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

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(Received - May 1, 2003)

NIFS-DATA-76

May 2003

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Bibliography of Electron and Photon Cross Sections

With Atoms and Molecules

Published in the 20th Century

—— Sulphur Hexafluoride ——*

Makoto Hayashi

(Gaseous Electronics Institute)

A bibliography 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 sulphur hexafluoride (SF₆). About 920 papers were compiled. A comprehensive author index is included. The bibliography covers the period 1934 through 2000 for SF₆. Finally, author's comments for SF₆ electron collision cross section are given.

Keywords : SF₆ molecule, collision cross section, 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 sulphur hexafluoride SF₆. The review papers on this subject are also included. Some SF₆ molecule cluster papers are included. Some conference reports, company or agency reports and PhD thesis are included. SF₆ 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) electron swarm parameters (drift velocity, diffusion coefficient)
- 10) 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. Oldest papers in this list are given by A. Eucken (1934) and M. Yost (1934). So for this SF₆ bibliography, published papers from 1934 to 1999 are compiled by alphabetical order of the first author's surname of the paper. And the references published in 2000 and plus some old papers found very recently after compilation are added as "Addenda of References for SF₆ (1)". In total, about 920 papers are compiled in the sulphur hexafluoride SF₆ molecule 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 argon
- 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 SF₆ are divided into two parts :

- Part 1. 1980 - 1999 p. 1 - 40
- Part 2. 1901 - 1979 p. 41 - 61
- Part 3. Addenda of References (1) published in 2000, plus some old papers p. 62 - 74
- Part 4. Addenda of References (2) some old papers p. 75 - 78

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.

- Part 1. 1901 - 1999 p. 1 - 12
- Part 2. Addenda (1) p. 13 - 16

Some Comments on Electron Collision Cross Sections for SF₆

Acknowledgments

The author would like to say many thanks to :
Kazuo Takayanagi and Yukikazu Itikawa of ISAS, Tokyo and Sagami-hara,
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 SF₆ (1980 - 1999)

(Sulphur hexafluoride, Sulfur hexafluoride)

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

Some important papers published until 1979 are included in this part.

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Electron attachment coefficients determined using a flowing afterglow/Langmuir probe (FALP) apparatus.
[E, SF₆, CCl₄, CCl₃F, CCl₂F₂, CHCl₃, Cl₂; see D. Smith (1984)]
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A comparison of shape resonant behaviour in the inner-shell photo-absorption and valence-level photoelectron spectra of SF₆, SF₅Cl and SeF₆.
[E, h ν , SF₆, etc.; 21.2 - 215 eV]
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A comparison of valence level photoelectron cross sections for SF₆, SeF₆ and "F₆" from 21 eV to 100 eV photon energy. [E, h ν , SF₆, etc.]
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Line shape for attachment of threshold electrons to SF₆ and CFCl₃ : Threshold photoelectron (TPSA) studies of Xe, CO, and C₂H₂.
[E, SF₆, CFCl₃]
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[review, SF₆, O₂, SO₂, etc.]
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Doubly differential cross sections for the ionization of the SF₆ molecule by electron impact. [E, SF₆; 100, 200 eV]
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[T, SF₆, SF₆ + O₂]

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 H. Polyatomic gases. [E, SF₆, CCl₂F₂, N₂O, etc.]
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 A Isoliergasgemischen mit einer verbesserten Swarm-Methode.
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 Measurements of electron and ion transport data in SF₆ and SF₆/N₂ mixtures.
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E : Elastic collision,	R : Rotational excitation,
V : Vibrational excitation,	EX : Electronic excitation,
D : Dissociation,	I : Ionization,
A : Attachment, Detachment	QT : Grand total cross section,
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Some Comments on Electron Collision Cross Sections for SF₆

The pioneer work on electron collision cross section set for SF₆ is given by L. E. Kline in 1979. After that, many cross section sets for SF₆ are proposed by T. Yoshizawa (1979), H. Itoh (1980, 1990), J. P. Novak (1982, 1984), M. Yousfi (1982, 1985, 1987, 1994), M. S. Dincer (1983), M. Hayashi (1984, 1991), Th. Vassiliadis (1985) and A. V. Phelps (1988). The authors' conference preprint M. Hayashi (1991) is included at the end of this report. In this preprint, the author presented the improved cross section set using new experimental data. Recently, L. G. Christophorou (2000) reviewed the new data and recommended cross section set for SF₆ are shown in Fig. 47 of their paper.

Now author do not like these all cross section sets. In 1999, author discussed that SF₆ molecules used in the beam and swarm experiments are always mixture of SF₆(r) and SF₆(v). r and v mean rotationally and vibrationally excited one. At 300 K, the concentration of ground state SF₆(g) molecules are negligible small. SF₆(r_J) = 30.1 %, SF₆(v₆) = 17.2 %, SF₆(v₅) = 7.4 %, SF₆(2v₆) = 6.5 % and SF₆(v₄, v₂, v₁, v₃, etc.) = 38.8 %. The cross section sets for SF₆(r_J) and SF₆(v₁) are different each other. At least, we have to determine these many cross section sets for the exact calculations.

All molecules have the same component M(g), M(r), M(v) and M_n (n = 2), depend on the pressure and temperature conditions of the experiment. Most interesting experimental results occur in the triatomic molecules. The change from linear mode combination of three atoms to bend mode combination of three atoms, or vice versa, occur very easy by vibrational excitation. SF₆ molecule is an octahedral molecule belonging to the O_h group, with very high symmetry. So the difference of cross section sets for SF₆(r) and SF₆(v) are not so large compared with the difference of triatomic molecules. Then cross section sets given by many authors, assuming all SF₆ molecules are in the SF₆(g) or SF₆(r) or SF₆(v) state, can use for approximate calculations for SF₆.

Author would like to present our recent two conference preprints at the end of this report.

M. Hayashi and S. Hara : Joint Symposium on Electron and Ion Swarms and Low Energy Electron Scattering, Bond University, Australia 109-111 (1991)

M. Hayashi and Y. Nakamura : International Symposium on Electron-Molecule Collisions and Swarms, EMS-99, Tokyo 175-176 (1999)

ELECTRON COLLISION CROSS SECTIONS FOR SF₆

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We have determined a new set of elastic and inelastic electron collision cross sections for SF₆ using the data obtained by beam experiments mainly and electron swarm experiments a little.

There are many cross section sets for SF₆. We have the sets given by Kline(1979), Yoshizawa(1979), Dincer(1983), Novak(1982, 1984), Hayashi¹⁾(1984), and Yousfi(1985). In 1988, Phelps²⁾ and Itoh³⁾ reported the new sets, but these two cross sections are different each other. Last year we have discussed again the all cross sections, including the new experimental data. Important beam experiments after 1988 are as follows: for elastic scattering, Sakae⁴⁾, 20-700 eV, and Johnstone⁵⁾, 5-75 eV; for attachment, Fenzlaff⁶⁾, 0-19 eV, and Hunter⁷⁾, 0-10 eV; for grand total cross section Q_T , Dababneh⁸⁾, 2.8-500 eV, and Zecca⁹⁾, 92.5-4000 eV.

Present tentative conclusion is given in Figure 1. Present final values of momentum transfer cross sections q_m are compared with reference values as shown in Figure 2. White triangle points in Fig-

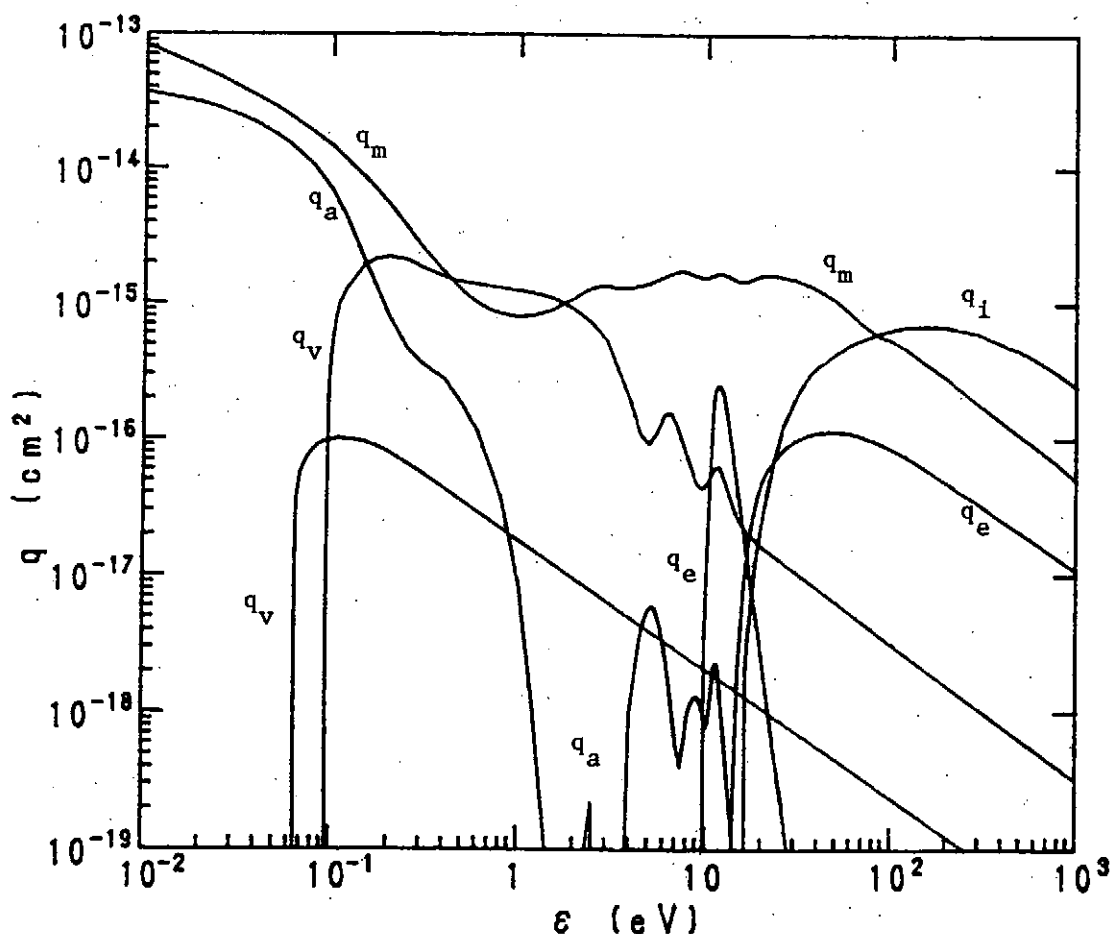


Figure 1. Electron collision cross sections for SF₆.

ure 2 are calculated from Rohr's DCS values. But we had to reduce the values of q_m for the electron energies from 1 to 5 eV by electron swarm data, as shown in Figure 2. The DCS values measured by Sakae⁴⁾ are much larger than Trajmar's one, especially at small scattering angles. We have used Sakae's data under some improvements by "smoothing method"¹⁰⁾. It was concluded that Johnstone's⁵⁾ new values at around 10 eV is good and have interesting structure, but the values at around 50 eV are smaller than true values. Then more exact DCS experiments are needed for the electron energies from 1 to 100 eV, especially 2, 3, 4, 30 and 50 eV of wide scattering angles.

In our old paper¹⁾, we have pointed out that the values of very small attachment cross sections q_a of F^- formation are important for the determination of electron swarm data, and also there is a large contradiction between measured Q_T and sum of all cross sections. Nobody discuss this latter problem in the literatures. From this study, we have found a solution of this problem approximately, for the first time, as shown in figure 3.

Electron swarm parameters have been calculated from the cross sections shown in Figure 1, using two term approximation of Boltzmann equation solution. Calculated electron drift velocities are almost coincide with Aschwanden's and Nakamura's¹¹⁾ values, and characteristic energies also almost fit with Naidu's and Maller's data. Ionization coefficients agree with Aschwanden's and our data below about

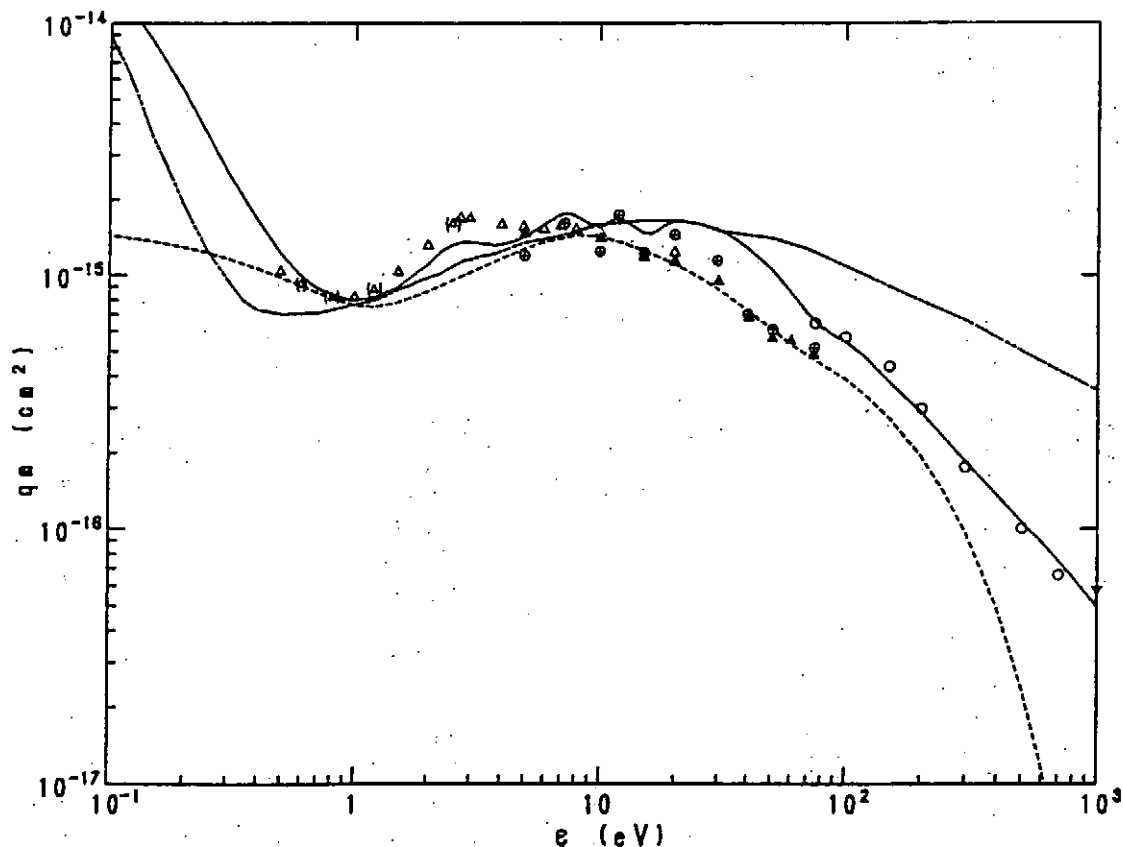


Figure 2. Momentum transfer cross sections q_m for SF_6 . Solid line is the present value. Dotted and line is Phelps' and dotted line is Itoh's value. Δ : Rohr, Θ : Johnstone, \blacktriangle : Trajmar, and \circ : Sakae. These values are integrated values from DCS experiments.

600 Td. More exact approximation is needed for the calculations, and slight improvements of cross section values are needed from the exact calculations of swarm parameters.

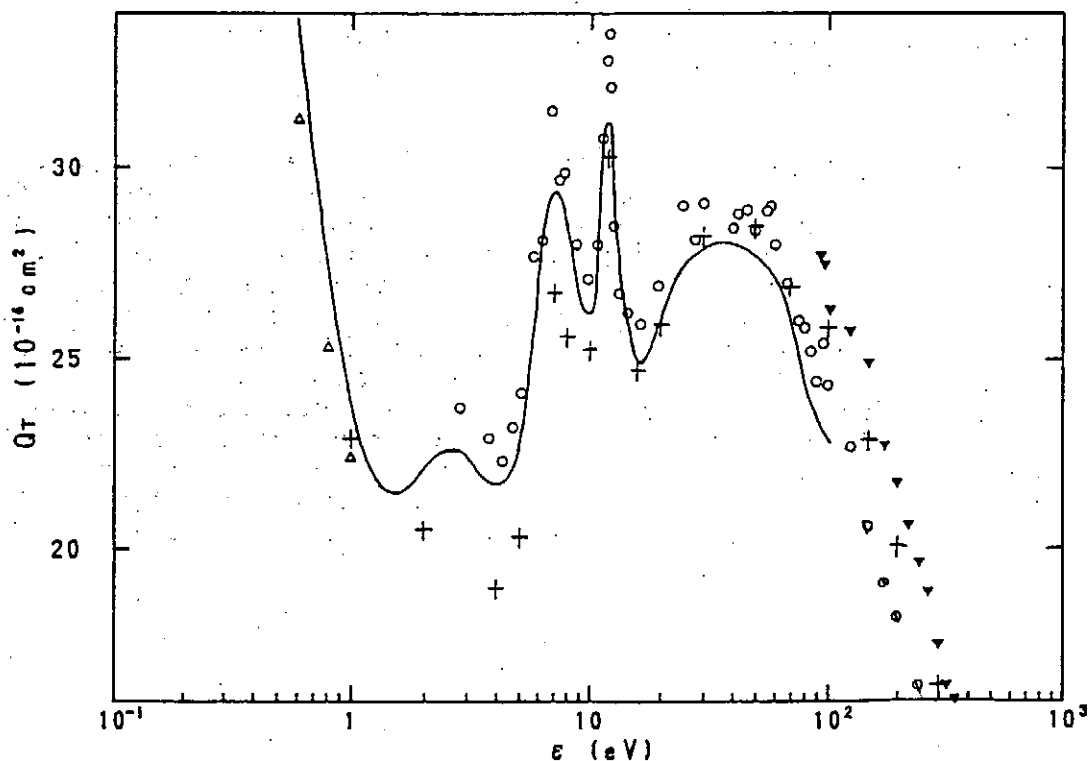


Figure 3. Grand total cross sections Q_T for SF_6 . + : sum of all cross sections given in Figure 1, but for elastic scattering, the values of integral elastic cross section q_t , instead of q_m , are summed. Solid line : Kennery, Δ : Ferch, O : Dababneh, and ∇ : Zecca.

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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 :

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

where $M(g)$, $M(r_j)$, $M(v_1)$ 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 $M(r_j)$ (except H_2 molecules) at 300 K. Then the molecule M is always mixture of $M(r_j)$ and $M(v_1)$, and the concentration of $M(r_j)$ 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 $M(r_j)$ and $M(v_1)$. In the case of H_2 , the target gas consists of $M(g)$ and $M(r_j)$, especially $M(g)$ and $M(r_1)$ at 78 K.

Most clear change of cross sections of $M(r_j)$ 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_{tg} 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 $M(r_j)$ 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_{aa} are quite different for $M(r)$ and $M(v)$, and $M(r)$ and $M(v)$ have the definite and individual cross sections, independent 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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Atoms (17)			Molecules (51)			
A + e.	A + hν		M + e.	M + hν.		
He 2	2170 *	2	H ₂ , D ₂	1870	5	CH ₄ 780
Ne 10	1140 *		N ₂	2240		
Ar 18	1960		O ₂	1700		CF ₄ 390
Kr 36	900		CO	1190		CCl ₄ 210
Xe 54	1040		NO	880		CCl ₂ F ₂ 250
						CH ₃ Cl 90
Li 3	450		F ₂	190		SiH ₄ 230
Na 11	800		Cl ₂	360		SiF ₄ 140
K 19	370		Br ₂	140		GeH ₄ 50
Rb 37	220		I ₂	240		
Cs 55	370				6	C ₂ H ₄ 370
			HF	260		CH ₃ OH 240
O 8	390		HCl	320		
			HBr	190		
F 9	90		HI	130	7	SF ₆ 920
Cl 17	130					
		3	CO ₂	1240		
					8	C ₂ H ₆ 260
Cu 29	180		H ₂ O	850		C ₂ F ₆ 150
Cd 48	210		O ₃	480		Si ₂ H ₆ 70
Ba 56	320		N ₂ O	450		
			NO ₂	300	9	C ₃ H ₆ 120
			H ₂ S	270		C ₂ H ₅ OH 60
Hg 80	600		SO ₂	260		
			CS ₂	260		
			OCS	240	11	C ₃ H ₈ 190
not final, but finished mostly						C ₃ F ₈ 100
		4	C ₂ H ₂	390		
					12	C ₄ F ₈ 100
include electron swarm papers			NH ₃	400		C ₆ H ₆ 240
			NF ₃	110		C ₆ F ₆ 100
			BF ₃	110		
include review papers			BCl ₃	90	60	C ₆₀ 300
			PH ₃	80		
			H ₂ CO	180		M _r + M _v 850

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

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