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

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# Bibliography of Electron and Photon Cross Sections

with Atoms and Molecules

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

—— Hydrogen Halide Molecules ——\*

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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 hydrogen halide molecules (HF, HCl, HBr, HI). About 330 (HF), 420 (HCl) 220 (HBr) and 150 (HI) papers were compiled respectively. Comprehensive author indexes for each molecule are included. The bibliography covers the period 1903 through 2000 for HF-HI. Finally, author's comments for HBr electron collision cross sections are given.

Keywords : HF, HCl, HBr, HI 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

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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 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 halide molecules HF, HCl, HBr, and HI. The review papers on this subject are also included. Some hydrogen halide molecule cluster papers are included. Some conference reports, company or agency reports and PhD thesis are included. Hydrogen halide molecules 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 paper in this list is given by J. S. Townsed (1903) for HCl. Oldest papers for other hydrogen halide molecules are shown in each molecules. So for this bibliography, published papers from 1903 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 each Hydrogen Halide Molecule". In total, about 330 for HF, 420 for HCl, 220 for HBr and 150 for HI papers are compiled in the four hydrogen halide 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	: <u>E</u> lastic collision	QT	: grand <u>T</u> otal cross section
R	: <u>R</u> otational excitation		(sum of elastic and inelastic
V	: <u>V</u> ibrational excitation		electron cross sections).
EX	: electronic <u>EX</u> citation		<u>Q</u> came from Querschnitt
D	: <u>D</u> issociation		
I	: <u>I</u> onization		
A	: <u>A</u> ttachment		
ME	: <u>ME</u> tastable molecules		
S	: electron <u>S</u> warm		
O	: <u>O</u> thers (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.

Bibliographies for HF, HCl, HBr, and HI are divided into two parts :

HF

Part 1. 1924 - 1999 p. 1 - 22

Part 2. Addenda of References published in 2000, plus some  
old papers p. 23 - 28

HCl

Part 1. 1903 - 1999 p. 1 - 27

Part 2. Addenda of References published in 2000, plus some  
old papers p. 28 - 36

HBr

Part 1. 1913 - 1999 p. 1 - 17

Part 2. Addenda of References published in 2000, plus some  
old papers p. 18 - 23

HI

Part 1. 1916 - 1999 p. 1 - 11

Part 2. Addenda of References published in 2000, plus some  
old papers p. 12 - 14

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.

HF p. 1 - 5

HCl p. 1 - 7

HBr p. 1 - 4

HI p. 1 - 4

Each author index of four hydrogen halide molecules follows each bibliography.

Some Comments on Electron Collision Cross Sections for HBr

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Hydrogen Fluoride HF

References for HF, DF (1900 - 1999)

(Hydrogen fluoride)

[Hydrogen halide, Halogen acid]

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 information,
		E	: Exp., T : Theory.

The oldest paper in this list is given by J. Simons (1924).

- A R. Abouaf and D. Teillet-Billy : 10th ICPEAC, Paris 2, 792-793 (1977) ·  
Electron attachment to polar molecules : Structure in the dissociative attachment cross sections for HCl, HBr, HF. [E, HF, HCl, HBr]
- A R. Abouaf and D. Teillet-Billy : Chem. Phys. Lett. 73, 106-109 (1980a) K  
Fine structure in the dissociative attachment cross sections for HBr and HF. [E, HF, HBr; 2 - 3.8 eV for HF]
- A R. Abouaf and D. Teillet-Billy : J. Phys. B13, L275-L279 (1980b)  
Predissociation of Feshbach resonances in hydrogen fluoride.  
[E, HF; 10 - 15 eV, Feshbach resonance at 12.8 - 14 eV]
- A R. Abouaf, D. Teillet-Billy, R. Azria and P. Girard : J. Phys. B18, 3017-3024 (1985)  
Resonances in HF : H<sup>-</sup> formation around 10 eV. [E, HF]
- A N. G. Adams, D. Smith, A. A. Viggiano, J. F. Paulson and M. J. Henchman : J. Chem. Phys. 84, 6728-6731 (1986) K  
Dissociative attachment reactions of electrons with strong acid molecules.  
[E, HF - HI, HNO<sub>3</sub>, H<sub>2</sub>SO<sub>4</sub>, etc.]
- O J. R. Airey and I. W. M. Smith : J. Chem. Phys. 57, 1669-1676 (1972)  
Quenching of infrared chemiluminescence : Rates of energy transfer from HF ( $v \leq 5$ ) to CO<sub>2</sub> and HF, and from DF ( $v \leq 3$ ) to CO<sub>2</sub> and HF.  
[E, HF; H + F<sub>2</sub> → HF + F, etc.]
- E Y. Alhassid and B. Shao : Phys. Rev. A46, 3991-4002 (1992) ·  
R Algebraic eikonal approach to electron-molecule scattering. II.  
V Rotational-vibrational excitations.  
[T, HF, HCl, LiF; 0.63 - 10 eV for HF]



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Dissociative attachment from vibrationally and rotationally excited HCl and HF. [E, HF, HCl; 300 - 1180 K]
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Selective excitation of the vibrational-rotational states and dissociation of diatomic molecules by picosecond infrared laser pulses : Modeling for HF in the ground electronic state. [T,  $h\nu$ , HF]
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Electron molecule collision at low energy resonance and threshold phenomena. [review, HF, HCl, HBr, HI]
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The electron density distributions in hydride molecule. III. Hydrogen fluoride. [T, HF]
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The nature of the chemical bond in lithium hydride and hydrogen fluoride. [T, HF, LiH; Hartree-Fock charge distribution]
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The electronic structure of hydrogen fluoride. [T, HF]
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X-ray photoemission molecular orbitals of hydrogen fluoride and the fluorinated methanes. [E,  $h\nu$ , HF, CH<sub>4</sub>, CH<sub>3</sub>F, CH<sub>2</sub>F<sub>2</sub>, CHF<sub>3</sub>, CF<sub>4</sub>]
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Molecular photoelectron spectroscopy at 132.3 eV. The second-row hydrides. [E,  $h\nu$ , HF, H<sub>2</sub>O, NH<sub>3</sub>, CH<sub>4</sub>, Ne]
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Variational calculations of vibrational-rotational properties of HF in the X<sup>1</sup>Σ<sup>+</sup> and B<sup>1</sup>Σ<sup>+</sup> electronic states. [T, HF]
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The ultra-violet spectrum of a diatomic hydride excited in hydrogen-potassium fluoride hollow-cathode discharges. [E, H<sub>2</sub> + KF; HF as possible emitter]
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Direct observation of the effect of enhanced vibrational excitation on fragmentation in a mass spectrometer. [E, HF]

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Spectra of stimulated emission in the hydrogen-fluorine reaction process and energy transfer from DF to CO<sub>2</sub>. [E, HF]
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Thermochemical tests of a kinetic-energy dependent exchange-correlation approximation. [T, HF, Cl<sub>2</sub>, SiH<sub>4</sub>, etc.]
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- I Electron-impact ionization and dissociative excitation of halogen-containing molecules.  
[comments. HF, SF<sub>6</sub>, CF<sub>2</sub>Cl<sub>2</sub>, CF<sub>4</sub>, HCl, HBr, CF<sub>3</sub>H, CF<sub>3</sub>Cl, etc.]
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Correlation energy and molecular properties of hydrogen fluoride.  
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Theoretical study of several electronic states of the hydrogen fluoride molecule. [T, HF]
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NH<sub>3</sub>, CH<sub>4</sub>, CO<sub>2</sub>, COS, CS<sub>2</sub>, N<sub>2</sub>O]
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[compilation, HF - HI, F<sub>2</sub> - I<sub>2</sub>, H<sub>2</sub>, N<sub>2</sub>, O<sub>2</sub>, CO, NO, CO<sub>2</sub>]
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Hydrogen Chloride HCl

References for HCl, DCl (1900 - 1999)

(Hydrogen chloride, Hydrochloric acid)

[Hydrogen Halide, Halogen acid]

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 information,
	E : Exp., T : Theory.

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Hydrogen Bromide HBr

References for HBr, DBr (1900 - 1999)

(Hydrogen bromide)

{Hydrogen halide, Halogen acid}

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 information,
	E : Exp., T : Theory.

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Hydrogen Iodide HI

References for HI, DI (1900 - 1999)

(Hydrogen iodide)

[Hydrogen halide, Halogen acid]

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 information,
		E	: Exp., T : Theory.

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## Some Comments on Electron Collision Cross Sections for HBr

We have determined the electron collision cross section set for HCl (Hayashi (1987)), assuming that all HCl molecules are in the ground state. This assumption is not true, so we do not like our cross section set of HCl.

As an example, we discuss the electron cross sections for HBr here. Experimental and theoretical studies on electron collision cross sections of HBr are summarized as follows :

On the study of electron scattering cross sections for HBr

### grand total cross section $Q_T$

no work

### elastic experiment

no data

(F. Linder                      1977)

### elastic theory

M. E. Riley	1975	
Y. Itikawa	1978	< 1 eV
E. Estrada	1984	general theory
S. Pozdneev	1988	
L. Malegat	B 1990	
R. Fandreyer	B 1993	0.1 - 11 eV
T. N. Rescigno	C 1996	0 - 10 eV, DCS
I. M. Smith	B 1998	

### rotational excitation experiment and theory

no work

vibrational excitation experiment

J. P. Ziesel	C 1975	○	
K. Rohr	B 1977a		DCS at 0.41 eV
K. Rohr	B 1978	○	th. - 7 eV for $v = 0 \rightarrow 1$
R. Azria	B 1980		
S. Cvejanovic	1993		
A. -C. Sergenton	1999		0.3 - 2.7 eV
M. Cizek	P 2001	○	0 - 4 eV
G. P. Karwasz	2001		compilation
M. Cizek	2002		

vibrational excitation theory

F. A. Gianturco	1977		
H. Estrada	1984		
S. Pozdneev	1988		
F. Fandreyer	B 1993		th. - 4.5 eV
J. Horacek	P 1996		
J. Horacek	2000		
S. A. Pozdneev	2000		
M. Cizek	P 2001	○	0 - 4 eV

electronic excitation experiment

G. R. Mohlmann	1979		
P. A. Shaw	B 1984		1500 eV
S. Cvejanovic	B 1987		
K. England	1987		0.5 - 50 eV
K. England	B 1990	○	0.5 - 50 eV
K. H. Becker	1994		
D. Cubric	B 1994		

electronic excitation theory

T. N. Rescigno (V. McKoy)	C 1996		th. - 25 eV
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ionization experiment

K. H. Becker	1994		
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ionization theory

H. Deutsch	1997		
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attachment experiment

H. Gutbier	1954		
D. C. Frost	C 1958		
I. S. Buchelnikova	1959		
L. G. Christophorou	C 1968a		
L. G. Christophorou	C 1968b		
K. G. Mothes	1972		
A. A. Christodoulides	1974	$\leq$	0.4 eV
O. H. Crawford	C 1974		
S. S. Nagra	1975		
J. P. Ziesel	C 1975	○	Br <sup>-</sup> formation, 0 - 1.9 eV
R. Abouaf	1977		
N. A. Burdett	1977		
D. W. Trainor	1978		
R. Abouaf	1980		0.05 - 2 eV
R. Azria	1982		
Y. Le Coat	B 1982	○	H <sup>-</sup> formation, 5 - 10 eV
N. G. Adams	C 1986		
D. Smith	B 1987		
W. C. Wang	1988a		
M. Cizek	P 2001	○	
G. P. Karwasz	2001		compilation
J. B. A. Mitchell	2001		
T. Speck	2001		

attachment theory

S. A. Pozdneev	1982
A. U. Hazi	B 1983
S. A. Pozdneev	1988
J. Horacek	P 1996
S. A. Pozdneev	2000
K. Houfek	2001
K. Houfek	P 2002

We need more experimental studies of cross sections and other processes, especially grand total cross section, elastic scattering cross section, ionization cross section and electron swarm parameters, for the determination of tentative and approximate cross section set for HBr.

We cannot determine the exact value of cross section set for molecules. The HBr molecules are always mixture of HBr(r) and HBr(v) at given experimental conditions. And cross section sets for HBr(r) and HBr(v) are different.

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  $Q_{ms}$ ,  $Q_{mr}$ ,  $Q_{mv}$ ,  $Q_{rs}$ ,  $Q_{rr}$ ,  $Q_{rv}$ ,  $Q_{vs}$ ,  $Q_{vr}$ , 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  $Q_{ms}$ ,  $Q_{mr}$ ,  $Q_{rs}$ ,  $Q_{rr}$  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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Atoms (17)		Molecules (51)			
A + e.	A + hν		M + e.	M + hν.	
He 2	2170 *	2 H <sub>2</sub> , D <sub>2</sub>	2200 ○	5 CH <sub>4</sub>	800
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	330 ○	6 C <sub>2</sub> H <sub>4</sub>	370
		HCl	420 ○	CH <sub>3</sub> OH	350
O 8	390	HBr	220 ○		
		HI	150 ○	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>	700	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>60</sub>	300
		PH <sub>3</sub>	120		
		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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