Electron capture in $H^+ + H_2$

V. Heckman, S. J. Martin, J. Jakacky, Jr., and E. Pollack
Department of Physics, University of Connecticut, Storrs, Connecticut 06268
(Received 13 July 1984)

Electron capture in $H^+ + H_2$ collisions is studied at energies of 1.0, 2.0, and 3.0 keV in the reduced angular range $\tau \leq 3.0$ keV deg. Time-of-flight techniques are used for state identification, and the probability of electron capture to $H(1s) + H_2^+(^2\Sigma_g^+)$ in an exchange collision is determined. This is shown to be the dominant exchange channel at small scattering angles. The "summed" exchange channels have a reduced cross section that is found to peak in the forward direction and shows no structure, while the cross section for capture to final ground-state channels shows some small structure at 3.0 keV for $\tau \geq 1.5$ keV deg. The reduced cross section, at 1.0 keV, for capture to excited states of H (with the H_2^+ in its ground state) is found to have a maximum at $\tau = 1$ keV deg. The results are in agreement with a previously proposed model for ion-molecule charge exchange.

INTRODUCTION

Electron capture by H^+ has been extensively investigated both theoretically and experimentally. To date most of the work has involved electron capture from atomic targets where the underlying processes are reasonably well understood. Discussions of electron capture by H^+ from atomic targets are included in several review articles. References 1 and 2 address the general ion-atom charge-transfer problem at low and high energies, respectively. There is currently a growing interest in ion-molecule interactions and for these more complex systems the $H^+ + H_2$ collision poses a fundamental and challenging problem. In $H^+ + H_2$ the small-angle electronically elastic collision channel primarily involves the ground-state potential energy surface, and the differential cross sections for elastic scattering therefore provide information on this surface for H_3^+. The $H^+ + H_2 \rightarrow H(1s) + H_2^+(^2\Sigma_g^+)$ exchange collision involves both the ground- and lowest-lying excited-state surfaces of the H_3^+ molecular ion. Experimental studies of electron capture to the ground-state channel can therefore serve as a test of the two lowest-energy surfaces in H_3^+ and the dynamical couplings between these two surfaces that result in the electron transfer. Electron capture in $H^+ + H_2$ is also of current interest since there are experiments using fast H projectiles in progress in many laboratories and it is important to have information on the states present in the incident beams (which are conveniently obtained by using H_2 as a charge-exchange gas in many cases).

In an early experiment using molecular targets, it was shown that the probability of electron capture (to all final states) in $H^+ + H_2$ oscillates with energy up to 50 keV at a fixed scattering angle of 3°.[3] A particularly striking result of these early studies is that the peaks in the electron-capture probability occur at the same energies for both the H and H_2 targets. In an early test of the theory,[4] the electron capture probability was calculated at large scattering angles for $1 < E < 20$ keV and compared to the experimental results. Reasonably good agreement was obtained. Electron capture in $H^+ + H_2$ was most recently addressed[5] using a two-state model which included translation factors and reproduced the essential features of the experiment in Ref. 3.

The present study is a continuation of our work on the small-angle scattering in the hydrogen system. We have previously reported on the direct scattering[6] in $D^+ + H_2 \rightarrow D^+ + H_2$ and on[7] $D^+ + H_2 \rightarrow D^0$ collisions. Our earlier results reported on electron capture into all final channels. Using a new apparatus having increased energy resolution for time-of-flight measurements we investigate the $H^+ + H_2 \rightarrow H(1s) + H_2^+(^2\Sigma_g^+)$ collision. The probability for a transition to this channel is presented at energies of 1.0, 2.0, and 3.0 keV for $\tau \leq 3$ keV deg. In addition we report ρ (the reduced cross sections) for the summed capture channels at 2.0 keV, for capture to the ground-state channel at 3.0 keV, and for $H^* + H_2^+(^2\Sigma_g^+)$ at 1.0 keV.

THE EXPERIMENTAL ARRANGEMENT

The present work uses a new experimental arrangement which is described elsewhere.[8] Briefly, H^+ is extracted

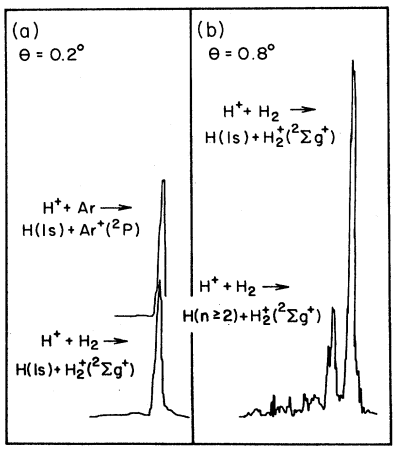

FIG. 1. Spectra showing electron capture in $E = 1.0$ keV H^+ collisions. (a) The $H^+ + Ar \rightarrow H(1s) + Ar^+(^2P)$ ($Q = 2$ eV) reference peak is used to identify the final channels as $H(1s) + H_2^+(^2\Sigma_g^+)$ ($Q = 2$ eV). (b) A typical spectrum. Separation between the maxima of the two peaks is 10 eV.

 ©1984 The American Physical Society

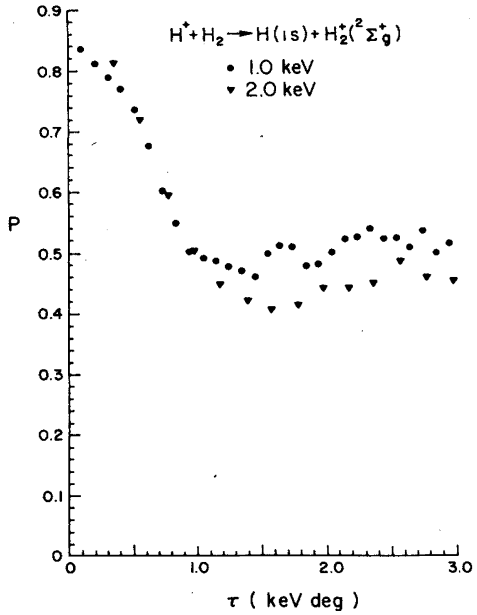

FIG. 2. Probability of electron capture to $H(1s) + H_2^+(^2\Sigma_g^+)$ as a function of reduced scattering angle in an exchange collision. Figure shows that capture to the ground states is the dominant process at small scattering angles. Results are accurate to 5%.

from a glow-discharge source, focused, and passed through a set of plates where it is "chopped" by a voltage pulse (amplitude of 20 V, frequency of 100–300 kHz, and width of 0.05 μsec). The H^+ beam then passes through a Wien velocity filter, is collimated and enters a cell containing H_2 target gas. The scattered H^0 resulting from $H^+ + H_2 \rightarrow H^0 + H_2^+$ collisions traverses a 4-m-long

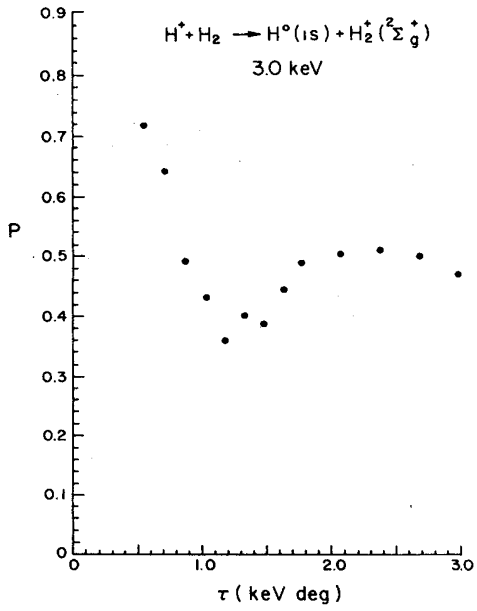

FIG. 3. Probability of electron capture to $H(1s) + H_2^+(^2\Sigma_g^+)$ as a function of reduced scattering angle at 3.0 keV. Results are accurate to 5%.

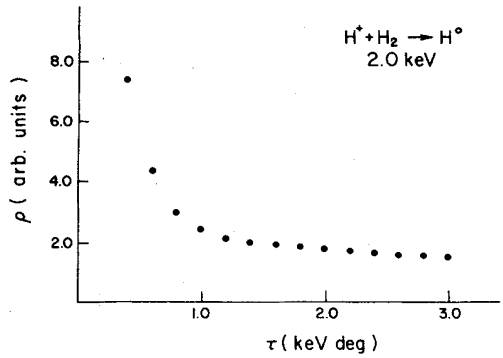

FIG. 4. Reduced cross section as a function of reduced scattering angle for the summed processes (electron capture into all final channels). The plot shows no structure and is typical of the cross sections at the other energies.

drift region positioned at an angle θ with respect to the incident beam and is energy analyzed using time-of-flight techniques.[9]

In $H^+ + H_2$ collisions the projectile changes charge state and therefore there is no reference channel from which absolute energy losses can be determined. An energy reference is obtained from electron capture in $H^+ + Ar$ where the dominant process[10] at small-θ results in $H^0(1s) + Ar^+(^2P)$. Figure 1(a) shows energy spectra of H^0 at 1.0 keV for $H^+ + Ar$ and $H^+ + H_2$ collisions ($\theta = 0.2°$). Using the peak from the Ar target as a reference and the known energy calibration of our detector, the peak in $H^+ + H_2$ is due to $H^0(1s) + H_2^+(^2\Sigma_g^+)$. Figure 1(b) shows a typical energy spectrum (1.0 keV, $\theta = 0.8°$) with the dominant peak corresponding to final ground-state products and the weaker peak at this angle resulting primarily from capture to $H^0(n \geq 2) + H_2^+(^2\Sigma_g^+)$. The additional weak structure seen may result from electronically excited[11] and/or repulsive states in H_2^+.

EXPERIMENTAL RESULTS

Figure 2 shows P, the probability of electron capture to $H(1s) + H_2^+(^2\Sigma_g^+)$ final states in an exchange collision at

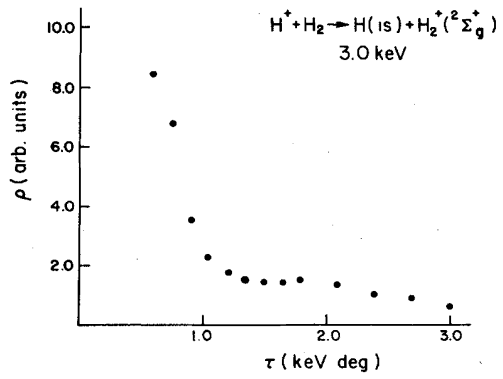

FIG. 5. Reduced cross section as a function of reduced scattering angle for 3.0-keV $H^+ + H_2 \rightarrow H(1s) + H_2^+(^2\Sigma_g^+)$ collisions. The results at this energy best show the weak structure for $\tau \geq 1.5$ keV deg in the cross section for the ground-state channels.

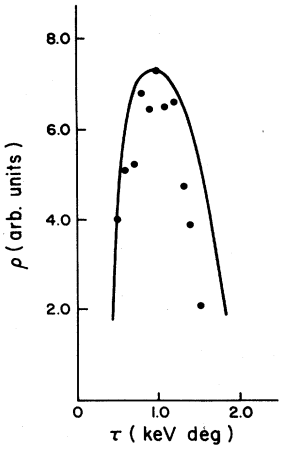

FIG. 6. The reduced cross section at 1.0 keV for $H^+ + H_2 \rightarrow H^* + H_2^+(^2\Sigma_g^+)$. Solid curve is for $E=3$ keV, $D^+ + H_2 \rightarrow D^+ + H_2^*$ ($Q=13$ eV) from Ref. 6. The peaks in the cross sections, each plotted in arbitrary units, occur near $\tau=1$ keV deg. The basic similarity in these cross sections suggests that a common primary interaction is responsible for the direct inelastic and these exchange channels in the hydrogen collision system.

energies of 1.0 and 2.0 keV for $\tau \leq 3$ keV deg. The results at 1.0 keV show some structure since the resolution in τ is better at lower energy. Figure 3 shows a similar plot at 3.0 keV. It may be seen that capture to final ground states is the dominant process at small scattering angles. At the larger angles capture to $H(n \geq 2) + H_2^+(^2\Sigma_g^+)$ becomes important and these channels then account for about one-half of the charge-exchange collisions. The reduced cross section for the summed channels is shown in Fig. 4, at 2.0 keV. This plot is typical of the cross sections at the other energies, peaking in the forward direction and exhibiting little or no structure (in agreement with our earlier results[7]). Figure 5 shows a ρ versus τ plot for capture to final ground states at 3.0 keV. The basic angular dependence of this cross section is quite similar to that for elastic scattering in $D^+ + H_2$ which is given in Fig. 10 of Ref. 4. Figure 5 shows some weak structure in the cross section for $\tau \geq 1.5$ keV deg. The better energy and angular resolutions at 1.0 keV allow identification of the channels corresponding to $H(n \geq 2) + H_2^+(^2\Sigma_g^+)$. The reduced cross section for capture to excited states of H is shown in Fig. 6. The figure also shows (at energies near 3 keV) the reduced cross section for the direct inelastic channel in $D^+ + H_2$ ($Q=13$ eV) from Ref. 6. The two cross sections (each plotted in arbitrary units and determined from data taken on different apparatuses) are seen to exhibit a similar behavior. The figure confirms that τ, which has approximately the same value in the laboratory and center-of-mass frames,[12,13] is a useful parameter for the hydrogen collision system.

CONCLUSIONS

The dominant small-angle channel in $H^+ + H_2$ exchange collisions is found to be $H(1s) + H_2^+(^2\Sigma_g^+)$. The cross section for this channel is peaked in the forward direction as expected[9] since, at large interparticle separation, the incident channel lies close in energy to this exchange channel ($Q=2$ eV). At the larger τ values studied approximately one-half the exchange collisions still result in ground-state products. This finding may account for the reasonably good agreement between a two-state theory[4,5] and experimental results on the summed channels.[3] The maximum in the cross section for capture into excited states of H (with the H_2^+ in its ground state) occurs at approximately the same τ value at which the cross section for the direct inelastic channel[6] exhibits a maximum. This finding suggests a common primary excitation mechanism followed by couplings between the direct inelastic and close-lying exchange channels.[9]

ACKNOWLEDGMENTS

This work was supported by the National Science Foundation under Grant No. PHY-8303618 and the University of Connecticut Research Foundation.

[1]J. B. Hasted, Adv. At. Mol. Phys. **15**, 205 (1979).
[2]Dž. Belkić, R. Gayet, and A. Salin, Phys. Rep. **56**, 279 (1979).
[3]G. J. Lockwood and E. Everhart, Phys Rev. **125**, 567 (1962).
[4]R. D. Piacentini and A. Salin, J. Phys. B **11**, L323 (1978).
[5]O. Yenen, D. H. Jaecks, and J. Macek, Bull. Am. Phys. Soc. **29**, 816 (1984).
[6]M. Vedder, H. Hayden, and E. Pollack, Phys. Rev. A **23**, 2933 (1981).
[7]R. S. Peterson, M. Vedder, and E. Pollack, in *Abstracts of the Eleventh International Conference on the Physics of Electronic and Atomic Collisions, Kyoto 1979,* edited by K. Takayanagi and N. Oda (Society for Atomic Collision Research, Japan), p. 826.
[8]J. Jakacky, Jr., E. Pollack, R. Snyder, and A. Russek (unpublished).
[9]W. L. Hodge, Jr., A. L. Goldberger, M. Vedder, and E. Pollack, Phys. Rev. A **16**, 2360 (1977).
[10]C. Benoit, C. Kubach, V. Sidis, J. Pommier, and M. Barat, J. Phys. B **10**, 1661 (1977).
[11]N. J. Kirchner, A. O'Keefe, J. R. Gilbert, and M. T. Bowers, Phys. Rev. Lett. **52**, 26 (1984).
[12]P. R. Jones, P. Costigan, and G. Van Dyk, Phys. Rev. **129**, 211 (1963).
[13]F. T. Smith, R. P. Marchi, and K. D. Dedrick, Phys. Rev. **150**, 79 (1966).