make it possible to observe the Ramsauer–Townsend minimum in the H-He system and to determine ϵ with considerable accuracy.

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Total Inelastic Cross Section for Collisions of H_2 with Fast Charged Particles*

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A sum rule due to Inokuti *et al.* for the Bethe inelastic cross section for fast-charged-particle collisions with atoms and molecules has been applied to H_2. Using an accurate two-center configuration-interaction wave function, the formula for nonrelativistic incident particles was found to be given as $\sigma_{tot}=4\pi a_0^2 z^2 (R/T)[1.5487 \ln(T/R)+2.2212]$ to within an error of 0.5% in σ_{tot} for incident-electron energies above 1 keV. Although the theoretical values are in good agreement with the summed experimental (i) total ionization (including dissociation ionization), (ii) total dissociative excitation, and (iii) most important discrete excitation cross sections, an apparent systematic trend suggests that one or more of the current experimental total cross sections for electron impact on H_2 may not be accurate and that omitted processes should be included for comparison in the incident energy range above 1 keV.

I. INTRODUCTION

A very accurate evaluation of the total inelastic cross section for high-incident-energy charged-particle collisions has been reported[1] for He, Li^+, and H^-. For the H_2 molecule, the theoretical evaluation of this inelastic cross section has not been reported because of the greater difficulties encountered in the evaluation of the optical quantity $L(-1)$, the oscillator-strength moment $S(-1)$, and the quantities I_1 and I_2 which were defined previously by Inokuti and Kim *et al.*[1] (see Sec. II). Recently the total inelastic differential cross sections[2] in the first Born approximation have been reported using five-term configuration interaction (CI)[3] and ten term CI[4] wave functions containing 95 and 97% of the binding energies, respectively. The quantity I_1 can be obtained from the calculated total inelastic differential cross sections. An estimate of the optical quantity $L(-1)$ has also recently been reported by Langhoff and Yates.[5] In addition, the quantity I_2 can be calculated by using the CI wave functions previously used for calculating I_1. Using these, a sum rule for the Bethe cross sections can be obtained with less than 1% uncertainty in the high-energy limit according to the method of Inokuti *et al.*[1] The experimental study of the impact phenomena of H_2 by fast charged

TABLE I. Comparison of values of M^2_{tot}.

	Fano (Ref. 15)	Platzman (Ref. 16)	Kamikawai *et al.* (Ref. 18)	Dalgarno and Williams (Ref. 17)	Victor and Dalgarno (Ref. 19)	Kolos and Wolniewicz (Refs. 20 and 21)	Present results 5 CI	10 CI
M^2_{tot}	1.65	1.65	1.58	1.576	1.757	1.5177 1.5487(vib)[a]	1.5515 1.5588(vib)[b]	1.4154

[a]The values of M^2_{tot} for the first four vibrational quantum states were obtained from Wolniewicz (Ref. 21) and the vibrational average of M^2_{tot} is $[M^2_{tot}]_{vib}=\langle M^2_{tot}\rangle_0$, where the contributions from the terms $\langle M^2_{tot}\rangle_\nu$ with ν greater than 0 are negligible at room temperature, where ν is the vibrational quantum number.

[b]The thermal vibrational average of M^2_{tot} can be expressed as $[M^2_{tot}]_{vib}=\langle M^2_{tot}\rangle_{R=1.4a_0}+\bar{x}(\partial/\partial R)\langle M^2_{tot}\rangle+\frac{1}{2}\bar{x}^2(\partial^2/\partial R)\langle M^2_{tot}\rangle+\cdots$. The values of M^2_{tot} are equal to 1.53, 1.55, and 1.57 for the internuclear distances $R=1.38$, 1.40, and 1.42 bohr, respectively, where the $\bar{x}$, $\bar{x}^2$ are the mean displacement and mean square displacement (Ref. 22) of H_2 at room temperature. The contribution of the third- or higher-order terms is negligible compared to the 2nd term.

particles is more complicated than in the case of He because of the additional dissociative processes that occur. The total ionization cross section,[6-8] the total dissociative excitation cross sections[9-12] and the summed discrete excitation cross section[14] have been separately reported and the sum of all these terms can be compared with the work reported here.

II. CALCULATIONS AND RESULTS

For a nonrelativistic incident charged particle, the total inelastic scattering cross section, using the notation of Inokuti *et al.*[1] can be written as

$$\sigma_{tot}=\frac{4\pi a_0^2 z^2}{T/R}\,M^2_{tot}\ln\left(\frac{4c_{tot}}{T/R}\right), \qquad (1)$$

TABLE II. The values of inelastic scattering factors for H_2 calculated by using the five-term CI wave functions.

K(Å^{-1})	S_{incl} (K)	$[S_{incl}$ (K)$]_{vib}$
0.0	0.0	0.0
1.00	0.3600	0.3676
1.25	0.5344	0.5444
1.50	0.7162	0.7283
1.75	0.8954	0.9091
2.00	1.0645	1.0792
2.25	1.2188	1.2338
2.50	1.3556	1.3706
2.75	1.4744	1.4888
3.00	1.5755	1.5907
3.50	1.7302	1.7416
4.00	1.8337	1.8426
4.50	1.9002	1.9068
5.00	1.9415	1.9462
5.50	1.9665	1.9698
6.00	1.9813	1.9835
6.50	1.9898	1.9912
7.00	1.9946	1.9956
7.50	1.9973	1.9979
8.00	1.9987	1.9991
8.50	1.9995	1.9996
9.00	1.9998	1.9999
9.50	2.0000	2.0000
10.00	2.0000	2.0000

and for a relativistic incident particle as

$$\sigma_{tot}=\frac{4\pi a_0^2 z^2}{T/R}\left\{M^2_{tot}\left[\ln\left(\frac{\beta^2}{1-\beta^2}\right)-\beta^2\right]+C_{tot}\right\}, \qquad (2)$$

where $T=\frac{1}{2}m_e v^2$, m_e is mass of electron, a_0 is the Bohr radius, z is the charge of the incident particle, R is the Rydberg energy, v is the velocity of the incident particle, c is the velocity of light, and $\beta=v/c$. Note also that $M^2_{tot}\ln c_{tot}=-2L(-1)+I_1-I_2$, where $L(-1)$, I_1, and I_2 are defined in the previous works of Inokuti, Kim, and Briggs,[1] and $C_{tot}=M^2_{tot}\times(\ln c_{tot}+11.2268)$. All parameters M^2_{tot}, $M^2_{tot}\times\ln c_{tot}$ are evaluated and reported below.

(a) $M^2_{tot}=(1/3a_0^2)\langle(\vec{r}_1+\vec{r}_2)^2\rangle$, where $\langle\ \rangle$ is the ground-state expectation value of the electronic wave function and $\vec{r}_1$ and $\vec{r}_2$ are the position vectors for electrons 1 and 2. All the previously reported M^2_{tot} and the present results are shown in Table I. The value of M^2_{tot} obtained from Kolos and Wolniewicz[20] appears to be the most accurate one. The vibrational correction to M^2_{tot} has been obtained by using three of the five CI wave functions at different internuclear distances according to a previous work[2(b)] (see footnote b in Table I for the brief description). The most accurate value of M^2_{tot} including the thermal vibrational average is taken from Wolniewicz[21] as 1.5487.

(b) The quantity $L(-1)$ can be obtained from the mean-excitation energy estimates for H_2 reported by Langhoff and Yates.[5] Note that $L(-1)$ was obtained from information other than the ground-state wave function according to the definition $\ln I(-1)=L(-1)/M^2_{tot}$. The vibrational average of $L(-1)$ is taken to be approximately equal to $(M^2_{tot})_{vib}\ln I(-1)$ [i.e., $=0.27797\pm0.01548$, where $\ln(I(-1)\,\text{eV})=2.79\pm0.01$].

(c) We have

$$I_1=\int_1^\infty \frac{S_{inel}(K)}{(Ka_0)^4}\,d(Ka_0)^2 .$$

The integral was evaluated numerically by using the previously calculated inelastic scattering fac-

TABLE III. Values of I_1, I_2, and $[-2L(-1)+I_1-I_2]$ obtained from the five- and ten-term CI wave functions.

Wave function	I_1	I_2	I_1-I_2	$-2L(-1)^a+I_1-I_2$
ten-term CI	1.4698	0.5981	0.8718 ± 0.0598	0.2670 ± 0.0862
five-term CI	1.4711	0.8331	0.6380 ± 0.0128	0.0932 ± 0.0392
	1.4758[b]	0.8568[b]	0.6190 ± 0.0124[b]	0.0742 ± 0.0434[b]

[a] $L(-1)=0.27239\pm0.01318$ and $[L(-1)]_{vib}=0.27797\pm0.01549$.

[b] The values with thermal vibrational average.

tors, $S_{inel}(K)$ for H_2. The values for $S_{inel}(K)$ are shown in Table II. The thermal vibrational average of $S_{inel}(K)$ has been reported and was used to calculate the term I_1. It is denoted by $(I_1)_{vib}$. All the results with and without the vibrational average are given in Table III.

(d) We have

$$I_2=\int_0^1 \frac{M_{tot}^2-S_{inel}(K)/(Ka_0)^2}{(Ka_0)^2}\,d(Ka_0)^2 .$$

For the region close to the lower limit, the integral must be evaluated analytically according to Inokuti's suggestion.[23] The remaining part of the integral can be evaluated numerically using the same method as the one used to evaluate I_1.

The integral I_2 can be rewritten as

$$I_2=I_2'+\int_h^1 \frac{M_{tot}^2-S_{inel}(K)/(Ka_0)^2}{(Ka_0)^2}\,d(Ka_0)^2 ,$$

where

$$I_2'=\int_0^h [a+b(a_0K)^2+c(a_0K)^4+\cdots]d(a_0K)^2$$
$$=[ah+\tfrac{1}{2}bh^2+c/3h^3] ,$$

where the higher-order terms $O(h)$ can be neglected when $h\ll 1$. For example, if $h=0.25$ the third term contributes only 1% to the total value. The constants, a, b, and c can be derived in a straightforward manner by expanding the integrand in a power series. For example,

$$\langle a\rangle_{R=1.4a_0}=\tfrac{1}{5}\left[-\tfrac{1}{6}\langle\vec{r}_1^{\,4}\rangle-\langle\vec{r}_1^{\,2}\rangle^2\right.$$
$$\left.-\tfrac{2}{3}\langle\vec{r}_1^{\,2}(\vec{r}_1\cdot\vec{r}_2)\rangle+\tfrac{1}{2}\langle\vec{r}_1^{\,2}\vec{r}_2^{\,2}\rangle\right] ,$$

where

$$\vec{r}_1^{\,2}=x_1^2+y_1^2+z_1^2 , \qquad \vec{r}_1\cdot\vec{r}_2=x_1x_2+y_1y_2+z_1z_2 .$$

All expectation values of $\langle x_1^m\rangle$, $\langle z_1^m\rangle$, $\langle x_1^m x_2^m\rangle$, $\langle x_1^m z_2^n\rangle$, and $\langle z_1^m z_2^n\rangle$, where m, n are integers, can be evaluated by the moment calculational method given by Kuppermann[24(a)] and Yoranos.[24(b)] The vibrational average values of a, b, c (i.e., denoting $[a]_{vib}$, $[b]_{vib}$, $[c]_{vib}$) were obtained by the same methods as used for $(M_{tot}^2)_{vib}$. The values obtained by combining these two integrals with or without the vibrational average are given in Table III.

It is interesting to note that the value of (I_1-I_2) for He is of about the same magnitude as that for H_2, but it is ten times smaller than that for H^-. The reason might be due to the fact that while both of the targets H_2 and He have the same type of charge distribution, the target H^- has a different charge distribution.

The slow convergence of the values of I_2 with increasing CI expansion length was noted as compared with the values of I_1. The slow convergence is due to the incoherent scattering function for small Ka_0 which depends chiefly on the wave function for larger r, where the wave function obtained by the variational method is worse as r gets larger. This effect appears to be more noticeable in the case of molecules. This behavior was also discussed by Inokuti *et al.*[1(b)] for the case of He. Table IV shows all the moments for H_2 as compared with the most accurate values reported by Kolos and Wolniewicz.[20]

The values of $S^{\perp}(-1)$, $S^{\parallel}(-1)$, and $S(-1)$ obtained from the five-term CI wave function are in better agreement with the values of Kolos and Wolniewicz[20] than the ten-term results. It is believed that the uncertainty of the quantity (I_1-I_2) calculated using the five-term CI wave function might be less than that for the ten-term CI wave function. The total uncertainty (±0.0310) of $2L(-1)$ and the uncertainty (±0.0124) of the quantity (I_1-I_2) which in turn was based on a 2% uncertainty in M_{tot}^2 for the five-term CI wave function. The resulting sum rules calculated by using the five-term CI wave function for the nonrelativistic and relativistic incident particle

$$\sigma_{tot}=\frac{4\pi a_0^2z^2}{T/R}\left[1.5487\ln\left(\frac{T}{R}\right)\right.$$

TABLE IV. Comparison of the moments and the values of $S^{\perp}(-1)$ and $S''(-1)$ for H_2. The values are given at $R=1.40$ bohr.

	$\langle z^2\rangle$	$\langle x^2\rangle$	$\langle z_1z_2\rangle$	$\langle x_1x_2\rangle$	$S^{\perp}(-1)$	$S''(-1)$
Kolos and Wolniewicz (Ref. 20)	1.023 15	0.761 66	−0.1596	−0.055 10	1.41	1.73
10 CI	0.772 2	0.743 0	−0.028 92	−0.053 15	1.38	1.49
5 CI	0.816 8	0.7883	0.038 24	−0.034 97	1.49	1.65

$$+ (2.2212 \pm 0.0434)\Big] \quad (3)$$

for a nonrelativistic incident particle, and

$$\sigma_{tot} = \frac{4\pi a_0^2 z^2}{T/R}\Big[1.5487 \ln\Big(\frac{\beta^2}{1-\beta^2}\Big) + (17.4615 \pm 0.0434)\Big] \quad (4)$$

for a relativistic incident particle. Because $L(-1)$ and $(I_1 - I_2)$ may have 6 and 2% uncertainties, respectively, predictions using the sum rule in Eq. (3) have an uncertainty of 0.5% at 1 keV and above. The σ_{tot} of Eq. (4) for the relativistic incident particle is in error by less than 0.3%.

III. COMPARISON WITH EXPERIMENT

The experimental total inelastic cross section obtained by charged-particle impact on H_2 has not been reported. Many processes[25] are possible as a result of charged-particle scattering from H_2. They can be classified into three categories: ionization, [6–8] dissociative excitation, [9–12] and discrete excitation. [14] A summary of these processes for electron impact follows below accompanied by a review of experimental studies.

A. Ionization

There are two reaction products of the negative- and positive-ion states.

1. Negative-Ion States

We have

$$H_2 + e \rightarrow H_2^-[X + {}^2\Sigma_u^+(1\sigma_g 1s)^2(1\sigma_u 1s)],$$

where X is ground-state of H_2. The cross sections for formation of negative-ion states by electron impact were measured by Golden and Bandel[6] and were found to be larger at incident energies near the resonance threshold and negligible for incident energies above threshold. Therefore the ionization processes involving the formation of negative ions can be neglected.

2. Positive-Ion State

We have

$$H_2 + e \rightarrow H_2^+(X\,{}^2\Sigma_g^+ 1s\,\sigma_g) + 2e\ ,$$

$$H_2 + e \rightarrow H_2^{++} + 3e\ .$$

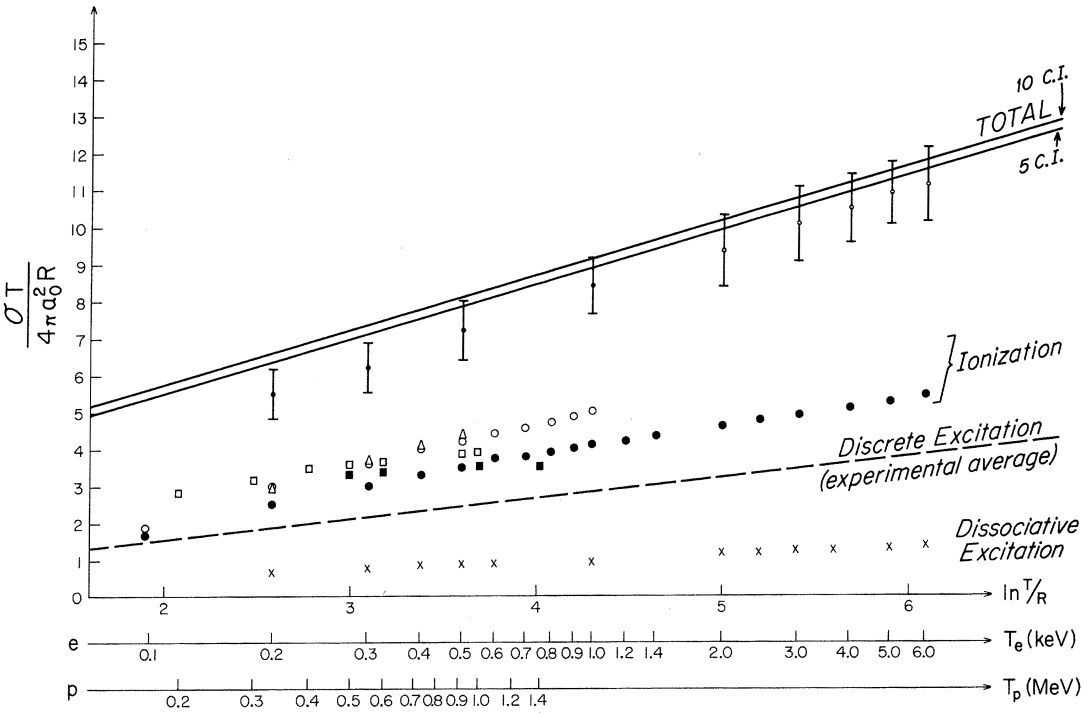


FIG. 1. Fano plot of the calculated total inelastic cross section for fast electron (—) impact on H_2 using Eq. (3) compared with that of experiment (Φ). Experimental total ionization cross sections alone are given by Rapp *et al.* (○), Brown (Δ), Schram *et al.* (●) for electron impact and by Hooper *et al.* (□) and Toburen and Wilson (■) for proton impact. The summed experimental discrete excitation cross sections obtained by Geiger for electron impact are shown by a dashed line (about 14% uncertainty). Experimental total dissociative cross-section data obtained by Vroom are shown by the curve (×××). Note that the uncertainty of $\sigma_i T/4\pi a_0^2 z^2 R$ was assumed to be ± 0.40 for all of the incident energies above 1 keV and that the dissociative ionization cross sections for the incident energies above 1 keV were obtained by extrapolation.

Three experimental total ionization cross sections ($\sigma_T = \sigma_{H_2^+} + 2\sigma_{H_2^{++}}$) have been reported by Brown,[7(a)] Rapp *et al.*,[7(b)] and Schram *et al.*[7(c)] In the case of proton impact these cross sections have been determined by Hooper *et al.*[8(a)] and by Toburen and Wilson.[8(b)] Fano[26] plots for these total ionization cross sections are shown in Fig. 1. The total ionization cross section with the experimental uncertainty can be expressed approximately as

$$\sigma_i = \frac{4\pi a_0^2 z^2 R}{T}\left[(0.71 \pm 0.02)\ln\left(\frac{T}{R}\right) + (1.30 \pm 0.40)\right] .$$

B. Discrete Excitation

For

$$H_2 + e \rightarrow H_2^*\,(\text{optically allowed transitions}) + e ,$$

the transition bands are $B(^1\Sigma_u^+ 2p\sigma)$, $B'(^1\Sigma_u^+ 3p\sigma)$ $B''(^1\Sigma_u^+ 4p\sigma)$, $C(^1\pi_u 2p\pi)$, $D(^1\pi_u 3p\pi)$, $D'(^1\pi_u 4p\pi)$, $D''(^2\pi_u 5p\pi)$, $V(^1\pi_u 4f\pi)$, etc. For

$$H_2 + e \rightarrow H_2^*\,(\text{optically forbidden transitions bands}) + e ,$$

the transition bands are E, $F(^1\Sigma_g^+ 2s\sigma + 2p\sigma^2)$, $H(^1\Sigma_g^+ 3s\sigma)$, $I(^1\pi_g 3d\pi)$, $G(^1\Sigma_g^+ 3d\sigma)$, $J(^1\Delta_g 3d\delta)$, etc. In general, $1s\sigma$ has been omitted from state designations in order to save space. The optically allowed transitions, the Lyman and Werner bands (B, B', C, D) have been experimentally studied by Geiger[14(a)] and by Geiger and Topschowsky[14(b)] using the electron-impact method with 25-keV incident electron energy. The discrete excitation cross sections were obtained from this experimental information by using the method of Miller and Platzman.[13]

The oscillator strength for the B and C bands is 0.57 ± 0.08, which is compatible with the theoretically calculated values of Mulliken and Rieke[27(a)] and Wolniewicz.[27(b)] The very accurate value of 0.67 reported by Wolniewicz suggests that cross-section values at the upper limit of the uncertainty are more reliable. This is also consistent with the fact that the calculated refractive index was in better agreement with that of experiment when one used the upper limit values of f_{B+C} for the polarizability calculations.[28] The experimental studies of optically forbidden transitions are too few to allow calculation of their cross section. However, these cross sections are, in general, small compared to the optically allowed ones. The Fano plot for the principle summed discrete excitation cross section is also shown in Fig. 1. It can be approximately expressed as

$$\sigma_{exc} = 4\pi a_0^2 z^2 \frac{R}{T}\left[(0.62 \pm 0.087)\ln\left(\frac{T}{R}\right) + (0.03 \pm 0.005)\right] .$$

C. Dissociative Excitation: Dissociative Ionization and Dissociative Discrete Excitation

1. Dissociative Ionization

It is well known that the electron-impact ionization of H_2 to form H_2^+ produces dissociative ionization to form H^+ and H from a repulsive state.[29] This is also true for all dissociative excitation processes. Negative-ion repulsive states are not appreciably excited at high incident energy.[9] The main contribution to dissociative ionization comes mainly from the repulsive state, $^2\Sigma_u^+$ rather than from the other repulsive states:

$$H_2 + e \rightarrow H_2^+(^2\Sigma_u^+) \rightarrow H^+ + H(1s) .$$

The dissociative ionization cross sections relative to the total ionization cross section were measured by Rapp *et al.*[9] and the ratio was found to be only 7% at 100 eV.

2. Dissociative Discrete Excitations

There are four processes:

(i) $H_2 + e \rightarrow H_2^*\,[b(^3\Sigma_u^+ 1s\sigma)] \rightarrow H(1s) + H(1s) + e$;

(ii) $H_2 + e \rightarrow H_2^*\,[a(^3\Sigma_g^+ 2s\sigma)] \rightarrow H(1s) + H(2s) + e$

(iii) $H_2 + e \rightarrow H_2^*\left(\begin{matrix} b(^3\Sigma_u 2p\sigma) \\ c(^3\pi_u 2p\pi) \end{matrix}\right) \rightarrow \begin{matrix} H(2p) + H(1s) + e \\ \qquad\qquad \rightarrow H(1s) + \text{Lyman } \alpha \end{matrix}$; $\rightarrow H(1s) + \text{Lyman } \alpha$;

(iv) $H_2 + e \rightarrow H_2^*\begin{bmatrix} b(^1\Sigma_g^+ 3s\sigma) \\ e(^3\Sigma_u^+ 3p\sigma) \\ d(^3\pi_u^+ 3p\sigma) \end{bmatrix} \rightarrow \begin{cases} H(3s) + H(1s) + e \rightarrow H(1s) + \text{Balmer } \beta \\ H(3p) + H(1s) + e \rightarrow H(1s) + \text{Balmer } \beta \\ H(ns \text{ or } np) + H(1s) + e \rightarrow \begin{matrix} H(1s) + \text{Balmer } \gamma, & n = 4 \\ H(1s) + \text{Balmer } \delta, & n = 5. \end{matrix} \end{cases}$

The cross sections for process (i) was determined by Corrigan,[10] who found that the cross section reaches a maximum at 40 eV and then decreased to a small value at high incident energies. Contributions from these states (i) were neglected in the high-incident-energy region. These observations might be true for all the high-energy equal dissociative excited atomic states, i.e.,

$$H_2 + e \rightarrow H(np) + H(ns) + e \ ,$$

where $n \geq 1$. The measurements of cross sections for (iii) has been performed by many investigators. For example, Fite and Brackman,[11(a)] Dunn *et al.*,[11(b)] Kauppila *et al.*,[11(c)] Mumma and Zipf,[11(d)] de Heer *et al.*,[11(e)] and Vroom and de Heer.[12] The cross sections for processes (ii)–(iv) were measured by Vroom and de Heer.[12] The dissociative exciton cross sections might contain significant errors. Mumma and Zifp found that their measurement of the emission cross section by observing Lyman-$\alpha(2p)$ lines contained a 20% cross-section contribution from emission of some higher molecular excited states. The experimental data by Vroom and de Heer[12] for all the processes from (ii) to (iv) were used here where the Lyman-$\alpha(2p)$ emission cross section has been reduced 20% before being added. The summed experimental disociative cross sections including dissociative ionization cross section are also shown in Fig. 1. These can be approximately expressed as

$$\sigma_d = \frac{4\pi a_0^2 z^2}{T} R\left[(0.18 \pm 0.02) \ln\left(\frac{T}{R}\right) + (0.25 \pm 0.06)\right] \ .$$

It is shown in Fig. 1 that impact ionization is the most favorable process, and that the dissociative excitations account for less than 10% of the electron-impact spectra. The total cross sections obtained by combining these three experimental cross sections with the uncertainty determined by their measurement are approximately expressed as

$$[\sigma_T]_{\text{expt}} = \frac{4\pi a_0^2 z^2 R}{T}\left[[M^2_{\text{tot}}]_{\text{expt}} \ln\left(\frac{T}{R}\right) + A\right] , \quad (5)$$

where $[M^2_{\text{tot}}]_{\text{expt}} = 1.51 \pm 0.13$ and $A = 1.58 \pm 0.46$.

Figure 1 shows the above total experimental cross section in comparison with the calculated total inelastic cross section of Eq. (3). It is apparent that the value of $[M^2_{\text{tot}}]_{\text{expt}}$ is too large if we believe the value of that f_{B+C} calculated by Wolniewicz[27(b)] to be accurate and use the upper limit value of the f_{B+C} reported by Geiger, and assume that the values of M^2_{exc} for all the optically forbidden transitions are negligibly small (see the case of He in Ref. 1). Therefore the sum of M^2_{ion} and M^2_{dis} is too large as reported. The value of A is too small compared to the value reported by Eq. (3). However, the values of A will increase when the sum of M^2_{ion} and M^2_{dis} decreases according to the above discussion. Moreover the small value of A might be due to the omission of the optically forbidden transitions because their contribution to the value of A might be in excess of 0.2, although the value of M^2_{exc} for those transitions is almost zero. For example, consider the E band[25] where $M^2_E \approx 0$ and $A_E = 0.15$. Although theory and experiment agree with respect to the values of the total inelastic cross section there is nevertheless a strong need for further and more accurate experiments, and for further experimental study of the contributions of optically forbidden transition to the total inelastic cross sections.

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Electron Loss by Helium Atoms Passing through Inert Gases and Molecular Hydrogen, Nitrogen, and Oxygen

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The Born approximation and free-scattering model have been used to calculate the electron-loss cross section from atomic helium incident on He, Ne, Ar, and Kr atoms and on H_2, N_2, and O_2 molecules. For the molecules the phase difference between the scattered wave emanating from the two atoms has been considered in the separated-atom approximation. The vibrational damping of the molecule is also taken into account. It is shown that the effect of phase is very small.

I. INTRODUCTION

Inelastic atom-atom and atom-molecule collisions have been topics of great interest in the study of the upper atmosphere and many physical problems in astrophysics. A projectile system A may suffer "electron loss" in an encounter with a target system B,

$$A+B\rightarrow A^*+e+B\,(\Sigma),$$