found to be less than 5% near the binary encounter peak and was subtracted from the electron count with H_2 gas in the cell. The beam was collected in a shielded Faraday cup with voltage suppression to insure proper beam integration. Further details of the apparatus can be found elsewhere [2, 13].

The beam energy differed slightly from 0.75 MeV/amu for each charge state due to stripping with a carbon foil. However, the cusp electrons have the same velocity as the incident projectiles, and the beam energy is then given by $E_p = t(M_p/m_e)$, where t is the cusp energy, M_p is the mass of the projectile, and m_e is the electron mass. High-resolution measurements in the region of the cusp were performed to accurately determine the cusp energy and thereby the beam energy. We also note that the absolute DDCS was obtained by normalizing the data for C^{6+}-H_2 collisions to the IA using the Rutherford scattering cross section where there is no contribution from electron exchange or the static potential.

The projectile frame DDCS is given in the impulse approximation by

$$\frac{d^2\sigma}{d\Omega\, d\varepsilon} = \left(\frac{d\sigma}{d\Omega}\right)\left(\frac{J(\mid Q \mid)}{V_P + Q}\right), \tag{1}$$

where $J(\mid Q \mid)$ is the experimental Compton profile of the H_2, V_P is the projectile velocity, and $Q = \sqrt{2}[\sqrt{(\varepsilon + B)} - \sqrt{t}]$. All quantities are in atomic units. Here, B is the binding energy of the electron in the target. $\frac{d\sigma}{d\Omega}$ is the elastic-differential cross section for the electron of energy ε colliding with C^{q+} ions. The radial wave function of the scattered state of the incident electron (energy $\varepsilon=\frac{1}{2}k^2$ and orbital angular momentum l) is a solution of the second-order coupled integro-differential equation of the form

$$\left(\frac{d^2}{dr^2}+\frac{l(l+1)}{r^2}-2V_s(r)-2V_p(r)+k^2\right)u_l(r)=\chi_l(r). \tag{2}$$

The static and polarization potentials are given by $V_s(r)$ and $V_p(r)$, respectively. The contribution of the polarization potential was neglected since the dominant interaction is governed asymptotically by the static potential. The static potential, the nonlocal two-electron exchange contributions, and $u_l(r)$ were calculated in a self-consistent Hartree-Fock atomic model. The phase shifts were computed up to a maximum l value beyond which there were negligible contributions to the scattering amplitude.

The predicted DDCS, with (solid line) and without (dotted line) electron exchange, for an impact of C^{2+} ion on H_2 is shown in Fig. 1 together with the pure Coulomb calculation (dot-dashed line). The electron exchange is found to increase the calculated DDCS over the entire range of the electron energy. However, it has a maximum contribution near the binary encounter peak. Furthermore, in the region of the binary encounter peak, the DDCS calculated with exchange is found to be in excellent agreement with the experimental data. The relative cross section at the binary peak is measured to better than 4% while the static potential contributes an additional 42% and the exchange contributes an additional 23% to the zero-degree DDCS. Similar results were observed for the other charge states. The pronounced peaks in the C^{2+} and C^{3+} spectra are due to the K-shell Auger electron decay from K-vacancy production mechanisms (i.e., K-shell ionization and excitation) which are not included in the present calculation.

The calculated values of the DDCS for C^{q+}-H_2 (q=3–6) collisions are compared with the experimental data in Fig. 2. An excellent agreement between the predicted BEE production cross section and the experimental data

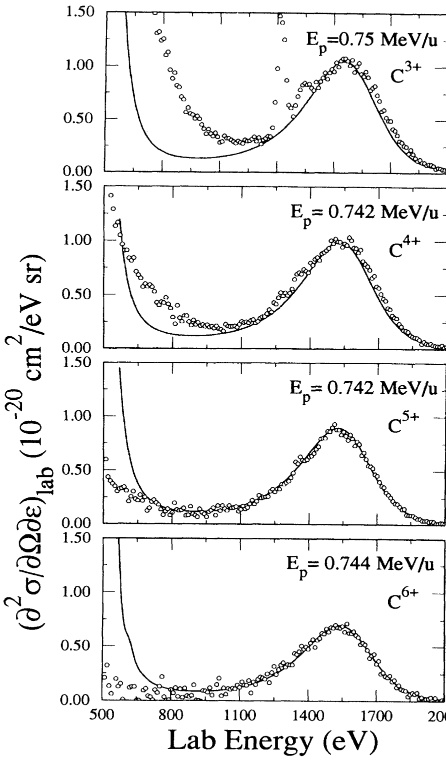

FIG. 2. Comparison of the predicted DDCS with experiment as a function of laboratory-frame electron energy for different charge states of carbon ions on H_2. E_p is the beam energy per amu for each collision system. Solid line, theory incorporating static and exchange. Circles, experimental data.

is found for all charge states. Furthermore, the calculated DDCS for the production of low-energy continuum electrons in C^{q+}-H_2 (q=2–6) collisions agrees with the data over a wider energy range as the projectile charge state increases. A large discrepancy between the calculated and the measured DDCS is evident for low-energy electrons. This is due to the electrons ejected either from the target or the projectile in soft encounters. These low-energy δ electrons are produced in soft encounters

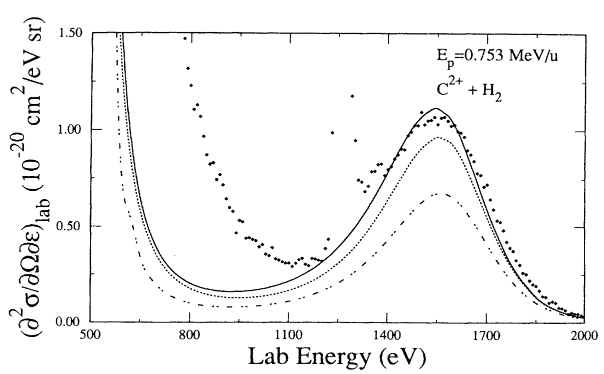

FIG. 1. Comparison of the predicted DDCS with experiment as a function of laboratory-frame electron energy. E_p is the beam energy per amu for the collision system. Theory: dotted line, static; solid line, static plus exchange; dot-dashed line, pure Coulomb potential. Experiment: diamonds.

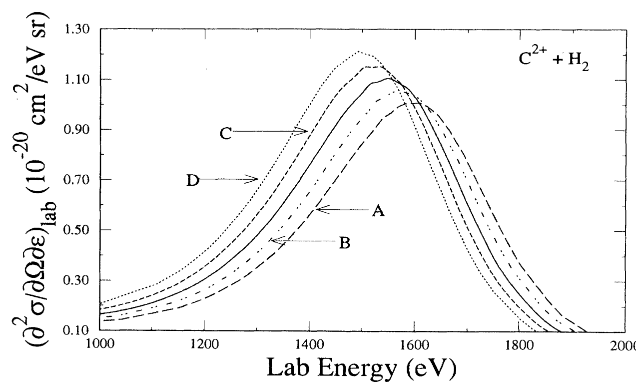

FIG. 3. Calculated DDCS as a function of laboratory-frame electron energy and for different beam energies. Solid line, beam energy (0.75 MeV/amu). Beam energy increased by 1.5% (B) and 3.5% (A), and decreased by 1.5% (C) and 3.5% (D).

between the projectile and the target, and originate either from the target (direct ionization) or from the projectile (electron loss to continuum). These processes are not included in the present theoretical approach.

The magnitudes of the BEE cross section as well as the peak position depend sensitively on the ion velocity. This is demonstrated in Fig. 3 where the calculated cross sections are given for beams of 0.75-MeV/amu C^{2+}-H_2, and for energies shifted by $\pm$ 0.011 and $\pm$ 0.026 MeV/amu. The peak cross sections are seen to vary by $\pm10\%$ in the extreme cases shown in Fig. 3. In the present experiments the beam energy was determined to an accuracy of $\pm$ 0.002 MeV/amu by measuring the energy of the cusp electrons to an uncertainty of 1 eV.

The production of BEE's in collisions of 0.75-MeV/amu C^{q+} ions with molecular hydrogen has been investigated, both theoretically and experimentally. The measured DDCS at a 0° laboratory angle is in excellent agreement with the corresponding theoretical values calculated using the impulse approximation and incorporating exchange contributions of the continuum and bound orbitals in addition to the static potential. This agreement between experiment and theory shows that the contribution of electron exchange must be included to properly describe BEE production.

This work was supported by the Division of Chemical Sciences, Office of Basic Energy Sciences, Office of Energy Research, U.S. Department of Energy.

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