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Bibliography of Electron and Photon Cross Sections  
with Atoms and Molecules  
Published in the 20<sup>th</sup> Century  
– Water vapour –

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# Bibliography of Electron and Photon Cross Sections

with Atoms and Molecules

Published in the 20<sup>th</sup> Century

—— Water vapour ——\*

Makoto Hayashi

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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 water vapour (H<sub>2</sub>O, D<sub>2</sub>O and HDO). About 1200 papers were compiled. A comprehensive author index is included. The bibliography covers the period 1915 through 2000 for H<sub>2</sub>O. Finally, author's comments for electron collision cross sections and photodissociation processes of H<sub>2</sub>O are given.

Keywords : H<sub>2</sub>O molecule, 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

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## 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 Insititute, 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 water vapour  $H_2O$ . The review papers on this subject are also included. Some water vapour molecule cluster papers are included. Some conference reports, company or agency reports and PhD thesis are included. Water vapour 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 nitrogen 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. Oldest paper in this list is given by J.S.Townsend (1915). So for this water vapour bibliography, published papers from 1915 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 H<sub>2</sub>O (1) and (2) ". In total, about 1200 papers are compiled in the water vapour 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 H<sub>2</sub>O are divided into two parts :

- Part 1. 1915 - 1999 p. 1 - 78  
Part 2. Addenda of References (1) and (2) published in 2000, plus  
some old papers p. 79 - 104

#### 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. 1915 - 1999 p. 1 - 13  
Part 2. Addenda (1) p. 14 - 17

Some Comments on Electron Collision Cross Sections and  
Photodissociation Processes for H<sub>2</sub>O

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References for H<sub>2</sub>O, HDO and D<sub>2</sub>O

and radical OH and OD (1900 - 1999)

(Water vapour, Deuterated water, Heavy water)

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,	$\alpha$	: Ionization coefficient,
O	: The others,	[ ]	: Additional informations,
		E	: Exp., T : Theory.

The oldest paper in this list is given by J. S. Townsend (1915).

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Semiclassical approach to the abnormal rotation of OH(A<sup>2</sup>Σ<sup>+</sup>) resulting  
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CO<sub>2</sub>, NH<sub>3</sub>, CH<sub>4</sub> - C<sub>5</sub>H<sub>12</sub>, etc.]
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Author Index for H<sub>2</sub>O References

- H. Aachi 57  
C. N. Abeyta 42  
H. Abgrall 8  
E. H. Abramson 1  
Y. Achiba 35, 36  
A. Adamczyk 45  
H. Agren 1, 34, 50  
R. Akamatsu 1  
N. Aktekin 59  
R. G. Albridge 35  
M. I. Al-Jobury 1  
A. Alkaa 77  
J. E. Allen 14  
L. J. Allen 42  
A. C. Allison 72  
S. Altshuler 1, 46  
R. D. Amado 6  
K. Amos 42  
R. D. Amos 1  
T. Anderson 53  
P. Andresen 1, 2, 20, 60  
L. Andric 16  
V. Ya. Antonchenko 2  
Th. Antoni 35  
J. Appell 2  
M. B. Arfa 2  
E. Arie 33  
A. T. Armstrong 12  
R. L. Armstrong 76  
M. N. R. Ashfold 2, 3, 30  
O. Ashihara 3  
N. Astoin 3, 34  
S. H. Autler 5  
F. W. Averill 57  
D. L. Azevedo 72  
R. Azria 3, 71  
  
D. S. Baer 48  
M. A. Baig 14  
T. L. Bailey 3, 48  
V. A. Bailey 3  
A. D. Baker 3  
G. G. Balint-Kurti 3, 60  
J. Ballard 33  
M. S. Banna 4  
  
I. Bar 16  
A. Barbe 24, 33, 57  
R. S. Barbieri 14  
J. B. Barriol 56  
G. Basavaraju 4  
H. Basch 64  
A. M. Bass 6  
A. Bauer 4  
D. L. Baulch  
W. Baumann 4, 23, 45  
A. O. Bawagan 4  
K. D. Bayes 4  
J. M. Bayley 3, 30  
V. I. Bazhanov 5  
T. V. Bazhenova 5  
E. C. Beaty 24, 51, 52  
G. E. Becker 5  
K. Becker 5, 18, 67  
C. I. M. Beenakker 5, 47  
M. J. M. Beerlage 5  
D. S. Belic 5  
S. Bell 5  
M. D. Benabdessadok 77  
J. Benard 11  
M. Ben Arfa 2, 5  
W. S. Benedict 6, 25, 46, 49, 67  
D. C. Benner 57  
T. Bergmark 35  
J. L. Berkosky 55  
J. Berkowitz 38  
P. Bernath 73  
P. F. Bernath 54  
M. H. F. Bettega 72  
V. Beushausen 2  
K. D. Beyer 6  
K. Bhanuprakash 6  
S. M. Bharathi 4  
K. G. Bhushan 4  
S. F. Biagi 6  
F. Biggs 56  
R. Bijker 6  
T. P. Birbeck 38, 39  
D. M. Bishop 7  
G. Bjoraker 33

G. Black 64  
 J. H. Black 64  
 A. J. Blake 7  
 K. Blum 40, 41  
 M. Bobeldijk 7  
 F. W. Bobrowicz 76  
 A. J. H. Boerboom 62  
 L. Boesten 59  
 L. P. Boivin 7  
 R. C. Bolden 7  
 M. A. Bolorizadeh 7  
 K. Bonhoff 40, 41  
 S. Bonhoff 40, 41  
 B. Bonnet 33  
 T. E. Bortner 31  
 N. Bose 7  
 R. Botter 8  
 L. Bouby 8  
 Y. Bouteiller 8  
 C. Boyle 21  
 F. P. Boynton 42  
 N. E. Bradbury 8  
 J. E. S. Bradley 18  
 A. M. Bradshaw 61  
 S. L. Bragg 8  
 J. W. Brault 43  
 J. M. Braut 28  
 M. Braunstein 42, 65  
 B. Brehm 8  
 M. Breitenstein 8  
 D. J. Brenner 8, 77  
 L. M. Brescansin 8, 40, 41, 42, 43  
 W. W. Brim 49  
 C. E. Brion 4, 8, 9, 13, 19, 24, 30,  
 51, 67, 75, 78  
 J. P. Bromberg 9  
 H. H. Brongersma 37  
 L. R. Brown 9, 33, 57, 70  
 C. R. Browne 19  
 R. Browning 19  
 E. Bruche 9  
 C. R. Brundle 3, 9  
 M. J. Brunger 10, 20  
 R. Brusa 66  
 R. S. Brusa 77  
 W. A. Bryan 59  
 Th. Bubel 47  
 I. S. Buchel'nikova 10  
 S. J. Buckman 10  
 R. J. Buenker 6, 10, 68  
 W. E. Bull 46  
 P. Bundgen 30  
 J. Busler 73  
 J. R. Busler 54  
 B. L. Bytchkov 10  
 I. Cacelli 10, 11  
 V. E. Cachorro 11  
 I. Cadez 38, 56  
 I. M. Cadez 18  
 C. Cahen 11  
 R. B. Cairns 11  
 R. Camilloni 11  
 C. Camy-Peyret 10, 11, 12, 13, 21, 22,  
 33, 43, 53, 57, 69  
 N. M. Cann 51  
 C. G. Cannon 18  
 J. Carlier 4, 8  
 T. A. Carlson 12, 46  
 F. Carnovale 9  
 V. Carravetta 1, 10, 11  
 T. Carrington 12, 30  
 D. G. Carroll 12  
 P. Carsky 13  
 J. H. Carver 7  
 J. L. Casanova 11  
 M. E. Casida 19  
 C. Chabalowski 6  
 P. Chandra 6  
 Y. S. Chang 13  
 C. T. Chen 61  
 D. -W. Chen 22  
 X. J. Chen 42  
 B. Cheung 13  
 L. M. Cheung 7  
 J. -P. Chevillard 12, 13, 43  
 M. S. Child 13, 26, 30, 53, 73  
 S. L. Chin 17  
 H. Cho 13  
 S. Y. Cho 63  
 D. P. Chong 19  
 S. Chou 72  
 S. I. Chou 48  
 A. A. Christodoulides 14  
 L. G. Christophorou 14  
 A. Chutjian 14, 71  
 H. H. Claassen 6  
 H. Clasen 49  
 C. R. Claydon 14  
 P. Cloutier 14

R. J. Cody 14  
 R. Cohen 14  
 D. Coimbra 14  
 J. E. Collin 24  
 L. A. Collins 6  
 D. Combecher 14  
 R. N. Compton 14, 36, 75  
 G. Comtet 22  
 J. P. Connerade 14  
 G. R. Cook 45  
 G. Cooper 13, 51, 78  
 M. A. Coplan 15  
 R. B. Cordaro 15  
 M. Cottin 15  
 J. D. Craggs 15, 55  
 T. E. Cravens 15, 37, 63  
 O. H. Crawford 15, 75  
 F. F. Crim 15, 20, 61  
 R. W. Crompton 15, 31  
 D. Cubric 35  
 M. G. Curtis 16  
 D. Cvejanovic 16, 35  
 S. Cvejanovic 35  
  
 F. W. Dalby 16  
 A. Dalgarno 16, 72  
 N. Damany 18  
 A. Danjo 16  
 F. J. da Paixao 16  
 M. Darrach 16  
 D. David 16  
 V. A. Davidenko 17  
 E. R. Davidson 4, 21, 78  
 W. F. Davidson 7  
 F. J. Davis 75  
 G. R. Davis 17  
 L. I. Davis 73  
 D. J. Dawson 77  
 Dayashankar 17, 27  
 T. P. Debies 17, 55  
 D. P. De Bruijn 22  
 J. Debyshire 17  
 J. E. Decker 17  
 P. Decleva 42  
 A. M. de Frutos 11  
 F. J. de Heer 5, 17, 47, 62, 71, 73  
 J. L. Dehmer 55  
 P. M. Dehmer 17, 55  
 F. C. de Lucia 17  
 F. C. De Lucia 53  
  
 J. Delwiche 24  
 D. M. Dennison 56  
 J. Derbyshire 17, 36  
 L. de Reilhac 18  
 C. Desfrancois 8  
 H. Deutsch 18, 44, 67  
 V. M. Devi 57  
 R. V. de Vore 49  
 M. J. S. Dewar 18  
 S. Dey 18  
 V. H. Dibeler 18  
 M. A. Dillon 39, 64  
 T. A. Dillon 41  
 R. B. Diniz 72  
 R. W. Ditchburn 18  
 A. J. Dixon 18  
 R. N. Dixon 3, 30  
 N. Djuric 18  
 N. Lj. Djuric 18  
 M. P. Docker 18  
 J. P. Doering 15, 19  
 T. J. Dolan 19  
 B. A. Dolgoshein 17  
 F. H. Dorman 19  
 A. A. Dougal 67  
 M. Doumont 19  
 D. Yu. Dubov 73  
 P. Duffy 19  
 A. B. F. Duncan 41  
 W. E. Duncanson 3  
 K. F. Dunn 19  
 T. H. Dunning 19  
 J. Durup 2  
 J. Dutton 19, 24  
 O. Dutuit 19  
  
 E. D. Earle 7  
 F. Edard 5  
 D. A. Edmonson 19  
 D. P. Edwards 58  
 F. Egger 44  
 H. Ehrhardt 19, 35  
 M. T. Elford 13, 20  
 D. E. Ellis 57  
 F. O. Ellison 55  
 M. W. Elsasser 20  
 A. El-Zein 20, 59  
 R. Emery 20  
 V. Engel 20, 60



V. F. Erko 54  
 P. Erman 76  
 D. D. Errett 21  
 M. P. Esplin 21

I. I. Fabrikant 21  
 S. Falk 62  
 C. B. Farmer 9, 69  
 D. Feil 5  
 J. Feldhaus 61  
 D. Feller 4, 21  
 W. S. Felps 74  
 L. G. Ferreira 72  
 T. A. Ferrett 9  
 C. C. Ferriso 42  
 F. H. Field 38  
 W. H. Fink 31  
 F. Fiquet-Fayard 3, 21, 71  
 G. Fischer 61  
 B. M. Fizgeer 54  
 M. R. Flannery 45  
 J. M. Flaud 11, 21, 69  
 J. -M. Flaud 10, 11, 12, 13, 21, 22,  
 43, 53, 57, 58, 69  
 F. Flouquet 22, 31  
 J. Fournier 22  
 P. G. Fournier 22  
 S. A. Francis 39  
 J. L. Franklin 38  
 G. R. Freeman 25  
 K. Freudenberg 4, 23  
 R. S. Freund 23  
 A. A. Fridman 58  
 W. Frisch 26  
 H. Frohlich 19  
 G. Fronzoni 42  
 D. C. Frost 23  
 K. Fujima 59  
 T. Fujita 23, 24  
 N. I. Furashov 58  
 M. Furlan 24  
 K. Furuya 24

N. Gailar 6  
 J. W. Gallagher 24  
 R. R. Gamache 24, 25, 57  
 D. Garg 34  
 W. R. S. Garton 14  
 R. H. Garvey 27  
 J. P. Gauyacq 67

A. Gedanken 25  
 N. Gee 25  
 U. Gelius 50  
 S. Geltman 67  
 B. Gentry 26, 75  
 R. B. Gerber 28  
 K. R. German 25  
 F. A. Gianturco 11, 25, 26, 33, 60, 69  
 T. L. Gibson 8, 41  
 T. J. Gil 26  
 R. D. Gilbert 26, 73  
 N. Ginsburg 56, 59  
 L. P. Giver 26, 75  
 N. V. Gloskovskaya 2  
 A. W. Goddard III 76  
 W. A. Goddard III 26, 31  
 M. Godon 4  
 A. Goldman 57, 58  
 V. F. Golovko 65  
 T. I. Gombosi 37  
 J. -C. Gomet 26  
 T. I. Gomvosi 15  
 D. M. Goodall 26, 37  
 J. M. Goodings 27  
 B. Gou 27  
 Q. Gou 27  
 S. Goursaud 71  
 A. Grafe 63  
 E. R. Grant 40  
 W. B. Grant 27  
 A. E. S. Green 17, 27, 51  
 D. A. Greenhalgh 56  
 R. C. Greenhow 26, 37  
 R. Greer 27  
 J. K. Gregory 27  
 B. E. Gribov 37  
 H. E. Griesinger 64  
 R. Grisenti 66, 77  
 B. E. Grossmann 11, 27  
 G. Guelachvili 11, 12, 22, 27, 43  
 A. G. Guidoni 11  
 R. J. Gulley 10  
 J. R. Gunn 74  
 B. Guo 54, 73  
 M. V. Gur'ev 66  
 P. Gurtler 27  
 P. M. Guyon 19, 21, 45

G. N. Haddad 28  
 R. I. Hall 5, 14, 16, 28, 71

W. H. Hamill 41  
 A. Hamnett 30  
 R. K. Hanson 2, 38, 39, 48  
 Y. Harada 28  
 J. W. Harder 28  
 P. W. Harland 72  
 H. Harrison 11  
 P. Harteck 68  
 H. J. Hartfuss 28  
 J. N. Harvey 28  
 J. B. Hasted 44  
 Y. Hatano 29, 32, 37, 44  
 Ya. Hatano 28, 50  
 Yo. Hatano 28  
 D. Hausler 2, 60  
 P. J. Hay 31  
 G. Hayakawa 28  
 M. Hayashi 28, 29  
 A. N. Hayhurst 27  
 M. S. Hegde 55  
 I. Heiber 41  
 P. A. Heimann 9  
 K. Heinzinger 2  
 P. Helminger 17, 53  
 A. Henglein 19, 29  
 A. Hennad 77  
 S. Hennig 60, 74  
 H. J. Henning 29  
 E. Herbst 53  
 G. Herzberg 29  
 W. Hilgner 29  
 P. R. Hilton 29  
 K. Hinkle 73  
 K. Hirao 29, 48  
 S. Hirokura 50  
 D. M. Hirst 30  
 A. Hodgson 18, 30  
 R. E. Hoffmeyer 30  
 Y. -S. Hoh 22  
 M. L. Hoke 21  
 D. M. P. Holland 17  
 K. W. Hollman 30  
 P. H. Hollosay 58  
 J. F. Holzwarth 26  
 S. T. Hood 30  
 T. Horie 30, 71  
 J. A. Horsley 22, 31  
 J. E. Houston 58  
 K. C. Hsieh 15  
 J. J. Huang 55  
 M. -J. Hubin-Franskin 24  
 B. Hudson 20  
 R. H. Huebner 14  
 R. E. Huffman 35  
 W. J. Hunt 26, 31  
 W. M. Huo 8, 39, 41  
 G. S. Hurst 31, 65  
 N. S. Hush 29  
 N. Husson 57  
 A. Hustrulid 43  
 L. G. H. Huxley 31  
 W. Hwang 31  
 I. Iga 56  
 S. Ihara 51  
 V. V. Ilyin 2  
 D. G. Imre 1, 77  
 E. C. Y. Inn 74  
 M. Inokuti 31, 36  
 S. Isaka 71  
 K. Ishibashi 35  
 E. Ishiguro 32  
 M. A. Ishii 31  
 Y. Ishikawqa 48  
 Y. Itikawa 31, 32, 50, 51  
 K. Ito 32, 37, 47  
 Y. Ito 69  
 T. Iwai 23, 24, 71  
 S. Iwata 32  
 C. F. Jackels 33  
 C. H. Jackman 27  
 N. Jacquinet-Husson 33  
 R. Jadrny 35  
 K. Jager 19  
 A. Jain 25, 33  
 A. K. Jain 33  
 D. K. Jain 33  
 D. R. James 14  
 H. J. Aa. Jensen 1  
 P. Jensen 34, 54, 61  
 Y. Jiang 42  
 A. Johannin-Gilles 3, 33, 34  
 J. W. C. Johns 26, 34  
 C. A. F. Johnson 34  
 H. L. Johnston 75  
 W. M. Johnstone 34  
 L. H. Jones 23, 75  
 D. Jonsson 34  
 P. Jørgensen 1

U. G. Jørgensen 34  
 R. L. Jory 15  
 K. N. Joshipura 34, 35, 46  
 D. L. Judge 40, 54, 76  
 J. S. Jun 13  
 J. O. Jung 28  
 K. Jung 35  
 Ch. Jungen 13  
 M. Jungen 35  
 J. Jureta 35  
 A. S. Jursa 74  
  
 U. Kaldor 35  
 L. D. Kaplan 6  
 A. Karawajczyk 76  
 K. Karlsson 35  
 M. Karplus 36  
 G. Karwasz 66, 77  
 G. P. Karwasz 44, 77  
 T. Kasuga 30  
 A. Katase 35  
 D. H. Katayama 35  
 Y. Katayama 66  
 S. Katsumata 35  
 W. E. Kauppila 35  
 H. Kawazumi 35, 51  
 K. Kaya 71  
 W. Kedzierski 17, 36  
 H. P. Kelly 72  
 S. D. Kelly 34  
 G. W. Kerby III 30  
 C. W. Kern 36  
 J. Kessler 29  
 G. A. Khachkuruzov 36  
 V. D. Khalimulina 65  
 S. P. Khare 33, 36, 59  
 S. V. Khristenko 36  
 L. J. Kieffer 36  
 S. S. Kim 13  
 Y. -K. Kim 31  
 K. Kimura 35, 36, 71  
 M. Kimura 31, 36, 59  
 W. H. Kirchhoff 17  
 S. M. Kishko 66  
 J. Kistemaker 62  
 P. G. Kistemaker 7  
 D. Kivelson 4, 69  
 R. B. Klemm 65  
 D. Kley 36  
 L. E. Kline 52

C. E. Klots 36  
 K. N. Klump 36  
 B. Knight 26, 37  
 R. J. Knight 53  
 F. W. E. Knoop 37  
 F. Koba 24  
 M. Kobayashi 69  
 U. Koble 76  
 P. H. Kobrin 71  
 E. E. Koch 27  
 K. -H. Kochem 35  
 I. V. Kochetov 37  
 M. R. Kodali 37  
 P. Koenig 66  
 J. Kolberbaur 14  
 A. Komornicki 18  
 A. Korosmezey 15, 37  
 W. S. Koski 41  
 A. D. Kotlyarov 5  
 N. Kouchi 32, 37  
 K. Kowari 37  
 J. U. Kozyra 15  
 M. O. Krause 46  
 M. Krauss 46  
 H. J. Krautwald 37  
 A. Kresling 19  
 E. Krishnakumar 38  
 T. Kroin 40  
 P. L. Kronebusch 38  
 H. B. Krop 5  
 A. N. Kuchenev 38  
 E. Kuffel 38  
 J. Kuhn 13  
 M. Kumar 38  
 A. Kuppermann 70  
 M. A. Kurbanov 38  
 M. Kurepa 38, 56  
 M. V. Kurepa 18  
 M. Kurtz 15  
 M. S. Kushwaha 59  
 Y. Y. Kwan 38  
  
 F. W. Lampe 38  
 M. Landau 5  
 N. F. Lane 38  
 P. W. Langhoff 18, 24, 75  
 A. J. Langley 59  
 S. Langlois 2, 38, 39  
 S. R. La Paglia 39  
 R. J. Larkin 52

F. P. Larkins 39  
 E. N. Lassetre 36, 39, 64  
 Z. Latajka 8  
 C. J. Latimer 19  
 A. H. Laufer 39  
 J. A. La Verne 47  
 J. A. LaVerne 39  
 G. M. Lawrence 40  
 G. Leboudec 11  
 J. S. Lee 19, 40  
 L. C. Lee 40, 54, 76  
 L. Y. Lee 4  
 M. -T. Lee 8, 40, 43, 74  
 S. H. Lee 13  
 Y. T. Lee 52, 73  
 D. Lefaivre 40  
 J. Lehmann 40, 41  
 S. W. Leifson 41  
 B. H. Lengsfeld III 26  
 B. N. Lengsfeld 56  
 G. Leroy 59  
 J. L. Lesne 11  
 K. T. Leung 4  
 H. Lew 41  
 D. Lewis 41  
 J. Li 41  
 J. -M. Li 50  
 Z. Li 42  
 H. J. Liebe 41  
 M. Lima 41  
 M. A. P. Lima 8, 16, 41, 42, 43, 55, 72  
 T. F. Lin 41  
 E. Lindemann 41  
 F. Linder 44, 62  
 E. Lindholm 41  
 D. W. Lindle 9, 71  
 B. G. Lindsay 66  
 H. T. Lion 51  
 A. Lisini 42  
 Y. Liu 42  
 W. Livingston 73  
 D. T. Llewellyn-Jones 53  
 Yu. S. Lobastov 5  
 S. N. Lopatin 72  
 A. J. Lorquet 42  
 J. C. Lorquet 42  
 J. Los 22  
 J. A. Lotoski 54  
 J. J. Lowke 42  
 W. W. Lozier 42  
 R. R. Lucchese 26  
 C. B. Ludwig 42  
 H. W. Lulf 2  
 A. Lun 42  
 Z. P. Luo 41  
 Q. Ma 4  
 Y. Ma 10, 12, 13, 22, 35, 43, 61  
 C. J. MacCallum 56  
 C. J. F. MacDonald 77  
 L. E. Machado 8, 40, 42, 43  
 K. Maciag 66  
 R. G. A. R. MacLagan 72  
 M. T. Macpherson 43  
 T. E. Madey 58  
 S. Madzunkov 38  
 K. Maeda 47  
 S. Maezono 35  
 G. Magyar 43  
 J. P. Maillard 22  
 S. Maji 4  
 S. V. Makarov 65  
 H. Maki 35  
 Yu. S. Makushkin 10, 43  
 W. Malkmus 42  
 C. Malone 36  
 K. F. Mamedov 38  
 J. -Y. Mandin 10, 12, 13, 22, 43  
 M. M. Mann 43  
 S. T. Manson 30, 45, 46  
 C. Maralejo 14  
 N. H. March 44  
 E. Marcinkowska 45  
 J. S. Margolis 69  
 D. Margreiter 44  
 B. Marinkovic 66  
 T. D. Mark 18, 44  
 V. N. Markov 44  
 P. Marmet 40  
 N. Martensson 50  
 A. I. Maslov 36  
 S. T. Massie 57, 58  
 H. Masuko 32  
 R. A. Mathis 14  
 R. F. Mathis 44  
 D. Mathur 44  
 Y. Matsumoto 35  
 L. Mattsson 35  
 R. J. Mawhorter 8  
 D. J. McCaa 44

I. E. McCarthy 18, 44  
 J. W. McConkey 16, 17, 36, 44  
 K. E. McCulloh 44  
 C. W. McCurdy 26, 45  
 E. W. McDaniel 45  
 C. A. McDowell 15, 23  
 S. P. McGlynn 12, 14, 74  
 J. W. McGowan 45  
 G. E. McGuire 12  
 L. C. McIntyre 15  
 V. McKoy 8, 18, 40, 41, 42, 43, 55,  
 65, 66, 74, 75, 76  
 J. R. McNesby 39  
 W. J. Meath 36, 77  
 R. Mecke 4, 23, 45  
 S. Meloni 26  
 C. E. Melton 45, 58  
 D. A. Mendis 37  
 J. E. Mentall 45, 47  
 R. P. Messmer 57  
 P. H. Metzger 45  
 H. Meyer 8  
 V. D. Meyer 64  
 W. Meyer 45, 75  
 L. Michalak 45  
 M. Michaud 46  
 S. R. Mielczarek 46  
 J. H. Miller 30, 46  
 K. J. Miller 46  
 M. H. Mittleman 46  
 R. Mocca 46  
 R. Moccia 10, 11, 46  
 W. E. Moddeman 46  
 M. Mohan 62  
 S. Mohanan 46  
 O. C. Mohler 46  
 G. R. Mohlmann 5, 45, 47, 71  
 G. Mollenstedt 47  
 J. E. Monahan 65  
 J. H. Moore 15  
 H. D. Morgan 47  
 L. A. Morgan 47, 68  
 S. Mori 66  
 Y. Morioka 32, 47  
 M. Morishita 36  
 J. L. Moruzzi 52  
 J. T. Moseley 51  
 H. R. Moustafa 62  
 A. Mozumder 47  
 R. Muller 35  
 U. Muller 47  
 G. Munday 18  
 L. A. Munoz 48  
 E. Murakami 35  
 W. F. Murphy 48  
 J. N. Murrell 28  
 E. E. Muschlitz 3, 48  
 S. Nagakura 32, 71  
 V. Nagali 48  
 S. Nagano 41  
 K. Nagesha 63  
 T. Nagura 30  
 A. F. Nagy 15, 37  
 M. S. Naidu 57  
 K. Nakamo 48  
 M. Nakamura 32  
 Y. Nakamura 29  
 K. Nakashima 51  
 H. Nakatsuji 29, 48  
 T. Namioka 47  
 K. Narahari Rao 22, 23, 49, 55, 75  
 A. P. P. Natalense 72  
 G. A. Natanson 49  
 O. Naumenko 10, 12, 22  
 G. A. Neece 45  
 D. R. Nelson 75  
 R. C. Nelson 49  
 I. Nenner 19  
 K. F. Ness 49  
 H. Neuert 49  
 H. Neujmin 68  
 W. R. Newell 20, 34, 59  
 A. J. C. Nicholson 49  
 C. A. Nicolaidis 68  
 H. H. Nielsen 16, 49  
 K. Niira 49  
 A. Nilsson 50  
 F. Nishimura 50  
 H. Nishimura 16, 50  
 T. Nishimura 32, 50  
 A. -F. Niu 50  
 N. Noda 50  
 T. Nomura 28, 50  
 D. W. Norcross 50  
 D. Nordfors 50  
 S. Nordholm 29  
 R. J. Nordstrom 68  
 P. Norman 34

C. L. O' Bryan 35  
 N. Oda 32, 37, 50  
 J. Oddershede 60  
 T. Ogawa 24, 35, 51  
 K. Ogura 23, 24  
 N. Ohashi 48  
 H. Okabe 51  
 Y. Okamoto 32, 51  
 L. B. O' Kelly 31  
 J. J. Olivero 27, 51  
 T. N. Olney 51  
 J. Olsen 1  
 K. Onda 32, 51  
 G. S. Ondrey 1, 2  
 P. F. O'Neill 19  
 Y. Ono 51  
 K. O-ohta 1  
 L. J. Oosterhoff 37  
 C. B. Opal 51, 52  
 L. Oren 40  
 O. J. Orient 52  
 T. M. Orland 63  
 S. Oss 66, 77  
 N. S. Ostlund 66  
 M. Otsuka 30  
  
 J. L. Pack 52  
 R. H. Page 52  
 P. Paiolletti 26  
 C. H. Palmer 52  
 N. Papineau 12  
 L. Parenteau 63  
 H. G. Paretzke 52  
 J. H. Parker 42  
 W. H. Parkinson 64  
 J. E. Parr 52  
 H. Partridge 53  
 R. W. Patch 53  
 P. M. Patel 34  
 S. H. Patil 4  
 W. A. Payne 65  
 J. C. Pearson 53  
 J. E. Pearson 53  
 D. Peeters 59  
 S. S. Penner 53, 72  
 W. K. Peterson 51, 52  
 A. I. Petrova 43  
 T. Petrova 10, 22  
 Z. Lj. Petrovic 53  
 I. D. Petsalakis 53, 68  
  
 S. D. Peyerimhoff 10, 68  
 A. V. Phelps 14, 52, 53, 65  
 E. Phillips 40, 54, 76  
 M. N. Piancastelli 9  
 M. H. Pickett 57  
 S. M. Pimblott 39  
 S. Pinchas 35  
 L. C. Pitchford 24  
 D. Pittman 14  
 E. K. Plyler 6, 49  
 G. N. Polyakova 54  
 O. L. Polyansky 54, 61, 73  
 A. W. Potts 54  
 R. L. Poynter 57  
 T. Pradeep 55  
 S. Prakash 36  
 A. N. Prasad 55  
 R. S. Prasad 63  
 S. T. Pratt 55  
 M. R. Predtechenshii 73  
 W. M. Preston 55  
 W. C. Price 54, 55  
 H. P. Pritchard 55  
 H. Pritchard 41  
 L. A. Pugh 55  
 B. P. Pullen 46  
  
 J. W. Rabalais 17, 55  
 E. Rachlew-Kallne 76  
 L. M. Raff 56  
 L. A. Rahn 56  
 H. M. Randall 56, 76  
 K. J. Randall 61  
 M. V. V. S. Rao 56  
 A. Rauk 56  
 R. V. Rechenmann 62  
 J. A. Rees 15, 42  
 R. R. Reeves 68  
 D. F. Register 71  
 P. W. Reihardt 14  
 Z. Reljic 56  
 T. N. Rescigno 18, 26, 56  
 E. M. S. Ribeiro  
 P. L. Richards 56  
 M. E. Riley 56  
 C. P. Rinsland 9, 57, 58  
 D. E. Rio 27  
 A. V. Risbud 57  
 J. S. Risley 57, 72

A. Rizzo 11, 46  
 M. B. Robin 57  
 R. E. Robson 49  
 M. Roche 57  
 J. Roeke 78  
 K. Rohr 57  
 A. Rosen 57  
 H. M. Rosenstock 18  
 S. Rosenwaks 16  
 K. J. Ross 39  
 D. E. Rothe 44  
 E. W. Rothe 1, 2  
 L. S. Rothman 21, 24, 57, 58  
 H. Rotike 58  
 R. W. Rozett 41  
 M. E. Rudd 7, 30, 31, 46  
 H. Rudolph 65  
 P. S. Rudolph 58  
 K. Ruedenberg 58  
 V. D. Rusanov 58  
 J. R. Rusk 58  
 V. R. Rustamov 38  
 A. Rutscher 58  
 V. Ya. Ryadov 58  
 R. Rye 58  
 H. Ryzko 58  
  
 J. R. Sabin 60  
 A. J. Sadlej 72  
 T. Sagara 59  
 R. Z. Sagdeev 37  
 Z. Saglam 59  
 V. Saile 27  
 A. Saito 48  
 T. Sakae 35  
 V. Saksena 59  
 D. S. Salahub 57  
 F. Salvat 59  
 S. Salvini 59  
 J. A. R. Samson 24, 28  
 M. Sana 59  
 L. Sanche 14, 46, 59, 63  
 J. H. Sanderson 59  
 R. B. Sanderson 59  
 W. Sandner 58  
 N. Sanna 26  
 M. Sasanuma 32  
 H. Sato 36, 59  
 S. P. A. Sauer 60  
 A. Scherbakov 10, 22  
  
 J. P. Schermann 8  
 R. N. Schindler 61  
 R. Schinke 2, 20, 60, 61, 74  
 P. F. Schippnick 27  
 J. Schirmer 61  
 M. Schmidt 44  
 F. Schmieder-Oppau 61  
 A. Schmillen 28  
 W. Schnell 61  
 L. Schnieder 37  
 R. I. Schoen 11  
 K. Schofield 61  
 J. H. Schryber 61  
 E. Schultes 61  
 G. Schulz 5, 47  
 R. Schumacher 61  
 M. Schurgers 61  
 J. Schutten 62  
 J. M. Schwartz 27  
 A. Schweig 8, 18  
 G. K. Schweitzer 46  
 G. Schwemmer 26, 75  
 D. W. Schwenke 53, 62  
 S. Scialla 25, 26  
 J. L. Scott 61  
 G. A. Segal 14, 76  
 E. Segev 62  
 G. Seng 62  
 B. Senger 62  
 R. J. Sension 20  
 F. Sette 61  
 L. V. Shachkin 37  
 M. M. Shahin 62  
 M. Shapiro 62  
 V. D. Shapiro 37  
 B. S. Sharma 62  
 V. M. Shashkov 37  
 J. H. Shaw 6, 13  
 Y. R. Shen 52  
 V. I. Shevchenko 37  
 V. P. Shevelko 36  
 Z. Shi 78  
 K. H. Shima 47  
 I. Shimamura 62, 63  
 M. Shimizu 63  
 D. A. Shirley 4, 9, 71  
 G. V. Sholin 58  
 T. W. Shyn 63  
 K. Siegbahn 35  
 M. T. Sieger 63

B. Silvi 8  
 J. P. Simons 18, 30, 43, 63  
 W. C. Simpson 63  
 D. Sinclair 7  
 A. N. Singh 63  
 L. Sinitza 10, 12, 22  
 V. L. Sinnett 49  
 H. Sjogren 63, 64  
 A. Skerbele 39, 64  
 A. M. Skerbele 39, 64  
 T. G. Slinger 64  
 Yu. M. Smirnov 38  
 A. J. Smith 63  
 K. A. Smith 66  
 M. A. H. Smith 57  
 P. L. Smith 64  
 P. T. Smith 67  
 V. H. Smith 38  
 H. D. Smyth 64  
 L. C. Snyder 64  
 A. M. Sobolev 65  
 V. F. Sokolov 65  
 Yu. A. Sokolova 65  
 S. V. Somov 17  
 S. Southworth 71  
 F. E. Spencer 65  
 R. Spohr 65  
 S. K. Srivastava 38, 52, 56  
 W. Sroka 7  
 V. Staemmler 20, 35, 60  
 R. W. Stagat 27, 51  
 A. E. Stanevich 76  
 V. S. Stankevich 65  
 H. E. Stanton 65  
 V. I. Starikov 65  
 A. Yu. Starikovskii 78  
 V. N. Starosel'tsev 17  
 R. F. Stebbing 23, 66  
 E. Steel 29  
 T. S. Stein 35  
 J. A. Stephens 65  
 L. J. Stief 65  
 J. A. Stockdale 31, 65  
 R. S. Storey 7  
 H. C. Straub 66  
 V. N. Stroinoval 43  
 J. Strong 67  
 F. Stuhl 75  
 B. Stumpf 5  
 O. Sueoka 66  
 T. M. Sugden 55  
 Suk T. Suh 17  
 L. V. Sumin 66  
 J. Sun 42  
 I. V. Sushanin 66  
 M. Suto 40  
 S. Suzuki 69  
 S. Svensson 50  
 A. Szabo 66  
 K. Szego 37  
 C. Szmytkowshi 66  
 A. Tabche-Fouhaile 19  
 P. F. Taday 59  
 K. Takatsuka 66  
 K. Takayanagi 67  
 S. Takeda 67  
 K. H. Tan 67  
 S. Tanahashi 50  
 H. Tanaka 59  
 J. Tanaka 71  
 K. Tanaka 28, 50  
 M. Taniguchi 51  
 Y. Taniguchi 50  
 V. Tarnovsky 67  
 J. T. Tate 43, 67  
 H. E. Tatel 8  
 H. Tawara 67  
 H. S. Taylor 14  
 J. H. Taylor 67  
 G. D. T. Tejwani 67  
 J. Tennyson 54, 61, 68  
 A. Terenin 68  
 A. J. Thakkar 30  
 G. Theodorakopoulos 53, 68  
 W. Thiel 18  
 E. W. Thomas 45  
 M. E. Thomas 68  
 B. A. Thompson 68  
 D. G. Thompson 25, 33, 59, 69  
 J. P. Thomson 9  
 G. Thornton 71  
 R. Tice 69  
 R. H. Tipping 4, 57  
 I. Tokue 69  
 H. Tomura 51  
 R. G. Tonkyn 40  
 R. A. Toth 9, 11, 12, 15, 22, 57, 69, 70  
 J. S. Townsend 1, 70  
 S. Trajmar 14, 70, 71



A. N. Tripathi 33, 38, 62  
A. B. Trofimov 61  
M. Tronc 5, 71  
C. M. Truesdale 71  
C. Trump 58  
T. Tsuboi 32, 37  
H. Tsubomura 71  
S. Tsurubuchi 47, 71  
D. W. Turner 3, 9  
J. E. Turner 31  
T. W. Turner 1  
N. D. Twiddy 7  
Vl. G. Tyuterev 65

A. Untch 60  
M. Urban 72

C. Vallance 72  
P. J. M. van der Burgt 72  
Ph. E. van der Leeuw 67  
R. L. Vander Wal 20, 61  
M. J. van der Wiel 67  
W. J. van der Zande 7  
E. F. van Dishoeck 72  
M. C. van Hemert 72  
D. van Lith 74  
P. Varanasi 53, 67, 72  
M. T. do N. Varella 19, 72  
H. F. A. Verhaart 72  
L. Veseth 72  
F. I. Vilesov 72, 73  
M. Vinodkumar 34, 35  
I. P. Vinogradov 73  
S. Viti 54  
B. Vodar 3, 34  
J. Vogt 35  
R. E. von Holdt 46  
E. von Puttkamer 65, 73  
R. E. Voshall 52  
A. A. Vostrikov 73  
M. J. J. Vrakking 73  
D. A. Vroom 44, 45, 73

H. E. Wagner 58  
N. Wainfan 73  
I. C. Walker 16  
J. A. Walker 18  
W. C. Walker 73  
L. Wallace 54, 73  
A. D. Walsh 73  
L. Wan 42

C. C. Wang 73  
H. -t. Wang 74  
K. Wang 40, 74, 75  
Y. Wang 74  
J. M. Warman 74  
K. Watanabe 35, 74  
S. Watanabe 23, 24  
Y. Watanabe 23, 24  
R. B. Wattson 21  
L. R. Weber 56  
P. Wehinger 74  
H. Wei 30  
K. Weide 20, 60, 74  
E. Weigold 18, 44  
B. R. Weiner 48  
G. L. Weissler 73  
K. H. Welge 6, 37, 61, 75  
H. -J. Werner 75  
W. B. Westerveld 57, 72  
E. R. White 39, 75  
M. G. White 40, 74, 75  
R. T. Wiedmann 40, 74, 75  
G. R. Wight 75  
C. Wilante 59  
T. D. Wilkerson 26, 75  
P. G. Wilkinson 75  
G. R. J. Williams 18, 75  
J. F. Williams 45  
W. Williams 70  
J. G. Williamson 75  
J. F. Wilson 75  
R. H. Wilson 49  
W. E. Wilson 46, 77  
C. Winstead 75  
N. W. Winter 76  
S. Woefe 78  
S. C. Wong 4  
S. F. Wong 76  
M. H. Wood 76  
N. Wright 76  
A. A. Wu 7  
C. Y. R. Wu 76  
S. Wyckoff 74

G. Xu 17

I. Yamashita 76  
T. Yamazaki 36  
X. Yang 27  
K. Yano 50

N. G. Yaroslavsky 76  
K. Yasmin 76  
T. Yasuda 51  
D. Yeager 76  
N. Yonekura 51  
K. Yoshiki Franzen 76  
K. Yoshino 64  
M. Yousfi 77  
J. Yuan 77  
V. A. Yuroskii 10

R. Zahradnik 13  
M. Zaider 8, 77  
A. Zecca 44, 66, 77  
M. Zelikoff 74  
W.-H. Zhang 50  
J. Zhang 1, 77  
K. Zhang 54, 73  
Y. Zhang 50  
Z. Zhang 77  
Y. Zheng 78  
M. Zhou-lei 74  
N. F. Zobov 54  
A. P. Zuev 78

Author Index for H<sub>2</sub>O References. Addenda

- M. Allan 79  
L. C. Allen 89  
W. D. Allen 85  
J. R. Alvarez 89  
P. Andresen 87  
T. Arusi 82  
L. Asbrink 82, 85  
R. L. Asher 81  
M. N. R. Ashfold 82, 91  
R. Atkinson 82, 83
- D. S. Baer 82  
I. Bar 82  
A. J. Barnes 83  
R. J. Bartlett 92  
A. M. Bass 83  
D. L. Baulch 82, 83  
K. Becker 79  
Y. Ben Aryeh 83  
W. S. Benedict 89  
J. E. Bernard 81  
A. Bernas 83  
P. F. Bernath 81  
R. Bersohn 83, 93  
L. Bertrand 83  
J. A. Beswick 83  
J. R. Birch 83  
J. E. Boggs 91  
M. J. Bramley 83  
J. Brandao 79  
J. W. Brault 83  
M. Braunstein 83  
C. E. Brion 79  
H. P. Broida 93  
M. Brouard 84  
J. M. Brown 84  
R. J. Brudzynski 93  
P. J. Bruna 84  
M. J. Brunger 79, 80  
R. J. Buenker 89, 92  
W. J. Burroughs 83
- C. Camy-Peyret 92  
T. Carrington 83, 93  
P. Carsky 80  
S. Carter 91
- J. H. Carver 90  
M. Castillejo 82  
B. J. Cederholm 87  
G. A. Chamberlain 84  
C. Champion 79  
M. S. Child 84  
C. C. Chou 84  
Y. Cohen 82  
D. F. Coker 84  
J. -M. Colmont 84  
E. R. Comben 84  
F. J. Comes 87, 91  
R. L. Cook 84  
G. Cooper 79  
R. Corriveau 83  
R. A. Cox 82, 83  
J. A. Coxon 84  
F. F. Crim 94  
D. R. Crosley 85  
H. M. Crosswhite 85  
A. G. Csaszar 81, 85  
R. Curik 79
- A. Danjo 80  
D. David 82  
P. Decleva 81  
W. Dementroder 79  
D. M. Dennison 85  
H. Deutsch 79  
G. H. Dieke 85  
G. H. F. Diercksen 90  
S. Ding 82  
R. Ditchfield 85  
D. A. Dixon 81  
R. N. Dixon 80, 85, 91  
A. J. Dobbyn 85  
M. P. Docker 86  
T. H. Dunning 88  
R. Duren 88  
G. Duxbury 85  
K. G. Dyall 81
- F. Edery 79  
M. Ehara 93  
J. B. Elgin 86  
A. El-Zein 79, 80

A. A. A. El-Zein 80  
 R. J. Emergy 83  
 R. S. Eng 86  
 V. Engel 88  
 K. M. Evenson 92  
  
 D. Feller 81  
 J. S. Fender 83  
 J. A. Fernley 86  
 C. C. Ferriso 86  
 J. H. Fillion 82  
 F. Fiquet-Fayard 87  
 J. -M. Flaud 92  
 S. C. Foster 84  
 K. F. Freed 91  
 G. Fronzoni 81  
 E. R. Furlong 82  
 S. Furuya 80  
  
 R. R. Gamache 84  
 D. Garvin 83  
 W. M. Gelbart 83  
 J. A. Gelbwachs 90  
 K. -H. Gericke 91  
 F. A. Gianturco 79  
 R. Goldstein 86, 87  
 D. T. Goodhead 91, 94  
 J. D. Gorfinkiel 80  
 K. Goto 92  
 S. Goursaud 87  
 L. A. Gribov 87  
 A. U. Grunewald 87  
 G. Guelachvili 92  
 M. F. Guest 91  
 H. Guo 87  
  
 D. N. B. Hall 83  
 R. N. Hamm 94  
 R. F. Hampson 82, 83  
 N. C. Handy 95, 96  
 R. K. Hanson 82  
 J. Hanssen 79  
 T. Harb 80  
 L. B. Harding 81, 88  
 P. C. Hariharan 87  
 S. Harich 85, 89  
 S. A. Harich 80  
 A. J. Harrison 87  
 Y. Hatano 80  
 D. Hausler 87  
  
 H. Hayashi 81  
 K. T. Hecht 85  
 W. J. Hehre 85  
 T. Helgaker 87  
 E. J. Heller 87, 88, 90, 94  
 P. Helminger 84  
 S. Hennig 88  
 P. A. Hervieux 79  
 B. Hess 88  
 M. Higo 90  
 G. Hirsch 89  
 A. Hodgson 86  
 J. Horacek 80  
 G. A. Hornbeck 88  
 M. Hoshi 91  
 A. R. Hoy 88  
 B. S. Hudson 93  
 N. S. Hush 89  
 D. W. Hwang 82, 89  
 D. W. H. Hwang 80, 85  
 W. Hwang 82, 89  
  
 D. G. Imre 88, 89, 93, 96  
 M. Ingr 80  
 J. R. Izatt 89  
  
 D. A. Jennings 92  
 P. Jensen 89  
 J. J. Jimenez 92  
 J. W. C. Johns 88  
  
 K. Kameta 80  
 A. Kanaev 79  
 G. P. Karwasz 80  
 W. Kedzierski 80  
 M. Keil 79  
 J. A. Kerr 82, 83  
 B. J. Kerridge 89  
 G. V. Khovrin 87  
 D. A. L. Kilcoyne 89  
 H. F. King 92  
 W. Klopper 87  
 D. B. Knowles 89  
 P. J. Knowles 85  
 H. Koch 87  
 P. A. Kollman 89  
 N. Kouchi 80  
 K. Kuhl 88, 90  
 J. Kurawaki 90

K. S. Lam 90  
 S. R. Langford 84  
 M. -T. Lee 81  
 S. -Y. Lee 90  
 Y. T. Lee 90, 95  
 J. L. Lemaire 82  
 R. K. Lengel 85  
 S. R. Leone 90  
 H. B. Levene 90  
 B. R. Lewis 90  
 J. Li 80, 82, 85, 89  
 M. A. P. Lima 80  
 J. J. Lin 80, 82, 85, 89  
 J. L. S. Lino 80  
 I. V. Litvinyuk 79  
 J. G. Lo 84  
 K. A. Long 90  
 G. L. Loper 90  
 F. J. Lovas 90  
 J. E. Lowder 90  
 C. B. Ludwig 86  
  
 L. E. Machado 81  
 A. A. Madej 81  
 D. E. Manolopoulos 84  
 A. W. Mantz 86  
 T. D. Mark 79  
 L. Marmet 81  
 P. Marshall 80  
 S. Matt 79  
 I. E. McCarthy 79  
 J. W. McConkey 80  
 B. M. McLaughlin 80  
 U. Meier 88  
 K. Mikulecky 91  
 R. E. Miller 84  
 S. Miller 86  
 I. M. Mills 88, 91  
 J. -P. Monchalin 83  
 E. A. Moore 91  
 D. H. Mordaunt 91  
 O. Moreira 79, 80  
 L. A. Morgan 80  
 M. D. Morse 91  
 F. Muller-Plathe 90  
 R. S. Mulliken 91  
 J. N. Murrell 87, 91, 93  
  
 V. Nagali 82  
 K. Narahari Rao 92  
  
 D. J. Nesbitt 92  
 W. R. Newell 79, 80  
 M. E. Newfield 82  
 C. A. Nicolaidides 91  
 H. Nikjoo 91, 94  
 J. Noga 87  
 S. Nordholm 89  
  
 J. Oddershede 91  
 T. Ogawa 90  
 M. A. O'Neill 90  
 T. Ono 80  
  
 R. T. Pack 83, 91  
 A. Palma 93  
 N. Papineau 92  
 H. G. Paretzke 90, 94  
 J. F. Paulson 92  
 L. R. Peebles 80  
 A. A. Peshkov 82  
 F. R. Petersen 92  
 K. A. Peterson 81  
 S. D. Peyerimhoff 84  
 R. A. Phillips 92  
 M. Polasek 80  
 O. L. Polyansky 81  
 J. A. Pople 85, 87  
 C. R. Prasad 94, 95  
 D. Priem 84  
 L. A. Pugh 92  
 G. D. Purvis 92  
 P. Pyykko 81  
  
 J. W. Rabalais 82, 85  
 G. Rathenau 92  
 J. R. Reimers 84, 92  
 E. E. Remsberg 89  
 E. M. S. Ribeiro 81  
 W. G. Richards 91  
 C. M. A. Rio 79  
 C. D. Ritchie 92  
 R. H. Ritchie 94  
 S. Rosenwaks 82  
 M. J. Rossi 82  
 F. Rostas 82  
 L. S. Rothman 95  
 F. S. Rowland 84  
 J. Ruiz 82  
 B. Ruscic 81

H. Sakai 89  
 N. Sanna 79  
 S. Satyapal 93  
 R. Schinke 87, 88, 90, 93, 94, 95  
 R. Schroder 93  
 J. L. Scott 94  
 R. J. Sension 93  
 N. Shafer 93  
 N. Shafizadeh 82  
 M. Shapiro 93  
 T. Yu. Sheludyakov 82  
 Y. R. Shen 90, 95  
 T. Shirai 81  
 K. J. Siemsen 81  
 J. P. Simons 84, 86  
 M. Sizun 87  
 K. Soejima 80  
 K. S. Sorbie 93  
 V. Staemmler 88, 93  
 M. Stener 81  
 G. Strey 88  
  
 T. Tabata 81  
 M. Takahasi 81  
 I. Tanaka 93  
 D. Tannor 88  
 D. J. Tannor 94  
 M. M. Tarasenko 82  
 G. Tarczay 81  
 H. Tawara 81  
 G. D. T. Tejwani 95  
 J. Tennyson 80, 81, 86  
 M. A. Terwilliger 87  
 G. Theodorakopoulos 91  
 D. G. Thompson 80  
 A. L. Thomson 86  
 D. Toffoli 81  
 R. A. Toth 81  
 J. Troe 82, 83  
 T. B. Truong 83  
 S. Tsuchizawa 81  
 J. E. Turner 94  
  
 Y. Udagawa 81  
 S. Uehara 91, 94  
 K. Ueki 90  
 O. N. Ulenikov 94  
 K. Umemoto 80  
  
 J. J. Valentini 82, 90  
  
 R. L. Vander Wal 94  
 M. C. van Hemert 81  
 P. Varanasi 94, 95  
 A. C. Varandas 95  
 I. M. Vardavas 90  
 M. S. Vardya 95  
 F. I. Vilesov 95  
 O. K. Voltsekhovskaya 82  
 O. Votava 92  
  
 Y. Wada 81  
 A. F. Wagner 81  
 N. Watanabe 81  
 R. T. Watson 83  
 R. O. Watts 84, 92, 95  
 R. B. Wattson 95  
 K. Weide 88, 94, 95  
 J. S. Wells 92  
 H. Wenz 79  
 R. J. Whitehead 95, 96  
 T. A. Wiggins 96  
 S. O. Williams 96  
 R. Williamson 81  
 W. E. Wilson 91  
 G. Wlodarczak 84  
 N. C. Wong 96  
 H. A. Wright 94  
  
 D. Xie 96  
  
 K. Yamashita 93  
 G. Yan 96  
 X. Yang 80, 85, 89  
 X. F. Yang 82, 85  
  
 A. H. Zanganeth 82  
 A. Zecca 80  
 J. Zhang 88, 89, 93  
 Y. Zheng 79, 82  
 A. S. Zhilyakov 94  
 N. F. Zobov 81

Some Comments on Electron Collision Cross Sections and  
Photodissociation Processes for H<sub>2</sub>O

The pioneer work on electron collision cross section set for H<sub>2</sub>O is given by J. J. Lowke in 1969. I have compiled the same set for H<sub>2</sub>O including new data two times. An example was shown in M. Hayashi (1989). This cross section set is shown in Figure 1. The other cross section sets for H<sub>2</sub>O were presented by many authors, N. Gee (1983), M. Yousfi (1987), K. F. Ness (1988), S. F. Biagi (1989), T. J. Dolan (1993), M. Yousfi (1994, 1996) and so on.

Now I do not like these cross section sets. Reasonable and correct cross section set have to calculate the temperature dependence of electron drift velocities at high E/N by B. Eq. and MCS method. We have solved this problem in the case of CO<sub>2</sub> and reported at the 51th GEC Conference, Maui, as shown in this report.

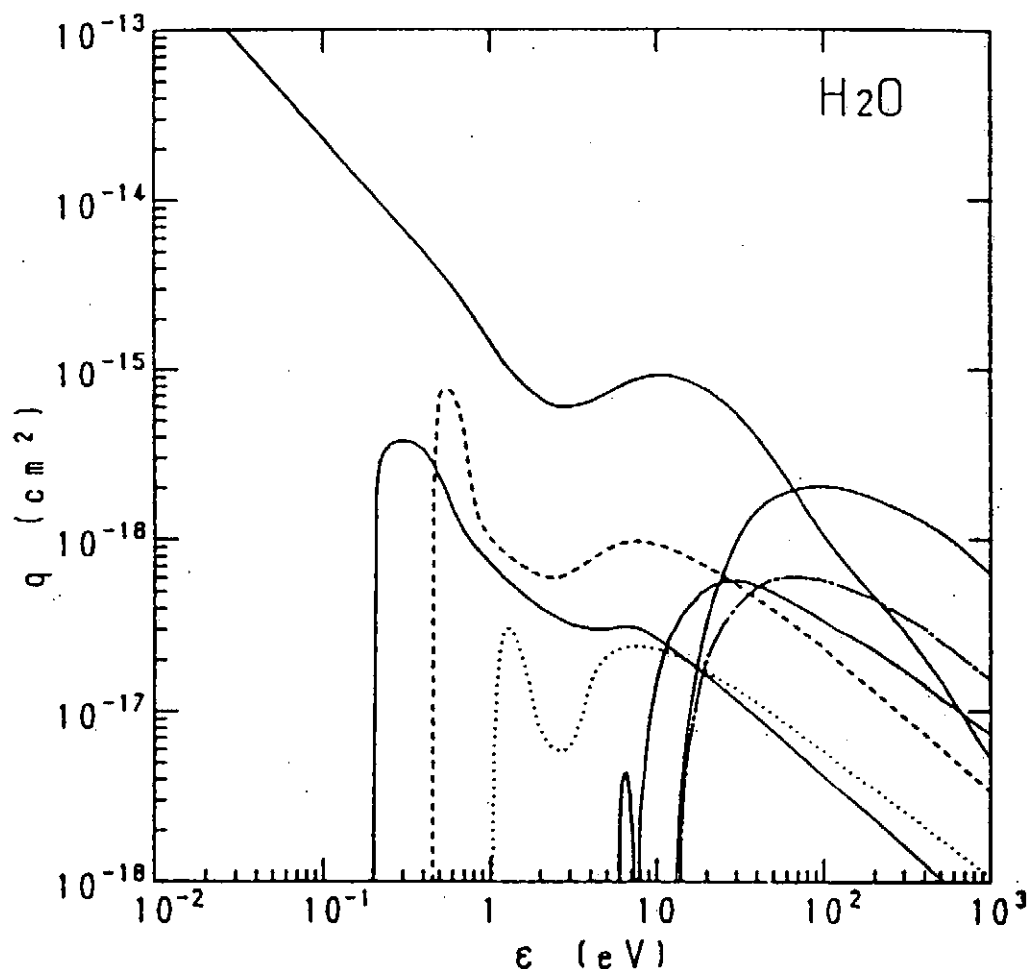


Figure 1. Electron collision cross section set for H<sub>2</sub>O, assuming all H<sub>2</sub>O molecules are in H<sub>2</sub>O(g) state (M. Hayashi, 1990). In all H<sub>2</sub>O + e experiments, H<sub>2</sub>O molecules are mixture of H<sub>2</sub>O(g), H<sub>2</sub>O(r) and H<sub>2</sub>O(v). So this cross section set is not applicable for exact calculations, and can use only for approximate applications.

In the case of H<sub>2</sub>O, the concentration of H<sub>2</sub>O(v) is small at 300 K. At high temperature, the effect of H<sub>2</sub>O(v) is important and interesting.

All molecules have the component M(g), M(r), M(v) and M<sub>n</sub> (n = 2), depend on the pressure and temperature condition 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 in the triatomic molecules by vibrational excitation.

Almost theoretical results of electron collision cross sections for molecules are for M(g). Theoretical studies involving the M(r) and M(v) are urgently required for many molecules.

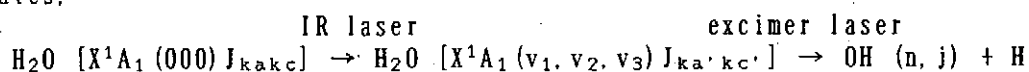
I would like to present our recent two conference reports at the end of this report.

M. Hayashi and Y. Nakamura : 51th GEC, Maui 265-266 (1998)

M. Hayashi and Y. Nakamura : EMS-99, Tokyo 175-176 (1999)

The photodissociation of H<sub>2</sub>O in the first absorption band has been studied in great detail by P. Andresen, R. Schinke, V. Engel, R. L. Vander Wal, V. Staemmler, F. F. Crim, D. Hausler, and so on, both experimentally and theoretically.

Photodissociation processes consist essentially of two steps. The first step is the absorption of a photon leading to the excited state. The second step is the subsequent dissociation of this complex to the products. This has been tested for several different initial vibrational and rotational states.



The experimental procedure require three lasers.

1. H<sub>2</sub>O is vibrationally excited to a well defined rotational state with a tunable IR laser. This IR excitation is used to prepare single rotational and vibrational states of H<sub>2</sub>O in the electronic ground state.
2. The prepared H<sub>2</sub>O is photodissociated using 193 nm ArF excimer laser.
3. A third probe laser is used to determine the vibrational state distribution of the OH product by laser induced fluorescence.

Details are not discussed here. Please find the selected papers from this bibliography. Photodissociation dynamics of H<sub>2</sub>O at 121.6 nm (Lyman- $\alpha$  wavelength) have been studied by some authors. The results are also interesting but complicated a little bit.

The author would like to expect that the similar studies on electron collision cross section experiments of single rotational and vibrational states of H<sub>2</sub>O in the electronic ground state.



## Temperature Dependence of Electron Drift Velocity and Electron Collision Cross Section Sets for Ground State and Vibrationally Excited State of the CO<sub>2</sub> Molecule

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The drift velocity of electrons in carbon dioxide have been calculated at gas temperatures ranging from 193 to 573 K and at E/N values up to 100 Td assuming that the gas was a mixture of the ground state molecules and the vibrationally excited molecules and its mix ratio depended on the temperature. The calculated drift velocities agreed well with the measurement of Elford (1980).

Generally, target molecule M in beam and swarm experiments consists of the mixture of different states:

$$M = M(g) + M(r_j) + M(v_i) + M_N,$$

where M(g), M(r<sub>j</sub>), M(v<sub>i</sub>) and M<sub>N</sub> represent the ground state molecules, the rotationally excited molecules, the vibrationally excited molecules and the van der Waals clusters consisting of N molecules (N≥2), respectively. It is known that the concentration of M(v<sub>i</sub>) increases with temperature. For example, the concentration of CO<sub>2</sub>(v<sub>i</sub>) in CO<sub>2</sub> has been calculated to be 8.4 % at 313 K and 26.5 % at 673 K, respectively [1,2]. This is due to the low threshold energy (0.083 eV) of the lowest vibrational excited level (010) mode. The concentrations of rotationally excited molecules are much larger than of the vibrationally excited molecules. The concentration of the clusters are important at low temperature and high pressure conditions.

Most of theoretical calculations of electron collision cross sections have been performed for pure M(g) target, not for the M(v) molecules.

A number of different electron collision cross sections for molecules have been determined with beam and swarm experiments. So far, in most of the experiments it is implicitly assumed that the target molecules are all in the ground state, or electron collision cross section set of M(g), M(r) and M(v) are almost the same. Strictly speaking, this assumption is not correct, and in particular, cannot be applied to the molecules which have temperature dependence in electron collision cross sections.

Take the CO<sub>2</sub> molecule. The ground state CO<sub>2</sub>(g) is linear, but CO<sub>2</sub>(010) is bent and this has a dipole moment. Electron collision cross section set

of CO<sub>2</sub>(g) and CO<sub>2</sub>(v) are expected to be different each other. In fact, Buckman [3], Ferch [1] and Strakeljahn [4] have determined the grand total cross section Q<sub>T</sub> for CO<sub>2</sub>(g) and CO<sub>2</sub>(v) and found that Q<sub>T</sub>(v) of CO<sub>2</sub> are larger than Q<sub>T</sub>(g) at the electron energies lower than about 10 eV.

It seems to be quite difficult to determine directly the electron collision cross section sets of CO<sub>2</sub>(g) and CO<sub>2</sub>(v) from the beam and swarm experiments. However, if the cross section sets of CO<sub>2</sub>(g) and CO<sub>2</sub>(v) are available, we can calculate the electron swarm parameters of a known concentration of CO<sub>2</sub>(g) and CO<sub>2</sub>(v) very easily. Momentum transfer cross sections q<sub>m</sub> for CO<sub>2</sub>(g) and CO<sub>2</sub>(v), which have been based on the compilation of Hayashi [5] and recent experiments of Nakamura [6] and Strakeljahn [4], are shown in Fig. 1. Tentatively, we have assumed that all other inelastic cross sections of CO<sub>2</sub>(g) and CO<sub>2</sub>(v) are practically the same [7,8]. At a given temperature, the concentrations of CO<sub>2</sub>(g) and CO<sub>2</sub>(v) are known, then we have calculated the values of electron drift velocity W in CO<sub>2</sub>. The results are shown in Fig. 2. The calculated W values at three temperatures are in general agreement with the experimental data of Elford [9].

Haddad [10] have discussed the importance of the populations of vibrationally excited CO<sub>2</sub> molecules already. They also have mentioned the contributions due to CO<sub>2</sub> molecules in rotational states and have concluded that such states are not likely to play a significant role compared with vibrationally excited molecules. But they could not reproduce their experimental data for W at high E/N from the analysis.

A similar analysis on H<sub>2</sub>(g), H<sub>2</sub>(r) and H<sub>2</sub>(v)

also have to be started. The  $H_2$  molecule have the famous long-standing controversy in the vibrational excitation cross section [11]. In the present paper, we propose to investigate and to measure the cross sections for molecules not only in the ground state but also in the excited states which should have different cross sections from those in the ground state. Although the difference among the cross section sets for  $H_2(g)$ ,  $H_2(r)$  and  $H_2(v)$  may be small compared with the  $CO_2$  molecule since the  $H_2$  molecule is diatomic. Theoretical studies involving the excited species are urgently required.

The term "temperature dependence of cross section" may not be appropriate. The molecules,  $CO_2(g)$ ,  $CO_2(r)$  and  $CO_2(v)$ , have the definite and individual cross section sets, and their concentrations change with temperature. The temperature dependence is caused through different concentration of the excited components at different temperatures. Attachment cross section of the excited molecules is quite different from the ground state molecules for many attaching gases.

We wish to thank Professor H. Tawara for valuable comments.

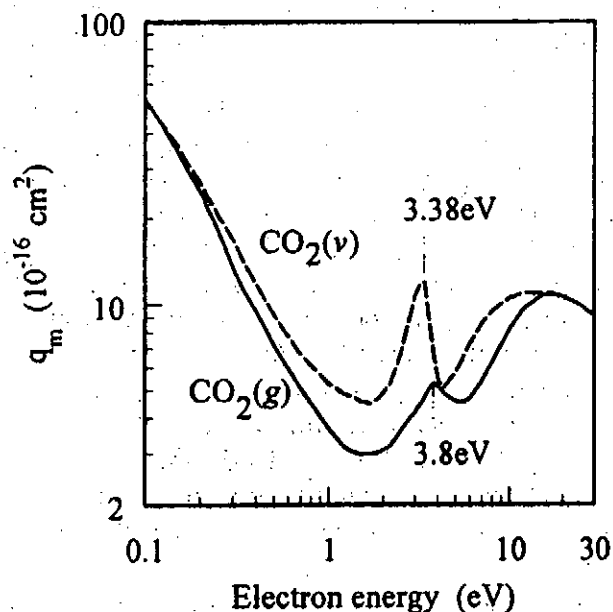


Fig. 1. The assumed elastic momentum transfer cross sections for the ground state (solid curve) and vibrationally excited  $CO_2$  molecules (broken curve).

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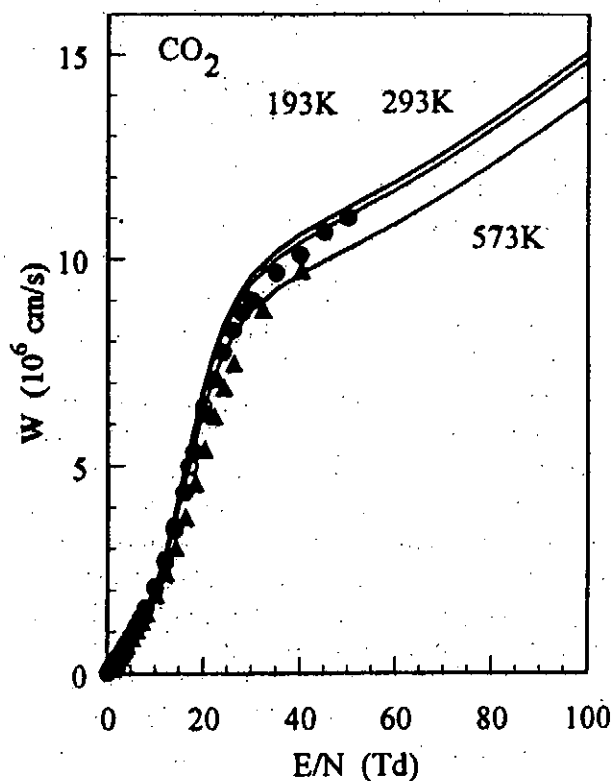


Fig. 2. Calculated electron drift velocities in  $CO_2$  at different temperatures. Open and closed circles and closed triangles show the measurements of Elford [9] at 193, 293 and 573 K, respectively.

# 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  $M(r_1)$  and  $M(v_1)$ , for most molecules. Theoretical studies involving the rotationally and vibrationally excited species are urgently required for many molecules. There is an 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 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 <sub>2</sub> , D <sub>2</sub>	2000	5 CH <sub>4</sub>	780
Ne 10	1140 *	N <sub>2</sub>	2240 ○		
Ar 18	1960 ○	O <sub>2</sub>	1700	CF <sub>4</sub>	390
Kr 36	1000	CO	1190	CCl <sub>4</sub>	210
Xe 54	1180 ○	NO	880	CCl <sub>2</sub> F <sub>2</sub>	250
				CH <sub>3</sub> Cl	90
Li 3	450	F <sub>2</sub>	190 ○		
Na 11	800	Cl <sub>2</sub>	360 ○	SiH <sub>4</sub>	230
		Br <sub>2</sub>	140 ○	SiF <sub>4</sub>	140
K 19	370	I <sub>2</sub>	240 ○	GeH <sub>4</sub>	50
Rb 37	220				
Cs 55	370	HF	260	6 C <sub>2</sub> H <sub>4</sub>	370
		HCl	320	CH <sub>3</sub> OH	350
O 8	390	HBr	200		
		HI	130	7 SF <sub>6</sub>	920 ○
F 9	90				
Cl 17	130	3 CO <sub>2</sub>	1240 ○		
		H <sub>2</sub> O	1200 ○	8 C <sub>2</sub> H <sub>6</sub>	260
Cu 29	180			C <sub>2</sub> F <sub>6</sub>	150
Cd 48	210	O <sub>3</sub>	480	Si <sub>2</sub> H <sub>6</sub>	70
Ba 56	340	N <sub>2</sub> O	450		
		NO <sub>2</sub>	350	9 C <sub>3</sub> H <sub>6</sub>	120
Hg 80	600	H <sub>2</sub> S	270	C <sub>2</sub> H <sub>5</sub> OH	60
		SO <sub>2</sub>	290		
		CS <sub>2</sub>	260		
		OCS	280	11 C <sub>3</sub> H <sub>8</sub>	190
not final, but finished mostly		4 C <sub>2</sub> H <sub>2</sub>	390	C <sub>3</sub> F <sub>8</sub>	100
include electron swarm papers		NH <sub>3</sub>	500	12 C <sub>4</sub> F <sub>8</sub>	100
		NF <sub>3</sub>	110	C <sub>6</sub> H <sub>6</sub>	240
		BF <sub>3</sub>	110	C <sub>6</sub> F <sub>6</sub>	100
include review papers		BCl <sub>3</sub>	90	60 C <sub>6</sub> O	300
		PH <sub>3</sub>	80		
		H <sub>2</sub> CO	180	M <sub>r</sub> + M <sub>v</sub>	850

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

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