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Target excitation in $H_2^+ + He$ collisions

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The direct scattering in $H_2^+ + He$ is studied at several energies in the range 1.0–3.0 keV. Excitation of the He target, primarily to $n = 2$ levels, is found even at small scattering angles. The probability of exciting the He is shown to be energy dependent and in our energy and angular ranges has a maximum value of about 0.1. The experimental results are not in agreement with predictions of an extended molecular-orbital model. The same model, however, provided substantial insight into the excitation processes in the direct and electron-capture channels in $He^+ + H_2$ collisions and for collisional dissociation in $H_2^+ + He \rightarrow H(2p) + H^+$. The excitation of the He in small-angle scattering suggests an interaction at moderate interparticle separation. Related theoretical work by Russek and Furlan [preceding paper, Phys. Rev. A **39**, 5034 (1989)] addresses the excitation process.

INTRODUCTION

The He-H_2 collision and its singly charged versions are among the most studied "three-center" systems. Since one of the collision partners is a molecule (or molecular ion) the underlying theory, even in this relatively simple case, is very much more complex than in the "simple" atom-atom and ion-atom cases. Because of the importance of the general three-center problem it is very useful to have simplified models which can provide some initial interpretation of experimental results and also guide the development of the theory. It is always essential to test the validity of models and this study addresses the applicability of the extended molecular-orbital (MO) model to the direct scattering in $H_2^+ + He$ collisions. This model was successfully used for describing the direct and electron-capture channels in $He^+ + H_2$ and in $H_2^+ + He \rightarrow H^+ + H(2p) + He$ dissociation.

The inverse $He^+ + H_2$ system has been the subject of many previous studies (see Ref. 1 for a review of some of the recent work). The angular dependence of the direct and exchange collision channels was first investigated in detail at low keV energies by Bray *et al.*[2] The experimental results showed selective excitation of the H_2 target as well as electron capture. Analysis of the direct and exchange collision channels provided an initial model[2,3] which suggested that the excitation processes in $He^+ + H_2$ were very similar to those in some ion-atom cases. The work of Dowek *et al.*[4] and of Sidis and Dowek[5] resulted in the "quasidiatomic MO" model which successfully explained one- and two-electron excitation processes and the selective population of $n = 2$ levels in the direct and exchange channels. In addition, it accounted for excitation in the neutral $He + H_2$ system. This extended MO model then served as a starting point for a more complex treatment involving three-dimensional correlation surfaces.[4,5] Later experimental results on $H_2^+ + He \rightarrow H^+ + H(2p) + He$ confirmed the applicability of the MO correlation picture to this collision channel.[6] The model predicts that there should be no (or only very weak) excitation of the He in the $H_2^+ + He$ case.[4,5] More recently several $(HeH_2)^+$ energy surfaces were determined by *ab initio* calculations.[7] Although the ground-state energy surface corresponding to the incident channel in our work was reported for interparticle separations $R > 1a_0$, the study primarily addressed two-electron rearrangement processes. The results were therefore applicable only to $He^+ + H_2$ collisions and no He excitation could be predicted.

EXPERIMENTAL ARRANGEMENT

The basic experimental arrangement is described in Ref. 8 and is only outlined here. Briefly H_2^+ is generated in a Colutron ion source, focused by an einzel lens and steered by shim fields through a Wien filter for velocity analysis. After collimation the H_2^+ beam enters a small cell containing He and scatters through an angle θ into a detector chamber where it is energy analyzed by a parallel plate electrostatic energy analyzer (resolution 0.5 eV

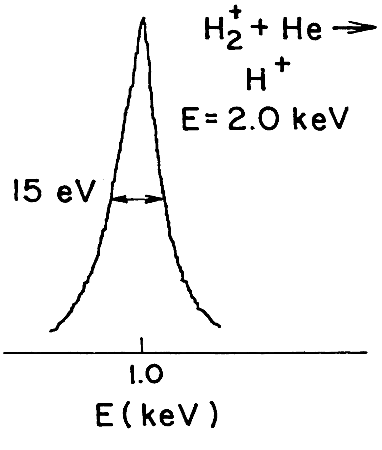

FIG. 1. A typical energy spectrum of the H^+ from 2.0 keV $H_2^+ + He \rightarrow H^+ + H + He$ collisions. The location of the peak at an energy of 1.0 keV confirms the incident beam to be H_2^+.

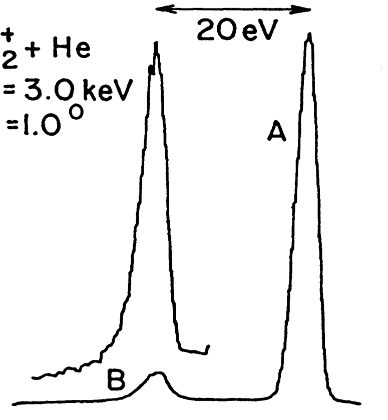

FIG. 2. An energy-loss spectrum for the direct scattering in $H_2^+ + He$ at 3.0 keV, $\theta = 1.0°$. Peak A corresponds to electronically elastic collisions and B results from excitation of He primarily to $n = 2$.

per 1.0 keV). Since the ion source generates H^+, H_2^+, and H_3^+ it is essential to confirm that the data are from $H_2^+ + He$ collisions. In the present work this is done by investigating the H^+ beam resulting from $H_2^+ + He \rightarrow H^+ + H + He$ dissociating collisions. Figure 1 shows a spectrum which is typical and routinely taken to confirm that the incident beam is indeed H_2^+. The location of the central H^+ peak, at an energy of 1.0 keV for a 2.0-keV H_2^+ beam, is consistent with the results of a recent study[9] at 6 keV. At this higher energy the dissociation resulted in a central H^+ peak at one-half the incident beam energy.

RESULTS AND CONCLUSIONS

A typical spectrum, from $H_2^+ + He$ collisions ($E = 3.0$ keV, $\theta = 1.0°$), is shown in Fig. 2. The peak labeled A is due to electronically elastic scattering. Peak B, which in the angular and energy range studied has its maximum at an energy loss $\Delta E = 20$ eV, is attributed primarily to excitation of He($n = 2$). The probability for the excitation of He in the direct scattering is shown as a function of $E\theta$ in Fig. 3. As defined here, P, the probability, is obtained from the ratio of the inelastic (B) to the total ($A + B$) H_2^+ signals. An energy dependence of this probability is clearly seen in the figure.

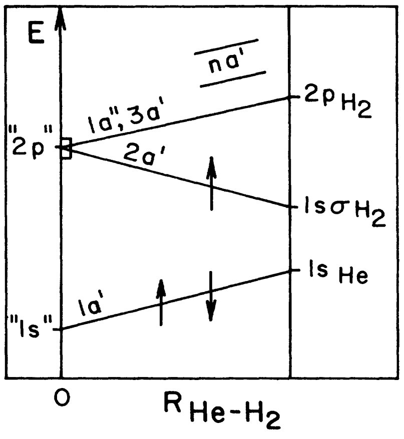

FIG. 4. A schematic quasidiatomic MO correlation diagram for $H_2^+ + He$ collisions. The two electrons correlating with He are tightly bound and therefore no He excitation is expected. The transition of an electron to the MO correlating with H_2^+ can result in He excitation but this process is weak because of the large energy separation (9 eV at infinity) between the orbitals.

As stated in the Introduction, the extended MO model successfully accounted for the experimental results in the direct and exchange collision channels in $He^+ + H_2$ and

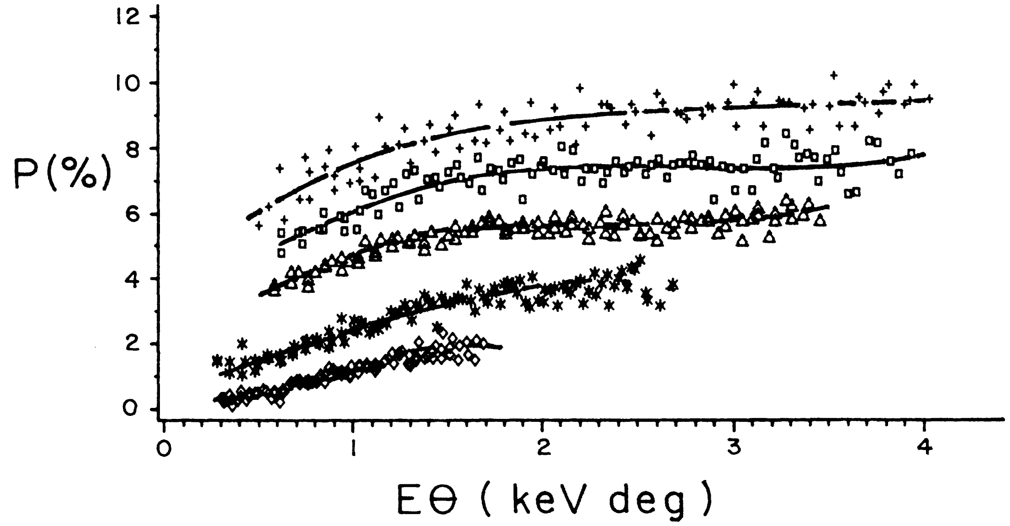

FIG. 3. The probability of He excitation as a function of reduced scattering angle at energies of 1.0 (◇), 1.5, (∗), 2.0 (△), 2.5 (□), and 3.0 (+) keV.

for dissociation to $H^+ + H(2p)$ in $H_2{}^+ + He$ collisions. The basic model for $H_2{}^+ + He$ collisions involves the MO correlation diagram shown in Fig. 4. As the collision progresses only the single electron correlating with the $H_2{}^+$ is excited since the He electrons are tightly bound. As can be seen the model does correctly predict the dissociation to $H(2p)$. In the $He^+ + H_2$ case there is an initial vacancy in the He MO with two electrons filling the upper level and thereby allowing excitation of the $n = 2$ processes observed.[4,5] Within the model, excitation of He in $H_2{}^+ + He$ can only occur following the transfer of an electron to the upper MO but this is at best expected to be a weak process because of the large energy separation between the MO's.

He excitation is expected from the results of a related theoretical study by Russek and Furlan[10] on diabatic energy surfaces of the $(HeH_2)^+$ triatomic molecular system. It is found that the ground state of $H_2{}^+ + He$ diabatically crosses an excited molecular state at $R = 0.7$ a.u. (smaller than the minimum interparticle separations reported in Ref. 7). The excited state diabatically separates as $He^*(n = 2) + H_2{}^+$. In this excitation process the full three-electron states must be considered. The individual orbitals (on which the MO model is based) by themselves do not exhibit this excitation.

In conclusion we find the dominant He excitation is to $n = 2$ levels. Excitation in $H_2{}^+ + He$ was previously investigated for principle quantum numbers $n = 3-6$, at energies in the range of 1–150 keV.[11] The optical emission cross sections reported in the study were typically 10^{-20} cm^2 in the energy range of the present experiment. Very weak excitation of the He was also seen in a study, at 8.0 keV, of an excited state of $H_2{}^+$.[12] The present doubly differential results show the excitation to be significant and also present in small-angle scattering. Since this inelastic channel involves a 20-eV excitation process it can strongly affect the dissociation and electron-capture channels and must therefore be considered in theoretical treatments of them.

ACKNOWLEDGMENTS

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