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DISSOCIATION AND IONIZATION OF H_2^+ BY ELECTRONS AND PROTONS

R. G. Alsmiller, Jr.

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ABSTRACT

The cross section for the dissociation and ionization of the H_2^+ molecule by electrons and protons is calculated using a method introduced by M. Gryzinski.[1]

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I. INTRODUCTION

In the evaluation of thermonuclear experiments such as DCX-1 and DCX-2, it is necessary to know the cross section for the dissociation of the H_2^+ molecule by electrons and protons.

These cross sections are known only in Born approximation[2,3] and are thus somewhat unreliable at low energies. Also the Born calculations are unsatisfactory in that they include only the contribution to the dissociation from the first excited state in the case of electrons and from the first and second excited states in the case of protons.

M. Gryzinski[1] has recently introduced a formalism for calculating the ionization and excitation of atomic systems by charged-particle impact. Since this theory appears to give reliable results in the low-energy region where the Born approximation is not accurate, it is used here to calculate the cross section for the dissociation and ionization of the H_2^+ molecule by both electrons and protons. The Gryzinski approximation is one in which the dissociation cross section includes the contribution from all excited states including the ionized state.

The results are compared with the Born approximation results. Appreciable differences are found between the present calculation and the Born approximation in the case of dissociation by electrons, but only minor differences are found in the case of dissociation by protons.

In an appendix the ionization of the H_2 molecule by protons is treated briefly and compared with experimental results.

II. METHOD OF CALCULATION

In doing the calculation we follow very closely the work of Gryzinski, hereinafter called I. All the formulas below are implicit in I, but they are reproduced here because in some cases they are not given explicitly in I and in some cases they differ from those given in I because of an algebraic error in the published text. The notation will be the same as that used in I.

We let $\sigma(\Delta E)$ be the cross section for a collision between an incident charged particle and a free electron such that the incident particle undergoes an energy loss ΔE. Then, using subscripts 1 and 2 to denote quantities associated with the target electron and the incident particle, respectively, we consider the two cases of an incident electron and an incident heavy particle.

Assuming that the free target electron has an isotropic velocity distribution, we have in the case of an incident electron, i.e., $m_1 = m_2$,

$$\sigma(\Delta E) = \frac{2\pi e^4}{m_1 v_2^2} \frac{1}{(\Delta E)^2} \left[\frac{v_2^2}{v_1^2 + v_2^2} \right]^{\frac{3}{2}} \tag{1}$$

$$\begin{cases} 1 - \dfrac{E_1}{E_2} + \dfrac{4}{3} \dfrac{E_1}{\Delta E} & \Delta E \leq E_2 - E_1 \\ \dfrac{1}{3}\left[1 + \dfrac{4}{3}\dfrac{E_1}{\Delta E} + \dfrac{2\Delta E}{E_2} - \dfrac{E_1}{E_2}\right] \left[\left(1 + \dfrac{\Delta E}{E_1}\right)\left(1 - \dfrac{\Delta E}{E_2}\right)\right]^{\frac{1}{2}} & \Delta E \geq E_2 - E_1 \end{cases}$$

while in the case of an incident heavy particle, i.e., $m_2 \gg m_1$ (the approximation involved here is that $E_2 \gg E_1$),

$$\sigma(\Delta E) \simeq \frac{2\pi z^2 e^4}{m_1 v_2^2} \frac{1}{(\Delta E)^2} \left[\frac{v_2^2}{v_2^2 + v_1^2} \right]^{\frac{3}{2}} \tag{2}$$

$$\begin{cases} 1 + \dfrac{4}{3} \dfrac{E_1}{\Delta E} & \Delta E \leq K_{12}E_2\left(1 - \dfrac{v_1}{v_2}\right) \\ \dfrac{1}{2}\left[\left(1 + \dfrac{\Delta E}{E_1}\right)\left(\dfrac{1}{3} + \dfrac{4}{3}\dfrac{E_1}{\Delta E}\right) + 1 + \dfrac{4}{3}\dfrac{E_1}{\Delta E} - \dfrac{1}{6}\dfrac{v_1}{v_2}\dfrac{(\Delta E)^2}{K_{12}E_1E_2}\right] & \Delta E \geq K_{12}E_2\left(1 - \dfrac{v_1}{v_2}\right) \end{cases}$$

where

z = charge of incident particle,

$$K_{12} = 4 \frac{m_1 m_2}{(m_1 + m_2)^2} \simeq 4 \frac{m_1}{m_2} .$$

The cross section for a collision with energy transfer greater than u, $Q(u, v_1, v_2)$, may be written

$$Q(u, v_1 v_2) = \int_u^{\Delta E_{max}} \sigma(\Delta E)\ d(\Delta E) \tag{3}$$

where

$$\Delta E_{max} = E_2 \qquad\qquad \text{if } m_1 = m_2$$

$$\simeq K_{12} E_2 \left(1 + \frac{v_1}{v_2}\right) \qquad\qquad \text{if } m_2 \gg m_1.$$

Carrying out the integration we have if $m_1 = m_2$

$$Q(u, v_1, v_2) = \frac{\sigma_0}{u^2}\, g\left[\frac{E_2}{u}, \frac{E_1}{u}\right] \tag{4}$$

$$g\left[\frac{E_2}{u}, \frac{E_1}{u}\right] = \left[\frac{v_2^2}{v_1^2 + v_2^2}\right]^{\frac{3}{4}}$$

$$\begin{cases} \frac{2}{3}\ \frac{E_1}{E_2} + \frac{u}{E_2}\left(1 - \frac{E_1}{E_2}\right) - \left(\frac{u}{E_2}\right)^2 & u + E_1 \leq E_2 \\ \frac{2}{3}\left[\frac{E_1}{E_2} + \frac{u}{E_2}\left(1 - \frac{E_1}{E_2}\right) - \left(\frac{u}{E_2}\right)^2\right]\left[\left(1 + \frac{u}{E_1}\right)\left(1 - \frac{u}{E_2}\right)\right]^{\frac{1}{2}} & u + E_1 \geq E_2 \end{cases}$$

and if $m_2 \gg m_1$

$$Q(u,v_1 v_2) = \sigma_0 z^2 \frac{1}{K_{12}E_2^2}\left[\frac{v_2^2}{v_1 + v_2^2}\right]^{\frac{3}{2}} \tag{5}$$

$$\begin{cases} \dfrac{K_{12}E_2}{u} + \dfrac{2}{3}\,\dfrac{E_1}{u}\,\dfrac{K_{12}E_2}{u} - 1 & u \leq K_{12}E_2\left(1 - \dfrac{v_1}{v_2}\right) \\ \left\{ -\dfrac{1}{3}\,\dfrac{E_1}{(\Delta E)^2}\left[1 + \left(1 + \dfrac{\Delta E}{E_1}\right)^{\frac{1}{2}}\right] - \dfrac{1}{2\Delta E}\left[1 + \dfrac{2}{3}\left(1 + \dfrac{\Delta E}{E_1}\right)^{\frac{1}{2}}\right] \right. & \\ \left. \qquad - \dfrac{1}{12}\,\dfrac{v_1}{v_2}\,\dfrac{\Delta E}{K_{12}E_1E_2} \right\}_{u}^{K_{12}E_2\left(1 + \frac{v_1}{v_2}\right)} & u \geq K_{12}E_2\left(1 - \dfrac{v_1}{v_2}\right) \end{cases}$$

where

$$\sigma_0 = \pi e^4 \frac{m_2}{m_1} .$$

For the purpose of numerical computation it is convenient to rewrite Eqs. 4 and 5 explicitly in terms of the velocities v_1 and v_2 and to use atomic units, i.e., units such that $m_1 = \hbar = e = 1$. In these units Eq. 4 becomes

$$Q(u,v_1,v_2) = \frac{1}{u^2}\left[\frac{1}{1 + \left(\frac{v_1}{v_2}\right)^2}\right]^{\frac{3}{2}} \tag{6}$$

$$\begin{cases} \dfrac{2}{3}\left(\dfrac{v_1}{v_2}\right)^2 + \dfrac{2u}{v_2^2}\left(1 - \dfrac{v_1^2}{v_2^2}\right) - \left(\dfrac{2u}{v_2^2}\right)^2 & 2u + v_1^2 \leq v_2^2 \\ \dfrac{2}{3}\left[\left(\dfrac{v_1}{v_2}\right)^2 + \dfrac{2u}{v_2^2}\left(1 - \dfrac{v_1^2}{v_2^2}\right) - \left(\dfrac{2u}{v_2^2}\right)^2\right]\left[\left(1 + \dfrac{2u}{v_1^2}\right)\left(1 - \dfrac{2u}{v_2^2}\right)\right]^{\frac{1}{2}} & 2u + v_1^2 \geq v_2^2 \end{cases}$$

and Eq. 5 becomes

$$Q(u, v_1 v_2) = \frac{z^2}{v_2^4}\left[\frac{1}{1+\left(\frac{v_1}{v_2}\right)^2}\right]^{\frac{3}{2}} \tag{7}$$

$$\begin{cases} \frac{2}{3}\left(\frac{v_1 v_2}{u}\right) + \frac{2v_2^2}{u} - 1 & u \leq 2v_2^2\left(1 - \frac{v_1}{v_2}\right) \\ \left\{ -\frac{1}{3}\left(\frac{v_1 v_2}{\Delta E}\right)^2 \left[1 + \left(1 + \frac{2\Delta E}{v_1^2}\right)^{\frac{1}{2}}\right] - \frac{v_2^2}{\Delta E}\left[1 + \frac{2}{3}\left(1 + \frac{2\Delta E}{v_1^2}\right)^{\frac{1}{2}}\right] \right. & \\ \left. \qquad - \frac{1}{6}\,\frac{\Delta E}{v_1 v_2} \right\}_{u}^{2v_2^2\left(1+\frac{v_1}{v_2}\right)} & u \geq 2v_2^2\left(1 - \frac{v_1}{v_2}\right) \end{cases}$$

Equations 6 and 7 were derived on the basis of two-body collisions between free particles. Following I we now assume that these equations may still be applied if the target electron is bound. The velocity v_1 is a particular velocity of the bound electron and the results are to be averaged over the quantum mechanical velocity distribution of the bound electron. We further assume that a particular quantum mechanical energy level of the bound electron cannot be excited unless the energy transfer is greater than the excitation energy of this level.

Using these assumptions we can now calculate the ionization and dissociation cross sections for the H_2^+ molecule. In the calculation the molecular protons are considered to be fixed force centers and a classical average over molecular orientation is performed. Since no spectra from the H_2^+ molecule are observed, all excited states of the electron must lead to dissociation. Thus the dissociation cross section may be identified with the total cross section for exciting all states of the molecule including the ionized states. This excitation cross section may be obtained directly from Eqs. 6 and 7 by setting u equal to the first excitation energy of the molecule and averaging over the velocity distribution of the bound electron.

Using the Q from Eq. 6 the cross section for dissociation by electrons is given by

$$\sigma_D(v_2) = 4\pi \int_0^\infty Q(u_1,v_1,v_2)\ f(v_1)\ v_1^2\ dv_1 \qquad E_2 > u_1 \tag{8}$$

$$= 0 \qquad \text{otherwise}$$

and using the Q from Eq. 7 the cross section for dissociation by protons is given by*

$$\sigma_D = 4\pi \int_L^\infty Q(u_1,v_1,v_2)\ f(v_1)\ v_1^2\ dv_1 \tag{9}$$

$$L = v_2 \left(\frac{u_1}{2v_2^2} - 1\right) \text{ or 0 whichever is larger}$$

where

u_1 = energy of the first excited state of the H_2^+ molecule,

$f(v_1)$ = velocity distribution of an electron in the ground state of the H_2^+ molecule.

The lower limit in Eq. 8 is zero because in the case of an incident electron the maximum energy transfer is independent of the velocity of the target electron. Thus an incident electron is capable of exciting all components of the velocity distribution or none of them. In the case of an incident proton the maximum energy transfer is

*Since $f(v_1)$ goes to zero very rapidly as v_1 gets large, the contribution to the integral from large v_1, where our Q is incorrect, is negligible.

$$2v_2^2\left(1 + \frac{v_1}{v_2}\right)$$

and since this increases with v_1 the incident particle may be capable of exciting some components of the distribution but not all of them. Thus in Eq. 9 one must include only those v_1 such that

$$2v_2^2\left(1 + \frac{v_1}{v_2}\right) \geq u_1$$

$$v_1 \geq v_2\left(\frac{u_1}{2v_2^2} - 1\right).$$

The ionization cross sections are given by the same expressions as the dissociation cross sections with u_1 replaced by the ionization energy. In defining the ionization of the H_2^+ molecule we use the vertical ionization energy 29.9 ev.

Note that Eq. 7 does not depend on the mass of the incident particle and varies as the charge of the incident particle squared so in these respects our cross sections agree with the Born approximation. On the other hand, in the high-energy limit Eqs. 6 and 7 give a cross section that goes as $1/v_2^2$ while the Born approximation cross section - which is known to be correct - goes as $1/v_2^2 \ln v_2^2$. Thus the present calculations cannot be trusted at very high energies.

III. VELOCITY DISTRIBUTION

The velocity distribution which occurs in Eqs. 8 and 9 is obtained by using the usual L.C.A.O wave function.[4] The wave function, ψ, may be written

$$\psi = N[u_a + u_b] \tag{10}$$

$$u_a = \sqrt{\frac{z^3}{\pi}}\; e^{-zr_a}$$

$$u_b = \sqrt{\frac{z^3}{\pi}}\; e^{-zr_b}$$

$$z = 1.228$$

r_a, r_b = coordinates of the electron with respect to the molecular protons

$$N^2 = \frac{1}{2(1 + S)}$$

$$S = (1 + zR + \frac{1}{3} z^2R^2)\; e^{-zR}$$

R = equilibrium separation distance between the molecular protons.

To find the velocity distribution we take the Fourier transform of ψ

$$\phi(\vec{v}_1) = \frac{1}{(2\pi)^{3/2}} \int e^{i\vec{v}_1\cdot\vec{r}}\; \psi\; d\vec{r}$$

$$= 2N \cos\left(\vec{v}_1 \cdot \frac{\vec{R}}{2}\right) \phi_N(v_1)$$

$$\phi_N(v_1) = \frac{1}{2\pi}\; \frac{2^{5/2}\; z^{5/2}}{(v_1^2 + z^2)^2}$$

and average $\phi^*(\vec{v}_1)\; \phi(\vec{v}_1)$ over molecular orientations; i.e., over all angles of $\vec{R}$, to obtain

$$f(v_1) = 2N^2 \phi_N^2(v_1) \left[1 + \frac{\sin v_1 R}{v_1 R} \right]$$

The quantity $\phi_N^2(v_1)$ is, of course, just the velocity distribution of an electron in the ground state of a hydrogen atom with nuclear charge z.

IV. RESULTS

The cross sections for dissociation and ionization by electrons are shown in Fig. 1. In Fig. 2 the dissociation cross section is compared to the Born approximation results of Ivash.[2] The two Born curves correspond to using no electron-electron exchange and to including the prior exchange terms. The use of the post exchange terms give a peak which is considerably larger than those shown in the figure.

The present calculation gives a somewhat smaller cross section than the Born approximation, particularly at the lower energies. In particular, if the present calculation is at all correct the large peaks due to exchange are completely fictitious. Of course, exchange effects are not included in the calculation done here, but Gryzinski[1] has calculated the ionization of the H_2 molecule by electrons using this theory and obtained very good agreement with the experimental results.

In Fig. 3 the cross sections for dissociation and ionization by protons are shown. Also shown is the dissociation cross section obtained by Born approximation.[3] The two cross sections are in reasonable agreement over the velocity range considered, but this does not necessarily mean that the cross sections can be trusted. One expects that the Born approximation is inaccurate at the lower velocities, and the agreement of the present calculation with the Born approximation may only mean that both are inaccurate.

It might also be mentioned that E. Gerjouy[5] has estimated the ionization cross section of H_2^+ by protons and obtained much larger values at the low velocities than those shown in Fig. 3.

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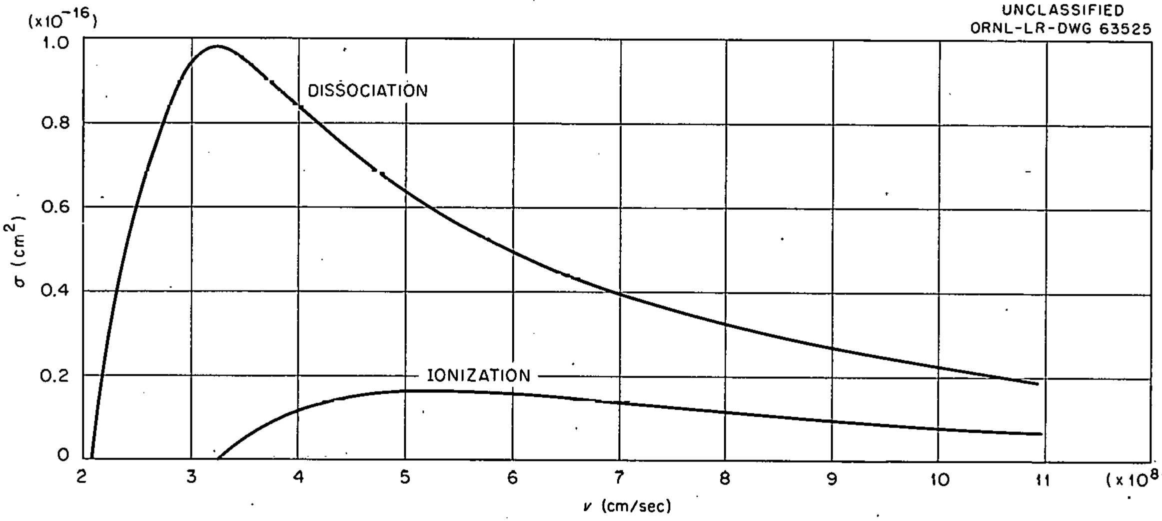

Fig.1. Dissociation and Ionization of H_2^+ by Electrons.

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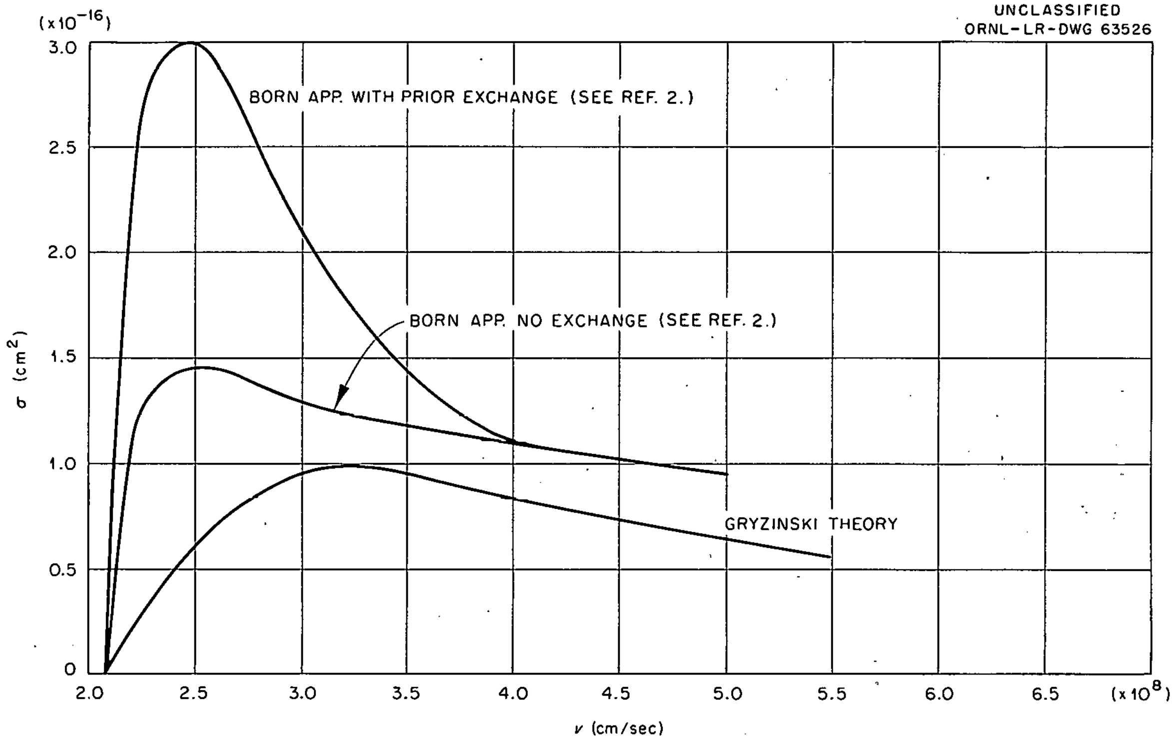

Fig. 2. Dissociation of H_2^+ by Electrons.

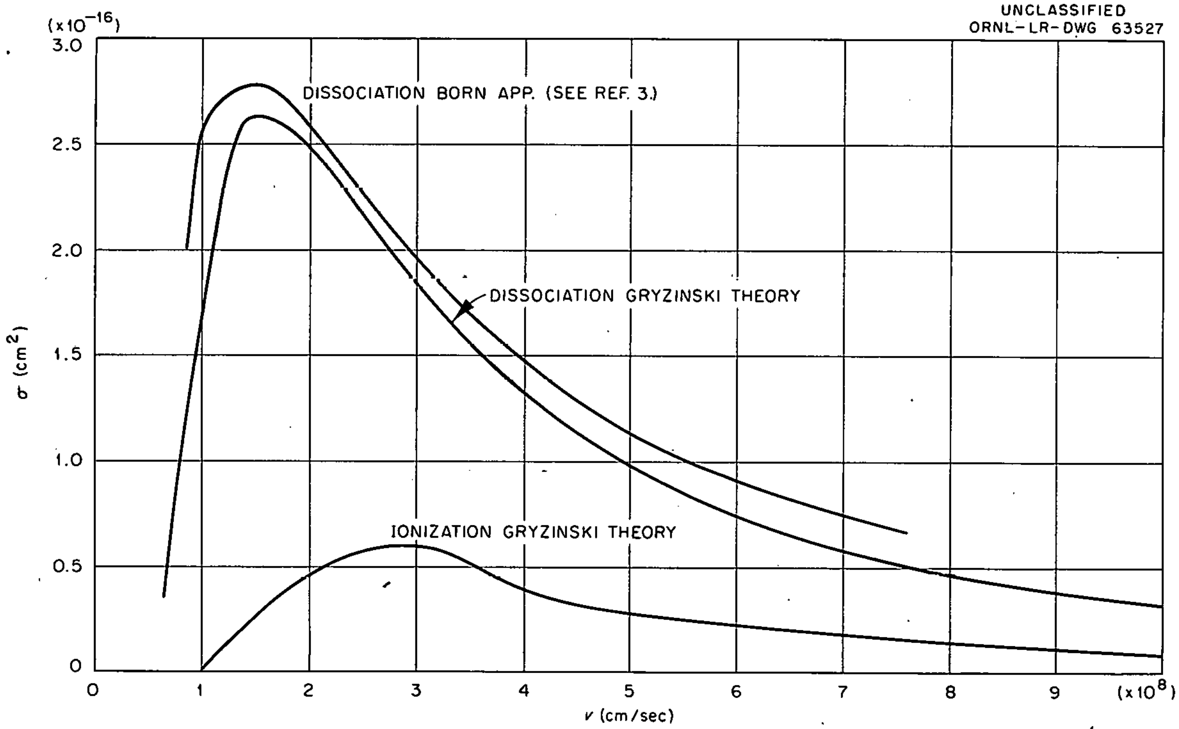

Fig. 3. Dissociation and Ionization of H_2^+ by Protons.

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Appendix 1

IONIZATION OF THE H_2 MOLECULE BY PROTONS

Because there is no data on the dissociation and ionization of H_2^+ by protons with which to compare our calculations, we calculate here the ionization of the H_2 molecule by protons and compare our results with the experimental data.

To carry out the calculation we need the distribution function of an electron in the H_2 molecule. Since Q, Eq. 7, is a slowly varying function of v_1 we can get a quick estimate of the cross section by using the simple distribution for

$$f(v_1) = 2 \frac{1}{4\pi v_1^2} \delta(v_1 - \bar{v}_1) \qquad (12)$$

where

$$\bar{v}_1 \simeq 1.07$$

for the H_2 molecule. This is the distribution function used in I - with good results - to calculate the ionization of the H_2 molecule by electrons.

The cross section obtained by using Eq. 12 in conjunction with Eqs. 6 and 9 is shown in Fig. 4. Also shown in the figure are some representative experimental points.[6,7] As can be seen, the calculated values are always too low.

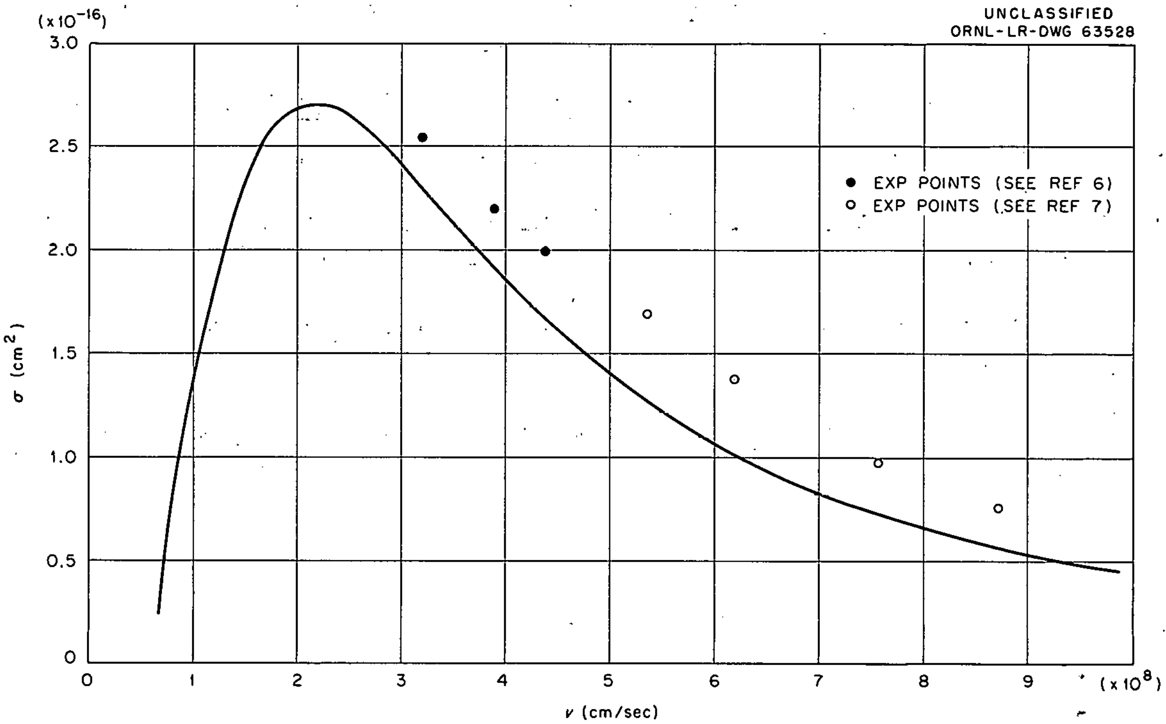

Fig. 4. Ionization of H_2 by Protons.

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