Cross Sections for Electron Collisions with Hydrogen Molecules

Jung-Sik Yoon,^{a)} Mi-Young Song, Jeong-Min Han, Sung Ha Hwang, Won-Seok Chang, and BongJu Lee

Data Center for Plasma Properties, National Fusion R&D Center, 52 Yeoeun-Dong, Yusung-Ku, 305-806 Daejeon,

Republic of Korea

Yukikazu Itikawab)

Institute of Space and Astronautical Science, Sagamihara 229-8510, Japan

(Received 4 June 2007; revised manuscript received 21 December 2007; accepted 3 January 2008; published online 31 March 2008)

Cross section data have been compiled for electron collisions with hydrogen molecules based on 71 references. Cross sections are collected and reviewed for total scattering, elastic scattering, momentum transfer, excitations of rotational, vibrational, and electronic states, dissociation, ionization, emission of radiation, and dissociative attachment. For each process, the recommended values of the cross section are presented for use. The literature has been surveyed through the end of 2006. © 2008 American Institute of Physics. [DOI: 10.1063/1.2838023]

Key words: cross section; dissociation; elastic scattering; electron collision; emission; excitation; H₂; hydrogen; ionization; momentum transfer; recommended data; total scattering.

COI	NTENTS			section	916
			2.	Recommended values of elastic scattering	
1.	Introduction	914		cross section	917
2.	Total Scattering Cross Section.	915	3.	Recommended values of momentum transfer	
3.	Elastic Scattering and Momentum Transfer	713		cross section	918
٥.	Cross Sections	915	4.	Recommended values of the rotational cross	
4.	Rotational Excitation.	918		section for $J=0 \rightarrow 2 \dots$	920
٠. 5.	Vibrational Excitation	919	5.	Recommended values of the vibrational cross	
5. 6.	Excitation of Electronic States	920		section for $v=0 \rightarrow 1$	921
0.			6.	Vertical excitation energy for the electronic	
	6.1. $b^{3}\Sigma_{u}^{+}$	921 922		state of H ₂ , considered in the present paper	921
			7.	Recommended values of the excitation cross	
	6.3. $c^3\Pi_{\rm u}$	922		section for the $b^{3}\Sigma_{u}^{+}$ state	921
	6.4. $B^{1}\Sigma_{\mathbf{u}}^{+}$ and $C^{1}\Pi_{\mathbf{u}}$	922	8.	Recommended values of the excitation cross	
	6.5. $E, F^{1}\Sigma_{g}^{+}$	922		section for the $B^{1}\Sigma_{u}^{+}$ and $C^{1}\Pi_{u}$ states	923
_	6.6. $e^{3}\Sigma_{\mathrm{u}}^{+}$.	923	9.	Recommended values of the excitation cross	
7.	Emission Cross Section	923		sections for the $E, F^{1}\Sigma_{g}^{+}$ state	924
8.	Dissociation	924	10.	Cross sections for the excitation of the $a^{3}\Sigma_{g}^{+}$,	
9.	Ionization	925		$c^{3}\Pi_{u}$, and $e^{3}\Sigma_{u}^{+}$ electronic states of H ₂ ,	
10.	Dissociative Attachment	926		measured by Wrkich et al. 40	924
11.	Summary and Future Problems	927	11.	Recommended values of the dissociation cross	
12.	Appendix: Electron Collisions with Hydrogen			section for the neutral products	925
	Molecules in Excited States	929	12.	Recommended values of total ionization cross	
	12.1. Collisions with vibrationally excited H ₂			sections	926
	(in its ground electronic state)	929	13.	Recommended values of partial ionization	
	12.2. Collisions with electronically excited H_2	930		cross section	927
13.	References	930	14.	Recommended values of dissociative	
				attachment cross section	928
	List of Tables				
				List of Figures	
1.	Recommended values of total scattering cross		1.	Potential energy diagrams for the singlet	
			1.	system of molecular hydrogen	915
"Elec	tronic mail: jsyoon@nfrc.re.kr		2.	Potential energy diagrams for the triplet	713
	tent address: 3-16-3 Miwamidoriyama, Machida 195-0055, Japa 08 American Institute of Physics.	n.	4.	system of molecular hydrogen	915
- 40	oo American hismuic of Fhysics.			system of molecular hydrogen	713

3.	Total scattering cross section for molecular	
	hydrogen	910
4.	Elastic scattering cross section for molecular	
	hydrogen	91′
5.	Momentum transfer cross section for	
	molecular hydrogen	91
6.	Rotational cross sections for the transition J	
	$=0 \rightarrow 2$	919
7.	Recommended values of the rotational cross	
	section Q_{rot} for $J=0 \rightarrow 2$	919
8.	Vibrational cross sections for the transition v	
	=0 → 1	920
9.	Cross sections for the excitation of the $b^{3}\Sigma_{u}^{+}$	
	electronic state of H ₂	92
10.	electronic state of H_2	
	electronic state of H ₂	92
11.	Cross sections for the excitation of the $B^{1}\Sigma_{u}^{+}$	
	electronic state of H ₂	92
12.	Cross sections for the excitation of the $C^{-1}\Pi_{n}$	
	electronic state of H ₂	92:
13.	Cross sections for the excitation of the	
	$E, F^{1}\Sigma_{g}^{+}$ electronic state of H_{2}	923
14.	Cross sections for the excitation of the $a^{3}\Sigma_{g}^{+}$,	
	$c^{3}\Pi_{u}$, and $e^{3}\Sigma_{u}^{+}$ electronic states of H_{2}	92
15.	Cross section for the emission of Paschen- α	
	line of H upon electron collision with H_2	92:
16.	Dissociation cross section and related	
	quantities	92:
17.	Recommended values (the present evaluation)	
	of ionization cross sections: total and the cross	
	sections for the production of H_2^+ and H^+	92
18.	Recommended values of dissociative	
	attachment cross section	92
19.	Dependence of the dissociative attachment	
	cross section on the vibrational state of the	
	hydrogen molecule	92
20.	Summary of the cross sections for electron	
	collisions with H ₂	929

1. Introduction

The hydrogen molecule (H₂) is the simplest molecule in nature. It is the most abundant molecule in universe, particularly in interstellar space. It is also the main constituent in the atmospheres of the outer planets. Plasmas containing H₂ are widely used in plasma technology for applications such as thin film deposition and material treatment. The H₂ plasma is a source of positive (H⁺) and negative (H⁻) ion beams. H₂ is known to be abundant in the edge region of fusion devices. The behavior of H₂ in the edge plasma is crucial in the understanding of the boundary condition, and hence the plasma-wall interaction, in the fusion plasma.

In many of the examples listed above, electron collisions with hydrogen molecules play an important role. In 1990, recognizing the importance, Tawara *et al.* published a comprehensive compilation of cross section data on the electron collision with H₂. (We refer to the paper as JPCRD90 here-

after.) Since then, a number of new theoretical and experimental results have been reported on the process. The present paper is the complete update of the previous data compilation 1 on the $e+H_2$ collision.

After the publication of JPCRD90, a review of the cross sections for the $e+\mathrm{H}_2$ collisions has been attempted several times. Zecca et al. ² and Brunger and Buckman ³ published a data compilation for electron collisions with various molecules, including H_2 . The latter authors, however, concentrated their compilation on the processes of elastic scattering and excitations of discrete states (i.e., nothing being included on ionization and dissociation). More recently an extensive data compilation has been reported on electron collisions with a large number of molecules. ⁴ The work included cross section data on total scattering, elastic scattering, momentum transfer, ionization, electron attachment, and excitation of rotational, vibrational, and electronic states. The present paper is partly based on this data compilation, ⁴ particularly for the processes for which no data are reported after its publication.

After reviewing available cross section data, we have determined a set of recommended values of cross section, as far as possible. The general criteria for the selection of preferred data are as follows:

- (i) In principle, experimental data are preferred to theoretical ones.
- (ii) The reliability of the experimental methods employed is critically assessed. Agreement between independent measurements of the same cross section is generally taken as an endorsement of the accuracy of the measured data. A strong emphasis is placed on the consistency of the results determined by different techniques.
- (iii) In cases where only a single set of data is available for a given cross section, those data are simply shown here (i.e., not designated as recommended), unless there is a strong reason to reject them. Even when multiple sets of data are available, no recommendation is made if there is a significant disagreement among them or they are fragmentary (i.e., only a few data points being reported).

In this way, the present paper aims to provide a more complete data set for electron collisions with H_2 than those published before. A survey of literature has been made mainly for those published after the publication of JPCRD90. The survey has been conducted through the end of 2006.

All the experimental data considered in the present paper are those obtained for the hydrogen molecule in its (vibrationally and electronically) ground state. In a H₂ plasma of practical use, many molecules are in their (vibrationally and, in some cases, electronically) excited states. Cross section data for the electron collisions with those excited molecules are often necessary to understand the behavior of such a plasma. At least at present, however, no experimental data are available on those cross sections. Instead many theoreti-

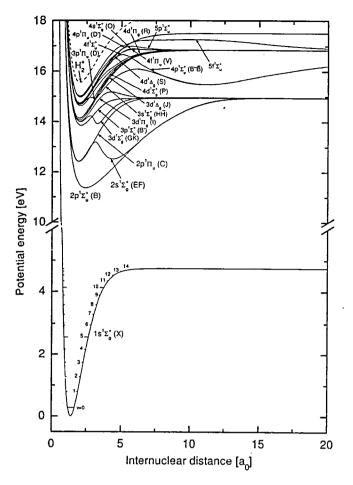


Fig. 1. Potential energy diagrams for the singlet system of molecular hydrogen. Adapted from Janev.⁵

cal works have been reported on this subject. For the readers' convenience, those theoretical studies are listed in the Appendix.

We show in Figs. 1 and 2 the potential energy diagrams of H_2 .⁵

2. Total Scattering Cross Section

Recently Karwasz et al. have made a survey of experimental data on the total scattering cross section (Q_T) for electron-molecule collisions. They have determined the recommended values of Q_T for various molecules. Their recommended cross section for H_2 is based on the results of several beam attenuation measurements. They also took into account one unpublished result of the experiment of Karwasz et al. Another recent data, but not considered by Karwasz et al., are those of Zhou et al. Although the aim of the experiment was a comparison of positron and electron collisions, they reported Q_T for electron- H_2 collisions at 1-300 eV. In Fig. 3, the Q_T of Zhou et al. are compared with the recommended values of Karwasz et al. The agreement is very good. Here we take the cross section of Karwasz et al. also as our recommended value. They are tabulated in Table 1.

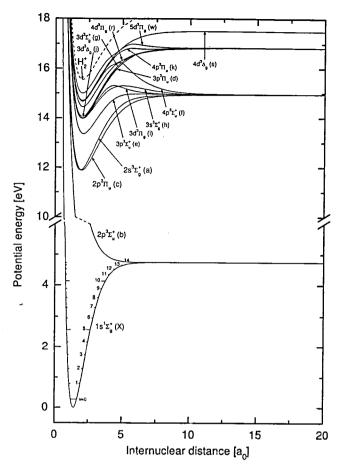


Fig. 2. Potential energy diagrams for the triplet system of molecular hydrogen. Adapted from Janey.⁵

By using a photoionization of Ar, Randell et al. ¹⁶ produced an electron beam of very low energy. With this electron beam, they obtained a backward scattering (i.e., the scattering at angles larger than 90°) cross section. From this cross section and the momentum transfer cross section $(Q_{\rm M})$ available at that time, they approximately derived the phase shifts of the first two partial waves. Using those phase shifts, they calculated $Q_{\rm T}$ for H_2 at 0.01-0.18 eV. The result was consistent with the beam attenuation measurement of Ferch et al., ⁸ but had a larger uncertainty than the latter.

JPCRD90 reports the total scattering cross section based on Hayashi's review published in 1981.¹⁷

3. Elastic Scattering and Momentum Transfer Cross Sections

Due to an insufficient energy resolution of electron beams, experimental results of elastic cross section ($Q_{\rm elas}$) normally include the effect of rotational transitions of the molecule. Hence the present section deals with the so-called vibrationally elastic cross section.

Buckman et al. 18 have determined the recommended value of $Q_{\rm elas}$ for H_2 at 0.02-100 eV after a critical survey of the available experimental data. Their recommendation was mainly based on the beam measurements of Refs. 20-24.

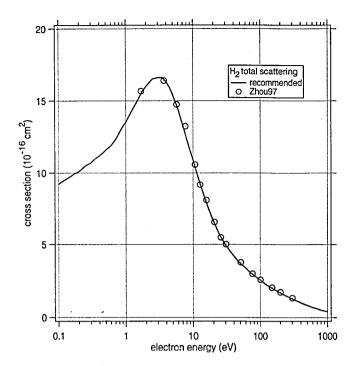


Fig. 3. Total scattering cross section for molecular hydrogen. The recommended values of Karwasz *et al.*⁶ are compared with the cross sections measured by Zhou *et al.*¹⁵

Below 0.05 eV, they took into account the total scattering cross section obtained by Ferch $et\ al.^8$ In this energy region, Q_T can be assumed to be equal to $Q_{\rm elas}$. Since no other experimental data are reported after the publication of Ref. 18, we take their values as the recommended data here. They are shown in Fig. 4 and Table 2. Buckman $et\ al.$ claimed that the cross section should be correct within $\pm 20\%$.

Buckman et al. gave no cross sections at the energies above 100 eV. The only comprehensive cross section data in the energy region were those reported by van Wingerden et al.24 They measured the elastic cross sections at 100-2000 eV. To see a general trend of $Q_{\rm elas}$, their values are also shown in Fig. 4. Their energy dependence is consistent with our recommended data in the lower energy region, but the absolute magnitude at 100 eV is by about 20% larger than the recommended value, van Wingerden et al. measured the elastic differential cross section (DCS) at the scattering angles between 5° and 50°. In order to obtain integral cross sections, they extrapolated the DCS to the forward and backward directions. They made the extrapolation with the help of other (fragmentary) experimental data and some simple analytic functions assumed for the energy dependence. They claimed 10% accuracy for their integral cross section, but it should be tested with more modern experiments.

JPCRD90 shows $Q_{\rm elas}$ derived from data given in Refs. 19, 20, 22, and 23. As a result, $Q_{\rm elas}$ in JPCRD90 are not much different from the present recommended values.

JPCRD90 reports no information about momentum transfer cross section ($Q_{\rm m}$). The momentum transfer cross section, however, is a basic physical quantity in the study of electron transport in a molecular gas. Elford *et al.* ²⁵ determined the

TABLE 1. Recommended values of total scattering cross section

	E 1. Recommended values of total scattering cross section	
Energy (eV)	Cross section (10 ⁻¹⁶ cm ²)	
0.1	9.23	
0.12	9.47	
0.15	9.76	
0.17	9.93	
0.2	10.1	
0.25	10.5	
0.3	10.7	
0.35	11	
0.4	11.2	
0.45	11.4	
0.5	11.6	
0.6	11.9	
0.7	12.3	
0.8	12.8	
0.9	13.2	
1	13.5	
1.2	14.2	
1.5	15 15.5	
1.7 2	16	
2.5	16.5	
3	16.6	
3.5	16.6	
4	16.3	
4.5	15.9	
5	15.4	
6	14.4	
7	13.3	
8	12.4	
9	11.6	
10	10.9	
12	9.61	
15	8.19	
17	7.46	
20	6.6	
25	. 5.61	
30	4.97	
35	4.54	
40	4.19	
45	3.91	
50	3.68	
60	3.36	
70	3.06	
80	2.86	
90	2.68	
100	2.54	
120	2.25	
150	1.98	
170	1.84	
200	1.66	
250	1.43	
300	1.24	
350	1.11	
400	1	
450	0.914	
500	0.841	
600	0.7	

TABLE 1. Recommended values of total scattering cross section—Continued

Energy (eV)	Cross section (10 ⁻¹⁶ cm ²)
700	0.614
800	0.516
900	0.464
1000	0.422

recommended value of $Q_{\rm m}$ for H₂. Their cross sections at the energies less than 2 eV were based on the swarm experiment of Schmidt *et al.*²⁶ Above 2 eV, Elford *et al.* considered the beam-type measurements of elastic scattering selected for the recommended values of $Q_{\rm elas}$ by the same group of authors.¹⁸ Those measurements also provided $Q_{\rm m}$.

In 1991, Ramanan and Freeman²⁷ determined $Q_{\rm m}$ from the measurement of electron mobilities in a hydrogen gas. First they measured the electron mobility over a wide range of electric field and gas temperature. From the measurement, they determined the mobility in the limit of zero field. Then they derived $Q_{\rm m}$ from a relationship between the zero-field mobility and $Q_{\rm m}$. It should be noted that the relationship is based on the thermal equilibrium between the electrons and the molecular gas. The measurement of mobility was done at the gas temperature of as low as 16 K. In this way, Ramanan and Freeman obtained the cross section at the electron energies down to 1 meV. Their result is compared in Fig. 5 with the recommended cross sections of Elford *et al.* The cross section of Ramanan and Freeman is consistent with the value of Elford *et al.*, but the agreement is not complete. The un-

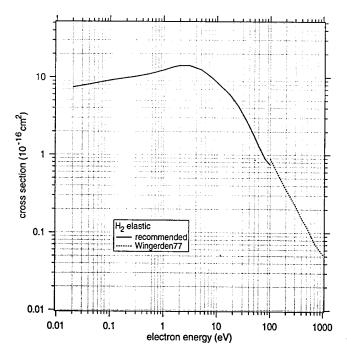


Fig. 4. Elastic scattering cross section for molecular hydrogen. The recommended values by Buckman *et al.*¹⁸ are shown at 0.02–100 eV. Above 100 eV, the cross section measured by van Wingerden *et al.*²⁴ is shown for a comparison.

TABLE 2. Recommended values of elastic scattering cross section

Energy (eV)	Cross section (10 ⁻¹⁶ cm ²)
0.02	7.41
0.03	7.71
0.04	8.08
0.05	8.32
0.06	8.51
0.07	8.69
0.08	8.84
0.09	8.99
0.1	9.13
0.12	9.33
0.15	9.55
0.2	9.83
0.25	10.04
0.3	10.24
0.4	10.61
0.5	10.95
0.6	11.28
0.7	11.59
0.8	11.88
0.9	12.16
1	12.36
1.25	13
1.5	13.55
2	14.11
3 4	14.12
5	13.2
6	12.51
8	11.45
10	9.85 8.58
12	7.61
14	6.92
16	6.32
18	5.78
20	5.26
25	4.23
30	3.4
35	2.81
40	2.36
50	1.73
60	1.31
70	1.06
80	0.89
90	0.81
100	0.74

certainty of the former cross section is not known. The measurement of mobility was accurately done. The procedure of extrapolation of the result to zero field and the deconvolution of the mobility formula to derive $Q_{\rm m}$ have some ambiguity. It is difficult, therefore, to evaluate the accuracy of the $Q_{\rm m}$ derived by Ramanan and Freeman. In conclusion, the recommended data of Elford *et al.*²⁵ are adopted here. They are tabulated in Table 3. According to Elford *et al.*, their uncertainties are estimated to be $<\pm5\%$ for 0.001-4 eVand $<\pm15\%$ for 4-100 eV.

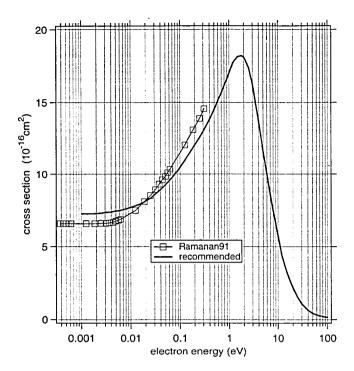


Fig. 5. Momentum transfer cross section for molecular hydrogen. The values derived from mobility measurement by Ramanan and Freeman²⁷ are compared with the recommended data from Elford *et al.*²⁵

4. Rotational Excitation

The present section is mainly concerned with the lowest transition of the rotational states in H_2 , $J=0 \rightarrow 2$ (J being the rotational quantum number of the molecule). Its transition energy is 44.1 meV. Other transitions are briefly mentioned at the end of this section.

England et al.²⁸ derived rotational cross sections from a swarm experiment. Their aim was to determine vibrational cross sections, but to be consistent with the newly determined vibrational cross sections, rotational cross sections were also determined. England et al. made a swarm experiment with parahydrogen at 77 K. Because of especially large separations of rotational levels of H2, almost all of the hydrogen molecules at the temperature are in the rotationally ground state. From the swarm experiment, the rotational cross section for $J=0 \rightarrow 2$ was accurately (within the error of ±5%) determined, as far as the electron energy was below the vibrational threshold (0.5 eV). They found that their rotational cross sections are in good agreement with the values obtained by a very elaborate calculation of Morrison et al. 29 England et al. then produced their recommended data by merging smoothly their swarm result for E<0.5 eV to the theoretical cross section of Morrison et al. for E>1 eV (see Fig. 6).

In 1994, Schmidt *et al.*²⁶ applied their new swarm techniques to the electron collision with hydrogen molecules. They developed two new techniques: swarm experiment with a long-length drift tube and that with crossed electric and magnetic fields. They reported their rotational cross section up to 0.7 eV. In this energy range, the recommended data of

TABLE 3. Recommended values of momentum transfer cross section

Energy (eV)	Cross section (10 ⁻¹⁶ cm ²)
0.001	7.25
0.0012	7.26
0.0015	7.26
0.0018	7.27
0.002	7.28
0.0025	7.3
0.003	7.35 7.38
0.004	7.38 7.45
0.005 0.006	7.43
0.007	7.54
0.007	7.59
0.009	7.64
0.01	7.7
0.012	7.78
0.015	7.9
0.018	8.04
0.02	8.14
0.025	8.33
0.03	8.56
0.04	8.93
0.05	9.27
0.06	9.54
0.07	9.79
0.08	10.04
0.09	10.25
0.1	10.47
0.12	10.86
0.15	11.35
0.18 0.2	11.78 12.02
0.25	12.02
0.23	13
0.4	13.81
0.5	14.52
0.6	. 15.16
0.7	15.66
0.8	16.17
0.9	16.58
1	17.01
1.2	17.7
1.5	18.15
1.8	18.22
2	18.11
2.5	17.4
3	16.28
4	13.7
5	11.59
6 7	10 8.59
8	7.48
9	6.58
10	5.78
12	4.396
15	3.275
18	2.529
20	2.154

TABLE 3. Recommended values of momentum transfer cross section—Continued

Energy (eV)	Cross section (10 ⁻¹⁶ cm ²)
25	1.476
30	1.077
40	0.636
50	0.417
60	0.311
70	0.243
80	0.2
90	0.169
100	0.149

England et al. 28 are consistent with the new measurement of Schmidt et al. Above 0.7 eV, we have no experimental data comparable to the values of England et al. From the theoretical points of view (see the review paper by Itikawa and Mason³⁰), the calculation of Morrison et al. 29 must be very accurate. In conclusion, we select the cross section of England et al. to be recommended for the rotational transition $J=0 \rightarrow 2$ in hydrogen molecules. Those recommended values are presented in Fig. 7 and Table 4.

JPCRD90 presents rotational cross sections based on an old swarm measurement. (Although published in 1990. JPCRD90 did not include the 1988 work of England *et al.*²⁸) Further, the cross section is shown only up to about 6 eV. It turns out, however, that the values in JPCRD90 are not much different from the cross sections recommended here.

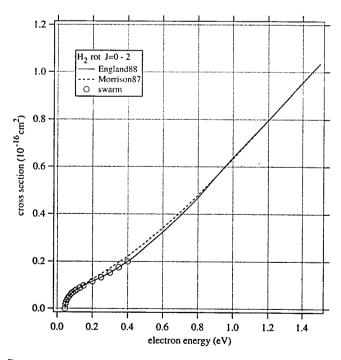


Fig. 6. Rotational cross sections for the transition $J=0\rightarrow 2$. The swarm cross sections (circles, Ref. 28) are compared with the theoretical values of Morrison *et al.* (dashed line, Ref. 29). The solid line is the cross section recommended by England *et al.*²⁸

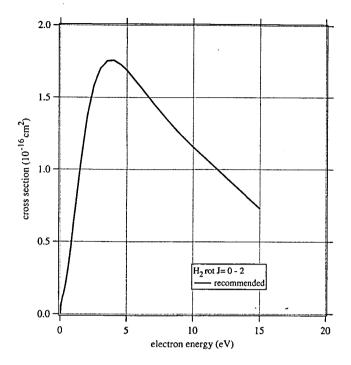


Fig. 7. Recommended values of the rotational cross section $Q_{\rm rot}$ for J=0 \rightarrow 2. Taken from England *et al.*²⁸

England et al.²⁷ also give the recommended cross sections for the rotational transitions $J=1 \rightarrow 3$, $2 \rightarrow 4$, and $3 \rightarrow 5$. There are no experimental determination of the cross section for a rotational transition with $|\Delta J| > 2$. Itikawa and Mason show in their article³⁰ that those higher-order transitions have a very small cross section.

5. Vibrational Excitation

Here the cross section for the vibrational excitation v=0 \rightarrow 1 is presented first. The transition energy for the process is 0.516 eV. The excitation of a higher state is discussed later. There is a rather old but very comprehensive measurement of the vibrational cross section by Ehrhardt et al. 31 This is a measurement of electron energy loss spectra (EELS) with a crossed beam method. The result of the measurement is in good agreement with the most recent beam data obtained by Brunger et al.21 The agreement is within the uncertainty (±20%) of the latter (see Fig. 8). In the energy range of 2-3 eV, the values of Brunger et al. are systematically smaller than the data of Ehrhardt et al. We thus recommend the cross sections of Ehrhardt et al.,31 but reduce the cross sections in the 2-3 eV range to be consistent with the data of Brunger et al.²¹ At the energies above 10 eV, the only available experimental data are those of Nishimura et al. 22 They made a beam-type measurement at the energies of 2.5-100 eV. When compared with the result of Ehrhardt et al., the cross sections of Nishimura et al. are too large in the energy region of 6-10 eV. The present recommended cross sections determined above for E<7 eV, however, are smoothly connected to the cross sections of Nishimura et al. at the energies above 15 eV (see Fig. 8). Then we extended the recommended cross sections to 100 eV by taking the

TABLE 4. Recommended values of the rotational cross section for $J=0\rightarrow 2$

Energy (eV)	Cross section (10 ⁻¹⁶ cm ²)
0.0439	0
0.047	0.0185
0.05	0.027
0.055	0.035
0.06	0.042
0.065	0.048
0.07	0.053
0.08	0.062
0.09	0.068
0.1	0.074
0.11	0.079
0.13	0.088
0.15	0.097
0.2	0.115
0.25	0.132
0.3	. 0.452
0.35	0.175
0.4	0.2
0.45	0.228
0.5	0.26
0.6	0.323
0.7	0.394
0.8	0.469
0.9	0.555
1	0.638
1.2	0.796
1.5	1.036
2	1.37
2.5	1.585
3	1.704
3.5	1.755
4	1.758
4.5	1.732
5	1.689
6	1.579
7	1.462
8	1.35
9	1.248
10	1.156
15	0.73

cross sections of Nishimura et al. for E > 15 eV. The resulting recommended cross sections are shown in Fig. 8 and Table 5. The overall uncertainty of the present recommended values is probably less than $\pm 20\%$. JPCRD90 shows the cross section based on Ref. 31 up to 10 eV.

The vibrational cross sections have also been measured with a swarm technique (e.g., Ref. 28). However, the resulting values are in a large (as much as $\pm 60\%$) disagreement with the ones obtained with a beam measurement mentioned above. To solve this discrepancy, extensive efforts have been spent on the following attempts:

(i) Several different elaborate theories (e.g., Morrison and Trail³²) have been applied to calculate the vibra-

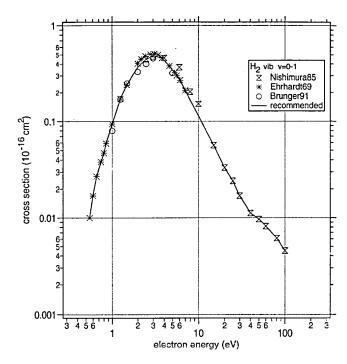


Fig. 8. Vibrational cross sections for the transition $v=0 \rightarrow 1$. A comparison is made for the results of the experiments by Ehrhardt *et al.*, ³¹ Nishimura *et al.*, ²² and Brunger *et al.* ²¹ The recommended cross section from the present evaluation is also shown.

tional cross section, but all of them failed to reproduce the swarm data.

- (ii) As is described in Sec. 4, Schmidt *et al.*²⁶ developed new swarm techniques. They obtained vibrational cross sections a little different from the old ones, but still a significant discrepancy from the beam data remains at the energies of 0.7–1.6 eV.
- (iii) A very detailed examination of the swarm analysis³³ was made, but no considerable error was found in the analysis.

For these reasons, no swarm data have been considered in determining the present recommended cross sections.

Ehrhardt et al. [31] also reported their experimental data on the cross section for the vibrational transitions $v=0 \rightarrow 2,3$. The magnitude of those cross sections is more than ten times smaller than the cross section for $v=0 \rightarrow 1$.

6. Excitation of Electronic States

After the publication of JPCRD90, a few comprehensive experimental measurements of the excitation cross section $Q_{\rm exc}$ of H_2 have been reported. Considering the results of those measurements, the evaluation of the cross section data was made to revise the cross sections reported in JPCRD90 for $b^3\Sigma_{\rm u}^+$, $a^3\Sigma_{\rm g}^+$, $c^3\Pi_{\rm u}$, $B^1\Sigma_{\rm u}^+$, $C^1\Pi_{\rm u}$, $E,F^1\Sigma_{\rm g}^+$, and $e^3\Sigma_{\rm u}^+$. For other states, no substantially new information is available. Table 6 gives the vertical excitation energy of the states considered here. The potential energy diagrams of H_2 are shown in Figs. 1 and 2.

TABLE 5. Recommended values of the vibrational cross section for $v=0 \rightarrow 1$

Energy (eV)	Cross section (10 ⁻¹⁶ cm ²)
0.55	0.01
0.6	0.017
0.66	0.027
0.74	0.038
0.8	0.047
0.85	0.059
1	0.094
1.25	0.172
1.48	0.24
2	0.367
2.46	0.442
3	0.486
3.8	0.461
4.6	0.38
5	0.343
5.3	0.324
5.6	0.302
6.1	0.27
7	0.21
15	0.056 5
20	0.033 2
25	0.024 2
30	0.017
40	0.011 2
50	0.009 68
60	0.008 17
80	0.006 09
100	0.004 51

6.1. $b^{3}\Sigma_{11}^{+}$

This is a repulsive state (see Fig. 2). Upon excitation of this state, hydrogen molecules promptly dissociate into two hydrogen atoms in the ground state. In an EELS, this excitation appears as a broad peak. Since the peak is rather isolated from others, the respective cross section can be derived from the measurement of EELS. Four different measurements ³⁶⁻³⁹ of the excitation cross section of this state

TABLE 6. Vertical excitation energy for the electronic state of H₂, considered in the present paper

State	Experimental (eV) ^{a,b}	Theory (R matrix) (eV) ^c	Figure ^d
$b^3\Sigma_u^+$ $B^1\Sigma_u^+$		10.45	9
$B^{1}\Sigma_{u}^{+}$	11.18	13.15	11
$c^{3}\Pi_{u}^{2}$ $a^{3}\Sigma_{g}^{+}$	11.76	12.6	14
$a^{3}\Sigma_{g}^{+}$	11.79	12.41	10 and 14
С¹П _u	12.29	13.11	12
$E_rF^1\Sigma_g^+$	12.3	13.25	13
$C_{i}^{1}\Pi_{u}^{i}$ $E,F_{i}^{1}\Sigma_{g}^{+}$ $e^{3}\Sigma_{u}^{+}$	13.23		14

Energy of the lowest vibrational state relative to $X^{1}\Sigma_{g}^{+}$ (v=0). Reference 34.

Theoretical result obtained with the R-matrix method. 35

Excitation cross sections shown.

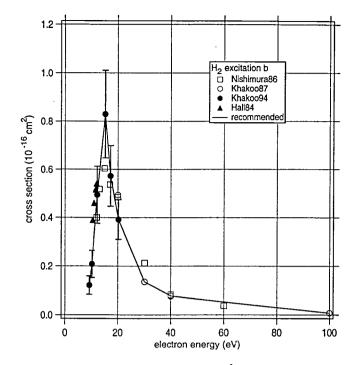


Fig. 9. Cross sections for the excitation of the $b^3\Sigma_{7}^+$ electronic state of H_2 . Results of four experiments (Nishimura and Danjo, Khakoo *et al.*, ³⁸ Khakoo and Segura, ³⁹ and Hall and Andric ³⁶) and the recommended cross sections from this evaluation are shown.

have been reported. The agreement among the four sets of data is fairly good (Fig. 9). Near the peak in the cross section at about 17 eV, there appears to be a large difference between the two sets of data by Nishimura and Danjo³⁷ and Khakoo and Segura.³⁹ Considering their uncertainties, however, they agree with each other. (Nishimura and Danjo did not explicitly show the uncertainty of the integral cross sections. However, they claimed the experimental errors of the DCSs to be up to $\pm 37\%$).

For the recommended data, we take the most recent values (i.e., Ref. 39) up to 20 eV and the cross sections previously obtained by the same group³⁸ for 30–100 eV. The resulting recommended cross sections are shown in Fig. 9 and tabulated in Table 7.

Table 7. Recommended values of the excitation cross section for the b $^3\Sigma_{\rm u}^+$ state

Energy (eV)	Cross section (10 ⁻¹⁶ cm ²)
9.2	0.121
10.2	0.208
12.2	0.494
15.2	0.83
17.2	0.573
20.2	0.392
30	0.135
40	0.0771
100	0.0073

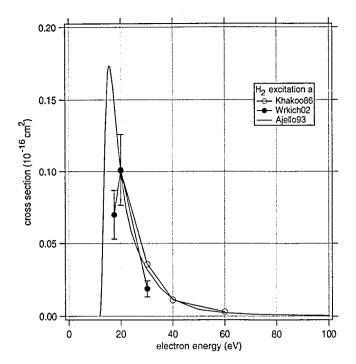


Fig. 10. Cross sections for the excitation of the $a^3\Sigma_g^*$ electronic state of H_2 . The results of two beam-type measurements (Khakoo and Trajmar²³ and Wrkich *et al.*⁴⁰) are compared with that of an emission measurement (Ajello and Snemansky⁴¹).

6.2. $a^{3}\Sigma_{\alpha}^{+}$

There are two results of the EELS measurement reported by the same group. 23,40 Ajello and Shemansky 41 derived $Q_{\rm exc}$ from their emission measurement. They obtained the cross sections in relative scale and normalized them with the $Q_{
m exc}$ measured by Khakoo and Trajmar.²³ Furthermore, to avoid possible cascade effects, they took the cross sections of Ref. 23 for the energies above 30 eV and connected them to their own $Q_{\rm exc}$ in the lower energy range. When we compare the resulting cross sections of Ajello and Shemansky with those of Wrkich et al., we see a large disagreement at the peak (around 17 eV) (Fig. 10). The difference might be a cascade effect in the emission measurement. Since Wrkich et al. 40 claimed a significant improvement of the measurement over their previous one,²³ we prefer the former here. In conclusion, we take the data of Wrkich et al. as the recommended ones for this excitation. The values are replotted in Fig. 14 and tabulated in Table 10.

6.3. $c^{3}\Pi_{u}$

There are two EELS measurements of the same group, 23,40 of which we prefer the newer one. 40 Mason and Newell 42 derived $Q_{\rm exc}$ for this excitation with detecting metastable hydrogen molecules. They assumed that only the $c^3\Pi_{\rm u}$ state contributes to their detected signal. Their cross sections were only reported in relative scale. Furthermore the cross section of Mason and Newell may include cascade contributions. Here we take the cross sections of Wrkich *et al.* 40 as the recommended values (shown in Fig. 14 and Table 10).

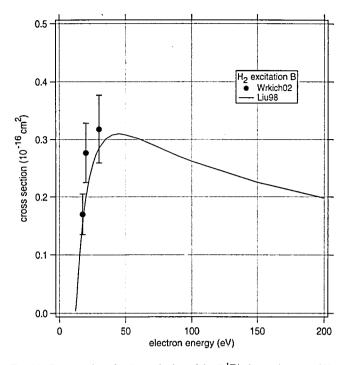


Fig. 11. Cross sections for the excitation of the $B^{1}\Sigma_{u}^{*}$ electronic state of H_{2} . The result of an EELS measurement by Wrkich *et al.*⁴⁰ is compared with that of an emission measurement of Liu *et al.*⁴⁴

6.4. $B^{1}\Sigma_{11}^{+}$ and $C^{1}\Pi_{11}$

Three different EELS measurements have been reported for the excitation of the $B^{1}\Sigma_{\rm u}^{+}$ state. The experiment by Srivastava and Jensen⁴³ is too old and the result of Khakoo and Trajmar²³ is superseded by a new measurement of the same group.⁴⁰ Liu *et al.*⁴⁴ derived $Q_{\rm exc}$ from their measurement of the B-X emission. They took much care about possible cascade effects and normalized their cross sections with the optical oscillator strength at the high-energy limit. The resultant $Q_{\rm exc}$ of Liu *et al.* agrees very well with the corresponding cross section obtained from the EELS measurement by Wrkich *et al.* (Fig. 11). We take the result of Liu *et al.* as the recommended values for the excitation (shown in Table 8). They estimated the errors of their cross sections to be $\pm (15-25)\%$ for 20-500 eV of electron energy, $\pm (7-15)\%$ for the energies above that, and $\pm 30\%$ for the energies below 20 eV.

We have the same situation for the excitation of the $C^{1}\Pi_{u}$ state as for the $B^{1}\Sigma_{u}^{+}$ state (Fig. 12). That is, we take the result of Liu *et al.*⁴⁴ for the recommended cross sections for the $C^{1}\Pi_{u}$ state (shown in Table 8).

6.5. *E*, $F^{1}\Sigma_{a}^{+}$

We have two different sets of $Q_{\rm exc}$ for this state. One is those from the EELS measurement by Wrkich *et al.*⁴⁰ and the other is those derived from an emission measurement by Liu *et al.*⁴⁵ These two sets of cross sections are in good agreement with each other (Fig. 13). We here take the result of Liu *et al.* as the recommended data (shown in Table 9). They claimed the experimental uncertainty of $\pm 25\%$.

Table 8. Recommended values of the excitation cross section for the $B^{1}\Sigma_{u}^{+}$ and $C^{1}\Pi_{u}$ states

Energy	$B^{1}\Sigma_{u}^{+}$ Cross section	$C^{1}\Pi_{u}$ Cross section
(eV)	(10 ⁻¹⁶ cm ²)	(10 ⁻¹⁶ cm ²)
12	0.003 51	0
12.2	0.006 4	0
12.4	0.010 3	0.000 68
12.6	0.015 1	0.002 07
12.8	0.020 6	0.004 81
13	0.026 6	0.008 73
13.3	0.036 3	0.015 9
13.6	0.046 4	0.024 2
14	0.059 8	0.036 1
14.5	0.076	0.051 2
15	0.091 3	0.065 7
15.5	0.106	0.079 3
16	0.119	0.092
16.5	0.131	0.104
17	0.143	0.115
17.5	0.154	0.126
18	0.164	0.135
18.5	0.174	0.145
19	0.183	0.153
20	0.199	0.169
22.5	0.232	0.201
25	0.255	0.224
27.5	0.273	0.242
30	0.285	0.254
35	0.301	0.27
40	0.308	0.278
45	0.31	0.281
50	0.308	0.281
60	0.301	0.276
70	0.291	0.267
80	0.281	0.258
90	0.271	0.25
100	0.262	0.241
150	0.225	0.208
200	0.198	0.184
250	0.177	0.165
300	0.16	0.149
350	0.146	0.136
400	0.134	0.125
450	0.124	0.116
500	0.115	0.108
600	0.101	0.094 9
700	0.090 7	0.085
800	0.082 3	0.077 1
900	0.075 4	0.070 7
1000	0.069 7	0.065 4

6.6. $e^{3}\Sigma_{11}^{+}$

One data set is available for the excitation of this state.⁴⁰ They are shown in Fig. 14 and Table 10. Without other experimental data for comparison, it is difficult to directly assess the reliability of the data. However, other cross-section data measured by the same group are generally reliable.

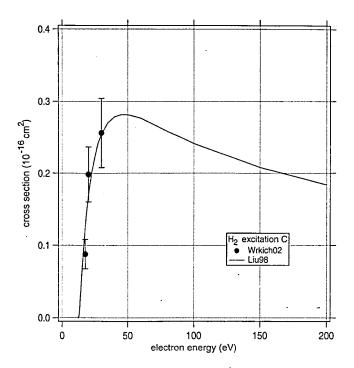


Fig. 12. Cross sections for the excitation of the $C^{\,1}\Pi_{\rm u}$ electronic state of ${\rm H}_{2}$. The result of an EELS measurement by Wrkich *et al.*⁴⁰ is compared with that of an emission measurement of Liu *et al.*⁴⁴

7. Emission Cross Section

JPCRD90 presented emission cross sections ($Q_{\rm emis}$) for various processes. The only $Q_{\rm emis}$ reported after the publication of JPCRD90 is that for the Paschen- α line of H atoms measured by Yonekura *et al.*⁴⁶ (except for the fragmentary

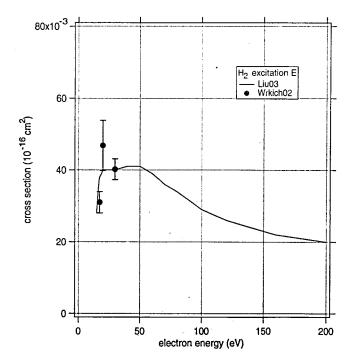


Fig. 13. Cross sections for the excitation of the $E,F^{1}\Sigma_{g}^{+}$ electronic state of H_{2} . An EELS measurement by Wrkich *et al.*⁴⁰ is compared with that of an emission measurement of Liu *et al.*⁴⁵

TABLE 9. Recommended values of the excitation cross sections for the $E, F^{1}\Sigma_{\bullet}^{*}$ state

Energy (eV)	Cross section (10 ⁻¹⁶ cm ²)
15	0.028
16	0.033
17	0.037
17.5	0.038
19	0.039
20	0.04
21	0.04
23.5	0.04
26	0.04
30	0.04
40	0.041
50	0.041
60	0.039
70	0.036
80	0.034
100	0.029
120	0.026
140	0.024
160	0.022
180	0.021
200	0.02
220	0.019
240	0.018
260	0.017
280	0.016
300	0.015
400	0.012
500	0.009 6
600	0.008
700	0.006 9
800	0.006 1
900	0.005 4
1000	0.004 9

data described below). They measured the line (at 1875 nm) emitted from H (n=4) upon electron collisions with H₂. Yonekura *et al.* obtained the relative intensities of the Paschen- α and the Balmer- β lines and then determined the absolute values of the $Q_{\rm emis}$ for the Paschen line with the use of a previous result for the Balmer line.⁴⁷ The resultant cross section is shown in Fig. 15. A typical error of the Paschen- α cross section was claimed to be $\pm 16\%$.

The Jet Propulsion Laboratory group has been engaged in a systematic study of electron-impact UV emission from hydrogen molecules (e.g., Liu et al. 48). As a result of the study, emission cross sections are reported for various lines but only at a few points of electron energy (e.g., James et al. 49 and Jonin et al. 50).

8. Dissociation

Here the dissociation cross section $Q_{\rm diss}$ is defined for the dissociation producing only neutral fragments. The dissociative ionization and the dissociative electron attachment are

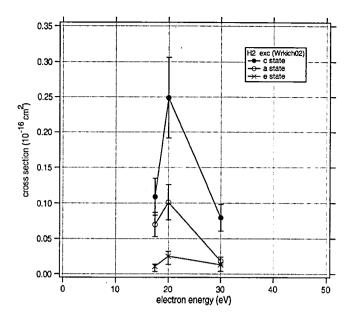


Fig. 14. (Color online) Cross sections for the excitation of the a $^3\Sigma_g^+$, c $^3\Pi_u$, and e $^3\Sigma_g^+$ electronic states of H_2 . Measured by Wrkich et al.

described in Secs. 9 and 10, respectively. Then it is difficult to obtain $Q_{\rm diss}$ experimentally. For hydrogen molecules, the only available data are the total dissociation cross section measured by Corrigan in 1965. He obtained the cross section by the measurement of pressure decrease in a closed system where the dissociation fragments are trapped on a getter (MoO₃) surface. As he claimed, his result includes the cross section for ionization. After subtracting our recommended values of $Q_{\rm ion}$ (tot) from Corrigan's data, we obtained the dissociation cross section shown in Fig. 16 and Table 11. The peak value of $Q_{\rm diss}$ is 9×10^{-17} cm² at 16.5 eV. Corrigan estimated the random error of this value to be $\pm 20\%$.

Many kinds of collision processes lead to the dissociation of H_2 . Near threshold, the excitation of the $b^3\Sigma_u^+$ state is expected to be the main contributor to the dissociation. In Fig. 16, we compare the dissociation cross section of Corrigan with our recommended $Q_{\rm exc}$ for the $b^3\Sigma_u^+$ state (in Sec. 6.1). At the energies below its peak, the dissociation cross section almost coincides with the $Q_{\rm exc}$ for the $b^3\Sigma_u^+$ state. Above the peak, excitations of highly excited states have a contribution to the dissociation, so that the $Q_{\rm diss}$ is much larger than the $Q_{\rm exc}$ for the b state. It should be noted that in JPCRD90, Corrigan's cross section was assigned to be the excitation cross section for the $b^3\Sigma_u^+$ state.

TABLE 10. Cross sections for the excitation of the $a^3\Sigma_{\rm g}^+$, $c^3\Pi_{\rm u}$, and $e^3\Sigma_{\rm u}^+$ electronic states of H₂, measured by Wrkich *et al.* ⁴⁰

Energy (eV)	$a^{3}\Sigma_{g}^{+}$ Cross section (10 ⁻¹⁶ cm ²)	c $^{3}\Pi_{\rm u}$ Cross section (10 ⁻¹⁶ cm ²)	$e^{3}\Sigma_{\rm u}^{+}$ Cross section (10^{-16} cm ²)
17.5	0.0699	0.109	0.0108
20	0.1011	0.2489	0.0252
30	0.0186	0.0796	0.0132

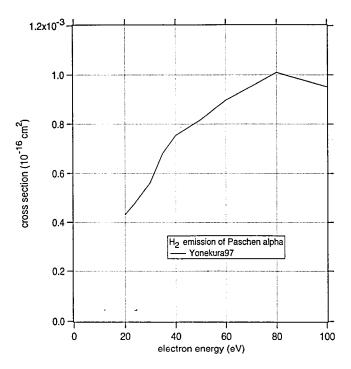


Fig. 15. Cross section for the emission of Paschen- α line of H upon electron collision with H₂. From Yonekura *et al.*⁴⁶

9. Ionization

Lindsay and Mangan⁵² carefully reviewed the experimental data on the ionization cross section (Q_{ion}) available for electron collisions with hydrogen molecules. Then they de-

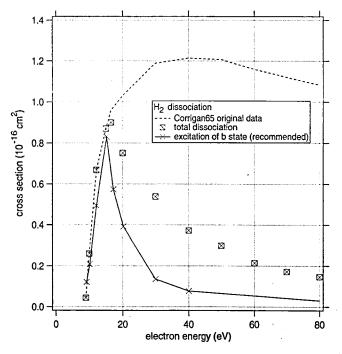


Fig. 16. Dissociation cross section and related quantities. The dashed line is the original result of Corrigan's experiment, ⁵¹ from which the ionization cross section is subtracted to give the neutral dissociation cross section (squares). For a comparison, the excitation cross section for the $b^3\Sigma_u^+$ state recommended by the present evaluation is also shown.

TABLE 11. Recommended values of the dissociation cross section for the neutral products

Energy (eV)	Cross section (10^{-16} cm^2)
9	0.044
10	0.26
12.2	0.668
15	0.87
16.5	0.9
20	0.751
30	0.538
40	0.373
50	0.299
60	0.215
70	0.172
80	0.147

termined the recommended values of $Q_{\rm ion}$ both for the productions of H_2^+ [i.e., $Q_{\rm ion}$ (H_2^+)] and H^+ [$Q_{\rm ion}$ (H^+)]. For that purpose, they selected the result of the experiment performed by Straub *et al.*, ⁵³ with a slight modification. Straub *et al.* used a time of flight mass spectrometer to detect product ions. They made their cross sections absolute without any normalization procedure. They took special care to have all the product ions collected. This is particularly important to obtain the partial cross section for H^+ , which may have a significant speed depending on the dissociation process. At the energy of 25 eV or less, Lindsay and Mangan took the cross sections measured by Krishnakumar and Srivastava and renormalized them to the cross section of Straub *et al.* at 25 eV. This is because Straub *et al.* measured their cross section only at a few points of energy in the region.

The total ionization cross section [defined by $Q_{\rm ion}$ (H_2^+) + $Q_{\rm ion}$ (H_2^+) and denoted by $Q_{\rm ion}$ (tot)] can be directly obtained with the measurement of the total ion current. From the partial cross sections they determined, Lindsay and Mangan obtained their $Q_{\rm ion}$ (tot). When it is compared with the value obtained from the ion-current measurement by Rapp and Englander-Golden, 55 the two sets of $Q_{\rm ion}$ (tot) at the energies above 25 eV agree with each other within the uncertainties of each experiment ($\pm 7\%$ for Ref. 55 and $\pm 5\%$ for Ref. 52). However, below 25 eV, there is some disagreement (see Ref. 52). This is probably due to a large uncertainty of the experiment of Krishnakumar and Srivastava. As for the total cross section at energies of 25 eV and below, therefore, Lindsay and Mangan preferred the value of Ref. 55 to their own result.

In the present paper, we recommend the partial and total cross sections determined by Lindsay and Mangan at the energies above 25 eV. At the energies of 25 eV and below, we take the $Q_{\rm ion}$ (tot) measured by Rapp and Englander-Golden. Since the dissociative ionization has a small contribution (less than 1%) in the low-energy region, the $Q_{\rm ion}$ (tot) can be regarded to be the same as $Q_{\rm ion}$ (H₂⁺) there. The present recommended values of ionization cross

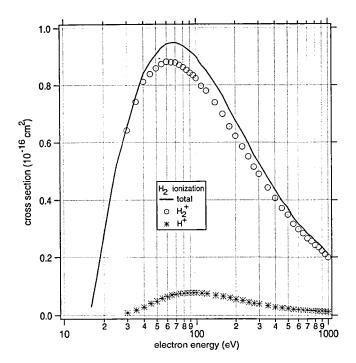


Fig. 17. Recommended values (the present evaluation) of ionization cross sections: total and the cross sections for the production of H₂⁺ and H⁺.

sections are shown in Fig. 17 and Tables 12 and 13. The best value of the ionization potential of H_2 is 15.426 eV, while the appearance energy of H^+ is 18.1 eV.

On the basis of the $Q_{\rm ion}$ (H₂⁺) of Lindsay and Mangan, Liu and Shemansky⁵⁶ obtained the ionization cross sections for the transitions between any discrete vibrational levels of the ground states of H₂ and H₂⁺. They analytically fitted the $Q_{\rm ion}$ (H₂⁺) of Lindsay and Mangan to determine the shape function (i.e., the energy dependence) of the ionization cross section. Combining the shape function and the optical oscillator strengths, they obtained the state-to-state ionization cross sections.

JPCRD90 reports the ionization cross section based on the review paper published in 1987. The recommended values there are slightly larger than the present ones.

10. Dissociative Attachment

Recently one of the present authors compiled cross sections for electron attachment to molecules. ⁵⁷ Here we take his recommended cross section for hydrogen molecules because no experimental data have been reported for the process after the completion of the compilation. The present cross sections, shown in Fig. 18 and Table 14, are based on the measurement by Drexel et al. ⁵⁸ for 3–5 eV and Rapp et al. ⁵⁹ for the energy region above that. JPCRD90 shows almost the same cross sections, but their values at the lower energy were taken from an older measurement.

The attachment in the region of 3-5 eV is known to be caused by a resonance through a negative ion state of $^2\Sigma_u$ symmetry. The resonance is strongly dependent on the vibrational state of the target molecule. Allan and Wong⁶⁰ detected H⁻ with changing the temperature of the H₂ gas. From the

TABLE 12. Recommended values of total ionization cross sections

Engrav	Cross section	
Energy (eV)	(10^{-16} cm^2)	
16	0.0299	
16.5	0.0607	
17	0.0924	
17.5	0.123	
18	0.156	
18.5	0.187	
19	0.22	
19.5	0.249	
20	0.28	
20.5	0.31	
21	0.336	
21.5	0.362	
22	0.39	
22.5	0.414	
23	0.439	
23.5	0.461	
24	0.484	
24.5	0.505	
25	0.524	
30	0.651	
35	0.76	
40	0.84	
45	0.88	
50	0.908	
55	0.931	
60	0.911	
65	0.948	
70	0.949	
75 75	0.944	
80	0.937	
85	0.928	
90	0.919	
	0.911	
95	0.9	
100	0.872	
110		
120	. 0.852	
140	0.806	
160	0.763	
180	0.714	
200	0.676	
225	0.636	
250	0.596	
275	0.556	
300	0.529	
350	0.477	
400	0.436	
450	0.398	
500	0.373	
550	0.339	
600	0.317	
650	0.302	
700	0.283	
750	0.272	
800	0.257	
850	0.248	
900	0.236	
950	0.222	
1000	0.211	
	<u> </u>	

analysis of their experiment, they found that the dissociative attachment cross section increases enormously with increasing the vibrational quantum number of the target H_2 . The ratio of the maximum cross sections for the vibrational state with v=4 to that for v=0, for example, was estimated to be about 4×10^4 . This ratio was confirmed theoretically. The absolute magnitude of the cross section for individual vibrational states (except for the values shown in Fig. 18, which are presumably the cross sections for the vibrationally ground state), however, has never been obtained experimentally. There have been many theoretical attempts to calculate the cross section (see the recent review by Fabrikant *et al.* 61).

TABLE 13. Recommended values of partial ionization cross section

- TABLE 13. RCCC	values of partial to	
Energy (eV)	H ₂ ⁺ Cross section (10 ⁻¹⁷ cm ²)	H ⁺ Cross section (10 ⁻¹⁸ cm ²)
30	6.42	0.86
35	7.42	1.76
40	8.12	2.87
45	8.39	4.08
50	8.59	4.82
55	8.74	5.72
60	8.82	6.25
65	8.8	6.82
70	8.79	7.05
75	8.71	7.37
80	8.63	7.39
85	8.53	7.51
90	8.43	7.54
95	8.35	7.61
100	8.24	7.59
110	7.97	7.44
120	7.8	7.24
140	7.39	6.71
160	6.99	6.39
180	6.55	5.92
200	6.22	5.45
225	5.85	5.05
250	5.51	4.5
275	5.15	4.12
300	4.9	3.92
350	4.43	3.39
400	4.07	2.94
450	3.72	2.6
500	3.49	2.41
550	3.17	2.11
600	2.98	1.97
650	2.84	1.81
700	2.66	1.71
750	2.56	1.59
800	2.42	1.49
850	2.34	1.37
900	2.22	1.35
950	2.1	1.25
1000	1.99	1.17

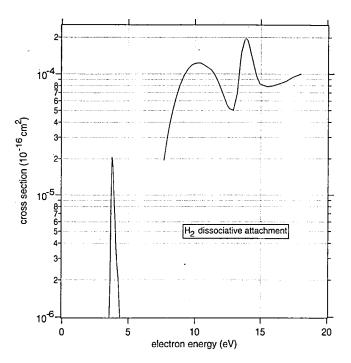


Fig. 18. Recommended values of dissociative attachment cross section.

Since correlations between electronic and nuclear motions have to be correctly taken into account, it is difficult to obtain reliable theoretical values. Figure 19 shows one of the recent theoretical results. The values in the figure are taken from the paper by Horacek et al.⁶² (they actually reported cross sections for v=0-12). They also showed a relatively large effect of rotational excitation of H₂ on the dissociative attachment cross section. It is not easy to compare these theoretical values to experiment. Experiments are performed at a finite temperature (e.g., 300 K) and with an electron beam of finite energy resolution (e.g., 0.1 eV). Taking consideration of the experimental condition, Horacek et al. claimed that their theoretical result is consistent with the experiment done by Allan and Wong. However, the consistency is not necessarily perfect (see Ref. 62). In conclusion, the dissociative attachment cross section of H₂, particularly the one in the energy region of 3-5 eV, is strongly dependent on the rovibrational state of the target molecule, but the absolute magnitude of the cross section for each state is still not known with certainty.

11. Summary and Future Problems

Cross sections for electron collisions with hydrogen molecules are summarized in Fig. 20. They are as follows:

- (i) total scattering cross section (Table 1),
- (ii) elastic scattering cross section (Table 2),
- (iii) momentum transfer cross section (Table 3),
- (iv) rotational cross section for the transition $J=0 \rightarrow 2$ (Table 4),
- (v) vibrational cross section for the transition $v=0 \rightarrow 1$ (Table 5),

TABLE 14. Recommended values of dissociative attachment cross section

TABLE 14. Recommended values	of dissociative attachment cross
Energy (eV)	Cross section (10 ⁻¹⁶ cm ²)
3.56	9.70 <i>E</i> -07
3.63	1.90 <i>E</i> -06
3.69	8.09 <i>E</i> -06
3.75	1.80 <i>E</i> -05
3.76	2.07E-05
3.81	1.94 <i>E</i> -05
3.88	1.29E-05
3.94	8.38 <i>E</i> -06
4	6.21 <i>E</i> -06
4.06	3.88E-06
4.13	2.80E-06
4.25	2.00E-06
4.375	9.70E-07
7.67	1.94 <i>E</i> -05
7.84	2.64 <i>E</i> -05
8.08	3.76E-05
8.3	
8.59	4.90E-05
8.87	6.51 <i>E</i> -05
	8.15 <i>E</i> -05
9.17	9.74 <i>E</i> -05
9.48	1.10 <i>E</i> -04
9.78	1.19E-04
9.99	1.22 <i>E</i> -04
10.2	1.23 <i>E</i> -04
10.4	1.23 <i>E</i> -04
10.6	1.20 <i>E</i> – 04
10.8	1.16 <i>E</i> -04
11	1.12 <i>E</i> -04
11.2	1.08 <i>E</i> -04
11.4	1.02 <i>E</i> – 04
11.6	9.29 <i>E</i> -05
11.8	8.27 <i>E</i> -05
12.1	6.80 <i>E</i> -05
12.4	5.57E-05
12.6	5.17 <i>E</i> -05
12.9	5.01E - 05
13.2	6.92E - 05
13.3	9.03E - 05
13.5	1.48 <i>E</i> -04
13.7	1.80 <i>E</i> -04
13.8	1.95 <i>E</i> -04
13.9	1.95 <i>E</i> -04
14	1.89 <i>E</i> -04
14.1	1.72E - 04
14.2	1.55 <i>E</i> -04
14.3	1.39 <i>E</i> -04
14.4	1.26 <i>E</i> -04
14.5	1.12 <i>E</i> -04
14.6	1.02 <i>E</i> -04
14.7	9.33 <i>E</i> -05
14.8	8.88 <i>E</i> -05
14.9	8.31 <i>E</i> -05
15.2	8.03 <i>E</i> -05
15.4	7.89 <i>E</i> -05
15.5	7.85 <i>E</i> -05
15.6	7.86 <i>E</i> -05
15.9	7.97E-05
	•

TABLE 14. Recommended values of dissociative attachment cross section-Continued

Energy (eV)	Cross section (10^{-16} cm^2)
16.4	8.29 <i>E</i> -05
16.9	8.70 <i>E</i> -05
17.4	9.41 <i>E</i> -05
18	1.00E - 04

- a few representative cross sections for the excitation of electronic states (i.e., the excitations of $b^{3}\Sigma_{\rm u}^{+}$, $B^{1}\Sigma_{\rm u}^{+}$, and $E, F^{1}\Sigma_{\rm g}^{+}$ states) (Tables 7–9), dissociation cross sections (Table 11),
- (viii) total ionization cross sections (Table 12), and
- (ix) ionization cross section for the production of H+ (Table 13).

To be consistent with each other, those cross sections should follow the relation

$$Q_T = Q_{clas} + Q_{ion}(tot) + Q_{att}(tot) + Q_{diss} + \sum_{i} Q_{i}$$

The last term on the right-hand side of the equation includes all the excitation cross sections of discrete (rotational. vibrational, electronic) states. It should be noted that the excitation of those states which are known to dissociate must be excluded in the summation. The Q_{elas} in Fig. 20 is the experimental value. That is, it is the vibrationally elastic cross section, which includes the contribution of rotational excitation. As is shown in Sec. 10, the magnitude of Q_{att} (tot)

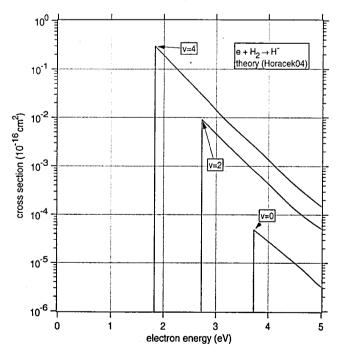


Fig. 19. Dependence of the dissociative attachment cross section on the vibrational state of the hydrogen molecule. The theoretical result of Horacek et al.62 is shown.

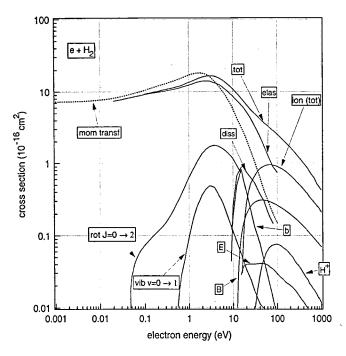


Fig. 20. Summary of the cross sections for electron collisions with H₂.

is smaller than 10^{-18} cm². Considering these facts, the cross sections shown in Fig. 20 satisfy the above relation within the uncertainties claimed for each cross section.

As is stated in the Introduction, the present paper serves as a complete update of the data compilation for the $e+H_2$ collisions, previously reported by one of the present authors and his colleagues (i.e., JPCRD90). Almost all of the cross sections have been revised. As is usual, however, further studies are still needed to make the cross section data more comprehensive and more accurate. In particular, the following problems should be addressed:

- (i) The rotational cross section has a large value at the energies up to a few tens of eV. However, no experimental data are available at the energies of about 1 eV and higher.
- (ii) Only one old set of measured values is available for the elastic cross sections at the energies of 100-1000 eV. They are not completely consistent with the recommended cross sections in the energy region below 100 eV.
- (iii) Although several sets of experimental cross sections are available for the excitation of electronic states, more detailed measurement should be done for the excitation of triplet states.
- (iv) The total dissociation cross sections are available with fair certainty. Further information is necessary for the details of the dissociation process.
- (v) Finally, as is described in the Appendix, cross section data for the target molecules in their excited states are of practical importance. Any experiment of the electron collision with excited hydrogen molecules would be very valuable.

12. Appendix: Electron Collisions with Hydrogen Molecules in Excited States

In a hydrogen plasma, vibrationally excited molecules (in its electronically ground state) are produced in several different ways. Besides the electron-impact direct excitation of the vibrational state, an excitation of particular electronically excited states results in the vibrational excitation of the ground state through emission of radiation. On the surface of plasma container or electrode, hydrogen molecules are produced through neutralization of H_2^+ or association of two hydrogen atoms. Some of the product molecules are in their vibrationally excited state. Since H_2 has no electric dipole moment, vibrationally excited H_2 has a long lifetime against radiative decay. Thus the collisions of those vibrationally excited H_2 with plasma particles (i.e., electrons, ions, or neutral particles) may have a non-negligible effect in the kinetic or transport phenomena in plasmas.

Electronically excited states (except for metastable one) of hydrogen molecules rapidly decay to the lower states by emission of radiation. For an application of detailed collisional-radiative model, however, information on the rate of collisional transition between those excited states is needed.

Almost all of the experiments of electron collisions with H₂ have been conducted with the target molecule in its ground (electronic and vibrational) state. All the experimental cross sections shown in the present paper (except for the dissociative attachment shown in Sec. 10) are the values obtained for the ground-state molecules. On the other hand, extensive effort has been spent on obtaining theoretical cross sections for the vibrationally or electronically excited targets. Since no corresponding experimental results are available, it is very difficult to evaluate the accuracy of those theoretical cross sections. For this reason, we do not make any recommendation on the cross section for the hydrogen molecules in their excited states. Instead we simply give here a list of those theoretical papers reporting cross sections for excited targets. To be consistent with the other parts of the present paper, we concentrate our list on the papers published in recent years.

Electron-impact dissociative attachment of H_2 has a peculiarity. Cross sections for the process strongly depend on the vibrational state of the target. Very extensive theoretical studies have been made for the process. They are mentioned in the section of dissociative attachment in the text (Sec. 10). The following list does not include the papers concerning the dissociative attachment process.

12.1. Collisions with vibrationally excited H₂ (in its ground electronic state)

Papers on the dissociative attachment are not included; see Sec. 10.

(i)
$$H_2(X,v) \to H_2^*(n) \to H + H$$

 $n=B^{-1}\Sigma_u^+, C^{-1}\Pi_u, B'^{-1}\Sigma_u^+, D^{-1}\Pi_u, B''^{-1}\Sigma_u^+, D'^{-1}\Pi_u,$

- $b^{3}\Sigma_{\rm u}^{+}$ (Ref. 63) $n=b^{3}\Sigma_{\rm u}^{+}$ (superseded by Ref. 65) (Ref. 64) $n=b^{3}\Sigma_{\rm u}^{+}$ (Ref. 65)
- $\begin{array}{l} H_{2}(X,v) \xrightarrow{u} H_{2}^{*}(n) \\ n = B^{1}\Sigma_{u}^{+}, C^{1}\Pi_{u}, B'^{1}\Sigma_{u}^{+}, D^{1}\Pi_{u}, B''^{1}\Sigma_{u}^{+}, D'^{1}\Pi_{u} \end{array}$ (ii)
- (iii) $H_2(X,v) \to H_2^+(n) \to H + H^+$
- $n = X^2 \Sigma_g^+$ (Ref. 63) $H_2(X, v) \to H_2^+(n) \to H_2(X, v') + h\nu$ (iv) $n = B^{1}\Sigma_{u}^{+}, C^{1}\Pi_{u} \text{ (Ref. 63)}$ $n = B^{1}\Sigma_{u}^{+}, C^{1}\Pi_{u}, B'^{1}\Sigma_{u}^{+}, D^{1}\Pi_{u} \text{ (Ref. 66)}$ $n = B^{1}\Sigma_{u}^{+}, D^{1}\Pi_{u} \text{ (Ref. 67)}$
- $H_2(X,v) \rightarrow H_2^*(n) \rightarrow H+H+h\nu$ (v) $n=B^{1}\Sigma_{u}^{+}, C^{1}\Pi_{u}$ (Ref. 63)
- $H_2(X,v) \rightarrow H_2^-(X^2\Sigma_u^+) \rightarrow H_2(X,v')$ (vi) (Ref. 68)

12.2. Collisions with electronically excited H₂

- $H_2^*(B^1\Sigma_u^+, v) \to H_2^*(n) \to H+H$ (i) $n = I \Pi_{g} (\text{Ref. 63})$
- $H_2^*(B^{1}\Sigma_u^+, v) \to H_2^*(n)$ $n=I^{1}\Pi_g$ (Ref. 63) (ii)
- $H_2^*(a^3\Sigma_g^+, v) \to H_2^*(n) \to H+H$ $n=d^3\Pi_u$ (Ref. 69) (iii)
- $H_2^*(a^3\Sigma_g^+, v) \rightarrow H_2^*(n)$ $n=d^3\Pi_u$ (Ref. 69) (iv)
- $H_2^*(c^{3}\Pi_u,v) \to H_2^*(n) \to H+H$ $n=g^{3}\Sigma_{g}^{+}, h^{3}\Sigma_{g}^{+}$ (Ref. 69)
- $H_2^*(c^3\Pi_u,v) \to H_2^*(n)$ $n=g^{3}\Sigma_{g}^{+}, h^{3}\Sigma_{g}^{+}$ (Ref. 69)
- $H_{2}^{*}(c^{3}\Pi_{u}) \rightarrow H_{2}^{*}(n)$ $n=a^{3}\Sigma_{g}^{+}, b^{3}\Sigma_{u}^{4}, c^{3}\Pi_{u}, X^{1}\Sigma_{g}^{+} \text{ (Ref. 70)}$
- (viii) $H_2^*(a^3\Sigma_g^+) \to H_2^*(n)$ $n=a^3\Sigma_g^+, b^3\Sigma_u^+, c^3\Pi_u, X^1\Sigma_g^+$ (Ref. 71)

13. References

- H. Tawara, Y. Itikawa, H. Nishimura, and M. Yoshino, J. Phys. Chem. Ref. Data 19, 617 (1990).
- ² A. Zecca, G. P. Karwasz, and R. S. Brusa, Rivista del Nuovo Cimento 19,
- ³ M. J. Brunger and S. J. Buckman, Phys. Rep. 357, 215 (2002).
- ⁴Photon and Electron Interactions with Atoms, Molecules and Ions, Landolt-Börnstein, New Series, Group I, Vol. 17, Pt. C, edited by Y. Itikawa (Springer, New York, 2003).
- ⁵R. K. Janev, D. Reiter, and U. Samm, FZ-Juelich Report No. 4105, 2003. ⁶G. P. Karwasz, R. S. Brusa, and A. Zecca, in Photon and Electron Interactions with Atoms, Molecules and Ions, Landolt-Börnstein, New Series, Group I, Vol. 17, Pt. C, edited by Y. Itikawa (Springer, New York, 2003). ⁷G. Dalba, P. Fornasini, I. Lazzizzera, G. Ranieri, and A. Zecca, J. Phys. B
- 13, 2839 (1980). ⁸ J. Ferch, W. Raith, and K. Schröder, J. Phys. B 13, 1481 (1980).
- ⁹B. van Wingerden, R. W. Wagenaar, and F. J. de Heer, J. Phys. B 13, 3481 (1980).
- 10 K. R. Hoffman, M. S. Dababneh, Y.-F. Hsieh, W. E. Kauppila, V. Pol, J. H. Smart, and T. S. Stein, Phys. Rev. A 25, 1393 (1982).
- ¹¹R. K. Jones, Phys. Rev. A 31, 2898 (1985).
- ¹²J. C. Nickel, I. Kanik, S. Trajmar, and K. Imre, J. Phys. B 25, 2427 (1992).

- ¹³C. Szmytkowski, K. Maciag and G. Karwasz, Phys. Scr. 54, 271 (1996). ¹⁴G. P. Karwasz, A. Piazza, R. S. Brusa, and A. Zecca (unpublished).
- ¹⁵S. Zhou, H. Li, W. E. Kauppila, C. K. Kwan, and T. S. Stein, Phys. Rev. A 55, 361 (1997).
- ¹⁶J. Randell, S. L. Lunt, G. Mrotzek, J.-P. Ziesel, and D. Field, J. Phys. B 27, 2369 (1994).
- ¹⁷M. Hayashi, Institute of Plasma Physics, Nagoya University, Report No. IPPJ-AM-19 1981.
- ¹⁸S. J. Buckman, M. J. Brunger, and M. T. Elford, in *Photon and Electron* Interactions with Atoms, Molecules and Ions, Landolt-Börnstein, New Series, Group I, Vol. 17, Pt. C, edited by Y. Itikawa (Springer, New York,
- ¹⁹ F. Linder and H. Schmidt, Z. Naturforsch. A **26a**, 1603 (1971).
- ²⁰S. K. Srivastava, A. Chutjian, and S. Trajmar, J. Chem. Phys. **63**, 2659 (1975).
- ²¹ M. J. Brunger, S. J. Buckman, D. S. Newman, and D. T. Alle, J. Phys. B 24, 1435 (1991).
- ²² H. Nishimura, A. Danjo, and H. Sugahara, J. Phys. Soc. Jpn. 54, 1757
- ²³ M. A. Khakoo and S. Trajmar, Phys. Rev. A 34, 138 (1986).
- ²⁴B. van Wingerden, E. Weigold, F. J. de Heer, and K. J. Nygaard, J. Phys. B 10, 1345 (1977).
- ²⁵ M. T. Elford, S. J. Buckman, and M. J. Brunger, in *Photon and Electron* Interactions with Atoms, Molecules and Ions, Landolt-Börnstein, New Series, Group I, Vol. 17, Pt. C, edited by Y. Itikawa (Springer, New York,
- ²⁶B. Schmidt, K. Berkhan, B. Götz, and M. Müller, Phys. Scr., T **T53**, 30 (1994).
- ²⁷G. Ramanan and G. R. Freeman, J. Chem. Phys. **95**, 4195 (1991).
- ²⁸ J. P. England, M. T. Elford, and R. W. Crompton, Aust. J. Phys. 41, 573
- ²⁹M. A. Morrison, R. W. Crompton, B. C. Saha, and Z. L. Petrovic, Aust. J. Phys. 40, 239 (1987).
- ³⁰ Y. Itikawa and N. Mason, Phys. Rep. 414, 1 (2005).
- ³¹ H. Ehrhardt, L. Langhans, F. Linder, and H. S. Taylor, Phys. Rev. 173, 222 (1968).
- ³²M. A. Morrison and W. K. Trail, Phys. Rev. A 48, 2874 (1993).
- ³³R. D. White, M. A. Morrison, and B. A. Mason, J. Phys. B 35, 605 (2002).
- ³⁴ K. P. Huber and G. Herzberg, Constants of Diatomic Molecules (data prepared by J. W. Gallagher and R. D. Johnson III) in NIST Chemistry WebBook, NIST Standard Reference Database Number 69, edited by P. J. Linstrom and W. G. Mallard, June 2005, National Institute of Standards and Technology, Gaithersburg, MD 20899 (http://webbook.nist.gov).
- 35 S. E. Branchett, J. Tennyson, and L. A. Morgan, J. Phys. B 23, 4625
- ³⁶R. I. Hall and L. Andric, J. Phys. B 17, 3815 (1984).
- ³⁷H. Nishimura and A. Danjo, J. Phys. Soc. Jpn. 55, 3031 (1986).
- ³⁸M. A. Khakoo, S. Trajmar, R. McAdams, and T. W. Shyn, Phys. Rev. A 35, 2832 (1987).
- ³⁹ M. A. Khakoo and J. Segura, J. Phys. B **27**, 2355 (1994).
- ⁴⁰ J. Wrkich, D. Mathews, I. Kanik, S. Trajmar, and M. A. Khakoo, J. Phys. B 35, 4695 (2002).
- ⁴¹ J. M. Ajello and D. E. Shemansky, Astrophys. J. **407**, 820 (1993).
- ⁴²N. J. Mason and W. R. Newell, J. Phys. B 19, L587 (1986).
- ⁴³S. K. Srivastava and S. Jensen, J. Phys. B 10, 3341 (1977).
- ⁴⁴X. Liu, D. E. Shemansky, S. M. Ahmed, G. K. James, and J. M. Ajello, J. Geophys. Res. A 103, 26739 (1998).
- ⁴⁵ X. Liu, D. E. Shemansky, H. Abgrall, E. Roueff, S. M. Ahmed, and J. M. Ajello, J. Phys. B 36, 173 (2003).
- ⁴⁶N. Yonekura, K. Furuya, K. Nakashima, and T. Ogawa, J. Chem. Phys. 107, 1147 (1997).
- ⁴⁷G. R. Möhlmann, F. J. de Heer, and J. Los, Chem. Phys. 25, 103 (1977). ⁴⁸ X. Liu, S. M. Ahmed, R. A. Multari, G. K. James, and J. M. Ajello,
- Astrophys. J., Suppl. Ser. 101, 375 (1995). ⁴⁹G. K. James, J. M. Ajello, and W. R. Pryor, J. Geophys. Res. 103E, 20113 (1998).
- ⁵⁰C. Jonin, X. Liu, J. M. Ajello, G. K. James, and H. Abgrall, Astrophys. J., Suppl. Ser. 129, 247 (2000).
- ⁵¹S. J. B. Corrigan, J. Chem. Phys. 43, 4381 (1965).
- ⁵²B. G. Lindsay and M. A. Mangan, in *Photon and Electron Interactions* with Atoms, Molecules and Ions, Landolt-Börnstein, New Series, Group I,

- Vol. 17, Pt. C, edited by Y. Itikawa (Springer, New York, 2003).
- 53 H. C. Straub, P. Renault, B. G. Lindsay, K. A. Smith, and R. F. Stebbings, Phys. Rev. A 54, 2146 (1996).
- ⁵⁴E. Krishnakumar and S. K. Srivastava, J. Phys. B 27, L251 (1994).
- 55 D. Rapp and P. Englander-Golden, J. Chem. Phys. 43, 1464 (1965).
- ⁵⁶X. Liu and D. E. Shemansky, Astrophys. J. **614**, 1132 (2004).
- ⁵⁷Y. Itikawa, in Photon and Electron Interactions with Atoms, Molecules and Ions, Landolt-Börnstein, New Series, Group I, Vol. 17, Pt. C, edited by Y. Itikawa (Springer, New York, 2003).
- ⁵⁸ H. Drexel, G. Senn, T. Fiegele, P. Scheier, A. Stamatovic, N. J. Mason, and T. D. Märk, J. Phys. B 34, 1415 (2001).
- ⁵⁹ D. Rapp, T. E. Sharp, and D. D. Briglia, Phys. Rev. Lett. **14**, 533 (1965). ⁶⁰M. Allan and S. F. Wong, Phys. Rev. Lett. **41**, 1791 (1978).
- 61 I. I. Fabrikant, J. M. Wadehra, and Y. Xu, Phys. Scr., T T96, 45 (2002). ⁶²J. Horacek, M. Cizek, K. Houfek, P. Kolorenc, and W. Domcke, Phys.
- Rev. A 70, 052712 (2004). 63 R. Celiberto, R. K. Janev, A. Laricchiuta, M. Capitelli, J. M. Wadehra,

- and D. E. Atems, At. Data Nucl. Data Tables 77, 161 (2001). (This is a summary of a series of calculations by the University of Bari group. Information of each original paper is included herein.)
- 64 D. T. Stibbe and J. Tennyson, Astrophys. J. 513, L147 (1999).
- 65 C. S. Trevisan and J. Tennyson, Plasma Phys. Controlled Fusion 44, 1263 (2002).
- 66 J. R. Hiskes, J. Appl. Phys. 70, 3409 (1991).
- ⁶⁷ A. Laricchiuta, R. Celiberto, F. Esposito, and M. Capitelli, Plasma Sources Sci. Technol. 15, S62 (2006).
- ⁶⁸ J. Horacek, M. Cizek, K. Houfek, P. Kolorenc, and W. Domcke, Phys. Rev. A 73, 022701 (2006).
- 69 A. Laricchiuta, R. Celiberto, and R. K. Janev, Phys. Rev. A 69, 022706 (2004).
- ⁷⁰C. S. Sartori, F. J. da Paixao, and M. A. P. Lima, Phys. Rev. A 55, 3243 (1997).
- ⁷¹C. S. Sartori, F. J. da Paixao, and M. A. P. Lima, Phys. Rev. A **58**, 2857 (1998).