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Excitation of Atomic Hydrogen to the $n = 2$ States by 15–200-keV Protons*

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Cross sections for the process $H^+ + H \rightarrow H^+ + H^*$ ($n=2$) are determined from the energy-loss spectra of 15–200-keV protons. After normalization at 200 keV to the Born approximation, the maximum value (1.07×10^{-16} cm^2 at 60 keV) lies below close-coupling calculations and above Glauber-approximation calculations. The agreement with low-energy (5–30-keV) data of others is very good.

The simplest ion-atom collision is a collision of a proton with an atomic hydrogen atom. This system has been intensively studied by theorists. Calculations using many different approximations are available; however, the range of validity of the various theoretical approaches is still uncertain. The number of experimental measurements is very sparse in spite of the obvious interest in the cross section. Prior to the present measurement, no data have been available at proton energies at which the cross section reaches its maximum. Excitation to the $n=2$ states in $H^+ + H$ collisions has been studied with crossed-beam techniques at low proton energies (5 to 30 keV). These studies, based on the detector developed by Fite and Brackman,[1] were first performed by Stebbings *et al.*[2] The cross section has been remeasured recently by Morgan, Geddes, and Gilbody[3] and by Kondow *et al.*[4] All of these data were normalized to the Born cross section for excitation to the $H(2p)$ state by electron bombardment.

We have measured the cross section for excitation to the $H(n=2)$ state by using heavy-ion energy-loss spectrometry. The apparatus and general method employed in measuring the cross section have been previously discussed in detail.[5-7] Protons produced in a Colutron ion source are mass analyzed by a Wien filter. Selected ions are then accelerated and steered through a collimator into a chamber containing the target gas. After traversing the scattering chamber, the ions pass through an exit collimator, and the beam is magnetically analyzed to remove any products of charge-changing collisions. Ions entering the decelerator are decelerated to 2000 V and analyzed by a 127° electrostatic analyzer. Spectra differential in energy loss are obtained by increasing the potential difference between the accelerator and decelerator terminals. Whenever the increased potential energy compensates for a discrete energy loss in the projectile-target system, a peak is detected in the spectrum. The energy-loss scale can be determined to an accuracy of ± 0.03 eV.[7] The target oven is constructed of tungsten tubes. Current flows coaxially along the oven wall and returns through an adjacent coaxial shield. We have not been able to detect any effect from magnetic fields produced by the currents in the oven.

With the target oven cold, the energy-loss spectrum of molecular hydrogen is obtained when hydrogen gas is introduced into the target cell. As the oven is heated, the spectrum begins to change. A peak at 10.2-eV energy loss appears and increases while the molecular peak at 12.5-eV energy loss decreases.

The energy-loss spectrum of atomic hydrogen

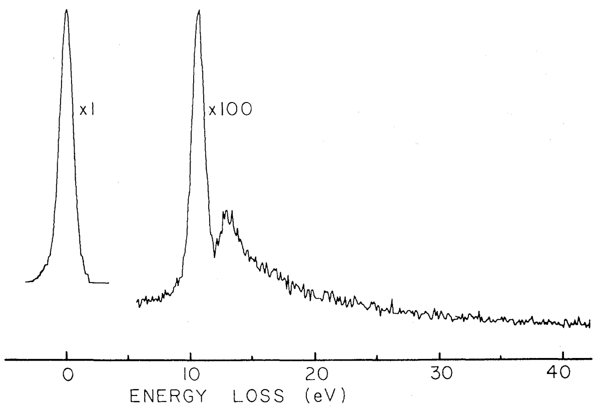

FIG. 1. The energy-loss spectra of 50-keV protons incident on atomic hydrogen.

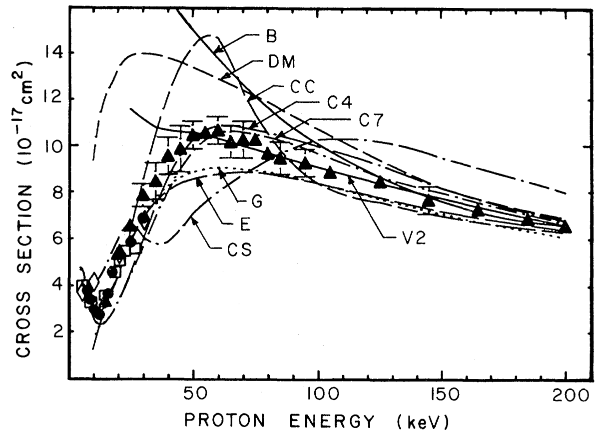

FIG. 2. The cross section for excitation of the $n=2$ state of atomic hydrogen by protons. Theory and experiment. ▲, present data; □, Morgan, Geddes, and Gilbody (Ref. 3); ◇, Young and co-workers (Refs. 2, 8); ●, Kondow *et al.* (Ref. 4). The H(2*s*) excitation cross sections of Ref. 3 are added to the H(2*p*) excitation cross sections measured in Refs. 2, 4, and 8 to yield the cross sections for excitation to the H($n=2$) state. Curve *B*, Born-approximation calculation (Ref. 9); curve *CC*, close-coupling, seven states with orthogonal pseudostates (Ref. 10); curve *C*4, four-state close coupling (Ref. 11); curve *C*7, seven-state close coupling (Ref. 11); curve *CS*, coupled-state calculation in the Sturmian representation (Ref. 12); curve *DM*, diagonalization method, twenty states (Ref. 13); curve *V*2, second-order-potentials calculation (Ref. 14); curve *E*, distorted-wave eikonal (Ref. 15); curve *G*, Glauber calculation (Ref. 16).

that is obtained with a hot oven is shown in Fig. 1. Clearly present is a peak at 10.2-eV energy loss that corresponds to the excitation to the $n=2$ state of atomic hydrogen. A secondary peak at 12.7 eV corresponds to the excitation to the $n=3$ state.

The determination of the cross section for the excitation to the H($n=2$) state is not dependent on the complete dissociation of the molecular hydrogen, because the 10.2-eV atomic peak is resolved from the molecular peak. We believe, however, that the molecular fraction is less than 3% during the data-acquisition period. This fraction is determined not only from pressure-temperature curves but also from plots of the ratio of the ion currents at 10.2- and 12.5-eV energy loss taken as a function of oven temperature. This ratio increases with temperature until it reaches a plateau. Higher oven temperatures do not make any further changes in the spectral shape.

A relative cross section can be obtained directly from the data.[6] Energy-loss spectra are measured in series. Consecutive spectrum measurements are taken at various energies from 200 keV down to 15 keV. During each series of spectrum measurements, the pressure in the chamber is held fixed to permit normalization to a single cross section at 200 keV. The cross sections obtained for the excitation to the $n=2$ state of atomic hydrogen are shown in Fig. 2. Averages of all the available data are given by the triangles. The error bars shown on the figure represent 1 standard deviation. They include only random errors. The averaged data are normalized at 200 keV to the Born-approximation calculation for proton excitation to the H($n=2$) state ($\sigma = 6.637 \times 10^{-16}$ cm^2).[9]

At low energies (5 to 30 keV) our data can be compared to the crossed-beam measurements. To obtain the cross section for the excitation to the $n=2$ state of atomic hydrogen the cross sections for both the H(2*s*) and H(2*p*) states have to be included. In the case of Young and co-workers[2,8] and of Kondow *et al.*,[4] the H(2*s*) excitation cross sections from Morgan, Geddes, and Gilbody[3] are added to the measured H(2*p*) excitation cross sections to give the excitation cross section for the H($n=2$) levels. Considering the major differences in technique and normalization, the agreement between our data and data from these crossed-beam experiments is unexpectedly good.

Examples of the various theoretical calculations are also shown in Fig. 2. The large number of theoretical techniques[9-28] applied to the proton–hydrogen-atom collision, many with several variations, cannot all be included in the figure. The Born-approximation calculations[9] (curve *B*) in general exhibit a peak that overestimates the observed cross sections and occurs at too low an energy. The results of the second-Born-approximation calculations for the direct excitation to the H* ($n=2$) state do not markedly improve the theoretical fit to the data over the first-Born-approximation calculations.[17-19] Impact-parameter formulations of the Born approximation similarly produce negligible improvement[20,21] in the theoretical fit to the data.

The distortion-approximation[22,23] agreement with the experimental measurements is poor but is better than for the Born approximation.

Impact-parameter coupled-state calculations have been undertaken by several groups. Unless exchange channels are included, the theoretical values are not in much better agreement with the experimental data than the distortion-approximation results.[24] The differences among the various four-state calculations are noticeable,[10,11,25,26] but the overall fit to the experimental data is roughly equivalent. The recent data of Rapp and Dinwiddie[10] are shown for both four-state (curve *C*4) and seven-state (curve *C*7) calculations. It is noted that the inclusion of the additional states does not produce any dramatic changes. The agreement between theory and experiment is quite good.

The best overall agreement at low energies is obtained by the seven-state close-coupling calculation of Cheshire, Gallaher, and Taylor[10] (curve *CC*). This calculation includes exchange and uses pseudostates to represent coupling to the higher states. Our measurements indicate the calculation in Ref. 10 tends to overestimate the cross section at the peak of the curve. Kondow *et al.*[4] also noted that at their highest energies the cross sections in Ref. 10 were larger than their experimental measurements.

Bransden and Coleman[27] have developed a technique in which they use second-order potentials to make allowance for states omitted in truncating the close-coupling expansion. The four-channel calculation that uses second-order potentials does not, however, provide a good fit to the data below 100 keV (curve *V*2). Gallaher and Wilets's coupled-state calculations, which use a Sturmian representation to form a complete basis set, are shown in curve *CS*.[12] The agreement with experiment is not good. No structure was detected in the experimental data that would correspond to the minimum in the cross section, which was obtained in this calculation at about 35 keV.

Baye and Heenen[13] have recently applied a diagonalization method, which includes twenty states. The cross sections obtained do not provide a good fit to the data at energies below 100 keV (see curve *DM*).

The Glauber approximation calculated by Franco and Thomas[16] (curve *G*) gives surprisingly good results in the energy range under study. The distorted-wave eikonal calculation of Joachain and Vanderpoorten[15] (curve *E*) is only slightly different from the Glauber approximation and fits the data equally well. The Glauber approximation is lower than our experimental measurement at the maximum in the curve of the cross section. The agreement with the low-energy measurements is not satisfactory below 10 keV. Nevertheless, the agreement is quite good over a large energy range, especially if one considers the relative simplicity of the Glauber approximation.

The agreement with the crossed-beam experiments at low energy is gratifying. Our data are normalized to the Born approximation; however, normalization at 200 keV to any of the other theoretical curves would not have produced any dramatic changes. Comparisons with theoretical results show the experimental measurements falling between the various theoretical cross-section curves. The close-coupling calculations are higher than the experimental values while the Glauber or eikonal calculations are lower; however, the differences between these theories and experiment are not large.

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Spectral Shape and Cross Section of Molecular-Orbital X-Ray Continua from Heavy-Ion Collisions

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We investigate molecular-orbital (MO) x-ray transitions resulting from collisions between 7–95-MeV sulfur ions and various thin, solid targets. MO radiation profiles beyond the united-atom limit are measured over several orders of magnitude in intensity, and absolute contributions of spontaneous and induced MO x rays are identified. We discuss formulations of MO theories which are in excellent agreement with our experimental spectral shapes and cross sections.

Observation of x rays from heavy-ion collisions has become an important tool to aid our still limited understanding of complex phenomena which occur in heavy-ion encounters. Careful measurements of collision-induced x rays have revealed that characteristic x-ray or satellite lines are always accompanied by relatively weak but distinct radiation continua. Almost at the same time, two mechanisms have been proposed to explain the production of such continua, molecular-orbital (MO)[1] and radiative-electron-capture (REC)[2,3] transitions. Since then, extensive further work has been reported especially on MO phenomena, but important features of this process such as precise spectral shapes and production cross sections remain poorly explained. It is the purpose of this Letter to clarify some experimental and theoretical questions on these radiation continua. In particular, we demonstrate that (i) MO and REC transitions can occur simultaneously in heavy-ion collisions and may give overlapping contributions to radiation continua, (ii) spectral shapes near and beyond the transition energy of the united (stationary) system, E_u, can be derived from a clarified formulation of the theory by Macek and Briggs[4] and are found to agree with experimental MO profiles over several orders of magnitude in intensity, and (iii) absolute MO production cross sections can be understood if one takes into account spontaneous and induced transitions.[5] We confine ourselves to the decay of K-shell vacancies and concentrate on MO tails beyond E_u which, in most cases, represent only a small though very distinct fraction of the total MO intensity. Our calculations for systems which need not be symmetric do not require detailed knowledge of the MO level diagram, and extension to initial vacancies in