PHYSICAL REVIEW A VOLUME 30, NUMBER 2 AUGUST 1984

# Angular differential and total cross sections for the excitation of atomic hydrogen to its $n=2$ level by 25—150-keV hydrogen molecular ions

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(Received 13 April 1983; revised manuscript received 20 March 1984)

Experimentally and theoretically determined differential and total cross sections are reported for excitation of atomic hydrogen to its $n=2$ level by 25—150-keV hydrogen molecular ions. The differential cross sections decrease 3—4 orders of magnitude over the measured center-of-mass scattering-angular range from 0 to 4.5 mrad. The results of a first Born approximation and two other theoretical calculations based upon the Glauber approximation are presented and compared with the experimental results. Both calculations based on the Glauber approximation agree fairly well with the experimental results. The Born approximation agrees moderately well with the experimental results at the very small scattering angles but is well below the experimental results at the larger scattering angles. None of the theoretical calculations presented agree well with the total cross section. However, the results for the total cross section of the two calculations based on the Glauber approximation agree with the experimental results in curve shape better than the Born-approximation results.

## INTRODUCTION

The collision of a hydrogen molecular ion with a hydrogen atom is the simplest atom-diatom collision system that one can investigate. However, there is little published information concerning this collision system. Prior to this paper, the only available experimental information consisted of the total charge transfer cross-section measurements for incident ${H_2}^+$ energies from 0.1—10.0 keV reported by Fite, Brackmann, and Snow[1] and the total proton production cross-section measurements for incident ${H_2}^+$ energies from 3.15—115.0 keV reported by McClure.[2] The only theoretical information available in the overlapping energy range of these experiments is the calculation of the total cross section for dissociation of the ${H_2}^+$ projectile with simultaneous excitation of the hydrogen target reported by Peek.[3]

In this paper experimental and theoretical differential cross-section results for the process

$$ {H_2}^+ + H(1s) \rightarrow {H_2}^+(\theta) + H^*(n=2) $$

are presented for an ${H_2}^+$ incident projectile energy range from 25—150 keV and center-of-mass scattering-angle range between 0.0—4.5 mrads. The total cross section obtained by integrating the differential cross sections is also presented. The theoretical calculations presented are the first Born approximation and two other approximations based upon the Glauber approximation.

## EXPERIMENTAL METHOD

The apparatus used for the present investigation and the method employed to extract differential cross sections for measured angular distributions of scattered particles are described in Refs. 4—9. Hydrogen molecular ions produced in a colutron ion source are extracted at 2000 V, momentum selected, and injected into an accelerating column. The accelerated beam is electrostatically steered through a tubular—joule-heated furnace which produces a hydrogen-atom target. The ion beam which exits the furnace is mass analyzed and decelerated to 2000 V. The decelerated beam is electrostatically analyzed by a 127° cylindrical analyzer to find the energy lost in the ion-target atom collision. The ion energy-loss scale of the decelerated beam can be established to an accuracy of $\pm 0.03$ eV. In the present experiment the energy resolution is 1.5 eV.

Angular distributions of scattered ions with a given energy loss are obtained by rotating the accelerating column and ion source about a pivot point centered under the hydrogen-atom—producing furnace. The scattering angle can be determined with an accuracy of $\pm 3.33\ \mu$rad. The full width at half maximum of the incident beam is 120 $\mu$rad measured in the laboratory. For a detailed discussion of the ion energy-loss measurement method see Refs. 4—9, and for a recent schematic of the present apparatus see Ref. 8.

The distribution of vibrational states in our incident ${H_2}^+$ beam has not been measured by us. McGowan and Kerwin[10] have determined the relative populations of the various vibrational levels of ${H_2}^+$ that are produced from bombarding $H_2$ by electrons at various energies. The ion source used for this experiment was always operated with an ionizing electron energy between 40 and 60 eV. This indicates that the vibrational levels in our incident ${H_2}^+$ beam correspond to the distribution at saturation.[10] The experiment does not separate out the various initial vibrational components of the incident hydrogen-molecular-ion beam nor does it measure the final vibrational distribution of the scattered hydrogen molecular ions.

Because the experiment does not resolve the vibrational states, the experimental results are compared to a theoreti-

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cal calculation that sums over all final vibrational states and statistically averages over all initial vibrational states of the incident $H_2^+$ projectile.

Any measurement of an angular distribution involves some convoluting effect of the measuring apparatus. One method for "unraveling" the effect of the apparatus on the experimentally determined differential cross section has been presented by Park *et al.* in Ref. 9. This method has been used to obtain the experimentally determined differential cross sections which are reported in this paper.

It is important to reiterate that the dissociation fraction of the present system is greater than 95% and that any residual molecular hydrogen in the target does not affect the integrity of the hydrogen $n=2$ state measurement as there are no hydrogen-molecular-ion states that have an energy loss of $10.2\pm1.5$ eV. The atomic hydrogen target density is normalized to the proton-impact-excitation measurements from Ref. 4.

## THEORY

The Born differential cross section for excitation is known to fall off more rapidly than experiment for proton-hydrogen scattering.[6] However, a first-Born-approximation calculation of $H_2^+ + H \rightarrow H_2^+(\theta) + H^*(n=2)$ was undertaken for comparison with the experimental results because the well-understood properties of the Born approximation make it useful as a benchmark in evaluating other theoretical approaches. Two different calculations based on the Glauber approximation[11] for $H_2^+ + H \rightarrow H_2^+(\theta) + H^*(n=2)$ are also presented. One Glauber-approximation calculation is based on the first Born approximation. The other is based on an expansion of the profile function that is similar to the treatment employed by Franco[12] for $He^+$-H excitation.

The interaction potential $V$ in atomic units between $H_2^+$ and H is given by

$$V=|\vec{r}+\tfrac{1}{2}\vec{R}|^{-1}+|\vec{r}-\tfrac{1}{2}\vec{R}|^{-1}-|\vec{r}+\vec{r}_0|^{-1}-|\vec{r}+\tfrac{1}{2}\vec{R}-\vec{r}_1|^{-1}-|\vec{r}-\tfrac{1}{2}\vec{R}-\vec{r}_1|^{-1}+|\vec{r}+\vec{r}_0-\vec{r}_1|^{-1}\ . \tag{1}$$

The vector $\vec{r}$ is from the hydrogen-atom nucleus to the center of the $H_2^+$ internuclear line, $\vec{r}_0$ is from the center of the $H_2^+$ internuclear line to the electron bound to $H_2^+$, $\vec{r}_1$ is from the hydrogen-atom nucleus to the electron bound to H, and $\vec{R}$ is the vector between the nuclei of $H_2^+$. Atomic units will be used throughout the theory section. We assume the Born-Oppenheimer separation of electronic and nuclear variables for $H_2^+$. Let $\Phi(\vec{r}_0,\vec{R})$ be the wave function for the ground electronic state of $H_2^+$. The nuclear wave function and subsequent matrix elements will be considered later. The initial and final wave functions for the hydrogen atom are $\psi_i(\vec{r}_1)$ and $\psi_f(\vec{r}_1)$, respectively. The momentum transfer is given by $\vec{q}=\vec{k}_i-\vec{k}_f$, where $\vec{k}_i$ and $\vec{k}_f$ represent the relative momenta of the collision system before and after the collision. Within the context of the first Born approximation[3] we define

$$G_{fi}^B=-\frac{\mu}{2\pi}\int d^3r_0\,d^3r_1\,d^3r\,|\Phi(\vec{r}_0,\vec{R})|^2\psi_f^*(\vec{r}_1)\times\psi_i(\vec{r}_1)V\exp(i\vec{q}\cdot\vec{r})\ , \tag{2}$$

where $\mu$ is the reduced mass for the $H_2^+$-H collision system. The mass of the electrons are ignored with respect to the nuclear masses. To obtain the scattering amplitude, the function $G_{fi}^B$ must be evaluated between the initial and final nuclear wave functions. The integration over $\vec{r}$ can be performed to yield[13]

$$G_{fi}^B=\left[2\cos\left[\frac{\vec{q}\cdot\vec{R}}{2}\right]-S_{H_2^+}(q)\right]f_{fi}^B(p,\mathrm{H})\ , \tag{3}$$

where

$$S_{H_2^+}(q)=\int d^3r_0\,|\Phi(\vec{r}_0,\vec{R})|^2\exp(-i\vec{q}\cdot\vec{r}_0) \tag{4}$$

is the form factor for the $H_2^+$ ground electronic state and $f_{fi}^B(p,\mathrm{H})$ is the first Born scattering amplitude for a "heavy proton" with a mass equal to the mass of $H_2^+$ and with a relative velocity $\vec{v}=\vec{k}_i/\mu$ colliding with a hydrogen atom. Thus in the first Born approximation, $G_{fi}^B$ consists of a factor depending upon the nuclear coordinate $\vec{R}$ and a factor independent of $\vec{R}$ which basically determines the angular distribution of the scattering. In the differential cross section the nuclear factor does not depend strongly upon $q$. Also the momentum transfer $q$ does not vary significantly over our range of angular scattering.

A simple Glauber approximation can be obtained that displays the same structure as the first Born approximation. This can most easily be achieved by replacing the first Born scattering amplitude by the Glauber scattering amplitude for the heavy proton scattering. Consider the first Born scattering amplitude which is given by

$$f_{fi}^B(p,\mathrm{H})=-\frac{\mu}{2\pi}\int d^3r_1\,d^3r\,\psi_f^*(\vec{r}_1)\psi_i(\vec{r}_1)V_{pH}(\vec{r}_1,\vec{r})\times\exp(i\vec{q}\cdot\vec{r})\ , \tag{5}$$

where $V_{pH}(\vec{r}_1,\vec{r})$ is the interaction potential between the heavy proton and the hydrogen atom. Let $\vec{r}=\vec{b}+\vec{z}$, where $\vec{b}$ and $\vec{z}$ are the components of $\vec{r}$ perpendicular and parallel to $\vec{v}$ which is the velocity of the projectile relative to the target.[12] Likewise define $\vec{r}_1=\vec{b}_1+\vec{z}_1$, where $\vec{b}_1$ and $\vec{z}_1$ are the components of $\vec{r}_1$ perpendicular and parallel to $\vec{v}$.[12] For small angle scattering we may assume $\vec{q}\cdot\vec{r}\approx\vec{q}\cdot\vec{b}$, i.e., $\vec{q}$ is perpendicular to the $\vec{z}$ direction.[14] The only remaining $z$ dependence is in the interaction potential $V_{pH}$. The $z$ integration can be related to the phase-shift function which is defined as[12]

$$\chi_{pH}(\vec{b},\vec{b}-\vec{b}_1)\equiv-\frac{1}{v}\int_{-\infty}^{\infty}V_{pH}(\vec{r}_1,\vec{r})\,dz\ . \tag{6}$$

Franco[15,12] has evaluated the phase-shift function for collisions between an ion and neutral hydrogen. The first Born scattering amplitude becomes

$$f_{fi}^B(p,\mathrm{H})=\frac{\mu v}{2\pi}\int d^3r_1\,d^2b\,\psi_f^*(r_1)\psi_i(\vec{r}_1)\times\chi_{pH}(\vec{b},\vec{b}-\vec{b}_1)\exp(i\vec{q}\cdot\vec{b})\ . \tag{7}$$

The profile function is defined as[12]

$$\Gamma_{p\mathrm{H}}(\vec{b},\vec{b}-\vec{b}_1)=1-\exp[i\chi_{p\mathrm{H}}(\vec{b},\vec{b}-\vec{b}_1)]\ , \tag{8}$$

which to lowest order becomes $-i\chi_{p\mathrm{H}}(\vec{b},\vec{b}-\vec{b}_1)$. The Glauber scattering amplitude for the heavy proton scattering is given by[11,12]

$$f_{fi}^{G}(p,\mathrm{H})=\frac{i\mu v}{2\pi}\int d^3r_1\, d^2b\, \psi_f^*(\vec{r}_1)\psi_i(\vec{r}_1)\Gamma_{p\mathrm{H}}(\vec{b},\vec{b}-\vec{b}_1)\times\exp(i\vec{q}\cdot\vec{b})\ . \tag{9}$$

The first Born scattering amplitude, Eq. (5), corresponds to keeping only the lowest-order term in the expansion for the profile function. Replacing the first Born scattering amplitude by the lowest-order Glauber scattering amplitude yields the following approximation for $G_{fi}$, namely,

$$G_{fi}^{G1}=\left[2\cos\left[\frac{\vec{q}\cdot\vec{R}}{2}\right]-S_{\mathrm{H}_2{}^+}(q)\right]f_{fi}^{G}(p,\mathrm{H})\ , \tag{10}$$

which has the same structure as the first Born approximation for $G_{fi}$.

A somewhat more complicated Glauber approximation can be obtained by expanding the profile function starting with the $\mathrm{H}_2{}^+$-H interaction potential. The interaction potential can be arranged to represent the interaction of the two protons and the electron of $\mathrm{H}_2{}^+$ with neutral hydrogen.[12] This leads to a similar form for the phase-shift function. As before, let $\vec{R}=\vec{B}+\vec{Z}$ and $\vec{R}_0=\vec{b}_0+\vec{z}_0$ where $(\vec{B},\vec{b}_0)$ and $(\vec{Z},\vec{z}_0)$ are the components of $(\vec{R},\vec{R}_0)$ perpendicular and parallel to $\vec{v}$. The phase-shift function is then given by

$$\chi=\chi_{p\mathrm{H}}(\vec{b}+\tfrac{1}{2}\vec{B},\vec{b}+\tfrac{1}{2}\vec{B}-\vec{b}_1)+\chi_{p\mathrm{H}}(\vec{b}-\tfrac{1}{2}\vec{B},\vec{b}-\tfrac{1}{2}\vec{B}-\vec{b}_1)+\chi_{e\mathrm{H}}(\vec{b}+\vec{b}_0,\vec{b}+\vec{b}_0-\vec{b}_1)\ , \tag{11}$$

where $\chi_{p\mathrm{H}}$ and $\chi_{e\mathrm{H}}$ are the phase-shift functions for proton-hydrogen and electron-hydrogen collisions, respectively. They are given explicitly by Franco.[12] Following Franco[12] the first-order profile function is given by

$$\Gamma^{(1)}=\Gamma_{p\mathrm{H}}(\vec{b}+\tfrac{1}{2}\vec{B},\vec{b}+\tfrac{1}{2}\vec{B}-\vec{b}_1)+\Gamma_{p\mathrm{H}}(\vec{b}-\tfrac{1}{2}\vec{B},\vec{b}-\tfrac{1}{2}\vec{B}-\vec{b}_1)+\Gamma_{e\mathrm{H}}(\vec{b}+\vec{b}_0,\vec{b}+\vec{b}_0-\vec{b}_1)\ , \tag{12}$$

where $\Gamma_{p\mathrm{H}}$ and $\Gamma_{e\mathrm{H}}$ are the corresponding profile functions for proton-hydrogen and electron-hydrogen collisions. In this approximation $G_{fi}$ is given by

$$G_{fi}^{G2}=\frac{i\mu v}{2\pi}\int d^3r_0\, d^3r_1\, d^2b\, |\Phi(\vec{r}_0,\vec{R})|^2\times\psi_f^*(\vec{r}_1)\psi_i(\vec{r}_1)\Gamma^{(1)}\exp(i\vec{q}\cdot\vec{b})\ . \tag{13}$$

Each of the terms in the profile function can be identified with a Glauber scattering amplitude if the origin of $\vec{b}$ is shifted appropriately in each term.[16] This yields

$$G_{fi}^{G2}=2\cos\left[\frac{\vec{q}\cdot\vec{B}}{2}\right]f_{fi}^{G}(p,\mathrm{H})+f_{fi}^{G}(e,\mathrm{H})\int d^3r_0\, |\Phi(\vec{r}_0\vec{R})|^2\exp(-i\vec{q}\cdot\vec{b}_0)\ , \tag{14}$$

where $f_{fi}^{G}(e,\mathrm{H})$ is the Glauber scattering amplitude for a heavy electron with a mass equal to the mass of $\mathrm{H}_2{}^+$ and with a relative velocity $\vec{v}=\vec{k}_i/\mu$ colliding with a hydrogen atom. In keeping with the assumption that $\vec{q}$ is perpendicular to the $\vec{z}$ direction we may take $\vec{q}\cdot\vec{B}\approx\vec{q}\cdot\vec{R}$ and $\vec{q}\cdot\vec{b}_0\approx\vec{q}\cdot\vec{r}_0$. Using this assumption gives the second Glauber approximation

$$G_{fi}^{G2}=2\cos\left[\frac{\vec{q}\cdot\vec{R}}{2}\right]f_{fi}^{G}(p,\mathrm{H})+S_{\mathrm{H}_2{}^+}(q)f_{fi}^{G}(e,\mathrm{H})\ . \tag{15}$$

In this approximation the nuclear coordinates are connected to the functions that determine the angular scattering distribution in a rather complicated way.

The quantity $G_{fi}$ for the three approximations considered here must be evaluated between the initial and final wave functions for the nuclear motion in order to obtain the scattering amplitude and ultimately the differential cross section. The nuclear motion is assumed to be that of a rigid rotator with the rotational and vibrational motion uncoupled. Let $\chi_v(R)$ be the vibrational wave function with vibrational quantum number $v$. The rotational wave function will be the spherical harmonic $Y_{jm}(\hat{R})$ with the rotational quantum numbers $j$ and $m$. The experimental results reported in this paper do not resolve the rotational or vibrational structure of $\mathrm{H}_2{}^+$. Therefore, we sum over the final vibrational state $v'$ and final rotational states $j',m'$ and average over the initial rotational state sublevel $m$. Thus the differential cross section for a particular approximation is given by

$$\frac{d\sigma^v}{d\Omega}=\frac{1}{2j+1}\sum_{m=-j}^{j}\sum_{j'=0}^{\infty}\sum_{m'=-j'}^{j'}\sum_{v'}\left[\frac{k_f}{k_i}\right]\langle v,j,m\,|\,G_{fi}^*\,|\,v',j',m'\rangle\langle v',j',m'\,|\,G_{fi}\,|\,v,j,m\rangle\ . \tag{16}$$

If we ignore energy conservation with regard to the rotational and vibrational states, we can carry out the $v',j',m'$ sums by using the closure relation. This gives

$$\frac{d\sigma^v}{d\Omega}=\frac{k_f}{k_i}\frac{1}{2j+1}\times\sum_{m=-j}^{j}\int d^3R\, |\chi_v(R)|^2|Y_{jm}(\hat{R})|^2|G_{fi}|^2\ . \tag{17}$$

The sum over $m$ can be carried out to yield a result which is independent of the initial rotational state $j$. Thus

$$\frac{d\sigma^v}{d\Omega}=\frac{k_f}{k_i}\frac{1}{4\pi}\int d^3R\, |\chi_v(R)|^2|G_{fi}|^2\ . \tag{18}$$

The differential cross section for a particular approximation is obtained by using the appropriate $G_{fi}$.

The differential cross section was averaged over the vibrational distribution of the incident $H_2^+$ beam. If $g_v$ is the fraction of $H_2^+$ molecular ions in vibrational state $v$ in the incident beam, the differential cross section averaged over the vibrational distribution of the incident $H_2^+$ beam is given by

$$\frac{d\sigma}{d\Omega}=\sum_v g_v \frac{d\sigma^v}{d\Omega} . \tag{19}$$

The normalized values for $g_v$ were determined by McGowan and Kerwin[10] for an ion source with our operating conditions.

The quantity $G_{fi}$ must be determined for the three approximations under consideration. One factor is $S_{H_2^+}(q)$ which involves the electronic wave function $\Phi(\vec{r}_0,\vec{R})$ for the ground state of $H_2^+$. A Gaussian basis function was chosen because of its simpler algebraic form. These basis functions have been used recently for electron-molecule scattering[17,18] in order to simplify the calculations. The electronic wave function is given approximately by

$$\Phi(\vec{r}_0,\vec{R})=\left[\left[\frac{\pi^3}{2a^3}\right]^{1/2}[1+\exp(-aR^2/2)]\right]^{-1/2} \times[\exp(-a\,|\,\vec{r}_0+\tfrac{1}{2}\vec{R}\,|^2) +\exp(-a\,|\,\vec{r}_0-\tfrac{1}{2}\vec{R}\,|^2)] . \tag{20}$$

The parameter $a$ is determined from a variational calculation to minimize the electronic energy at a given internuclear separation $R$ and thus it is a function of $R$. The value of the parameter $a$ varies from $a=32/9\pi$ a.u.$=1.132$ a.u. at $R=0$ to $a=8/9\pi$ a.u.$=0.282$ a.u. at $R=\infty$. It has a weak minimum value of 0.251 a.u. around $R=5.3$ a.u. The value of $a$ at $R=2.00$ a.u., the physical equilibrium distance of $H_2^+$, is 0.436 a.u. The variational calculation yields an equilibrium distance for $H_2^+$ of 2.06 a.u. and the value of $a$ for this distance is 0.427 a.u. Overall the variational calculation using Gaussian basis functions yields quite reasonable results for the bound electronic energy of $H_2^+$. The electronic wave function determined in this way was used to calculate the form factor $S_{H_2^+}(q)$ with the result that

$$S_{H_2^+}(q)=\left[\frac{\cos(\vec{q}\cdot\vec{R}/2)+\exp(-aR^2/2)}{1+\exp(-aR^2/2)}\right] \times\exp\left[-\frac{q^2}{8a}\right] . \tag{21}$$

The Glauber scattering amplitudes for a heavy proton or a heavy electron exciting a hydrogen atom are also needed to determine $G_{fi}$ for the two Glauber approximations to the $H_2^+$-H collision. Thomas and Gerjuoy[19] have given these in closed form in terms of hypergeometric functions for the excitation of hydrogen to a particular substate of its $n=2$ level. The Born scattering amplitude for the excitation of hydrogen to a particular substate of its $n=2$ level is, of course, straightforward to calculate.

Once $G_{fi}$ is determined for the various approximations, the expectation value of $|\,G_{fi}\,|^2$ for vibrational state $v$ must be calculated. Harmonic-oscillator wave functions were used for $\chi_v(R)$ with the parameters taken from Herzberg.[20] The angular integration can be carried out analytically. The remaining integral over $R$ was carried out numerically using standard numerical techniques.

## RESULTS AND DISCUSSION

The experimental results of the present investigation are summarized in Table I. The experimentally determined differential cross sections and the scattering angles are given in the center-of-mass system while the incident $H_2^+$ ion energies are given in the laboratory system. The total cross sections were obtained by numerically integrating the experimental differential cross sections. These are also given in Table I. All error bars in the table represent one standard deviation about the mean.

Figures 1 and 2 display the present results for the differential cross section for the excitation of atomic hydrogen to its $n=2$ level by singly charged hydrogen molecular ions at incident laboratory energies of 50 keV ($v=1.0$ a.u.) and 150 keV ($v=1.73$ a.u.), respectively. Also shown are the results of the Born and the two Glauber approximations discussed in the theory section. Both the simpler Glauber ($G1$) results and the more complicated Glauber ($G2$) results are in fairly good agreement with the experimental results over the measured range of scattering angles. In general the Born results are higher than either Glauber result at the very small scattering angles but at

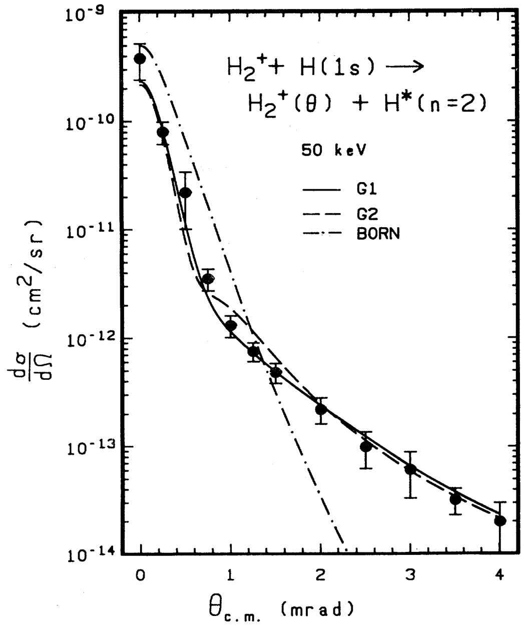

FIG. 1. Angular differential cross section for excitation of atomic hydrogen to its $n=2$ level by 50-keV hydrogen-molecular-ion impact. The solid circles with error bars are the experimental results. The error bars represent one standard deviation from the mean and include only random statistical error. The theoretical results for the approximations described in the text are the following: ——, $G1$; — — —, $G2$; and —·—·—·, Born.

TABLE I. Experimentally determined differential and total cross sections for the excitation of atomic hydrogen to its $n=2$ level by hydrogen-molecular-ion impact. The angle $\theta$ is given in the center-of-mass system in millirads. The differential cross section $d\sigma/d\Omega$ is given in the center-of-mass system in units of cm$^2$/sr.

| $\theta_{\text{c.m.}}$ (mrad) | 25 keV | 35 keV | 50 keV | 75 keV | 100 keV | 125 keV | 150 keV |
|---|---|---|---|---|---|---|---|
| 0.00 | $(4.7\pm0.9)\times10^{-11}$ | $(1.4\pm0.2)\times10^{-10}$ | $(3.8\pm1.4)\times10^{-10}$ | $(7.8\pm1.0)\times10^{-10}$ | $(6.9\pm0.6)\times10^{-10}$ | $(6.6\pm0.7)\times10^{-10}$ | $(9.1\pm1.7)\times10^{-10}$ |
| 0.25 | $(4.2\pm2.3)\times10^{-11}$ | $(6.4\pm0.5)\times10^{-11}$ | $(8.0\pm1.9)\times10^{-11}$ | $(2.1\pm0.4)\times10^{-10}$ | $(2.1\pm0.5)\times10^{-10}$ | $(2.2\pm0.3)\times10^{-10}$ | $(2.2\pm0.4)\times10^{-10}$ |
| 0.50 | $(2.0\pm0.5)\times10^{-11}$ | $(2.4\pm0.4)\times10^{-11}$ | $(2.2\pm1.2)\times10^{-11}$ | $(2.3\pm0.8)\times10^{-11}$ | $(2.9\pm0.6)\times10^{-11}$ | $(2.8\pm0.6)\times10^{-11}$ | $(2.3\pm0.6)\times10^{-11}$ |
| 0.75 | $(9.7\pm2.6)\times10^{-12}$ | $(8.5\pm3.1)\times10^{-12}$ | $(3.5\pm0.8)\times10^{-12}$ | $(4.3\pm2.6)\times10^{-12}$ | $(5.4\pm1.8)\times10^{-12}$ | $(5.0\pm1.9)\times10^{-12}$ | $(3.4\pm0.6)\times10^{-12}$ |
| 1.00 | $(4.8\pm1.2)\times10^{-12}$ | $(3.5\pm1.2)\times10^{-12}$ | $(1.3\pm0.3)\times10^{-12}$ | $(1.5\pm1.3)\times10^{-12}$ | $(1.7\pm0.6)\times10^{-12}$ | $(1.3\pm0.4)\times10^{-12}$ | $(9.6\pm2.8)\times10^{-13}$ |
| 1.25 | $(2.3\pm0.3)\times10^{-12}$ | $(1.5\pm0.5)\times10^{-12}$ | $(7.5\pm1.5)\times10^{-13}$ | $(9.2\pm5.7)\times10^{-12}$ | $(7.8\pm2.3)\times10^{-13}$ | $(6.0\pm1.7)\times10^{-13}$ | $(5.4\pm1.7)\times10^{-13}$ |
| 1.50 | $(1.4\pm0.3)\times10^{-12}$ | $(7.6\pm2.4)\times10^{-13}$ | $(4.8\pm1.0)\times10^{-13}$ | $(6.1\pm4.5)\times10^{-12}$ | $(4.8\pm1.6)\times10^{-13}$ | $(3.6\pm1.0)\times10^{-13}$ | $(3.4\pm0.9)\times10^{-13}$ |
| 2.00 | $(5.8\pm1.6)\times10^{-13}$ | $(3.1\pm0.8)\times10^{-13}$ | $(2.2\pm0.6)\times10^{-13}$ | $(2.8\pm2.0)\times10^{-13}$ | $(2.0\pm0.7)\times10^{-13}$ | $(1.5\pm0.6)\times10^{-13}$ | $(1.1\pm0.5)\times10^{-13}$ |
| 2.50 | $(3.2\pm0.6)\times10^{-13}$ | $(1.7\pm0.6)\times10^{-13}$ | $(9.9\pm3.7)\times10^{-14}$ | $(1.2\pm0.9)\times10^{-13}$ | $(8.8\pm3.2)\times10^{-14}$ | $(6.3\pm2.7)\times10^{-14}$ | $(5.1\pm2.8)\times10^{-14}$ |
| 3.00 | $(1.7\pm0.3)\times10^{-14}$ | $(8.6\pm3.3)\times10^{-14}$ | $(6.1\pm2.8)\times10^{-14}$ | $(6.1\pm3.0)\times10^{-14}$ | $(4.6\pm2.2)\times10^{-14}$ | $(4.7\pm1.1)\times10^{-14}$ | $(4.9\pm2.3)\times10^{-14}$ |
| 3.50 | $(8.5\pm1.2)\times10^{-14}$ | $(3.6\pm2.6)\times10^{-14}$ | $(3.2\pm0.9)\times10^{-14}$ | $(3.2\pm2.1)\times10^{-14}$ | $(2.8\pm1.2)\times10^{-14}$ | | |
| 4.00 | $(7.1\pm0.2)\times10^{-14}$ | | $(2.0\pm1.0)\times10^{-14}$ | | | | |
| 4.50 | $(6.8\pm2.5)\times10^{-14}$ | | | | | | |
| $\sigma_T$(cm$^2$) | $(7.3\pm1.7)\times10^{-17}$ | $(7.4\pm1.2)\times10^{-17}$ | $(8.2\pm2.6)\times10^{-17}$ | $(1.4\pm0.3)\times10^{-16}$ | $(1.4\pm0.1)\times10^{-16}$ | $(1.5\pm0.2)\times10^{-16}$ | $(1.4\pm0.2)\times10^{-16}$ |

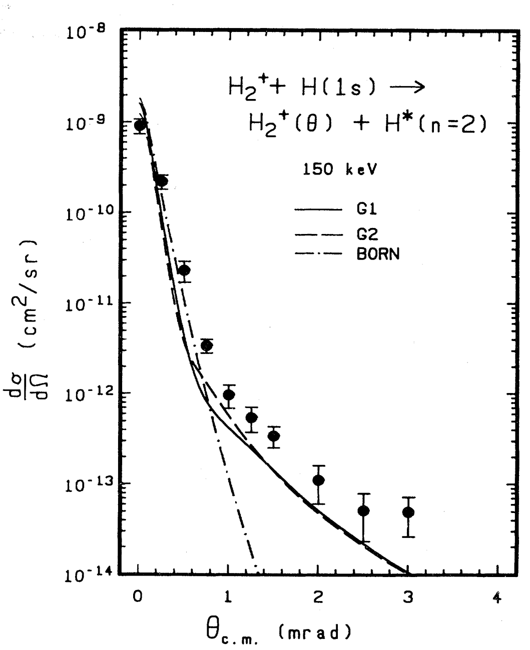

FIG. 2. Same as Fig. 1 except for 150-keV hydrogen-molecular-ion impact.

the larger scattering angles the Born results are well below either of the Glauber results or the experimental results.

It was found that the results for $d\sigma^v/d\Omega$ [Eq. (18)] were not very dependent upon the vibrational state $v$. For a fixed scattering angle $\theta$ or momentum transfer $q$ the various approximations for $\int d\Omega_R \mid G_{fi} \mid^2$ were slowly varying over the range of internuclear separation $R$ for which $\mid \chi_v(R) \mid^2$ is significant. To a fair approximation one could evaluate $\int d\Omega_R \mid G_{fi} \mid^2$ at the equilibrium internuclear separation for $H_2^+$. This would leave only the normalization integral for $\mid \chi_v(R) \mid^2$ which is, of course, equal to 1. Thus the results are not expected to change significantly even if a more sophisticated wave function than the harmonic-oscillator wave function were used for $\chi_v(R)$.

The experimental results for the excitation of atomic hydrogen to its $n=2$ level by an $H_2^+$ projectile are similar to the results for an $H^+$ projectile if the results are corrected for the change in reduced mass and compared at the same velocity. The experimental results for protons and deuterons exciting hydrogen to its $n=2$ level appear to be identical if the data is plotted in this manner.[21] The Glauber approximation agreed well with the experimental results.[21] In the context of the simpler Glauber approximation ($G1$) the differential cross section for the excitation of hydrogen to its $n=2$ level contains a factor, which depends on the internal structure of $H_2^+$, times the differential cross section that would be obtained if the projectile were a deuteron. This factor is basically the form factor for $H_2^+$, averaged over the nuclear wave function, and summed over final and averaged over initial vibrational and rotational states of the $H_2^+$. The factor, which is a function of the momentum transfer $q$, varies smoothly from 1.0 at $q=0$ to 2.0 for large $q$. It is essentially equal to 2.0 at $q=4.0$ a.u. Thus the differential cross section for the excitation of hydrogen to its $n=2$ level by $H_2^+$ is predicted to be the differential cross section for the excitation of hydrogen to its $n=2$ level by a deuteron projectile times a factor which is close to 1.0 at the very small scattering angles and becomes $\sim 2.0$ at the larger scattering angles. The fairly good agreement between the experimental results and the simpler Glauber results ($G1$) support this interpretation of the experimental results at these intermediate energies.

In Fig. 3 the total cross section for the excitation of atomic hydrogen to its $n=2$ level by singly charged hydrogen molecular ions is plotted versus the incident laboratory energy of the $H_2^+$ ion. The uncertainty in the total cross section obtained by integrating our experimentally determined differential cross sections include the errors inherent in the measurement of a differential cross section as well as any errors resulting from the numerical integration. As a result the uncertainty of the reported total cross section is larger than might be obtained from a less sophisticated experiment designed to measure only the total cross section. The Born and the two Glauber approximation results are also shown. The Born results obviously have the wrong curve shape and are significantly higher than the experimental results at the lower energies. The two Glauber results yield a better curve shape but they are both lower than the experimental results over the whole energy range. At the higher energies the Born results are closer in magnitude to the experimental results. This is due to the fact that most of the contribution to the total cross section at a given incident energy comes from the very small scattering angles. Thus even though the Born results for the differential excitation cross section are wrong for the larger scattering angles, they agree better with the experimental results at the very small scattering angles. It is for this same reason that the simpler Glauber results ($G1$) yield a higher total excitation cross section than the more complicated Glauber results ($G2$). On the semilog plots of the differential excitation cross sections the simpler Glauber results ($G1$) are only slightly higher than the more complicated Glauber results ($G2$). However, this difference yields a higher total excitation cross section for the simpler Glauber results ($G1$).

In conclusion it has been shown that a Glauber approximation ($G1$) that exhibits the same simple structure as the first Born approximation yields fairly good agreement with the experimental results for both differential and total excitation cross sections over the scattering-angular range and incident energy range considered.

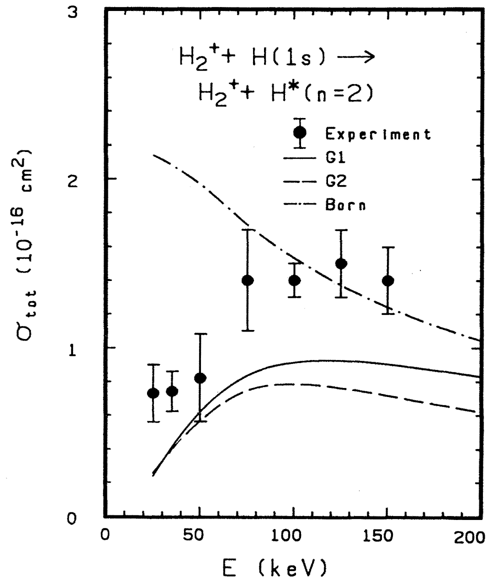

FIG. 3. Total cross section for excitation of atomic hydrogen to its $n=2$ level by hydrogen-molecular-ion impact. The solid circles with error bars are the results obtained by numerically integrating the experimentally determined differential cross sections. The mean value is obtained by averaging the total cross sections obtained from the individual experimental runs. The error bars represent one standard deviation from the mean and include only random statistical error. The theoretical results for the approximations described in the text are the following: ——, $G1$; — — —, $G2$; and —·—·—·, Born.

## ACKNOWLEDGMENTS

Two of us (J.L.P. and P.J.M.) would like to thank James M. Peek for helpful discussions. The authors would also like to thank E. Rille for reading the manuscript and useful suggestions. This work was supported in part by the National Science Foundation.

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