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Bibliography of Electron and Photon Cross Sections
with Atoms and Molecules
Published in the 20th Century
– Hydrogen molecules –

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(Received - Jan. 29, 2004)

NIFS-DATA-82

Feb. 2004

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Bibliography of Electron and Photon Cross Sections
with Atoms and Molecules

Published in the 20th Century

— Hydrogen molecules —*

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(Gaseous Electronics Institute)

Bibliographies of original and review reports of experiments or theories of electron and photon cross sections and also electron swarm data are presented for atomic or molecular species with specified targets. These works covered 17 atoms and 51 molecules. The present bibliography is only for hydrogen molecules (H_2 , HD, HT, D_2 , DT, T_2). About 2200 papers were compiled. A comprehensive author index is included. The bibliography covers the period 1901 through 2000 for H_2 . Finally, author's comments for H_2 electron collision cross sections are given.

Keywords : H_2 molecules, collision cross sections, electron, elastic scattering, rotational, vibrational and electronic excitations, dissociation, ionization photon, photoabsorption, photodissociation, photoexcitation, photoionization, electron swarm, drift velocity, diffusion coefficient, ionization coefficient, excitation and ionization energies, transition probabilities, lifetimes of excited states

* This work was carried out under the collaboration research program at National Institute for Fusion Science.

Introduction

History

This bibliography is the result of a continuing literature survey which was begun around 1970 and originally encompassed only electron collision cross section and electron swarm data. The organization responsible for continuing this survey is Nagoya Institute of Technology, Nagoya. From 1994, the work continued to Gaseous Electronics Institute, Nagoya. In 1997, the collection of photon cross section references was begun. The search for references in both cases was retrospective and included all papers reporting measurements, theoretical calculations or reviews and data compilations of such cross sections and electron swarm data.

Scope

This bibliography contains references to original research papers which report experiments or theoretical calculations of cross sections for electron and photon collisions with hydrogen molecules, H₂, HD, HT, D₂, DT, and T₂. The review papers on this subject are also included. Some hydrogen molecule cluster papers are included. Some conference reports, company or agency reports and PhD thesis are included. Hydrogen ion papers and positron collision papers are not included in principle.

Papers reporting the following data are included.

For electron collision cross section :

- 1) elastic scattering
- 2) rotational excitation
- 3) vibrational excitation
- 4) electronic excitation
- 5) dissociation
- 6) ionization
- 7) attachment
- 8) grand total scattering (sum of elastic and inelastic cross sections)
- 9) metastable hydrogen molecules
- 10) electron swarm parameters (drift velocity, diffusion coefficient)
- 11) excitation and ionization coefficients

For photon collision cross section :

- 1) photoabsorption
- 2) photoexcitation and fluorescence
- 3) photodissociation
- 4) photoionization

For some related data :

- 1) excitation and ionization energies
- 2) transition probabilities
- 3) lifetimes of excited states
- 4) others

The energy range for electron cross section data is usually 0 - 10 KeV, but some higher electron energy papers are included. The wavelength range for photon cross section data is from microwave to X-ray. Most papers are concerned with infrared, visible and ultraviolet ray region.

The bibliography includes the papers published in the 20th century, from 1901 to 2000. The oldest paper in this list is given by J. S. Townsend (1901). So for this hydrogen molecules bibliography, published papers from 1901 to 1999 are compiled in alphabetical order of the first author's surname of the paper. References published in 2000 and plus some old papers found very recently after compilation are added as "Addenda of References for Hydrogen Molecules". In total, about 2200 papers are compiled in the hydrogen molecules bibliography.

Organization

This report consists of four parts : introduction, the bibliography and its addenda, author index and some comments on electron collision cross sections.

Bibliography

In this section the complete citation for all references are given. At first following classifications are shown :

- E : Elastic collision
R : Rotational excitation
V : Vibrational excitation
EX : electronic EXcitation
D : Dissociation
I : Ionization
A : Attachment
ME : Metastable hydrogen
S : electron Swarm
O : Others (photon cross sections and the others)

All authors' initials and surname, journal name, volume, inclusive pages and year of publication are given as well as the title, and some additional information in the square bracket []. E and T in the square bracket mean experiment and theory.

Bibliography for H₂, D₂ and so on are divided into four parts :

- Part 1. 1990 - 1999 p. 1 - 29
- Part 2. 1980 - 1989 p. 30 - 65
- Part 3. 1901 - 1979 p. 66 - 169
- Part 4. Addenda of References (1) published in 2000, plus some old papers p. 170 - 183
- Addenda of References (2) published in 2000, plus some old papers p. 184 - 190

Author Index

In this section all authors are listed alphabetically by surname. After each author's name is a list of page numbers indicating which references he or she authored or coauthored. This author index are also divided into four parts :

- Part 1. 1990 - 1999 p. 1 - 6
- Part 2. 1980 - 1989 p. 7 - 13
- Part 3. 1901 - 1979 p. 14 - 25
- Part 4. Addenda of References (1) published in 2000, plus some old papers p. 26 - 29

Some Comments on Electron Collision Cross Sections for H₂

Acknowledgments

The author would like to say many thanks to :

Kazuo Takayanagi and Yukikazu Itikawa of ISAS, Tokyo and Sagamihara,
Hiroyuki Tawara of NIFS, Nagoya and Toki,
Yoshiharu Nakamura of Keio University, Kanagawa,
Yoshihiko Hatano of Tokyo Institute of Technology, Tokyo
for continuous support and encouragement.

The author also would like to say many thanks to the librarians of the following organizations :

Nagoya Institute of Technology, Nagoya
Nagoya University, Nagoya {five libraries}
Institute of Plasma Physics, Nagoya University
National Institute for Fusion Science, Toki
Institute for Molecular Science, Okazaki

Finally, the author would like to say many thanks to Kayo Hirono for longstanding support for the preparation of these bibliographies.

References for H₂, HD and D₂ (1990 - 1999)

(Hydrogen, Deuterium hydride, Deuterium)

E : Elastic collision,	R : Rotational excitation,
V : Vibrational excitation,	EX : Electronic excitation,
D : Dissociation,	I : Ionization,
A : Attachment,	QT : Grand total cross section,
S : Swarm,	α : Ionization coefficient,
O : The others,	[] : Additional informations,
	E : Exp., T : Theory.

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Study of electron-molecule collisions via the finite-element method and
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E : Elastic collision,	R : Rotational excitation,
V : Vibrational excitation,	EX : Electronic excitation,
D : Dissociation,	I : Ionization,
A : Attachment,	QT : Grand total cross section.
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(Hydrogen, Deuterium hydride, Deuterium, Tritium)

E	: Elastic collision.	R	: Rotational excitation.
V	: Vibrational excitation.	EX	: Electronic excitation.
D	: Dissociation.	I	: Ionization.
A	: Attachment.	QT	: Grand total cross section.
S	: Swarm.	α	: Ionization coefficient.
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Some Comments on Electron Collision Cross Sections for H₂

Electron collision cross section set of elastic, rotational excitation, vibrational excitation, electronic excitation, dissociation and ionization collision for hydrogen molecule are reported by many authors. An example is given by A. V. Phelps (1985a) and S. J. Buckman and A. V. Phelps (1985b). Another one is given by Y. Itikawa (1986). But vibrational excitation cross section has the problem as pointed out by R. W. Crompton (1993). See the following related papers : S. J. Buckman (1990), J. P. England (1988), M. A. Morrison (1987) (1991), T. N. Rescigno (1993), and Z. Lj. Petrovic (1987).

Recently, we have pointed out at International Symposium on Electron-Molecule Collisions and Swarms, Tokyo that we cannot measure the exact values of electron collision cross sections for all molecules at present (M. Hayashi (1999). See at the end of this report). For H₂, initial target molecules of beam and swarm experiments are mixture of H₂(g), H₂(r) and small amount of H₂(v) molecules depend on the temperature. Electron collision cross section sets for H₂(g), H₂(r) and H₂(v) are different each other. Hydrogen is the homonuclear diatomic molecule. Then differences of cross section sets for H₂(g), H₂(r) and H₂(v) are not so large, compared with triatomic or polyatomic molecules. But the initial collision cross section sets for three H₂ molecules are different. Probably, not sure now, the value of q_m(r) is larger than q_m(g) as discussed by P. K. Bhattacharyya (1985). The attachment cross section q_a(r) is larger than q_a(g), and q_a(v) is much larger than q_a(g), from the results of Y. Xu (2000) (2001a) (2001b), I. I. Fabrikant (2002) and J. Horacek (2003). If we want the exact values of cross section sets for H₂, we have to determine these three cross section sets of H₂(g), H₂(r) and H₂(v) separately and independently. We have to consider the formation of (H₂)₂ dimer at low temperature condition.

Theoreticians calculate the electron collision cross section set for M(g), not for M(r) and M(v) for most molecules. Theoretical values for M(r) and M(v) are urgently required for many molecules. Recently, some interesting theoretical (plus some experimental) papers on rotationally and vibrationally excited H₂ molecules are published as follows : M. Capitelli (1999), R. Celibert (1990a)-(1997) (2000a) (2000b) (2002), M. Cizek (1998), D. R. Flower (2000), G. A. Gallup (1998), R. I. Hall (1991), M.-T. Lee (2002), S. A. Pozdneev (2000a) (2000b) (2000c), and G. N. Sargsyan (1999).

We would like to have the information about the concentration of (H₂)₂ at liquid N₂ temperature in the swarm experiments of H₂.

I think that there are many uncompiled papers in this hydrogen molecules bibliographies, probably one hundred or more of photon collision papers. I would like to stop the collection of H₂ papers at the beginning of 2004.

May We Measure the Exact Values of
Electron Collision Cross Sections
for Molecules by Beam and Swarm
Experiments ?

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We cannot measure the exact values of DCS for molecules intrinsically. Of course, we can measure the approximate values of DCS for molecules, but can measure the exact values of DCS for atoms. The reason is very simple.

Target molecule M in both beam and swarm experiments consists of the mixture of different states :

$$M = M(g) + M(r_s) + M(v_1) + M_N$$

where $M(g)$, $M(r_s)$, $M(v_1)$ and M_N represent the completely ground state molecules, the rotationally excited molecules, the vibrationally excited molecules and the van der Waals clusters consisting of N molecules ($N \geq 2$), respectively. Usually beam and swarm experiments are carried out at about 300 K. The concentration of $M(g)$ is small compared to $M(r_s)$ (except H_2 molecules) at 300 K. Then the molecule M is always mixture of $M(r_s)$ and $M(v_1)$, and the concentration of $M(r_s)$ and $M(v_1)$ changes with temperature. And electron collision cross section sets from elastic to inelastic collision processes for $M(r)$ and $M(v)$ are different each other. The target molecules M in the beam and swarm experiments are always mixtures of different molecules $M(r_s)$ and $M(v_1)$. In the case of H_2 , the target gas consists of $M(g)$ and $M(r_s)$, especially $M(g)$ and $M(r_s)$ at 78 K.

Most clear change of cross sections of $M(r_s)$ and $M(v_1)$ will occur for triatomic molecules. CO_2 , N_2O and so on. Triatomic molecules can change from linear to bend, or vice versa easily. The authors [1] have presented the different elastic momentum transfer cross sections q_{mr} and q_{mv} for $CO_2(r)$ and $CO_2(v)$, where they assumed that all other inelastic cross sections of $CO_2(r)$ and $CO_2(v)$ are practically the same. Then they have calculated the electron drift velocity W as a function of gas temperature T. When T increases, concentrations of $CO_2(v)$ increases, then W decreases with T at the same E/N, the electric field over the gas number density, around 50 Td.

We have a comment to the interesting and important paper of W. Johnstone, et al. [2]. They have measured the temperature dependence of elastic DCS for CO_2 at 4.0 eV. Unfortunately, q_{mv} for $CO_2(v)$ at 4 eV is almost equal to q_{mr} for $CO_2(r)$ [1]. Then we propose the same experiments at about 3.4 eV for CO_2 , because the temperature dependence of DCS seems to be very large there.

Winstead and McKoy [3] calculated the elastic DCS for $N_2O(g)$ at low electron energies and compare the experimental DCS data for $N_2O(r) + N_2O(v)$ mixture at 300 K. We can see large discrepancy between them at lower than about 10 eV. We urge Winstead and McKoy to calculate the DCS

for $N_2O(v)$ and also $N_2O(r)$ for comparison. We can see the same discrepancy of DCS for CO_2 . [4] [5] at low electron energies..

H_2 molecules have the famous long standing controversy in the vibrational excitation cross section [6]. A possible way to solve the problem may be as follows. At first, theoreticians calculate the Q_{mg} , Q_{mr} , Q_{mv} , Q_{rg} , Q_{rr} , Q_{rv} , Q_{vg} , Q_{vr} , and Q_{vv} for $H_2(g)$, $H_2(r_1)$ and $H_2(v_1)$, as a function of electron energies. Using these data, we calculate the electron swarm parameters. From beam experiments, we cannot determine the values of Q_{mg} , Q_{mr} , Q_{rg} , Q_{rr} for $H_2(g)$ and $H_2(r_1)$ at the same time. It is clear that the threshold energies of q_r and q_v for $H_2(g)$ and $H_2(r_1)$ are different. Bhattacharyya, et al. [7] have shown that elastic integral cross sections Q_{tr} are larger than Q_{ts} for 20 to 200 eV for $H_2(g)$ and $H_2(r_1)$. We want the elastic DCS values for $H_2(g)$ and $H_2(r_1)$ at low electron energies lower than 10 eV. Swarm experiments also carried out in the mixtures of $H_2(g)$ and $H_2(r_1)$, except for para- $H_2(g)$ at 78 K (concentration of $H_2(g)$ is 99.3 %). We compare the experimental and calculated swarm parameters at given conditions.

Usually, theoreticians calculate the DCS for $M(g)$, not for $M(r_1)$ and $M(v_1)$, for most molecules. Theoretical studies involving the rotationally and vibrationally excited species are urgently required for many molecules. There is a interesting paper given by A. Jain [8].

If we have the cross section sets for excited inert gas clusters, we can calculate the electron swarm parameters of inert gases at high pressure and low temperature conditions. The concentration of the clusters for atoms and molecules are important at low temperature and high pressure conditions.

Most interesting temperature dependence occur for attachment cross sections q_a [9]-[13]. The values of non-dissociative q_{an} and dissociative q_{ad} are quite different for $M(r)$ and $M(v)$, and $M(r)$ and $M(v)$ have the definit and individual cross sections, independ on the temperature. Apparent temperature dependence of attachment cross section is caused through different concentration of the excited components $M(r)$ and $M(v)$ at different temperatures.

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published in the 20th Century

Atoms (17)				Molecules (51)			
	A + e,	A + hν		M + e,	M + hν,		
He 2	2170 *		2	H ₂ , D ₂	2200 ○	5	CH ₄ 800
Ne 10	1140 *			N ₂	2240 ○		
Ar 18	1960 ○			O ₂	1700	CF ₄ 390	
Kr 36	1000			CO	1190	CCl ₄ 210	
Xe 54	1180 ○			NO	880	CCl ₂ F ₂ 250	
						CH ₃ Cl 90	
Li 3	450			F ₂	190 ○		
Na 11	800			Cl ₂	360 ○	SiH ₄ 230	
				Br ₂	140 ○	SiF ₄ 140	
K 19	370			I ₂	240 ○	GeH ₄ 50	
Rb 37	220						
Cs 55	370			HF	260	6 C ₂ H ₄ 370	
				HC ₁	320	CH ₃ OH 350	
O 8	390			HBr	200		
				HI	130	7 SF ₆ 920 ○	
F 9	90						
Cl 17	130		3	CO ₂	1240 ○	8 C ₂ H ₆ 260	
				H ₂ O	1200 ○	C ₂ F ₆ 150	
Cu 29	180			O ₃	480	Si ₂ H ₆ 70	
Cd 48	210			N ₂ O	450		
Ba 56	340			NO ₂	350	9 C ₃ H ₆ 120	
Hg 80	600			H ₂ S	270	C ₂ H ₅ OH 60	
				SO ₂	290		
				CS ₂	260		
				OCS	280	11 C ₃ H ₈ 190	
not final, but finished mostly			4	C ₂ H ₂	390	C ₃ F ₈ 100	
include electron swarm papers				NH ₃	700	12 C ₄ F ₈ 100	
				NF ₃	110	C ₆ H ₆ 240	
				BF ₃	110	C ₆ F ₆ 100	
include review papers				BCl ₃	90	60 C ₆₀ 300	
				PH ₃	120		
				H ₂ CO	180	M _r + M _v 850	

* He(Ne) + e only. Not include He(Ne) + hν papers.

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