

# **Total and partial cross sections for electron scattering on atoms and molecules**

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IAEA –AMD, Vienna, 27/11/2019

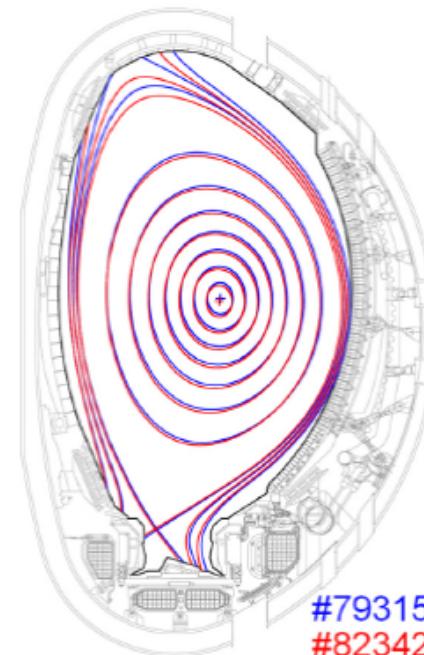
# Rationale: edge and divertor plasma

Influence of atomic physics on  
EDGE2D-EIRENE simulations of JET  
divertor detachment with carbon and  
beryllium/tungsten plasma-facing  
components

**Table 3.** Atomic and molecular reactions included in the physics models used in EIRENE (also valid for D).

NIMBUS-like model	Kotov-2008 model
(1) $e + H^0 \rightarrow 2e + H^+$	Same reactions as default plus:
(2) $H^+ + H^0 \rightarrow H^0 + H^+$	(9) $H_2 + H^+ \rightarrow H^+ + H_2$
(3) $e + C^0 \rightarrow 2e + C^+$	(10) $H_2 + H^+ \rightarrow H_2^+ + H^0$
(4) $e + H_2 \rightarrow 3e + 2H^+$	(11) $e + H_2 \rightarrow 2e + H_2^+$ (replacing (4))
(5) $e + H_2 \rightarrow e + 2H^0$	
(6) $e + H_2 \rightarrow 2e + H^+ + H^0$	(12) $e + H_2^+ \rightarrow e + H^0 + H^+$
(7) $e + H^+ \rightarrow H^0$	(13) $e + H_2^+ \rightarrow 2e + 2H^+$
(8) $2e + H^+ \rightarrow e + H^0$	(14) $e + H_2^+ \rightarrow 2H^0$
No CRM <sup>a</sup> for (4), (5) and (6)	CRM <sup>a</sup> for (11), (5) and (6)

<sup>a</sup> Collisional Radiative Model.



**Figure 1.** Magnetic equilibria for the shots #79315 and #82342 at 20 s and 13 s, respectively.

# Data needed:

## I Neutrals (H, C, C<sub>2</sub>, Be, BeH<sub>2</sub>, CH<sub>4</sub>)

### 1. Total cross section

### 2. Partial cross sections:

elastic scattering       $e+A \rightarrow e+A$

rotational excitation     $e+CH_4 (J=0) \rightarrow e+CH_4 (J=2)$

vibrational excitation     $e+AB(v=0) \rightarrow e+AB(v>0)$

electron attachment (dissociative)     $e+AB \rightarrow A^- + B$

electronic excitation     $e+A \rightarrow e+A^*$

emission lines:  $A^* \rightarrow A + h\nu$

neutral dissociation     $e+AB \rightarrow A + B + e$

emission from dissociation     $e + AB \rightarrow A^* + B + e + h\nu$

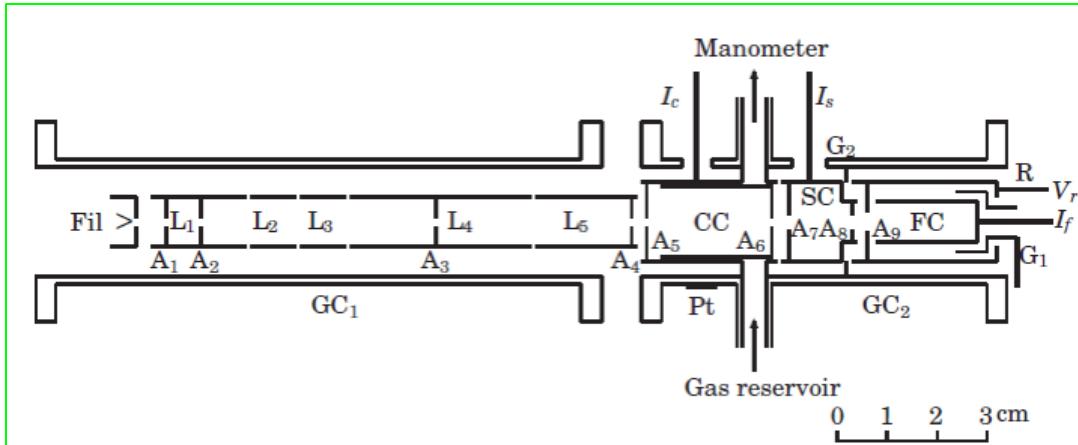
ionization                 $e+A \rightarrow A^+ + 2e$

dissociative ionization     $e+AB \rightarrow A + B^+ + 2e$

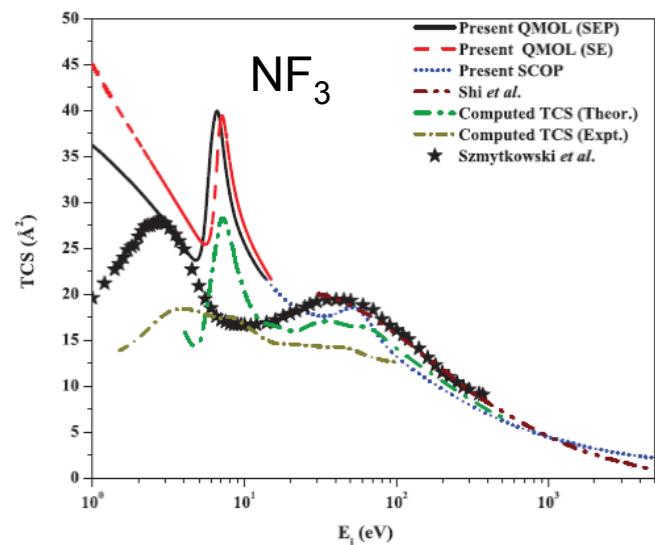
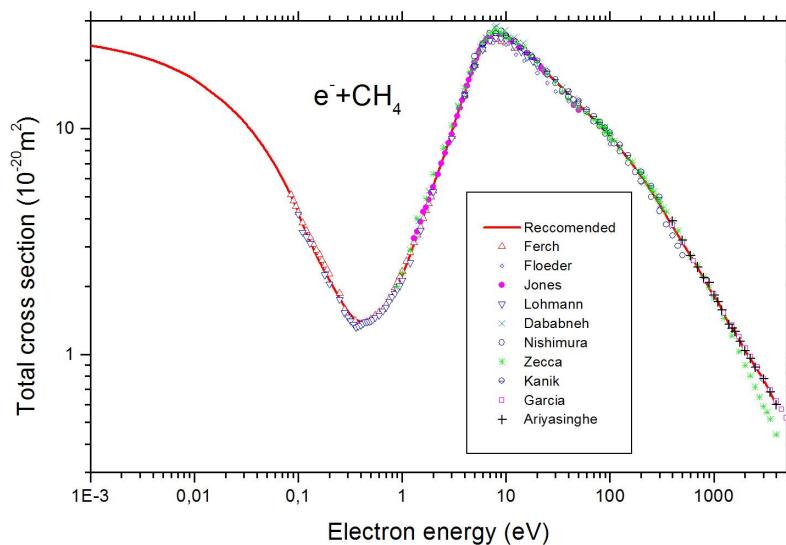
ionization into excited states     $e + A \rightarrow (A^*)^* + 2e$

# Experimental methods: total

attenuation method  $I = I_0 \exp(-\sigma n L)$ ; precision <5%

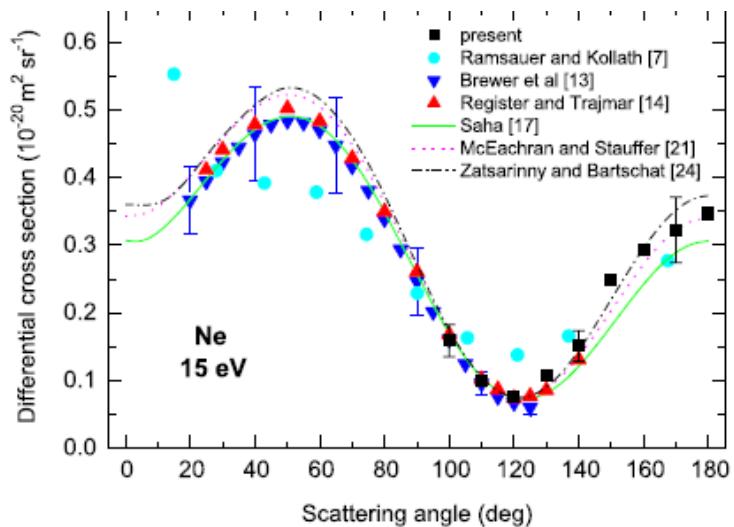
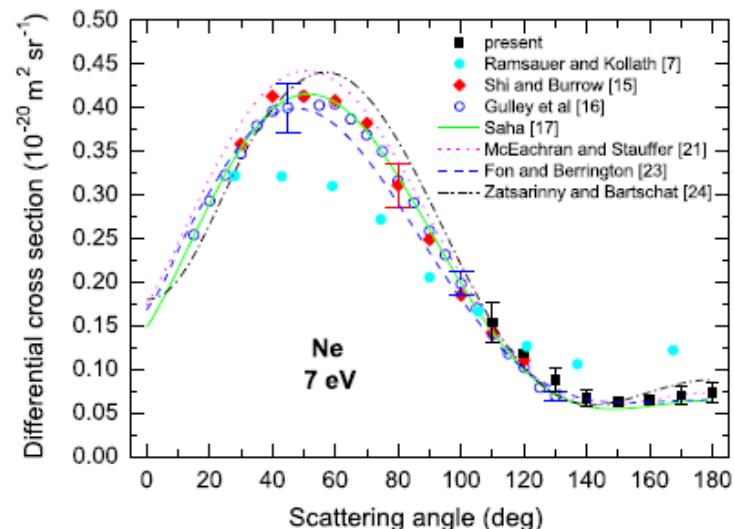
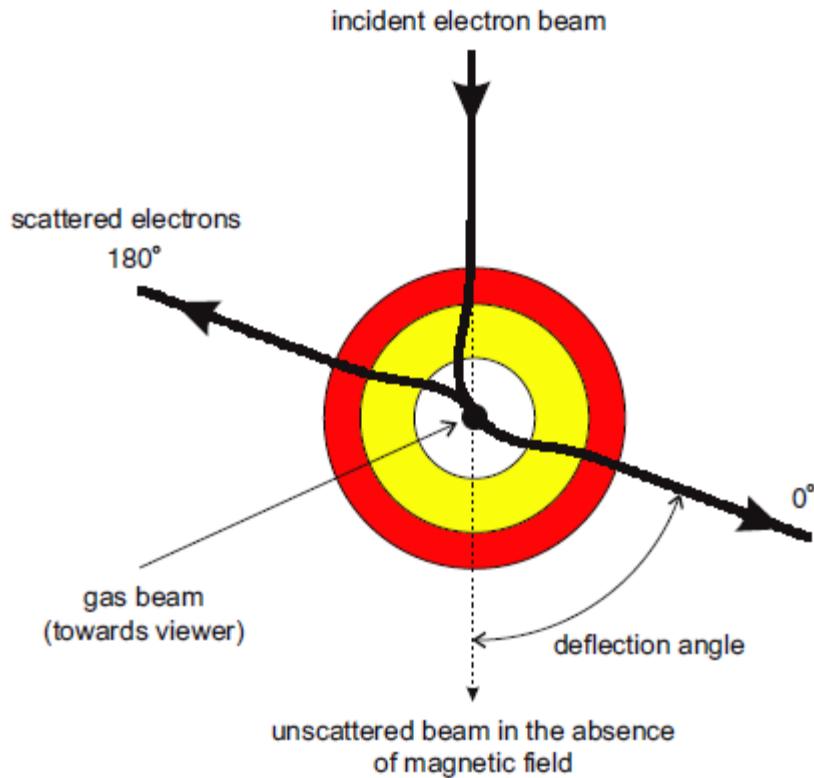


H. Nishimura et al.,  
J.Phys. Soc. Japan 72 (2003) 1080

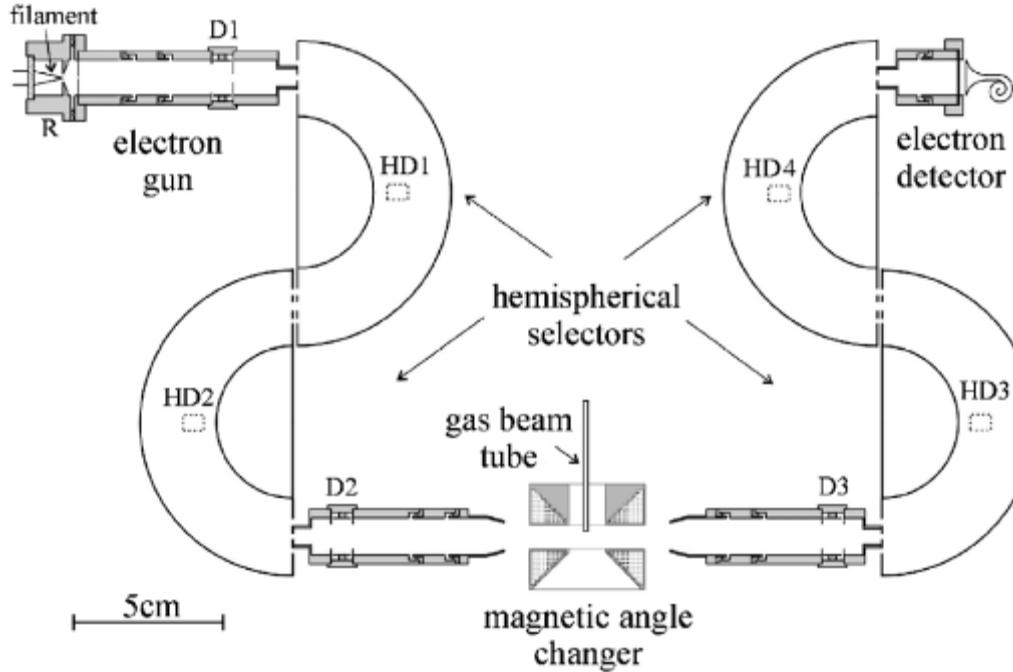


# Experimental methods: elastic

PHYSICAL REVIEW A 74, 042701 (2006)



# Experimental methods: excitation (electronic, vibrational)

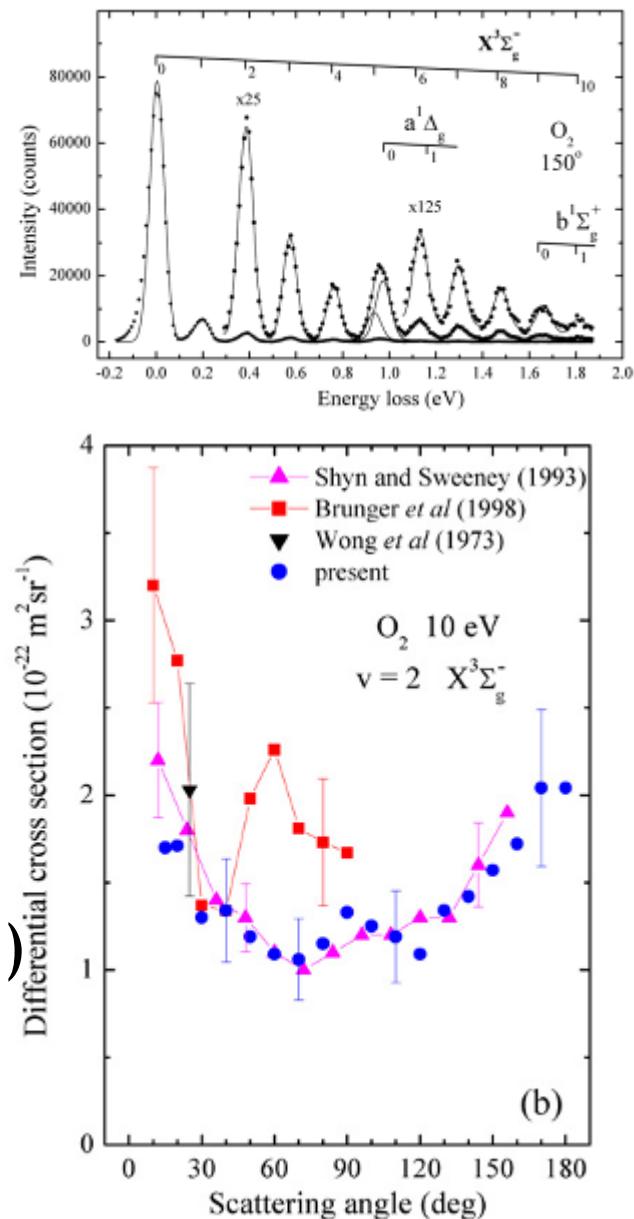


Experiments by:

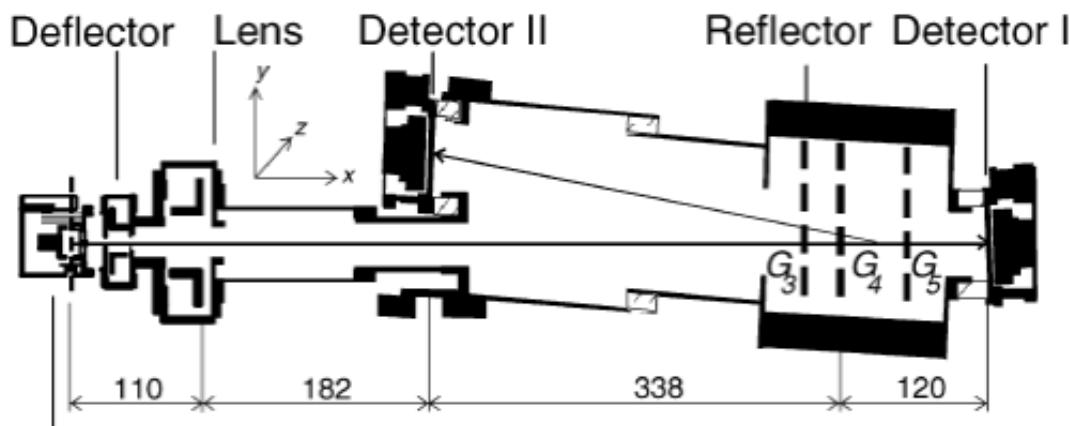
I. Linert, M. Zubek (Gdansk) J. Phys. B 39  
(2006)

M. Khakoo et al. (Fullerton California)

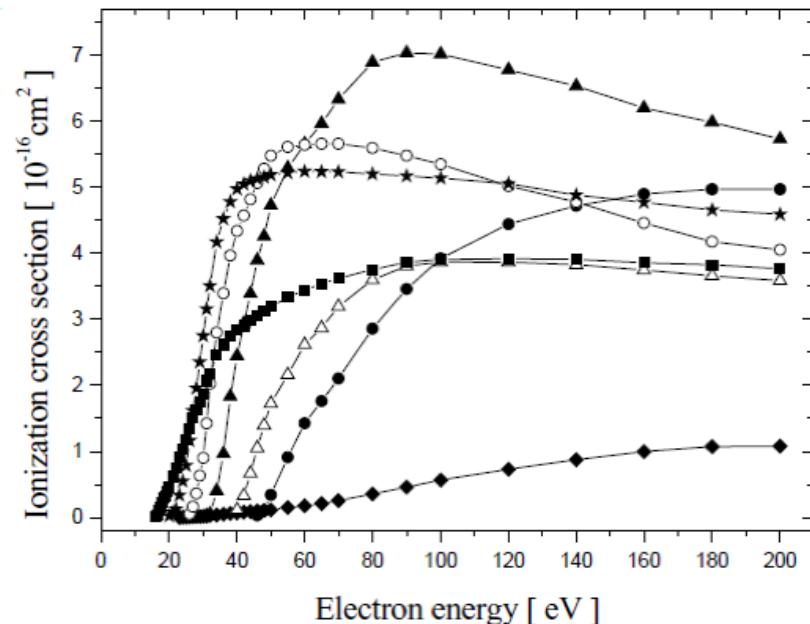
M. Allan (Freiburg University)



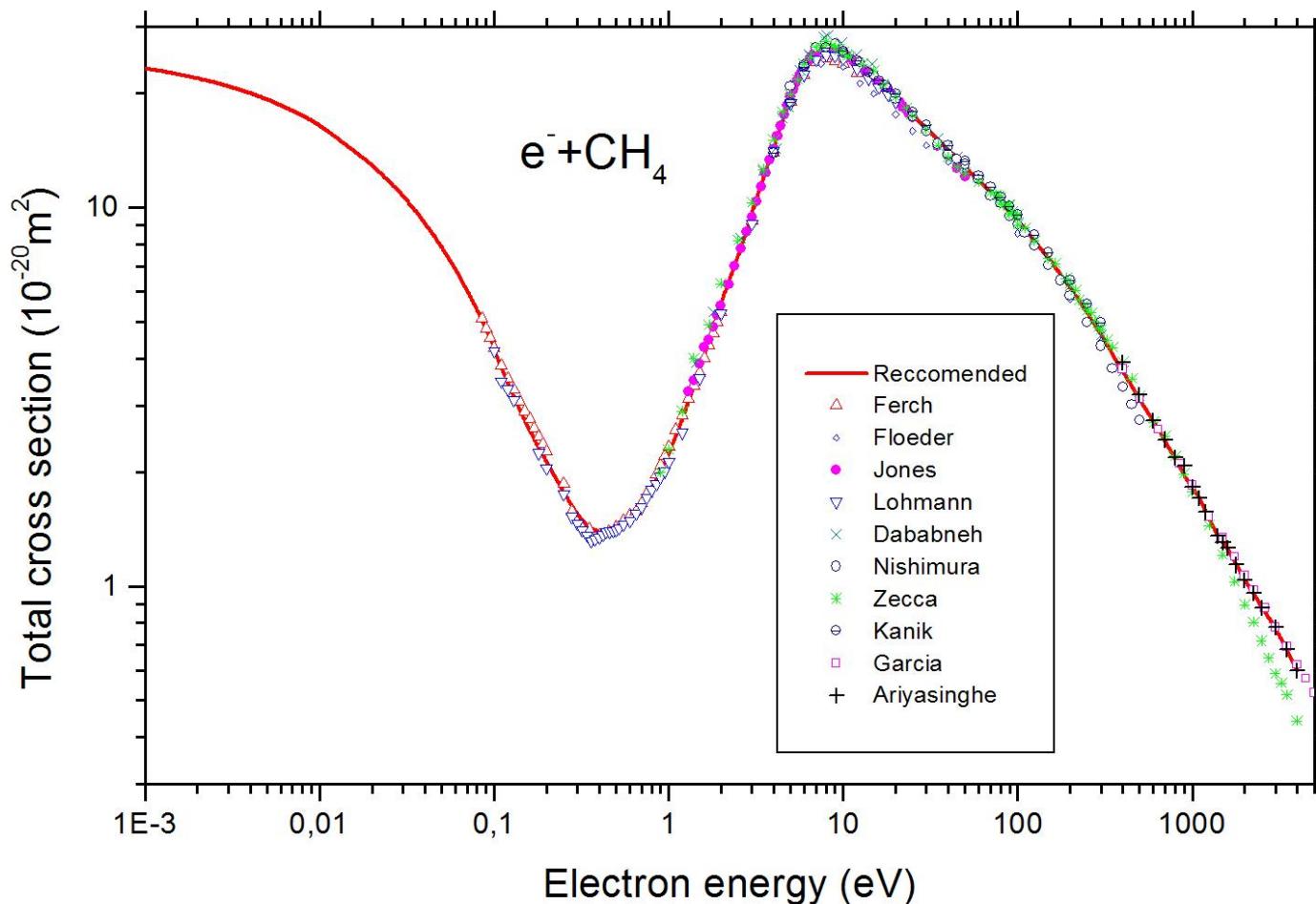
# Experimental methods: ionization



If two ions are formed  
(for example  $\text{CH}_4 \rightarrow \text{CH}_3^+ + \text{H}^+ + 2e^-$ )  
the ionization is counted twice



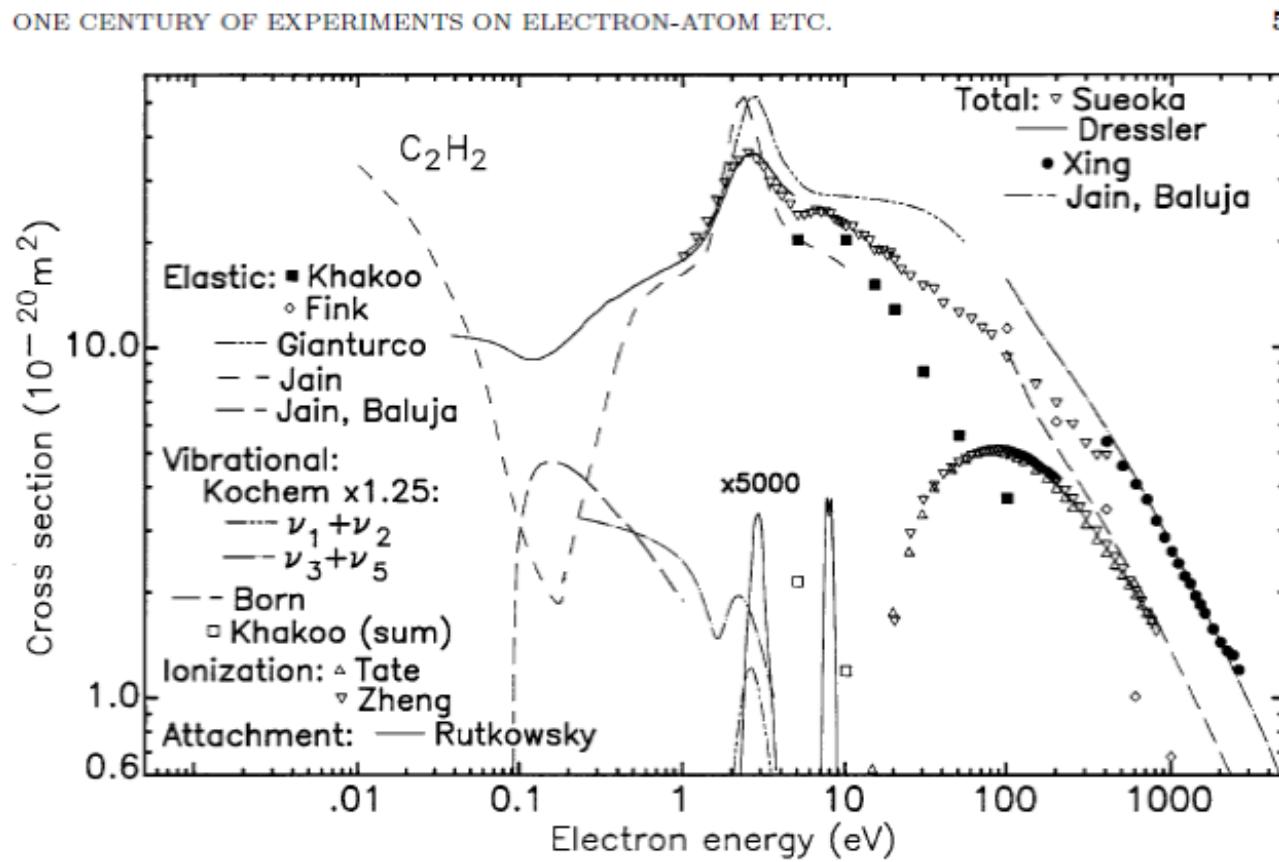
# Total cross sections: beam ( $\pm 5\%$ )



M.-Y. Song, Y.-S. Yoon, H. Cho, Y. Itikawa, G. P. Karwasz, V. Kokououline, Y. Nakamura, J. Tennyson, Journal of Physical and Chemical Reference Data **44**, 023101 (2015)

# „One century experiments on electron-atom and molecule scattering (2001)

3 volumes, some 50 molecules



# One century of experiments on electron-atom and molecule scattering: a critical review of integral cross-sections

## II. – Polyatomic molecules

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(ricevuto il 29 Marzo 2000)

3 volumes,  
some 50 molecules

G.P. Karwasz,  
R.S. Brusa, A. Zecca,  
*Riv. Nuovo Cimento*,

Vol. 19, No. 3 (1996)  
atoms & diatomic

Vol. 24, no.1 (2001)  
triatomeric etc.

Vol. no 4. (2001)  
hydrocabons

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1	1.	Introduction
1	1'1.	General remarks
2	1'2.	Review papers
2	1'3.	Updating references
4	1'4.	Aims of the paper
4	1'5.	Organization of the paper
12	2.	Tetrahedral hydrides
12	2'1.	Methane ( $\text{CH}_4$ )
22	2'2.	Silane ( $\text{SiH}_4$ )
29	2'3.	Germane ( $\text{GeH}_4$ )
34	3.	Hydrides
34	3'1.	Ammonia ( $\text{NH}_3$ )
41	3'2.	Water vapour ( $\text{H}_2\text{O}$ )
51	3'3.	Phosphine ( $\text{PH}_3$ )
52	3'4.	Hydrogen sulfide ( $\text{H}_2\text{S}$ )
58	3'5.	Hydrogen chloride ( $\text{HCl}$ )
66	3'6.	Other hydrogen halides ( $\text{HF}, \text{HBr}$ )
69	4.	Triatomic molecules
69	4'1.	Carbon dioxide ( $\text{CO}_2$ )
79	4'2.	Nitrous oxide ( $\text{N}_2\text{O}$ )
87	4'3.	Nitrogen dioxide ( $\text{NO}_2$ )
91	4'4.	Ozone ( $\text{O}_3$ )
97	4'5.	Carbonyl sulfide ( $\text{OCS}$ )
104	4'6.	Sulphur dioxide ( $\text{SO}_2$ )
112	4'7.	Chlorine dioxide ( $\text{ClO}_2$ )
114	4'8.	Carbon disulphide ( $\text{CS}_2$ )

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TABLE I. – *Integral cross-sections for electron scattering on methane (in  $10^{-20} \text{ m}^2$  units).*

Energy	Elastic	Vibrational	Electronic excitation	Ionization	Neutral dissociation	Summed	Total
0.6	0.92 S 1.1 BU	0.34 B				1.26 1.44	1.49 L 1.54 F
1.0	1.66 S 1.78 BU	0.24 B				1.90 2.16	2.13 L 2.34 F
2.0	5.61 BO 4.64 BU	0.21 B 0.28 BU				5.82 4.92 6.3 Z	5.24 L 5.5 J
2.5	6.06 S	0.18 B				6.24	8.2 Z
3.0	9.25 BO 7.70 BU 7.4 TA	0.46 T 0.45 BU				9.71 8.15 7.85	9.06 L 9.4 J 10.3 Z
5.0	18.0 BO 17.5 BU 13.7 TA	0.83 T 1.32 BU				18.8 18.8	18.9 K 19.9 Z
8.0	26.3 BO 19.6* TA	1.33 T				27.6	26.4 K 27.4 Z
10	23.0 BO 19.8 SH 18.4 TA	1.02 T		0.31 N		24.3	25.9 K
15	18.3 BO 17.6 SH 15.7 TA	0.45 T	1.1 KA	0.21 NI	(1.3) N	20.1	23.0 Z
20	14.4 BO 15.3 SH 17.6 V 14.3 TA	0.31 T	1.75 KA (1.5 VT)	1.22 NI	(2.0) N	17.7 18.6 20.6	20.0 K

Compared,  
checked,  
not recommended

# Electron-scattering database – UMK (2013)

European Physical Journal D | Causality in a quantum world | Magdalénien musique - Szukaj w | Electron Scattering Cross Section

Niezabezpieczona | dydaktyka.fizyka.umk.pl/ESCS/

## ELECTRON SCATTERING CROSS SECTIONS

Interactive data base (K. Fedus, K. Służewski, 2013) based on Rivista del Nuovo Cimento (G.P. Karwasz, R.S. Brusa, A. Zecca, 1996-2001)

Atoms	Diatomeric molecules	Hydrides	Triatomic molecules	Hydrocarbons	Halides
H	H <sub>2</sub>	CH <sub>4</sub>	CO <sub>2</sub>	C <sub>2</sub> H <sub>2</sub>	CF <sub>4</sub>
He	N <sub>2</sub>	SiH <sub>4</sub>	N <sub>2</sub> O	C <sub>6</sub> H <sub>6</sub>	CF <sub>3</sub> Cl
Li	CO	GeH <sub>4</sub>	NO <sub>2</sub>	C <sub>2</sub> H <sub>4</sub>	CF <sub>2</sub> Cl <sub>2</sub>
O	O <sub>2</sub>	NH <sub>3</sub>	O <sub>3</sub>	C <sub>2</sub> H <sub>6</sub>	CFCl <sub>3</sub>
Ne	NO	H <sub>2</sub> O	OCS	C <sub>3</sub> H <sub>8</sub>	CCl <sub>4</sub>
Na		PH <sub>3</sub>	SO <sub>2</sub>		CH <sub>3</sub> F
Ar		H <sub>2</sub> S	ClO <sub>2</sub>		CH <sub>3</sub> Cl
K		HCl	CS <sub>2</sub>		CH <sub>3</sub> Br
Kr		HF			CH <sub>3</sub> I
Rb		HBr			NF <sub>3</sub>
Xe					C <sub>2</sub> F <sub>6</sub>
Cs					C <sub>3</sub> F <sub>8</sub>
Hg					C <sub>6</sub> F <sub>6</sub>
					SF <sub>6</sub>
					UF <sub>6</sub>
					WF <sub>6</sub>
					SiF <sub>4</sub>

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<http://dydaktyka.fizyka.umk.pl/ESCS/>

# Electron-scattering database – UMK (2013)

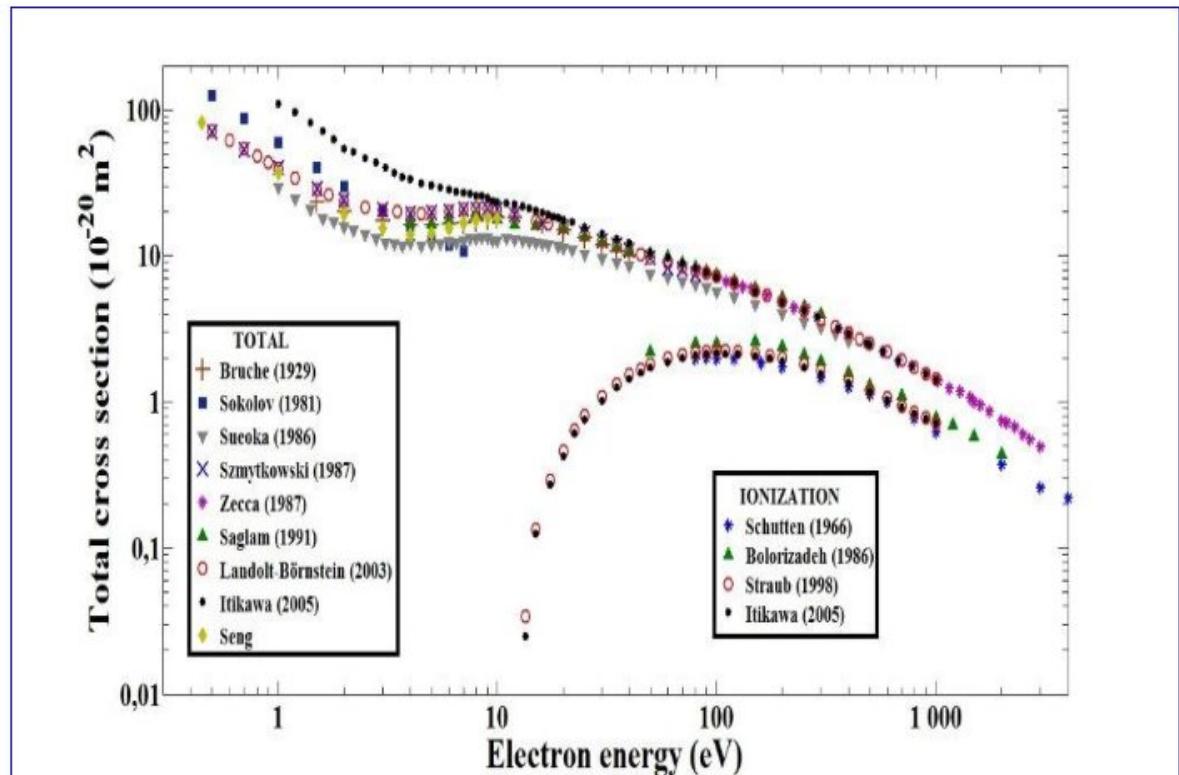
## ELECTRON SCATTERING CROSS SECTIONS

H<sub>2</sub>O

[Main Menu](#)

[Total](#)  
[Elastic](#)

Momentum transfer  
Vibrational excitation  
Rotational excitation  
Electronic excitation  
[Ionization](#)  
Electron attachment



Chosen integral cross sections

# Electron-scattering database – UMK (2013)

← → C ⓘ Niezabezpieczona | [dydaktyka.fizyka.umk.pl/ESCS/Hydrides/H2O/Ionization/index.html](http://dydaktyka.fizyka.umk.pl/ESCS/Hydrides/H2O/Ionization/index.html)

## ELECTRON SCATTERING CROSS SECTIONS

### H<sub>2</sub>O

#### Total

#### Elastic

Momentum transfer

Vibrational excitation

Rotational excitation

Electronic excitation

#### Ionization

Electron attachment

### Main Menu

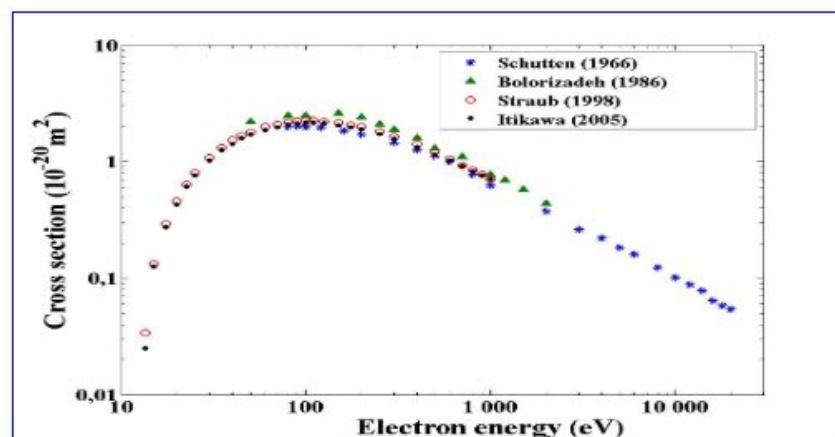
#### Data



[Integral and partial ionization](#)

H<sub>2</sub>O. Ionization – intergal cross sections

#### Graph



Integral ionization cross sections

#### References:

- SCHUTTEN J., de Heer F. J., Moustafa H. R., Boerboom A. J. H. and Kistemaker J., *J. Chem. Phys.*, 44 (1966) 3924.  
BOLORIZADEH M. A. and Rudd M. E., *Phys. Rev. A*, 33 (1986) 882.  
STRAUB H. C., Lindsay B. G., Smith K. A., and Stebbings R. F., *J. Chem. Phys.* 108, 109 (1998).  
ITIKAWA Y. and Mason N., *J. Phys. Chem. Ref. Data* 34, (2005) 1.

# Electron-scattering database – UMK (2013)

## H<sub>2</sub>O: elastic – differential cross sections

Microsoft Excel - H <sub>2</sub> O_elastic_DCS.xls															
Plik Edycja Widok Wstaw Format Narzędzia Dane Okno Pomoc Wpisz pytanie do Pomocy															
AL15	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
1	Katase86	energy (ev)	-	Shyn87	energy (ev)	energy (ev)	energy (ev)	energy (ev)	er						
2	angle(deg.)	100	200	300	400	500	700	1000	-	angle(deg.)	2.2	4.0	6.0	8.0	10
3	0	9,71	12	8,54	8,71	6,53	5,9	4,47	-	15	7,44	7,21	8,43	9	
4	5	8,34	9,7	6,99	6,88	5,23	4,74	3,67	-	30	2,77	3,37	3,36	3,17	
5	10	5,44	4,09	3,29	2,91	2,28	1,95	1,25	-	45	1,38	1,44	1,6	1,46	
6	15	2,96	2,02	1,64	1,27	0,957	0,767	0,5	-	60	0,74	0,99	1,05	1,12	
7	20	1,59	1,03	0,727	0,597	0,487	0,357	0,246	-	75	0,58	0,67	0,78	0,82	
8	30	0,573	0,329	0,232	0,204	0,17	0,125	0,0751	-	90	0,44	0,49	0,55	0,54	
9	40	0,228	0,158	0,114	0,0874	0,0744	0,0524	0,03	-	105	0,36	0,31	0,45	0,4	
10	50	0,129	0,0822	0,0595	0,046	0,0403	0,026	0,0148	-	120	0,35	0,29	0,37	0,42	
11	60	0,0785	0,0489	0,0381	0,0308	0,0255	0,0162	0,00872	-	135	0,33	0,38	0,5	0,62	
12	70	0,0498	0,0326	0,0283	0,0219	0,0163	0,0106	0,00534	-	150	0,46	0,58	1	1,25	
13	80	0,0286	0,0263	0,0218	0,0157	0,012	0,00724	0,00372	-	165	0,68	0,88	1,95	1,95	
14	90	0,0251	0,0254	0,0187	0,0128	0,00973	0,00535	0,00267	-						
15	100	0,0287	0,0245	0,0158	0,011	0,00831	0,00427	0,00214	-						
16	110	0,0388	0,0246	0,0151	0,0102	0,00711	0,00353	0,00172	-						
17	120	0,0531	0,0242	0,0145	0,00953	0,00629	0,00303	0,00148	-						
18	130	0,068	0,0245	0,0142	0,0091	0,00607	0,00269	0,00136	-						
19	140	0,0984	0,0293	0,0155	0,00915	0,00577	0,00255	0,0013	-						
20	150	0,132	0,0356	0,017	0,00924	0,00571	0,0025	0,001	-						
21	160	0,167	0,0429	0,0186	0,00938	0,00572	0,00251	0,00134	-						
22	170	0,192	0,0487	0,0198	0,00949	0,00575	0,00253	0,00137	-						
23	180	0,202	0,051	0,0203	0,00953	0,00576	0,00254	0,00138	-						
24									-						
25									-						
26									-						
27									-						
28									-						
29									-						
30									-						
31									-						

# Landolt-Börstein Data (2003)

[LB-SEARCH \(Springer\)](#)

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[GROUP I: Elementary Particles, Nuclei and Atoms](#)

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[Photon and Electron Interactions with Atoms, Molecules and Ions](#)

[SUBVOLUME C](#)

[Interactions of Photons and Electrons with Molecules](#)

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[2 Electron collisions with atoms \( See Vol. 17A\)](#)

[3 Electron collisions with atomic ions \( See Vol. 17B\)](#)

[4 Cross sections for photoabsorption, photoionization, neutral dissociation of molecules \(K. KAMETA, N. KOUCHI, Y. HATANO\)](#)

[4.1 Introduction](#)

[4.2 General comments](#)

[4.3 Glossary and abbreviation](#)

[4.4 Cross section data](#)

[CCl<sub>4</sub>](#)

[CF<sub>4</sub>](#)

[CH<sub>3</sub>OCH<sub>3</sub>](#)

[CH<sub>3</sub>OC<sub>2</sub>H<sub>5</sub>](#)

[CH<sub>3</sub>OH](#)

[CH<sub>4</sub>](#)

[CO](#)

[CO<sub>2</sub>](#)

[CS<sub>2</sub>](#)

[C<sub>2</sub>H<sub>2</sub>](#)

G.P.Karwasz, A.Zecca, R.S.Brusa, Electron Scattering with Molecules. Total. (in:) Landolt-Börnstein. Numerical Data and Functional Relationships in Science and Technology. New Series / Editor in Chief: W. Martienssen. Group I: Elementary Particles, Nuclei and Atoms. Volume 17. Photon and Electron Interactions with Atoms, Molecules and Ions. Subvolume C. Interactions of Photons and Electrons with Molecules. Chapter VI.1 , p. 6.1-6.51, Springer-Verlag, Berlin, Heidelberg, 2003

# Landolt-Börstein Data (2003)

6-14

## 6.1 Total scattering cross sections

[Ref. p. 6-4]

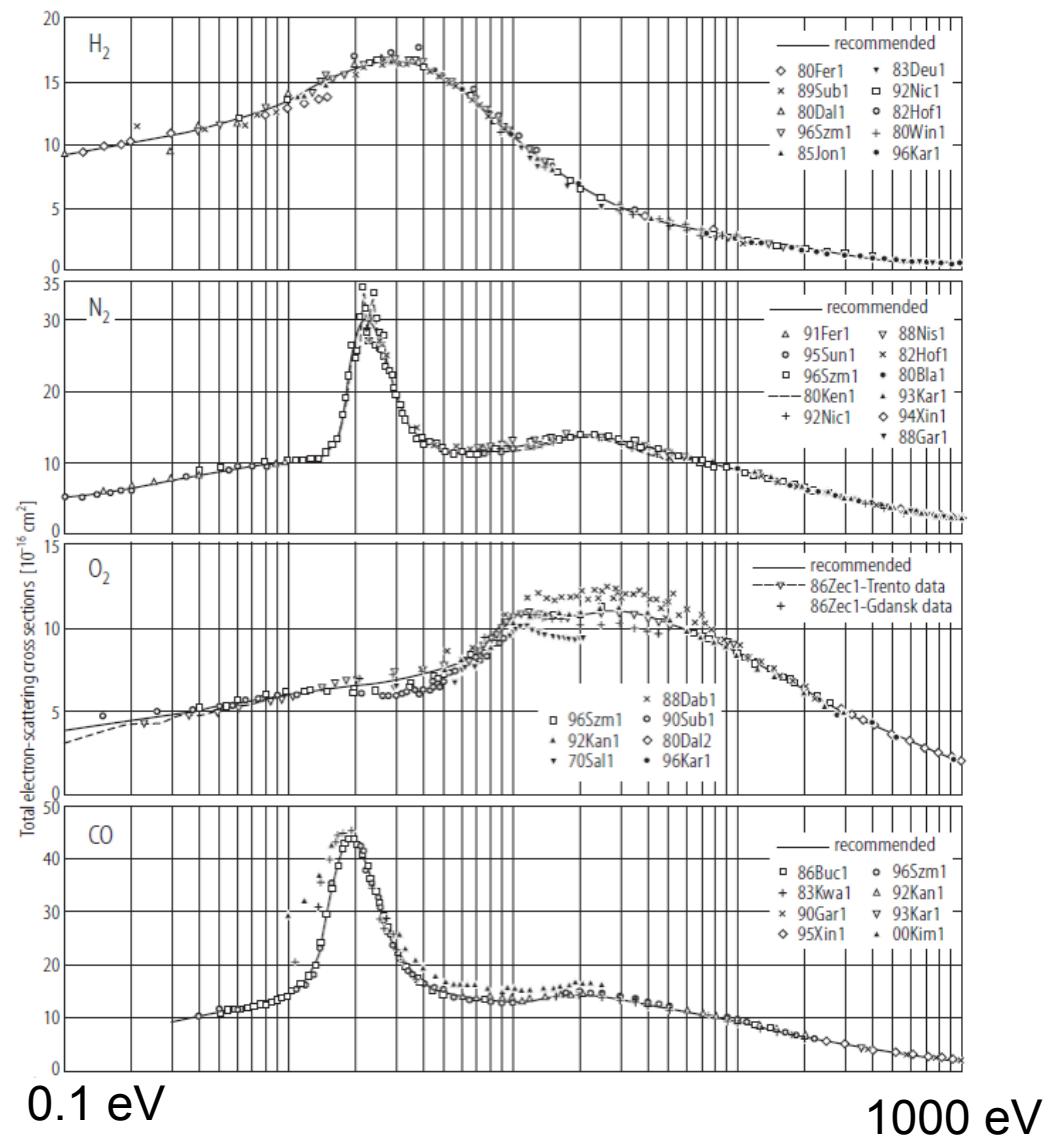


Table 6.1.2. Recommended total cross sections for diatomic molecules.

Energy [eV]	Cross section [10 <sup>-16</sup> cm <sup>2</sup> ]				
	H <sub>2</sub>	N <sub>2</sub>	O <sub>2</sub>	CO	NO
0.1	9.23	4.88	3.83 (c1)		
0.12	9.47	5.13	4.02 (d1)		
0.15	9.76	5.56	4.22		
0.17	9.93	5.85	4.33		
0.2	10.1	6.25	4.47		
0.25	10.5	6.84	4.65		
0.3	10.7	7.32	4.79	9.13	
0.35	11.0	7.72	4.91	9.69	
0.4	11.2	8.06	5.07	10.2	
0.45	11.4	8.33	5.20	10.6	
0.5	11.6	8.61	5.31 (c2)	10.9	
0.6	11.9	8.96	5.49	11.7	
0.7	12.3	9.25	5.64	12.2	
0.8	12.8	9.48	5.77	12.7	
0.9	13.2	9.66	5.87	13.3	
1.0	13.5 (a1)	9.85	5.97	14.1	
1.2	14.2	10.2	6.18	16.7	
1.5	15.0	11.2	6.36	29.1	
1.7	15.5	13.3	6.45	38.9	
2.0	16.0	25.7	6.56 (c3)	43.3 (d2)	
2.5	16.5	28.5 (b1)	6.68	33.3	9.70
3.0	16.6	21.0	6.84	23.8	9.47
3.5	16.6	14.6	7.01	18.9	9.32
4.0	16.3	13.2	7.18	16.4	9.25
4.5	15.9	12.3	7.36	15.2	9.22
5.0	15.4	11.8	7.55	14.5	9.23
6.0	14.4	11.4	7.93	13.7	9.32
7.0	13.3	11.4	8.39	13.5	9.48
8.0	12.4	11.5	9.16	13.6	9.68
9.0	11.6	11.7	9.91	13.5	9.92
10	10.9	12.0	10.4	13.2	10.2
12	9.61	12.4	10.8	13.3	11.0
15	8.19	13.2	10.7	13.9	11.5
17	7.46	13.5	10.7	14.3	11.6
20	6.60	13.7	10.8	14.5	11.4

# „Recommended” cross sections for electron scattering with molecules

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**Vяtcheslav Kokouline**

*Department of Physics, University of Central Florida, Orlando, USA*

**Yoshiharu Nakamura**

*6-1-5-201 Miyazaki, Miyamae, Kawasaki, 216-0033, Japan*

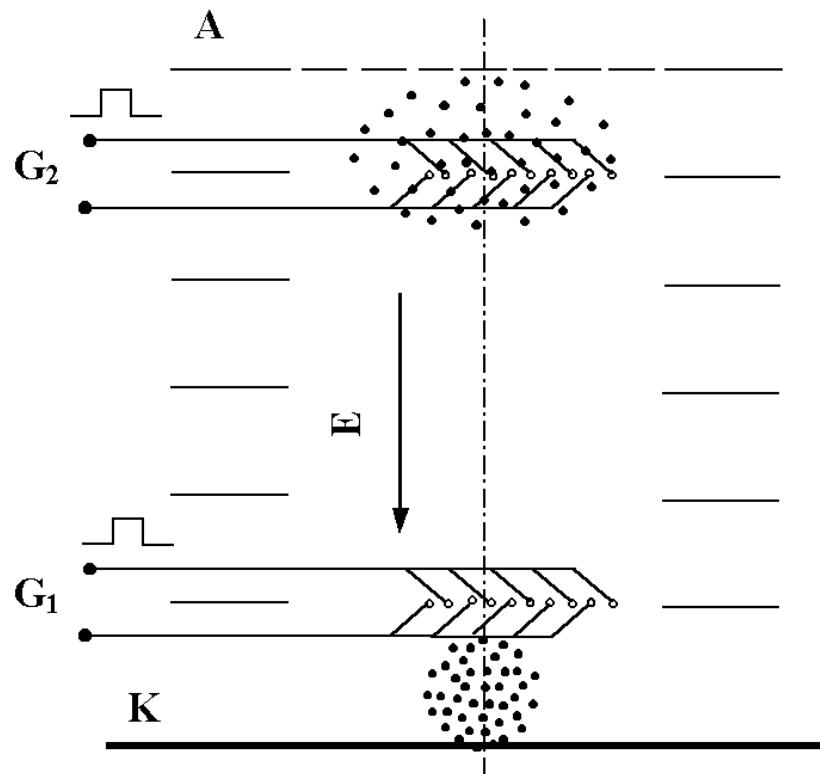
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# Swarm experiments: diffusion coefficients → cross sections

$$\frac{\partial}{\partial t} n_e(\mathbf{r}, t) = -w \frac{\partial}{\partial z} n_e(\mathbf{r}, t) + D_T \left[ \frac{\partial^2}{\partial x^2} n_e(\mathbf{r}, t) + \frac{\partial^2}{\partial y^2} n_e(\mathbf{r}, t) \right] + D_L \frac{\partial^2}{\partial z^2} n_e(\mathbf{r}, t)$$



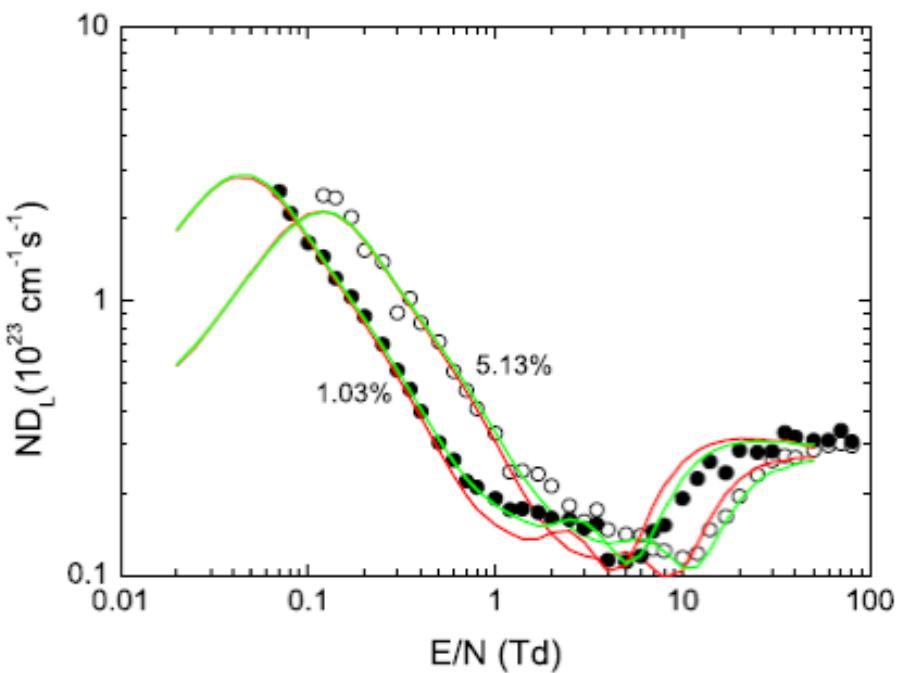
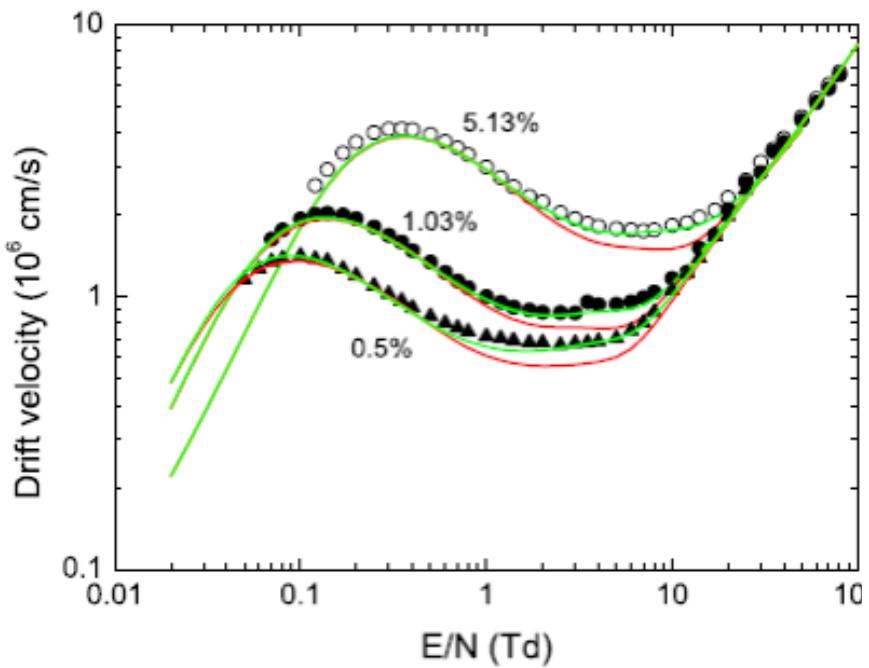
$$w = - \left( \frac{2}{m} \right)^{1/2} \frac{eF}{3N} \int_0^\infty \frac{E}{\sigma_m(E)} \frac{df_0(E)}{dE} dE$$

$$D_T = \left( \frac{2}{m} \right)^{1/2} \frac{1}{3N} \int_0^\infty \frac{E}{\sigma_m(E)} f_0(E) dE$$

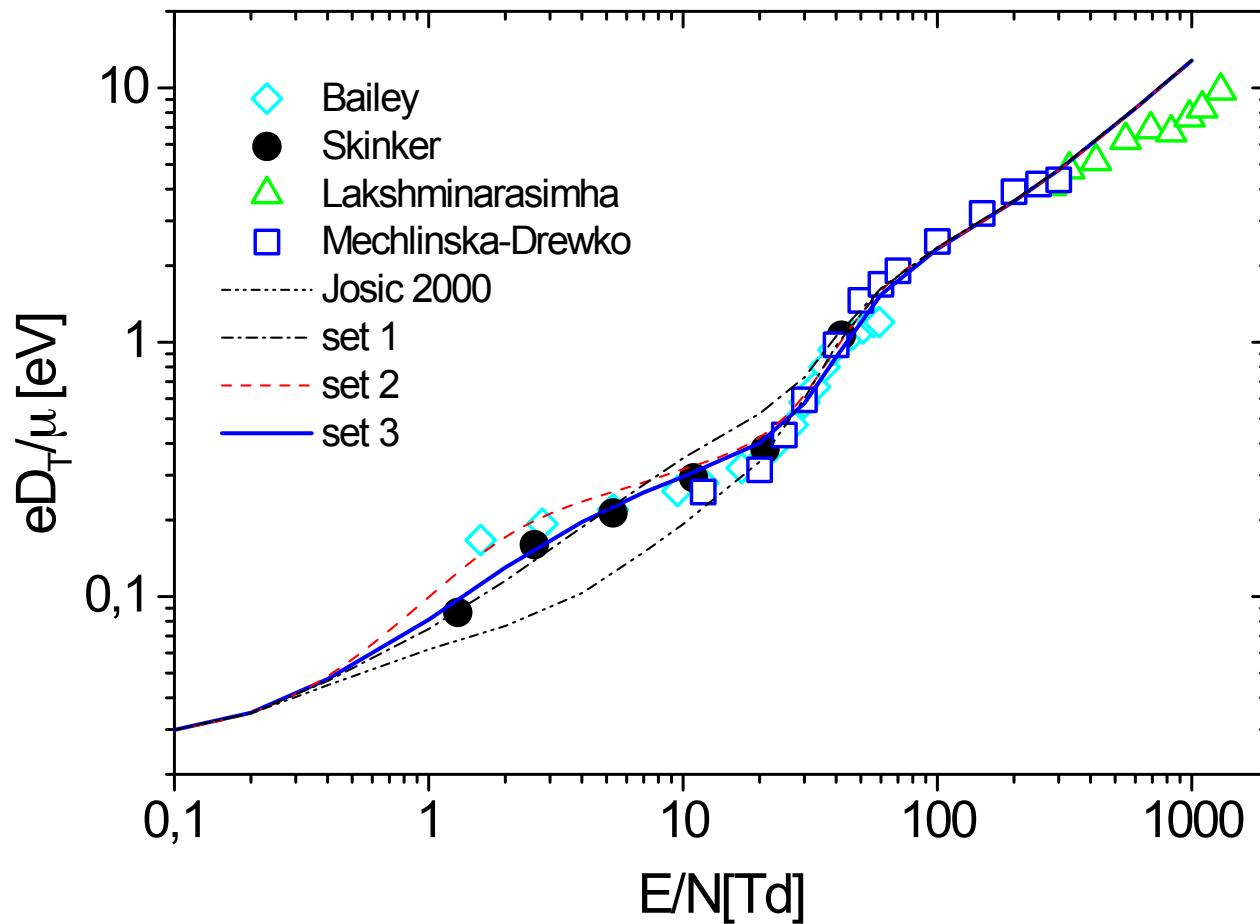
Experiment is simple, but requires guessing cross sections, that can form a non-unique set

# Vibrational: swarm cross-check

$\text{CH}_4$

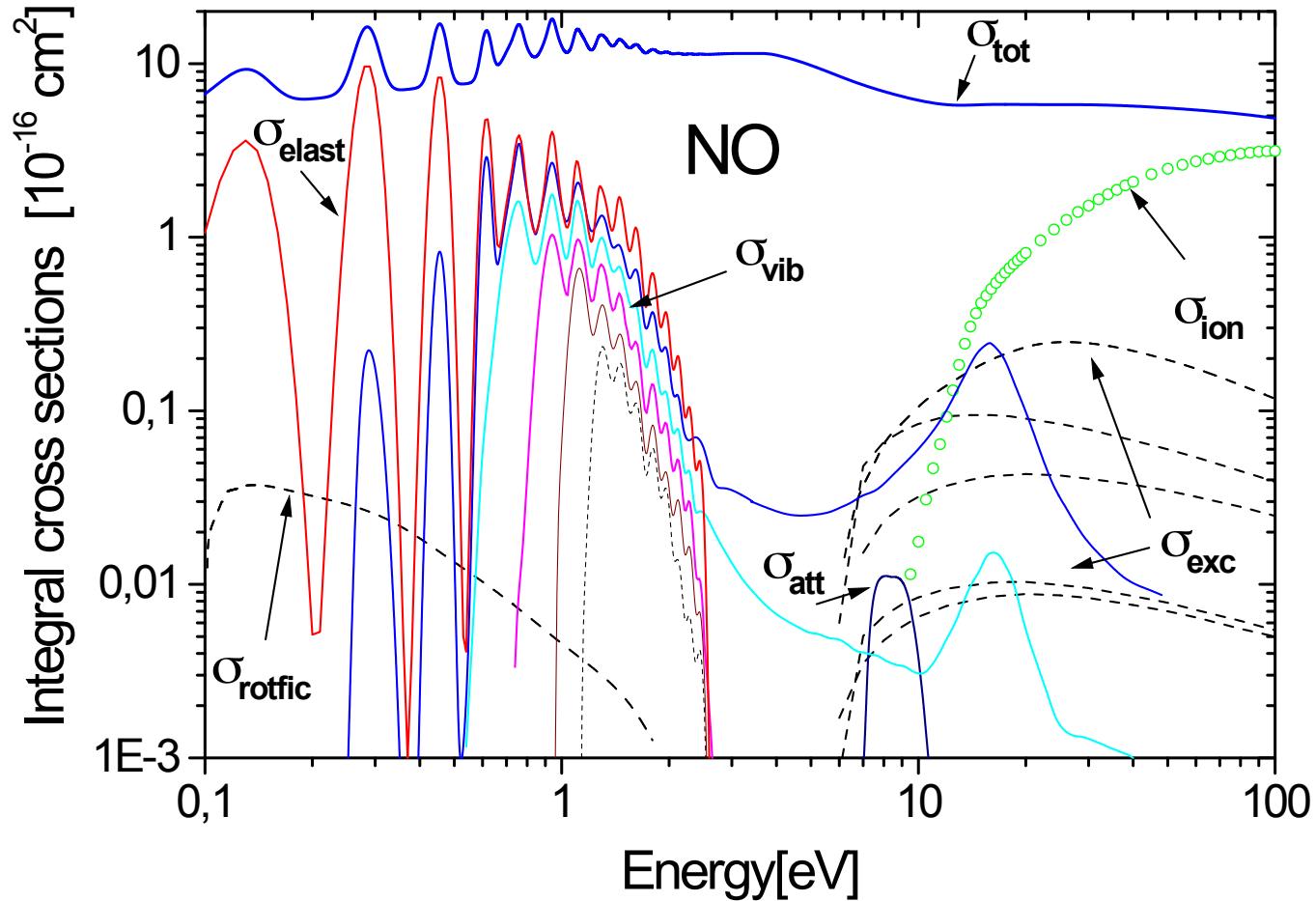


# NO swarm data



L. Josić, T. Wróblewski, Z.Lj. Petrović, J. Mechlińska-Drewko, G. Karwasz  
Chem. Phys. Lett. 350 (2001) 318

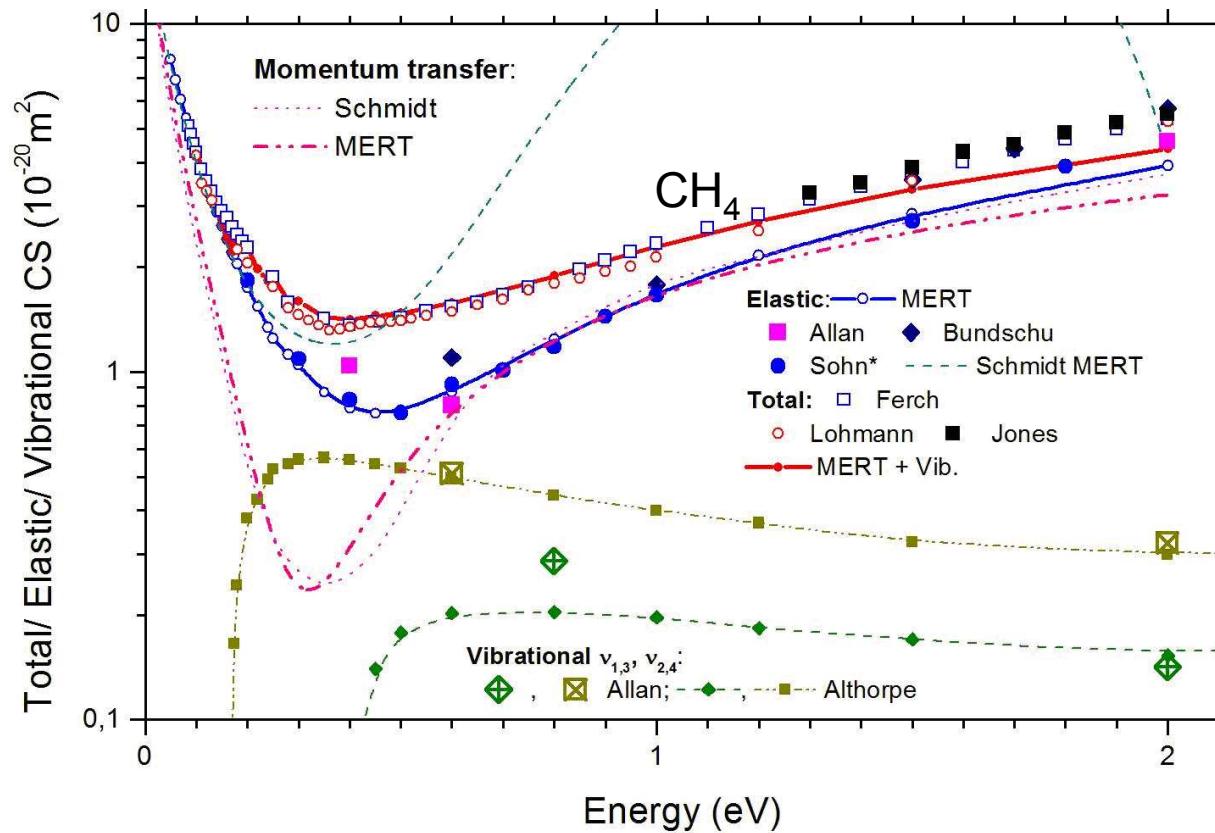
# NO – congruent set of cross sections



Confirmed by beam experiments (ANU Canberra, Fribourg Uni)

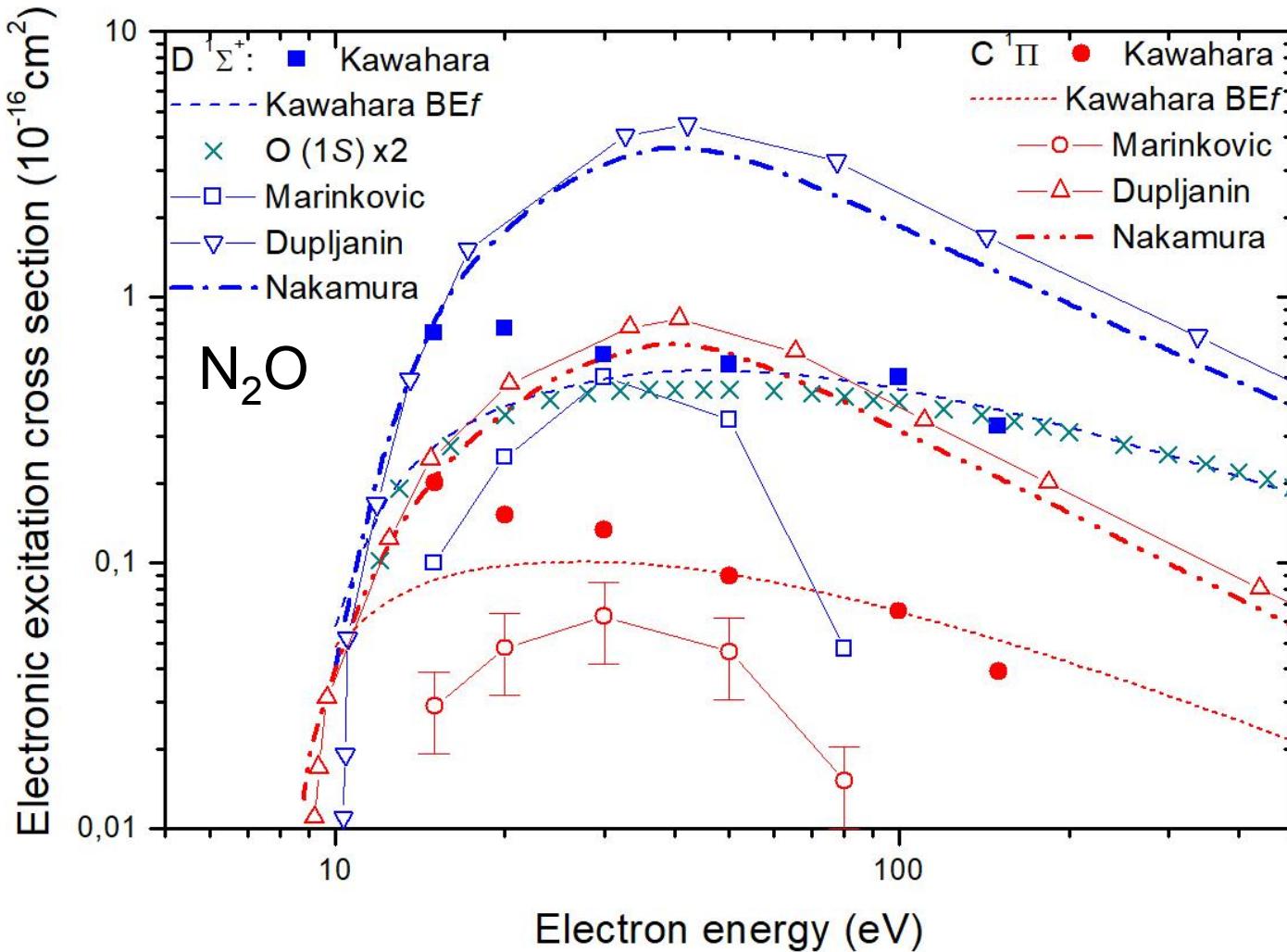
# Semi-empirical methods: elastic (MERT)

Link between elastic, total, MTCS: in some simple cases, and low energies

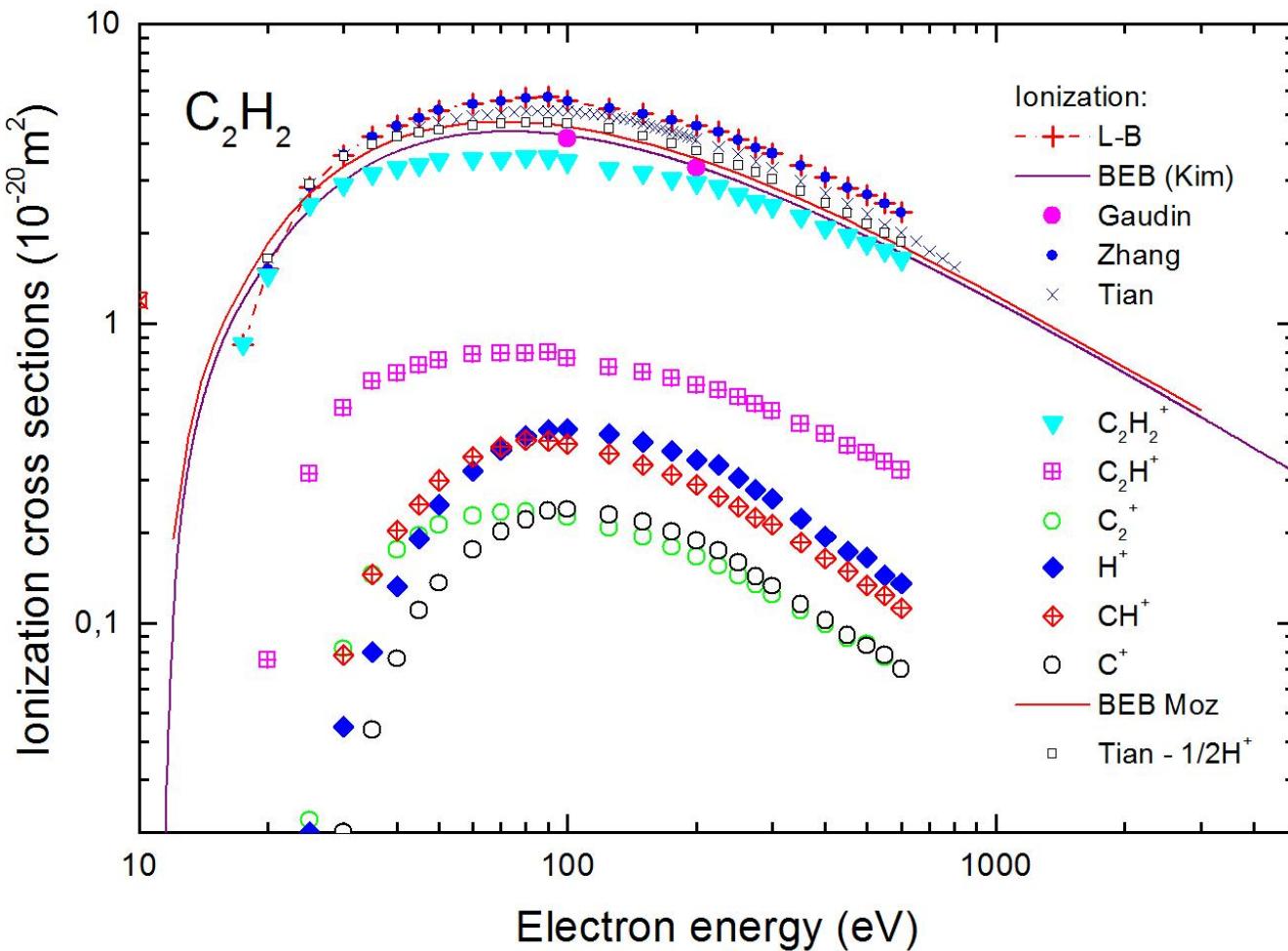


**MERT allows to links elastic, total, MTCS:**  
for atoms, spherical molecules @ energies <1 eV

# Electronic excitation: swarm, beam, theory

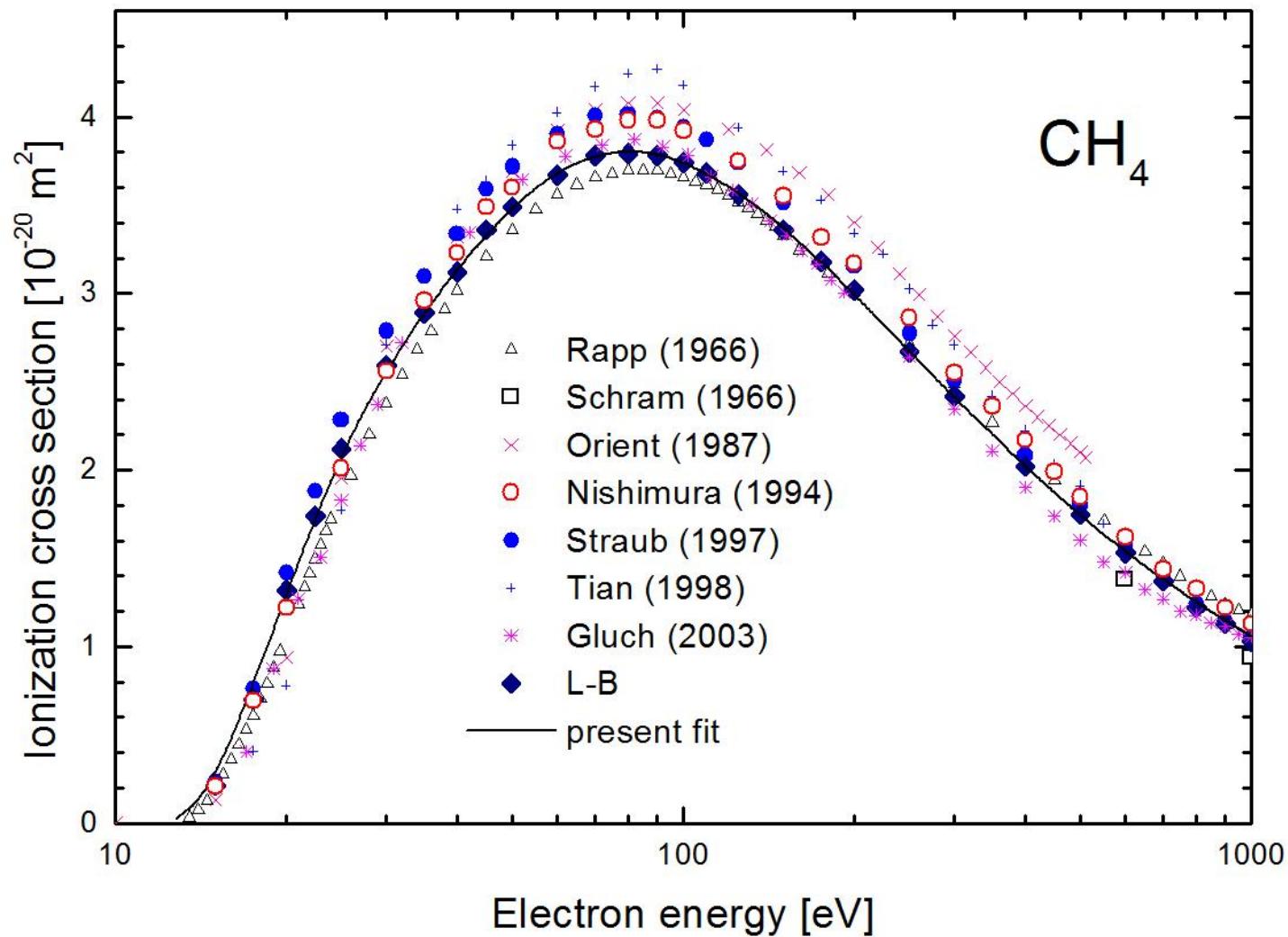


# Ionization: partial

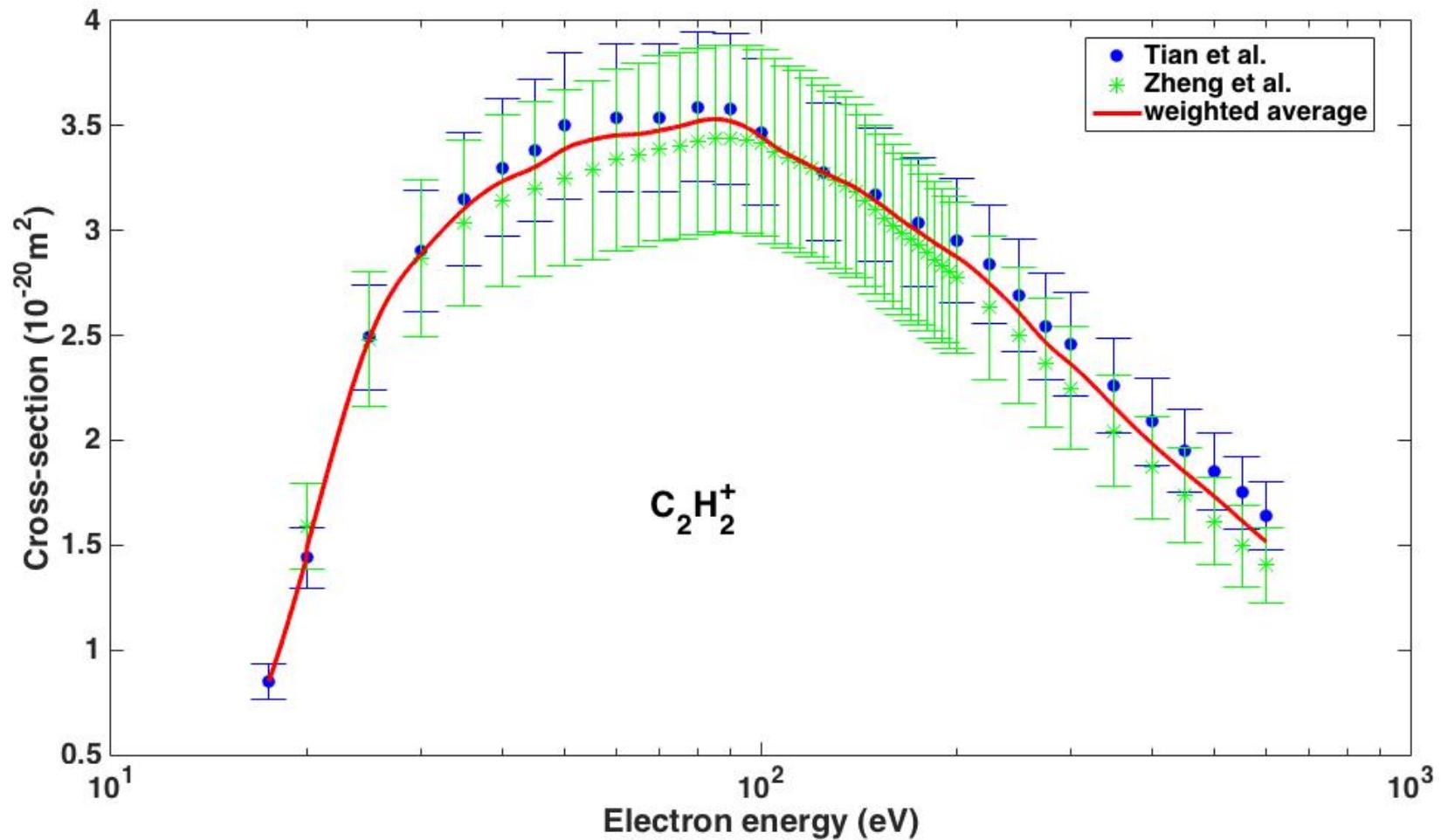


These data are from L-B, based on Tian and Vidal.  
Data by Feil et al. and King/Price change little on this picture

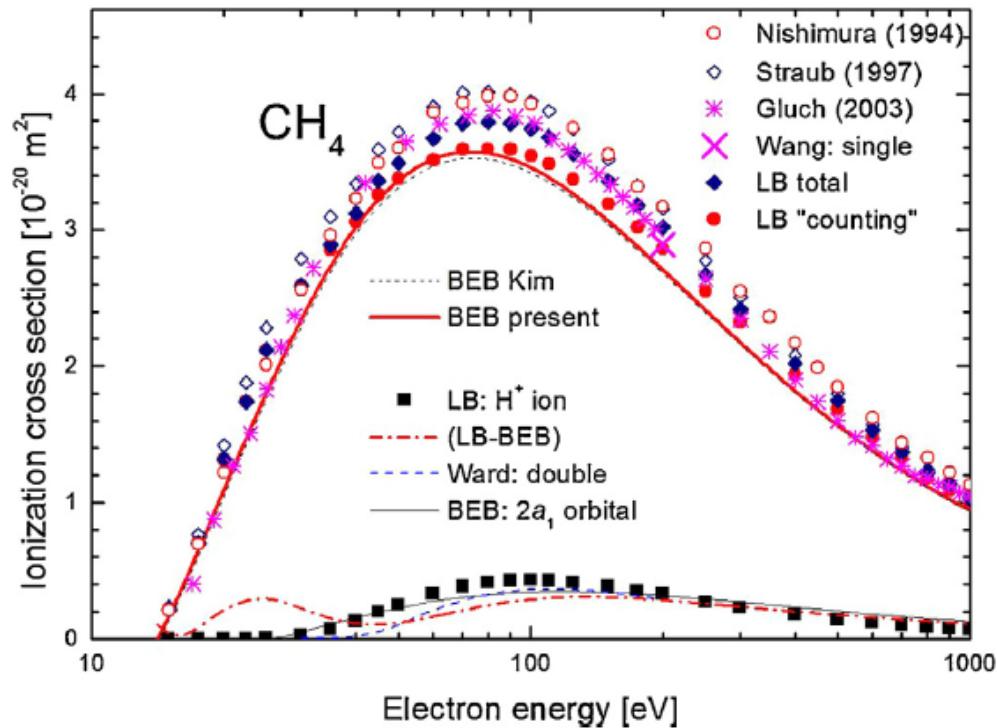
# Ionization: total ( $\pm 5\%$ )



# Ionization: partial ( $\pm 15\%$ )



# Ionization: BEB formula



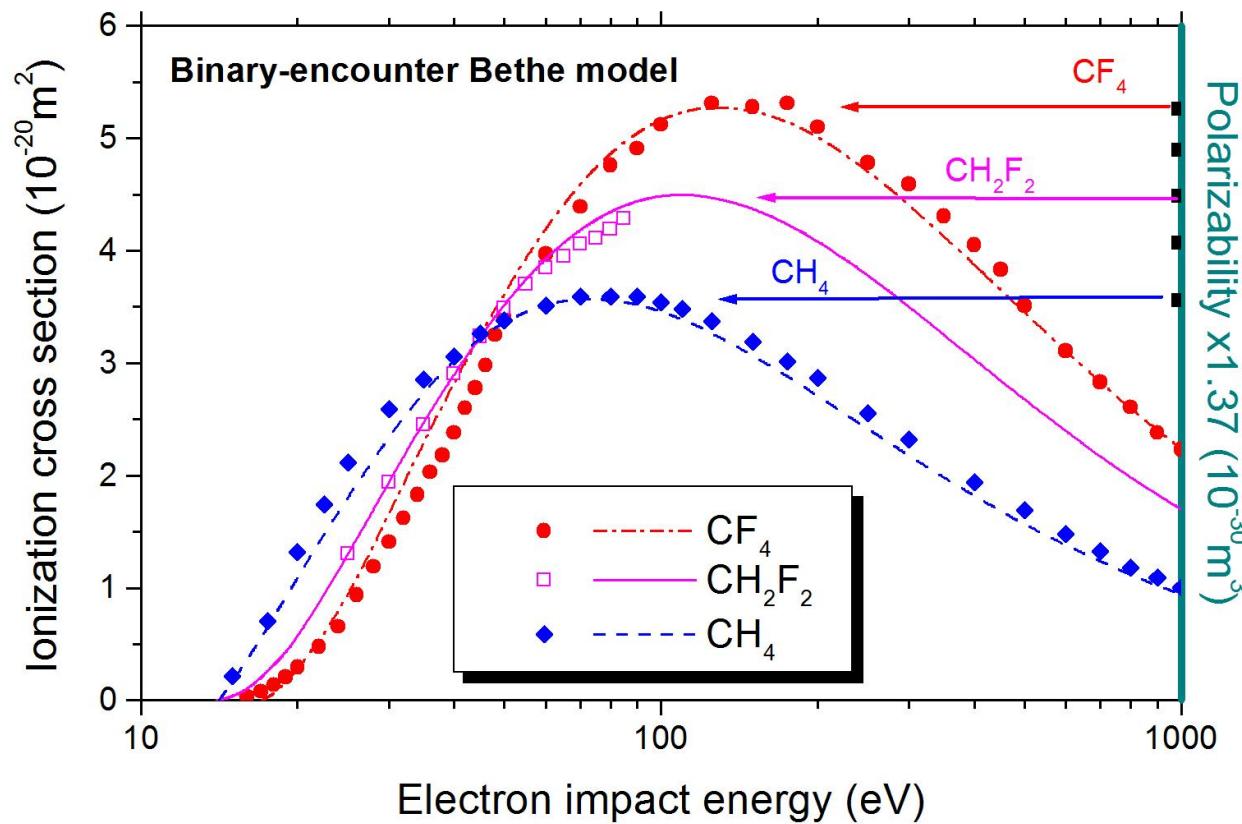
Experiment overestimates t*counting* ionization (due to dissociative ionization)

$$\sigma = \sum_n 4\pi a_0^2 \xi_n \left( \frac{R}{I_n} \right)^2 \frac{1}{t + u_n + 1} \left\{ 1 - \frac{1}{t} + \frac{\ln t}{2} \left( 1 - \frac{1}{t^2} \right) - \frac{\ln t}{t + 1} \right\}$$

Normalized energies:  $t = E/I_n$ ,  $u_n = E_{kin}/I_n$

Only two values needed from QCh

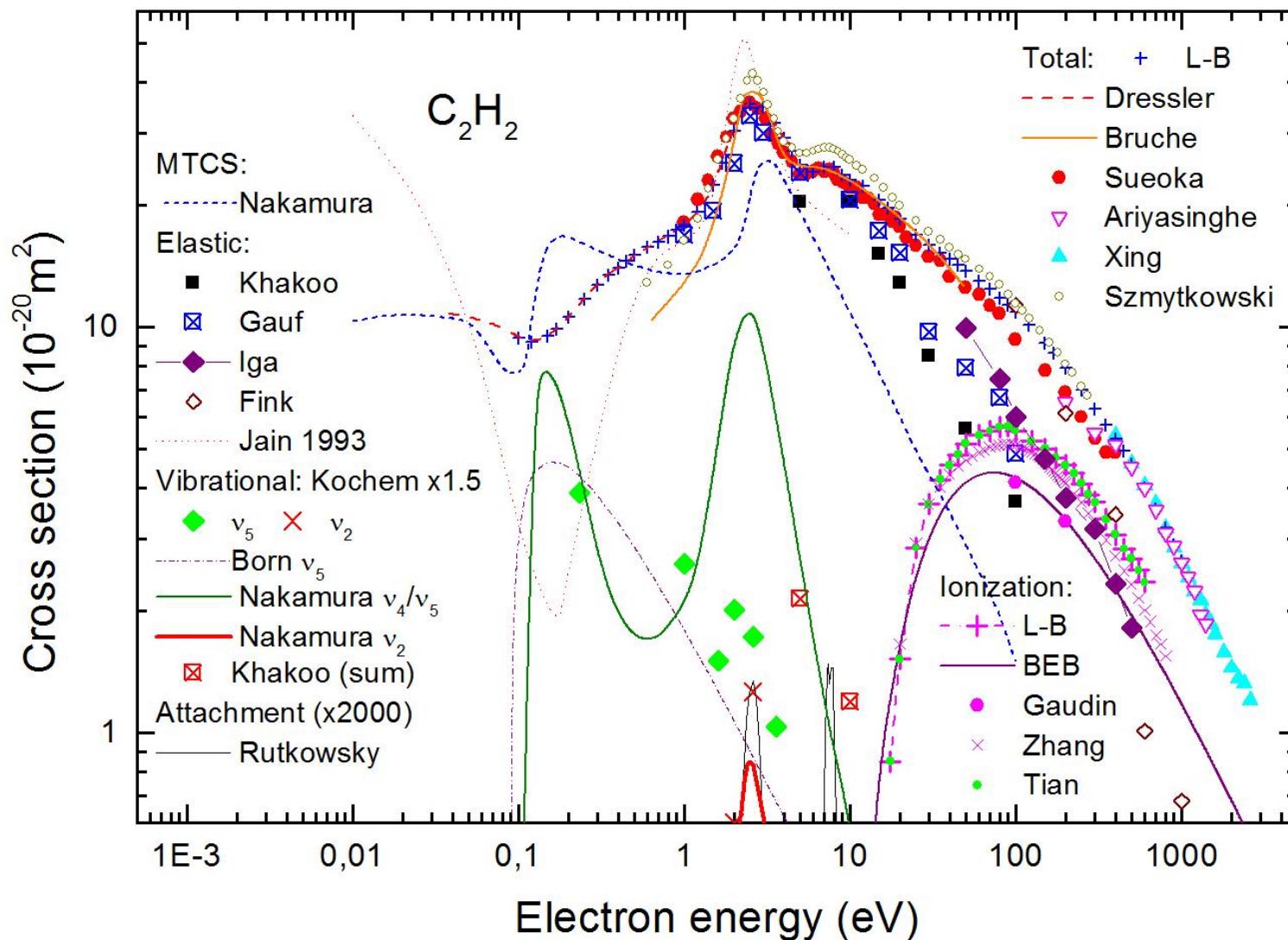
# Ionization (BEB): CH<sub>4</sub>, CH<sub>3</sub>F, ... CF<sub>4</sub>



Thumb rule (?)

$$\sigma_{\max} = 4/3 \alpha$$

# Total and partial: $\text{C}_2\text{H}_2$



# A+M Data Center Activities in National Fusion Research Institute

Mi-Young Song with Team Members

Plasma Technology Research Center  
National Fusion Research Institute



[http://www.adas.ac.uk/2016talks/2016\\_ADAS\\_MSong.pdf](http://www.adas.ac.uk/2016talks/2016_ADAS_MSong.pdf)

# NFRI – Republic of Korea

## Evaluated data (2007 ~ 2015)

	구분	total scattering	elastic scattering	momentum transfer	DCS	total ionization	partial ionization	TDCS	Neutral dissociation	Total attachment	Dissociative attachment	vibration excitation	rotational excitation	electronic excitation
		TCS	ES	MT	DCS	TICS	PICS	TDCS	NDCS	TACS	DACS	VI	RO	EX
1	H <sub>2</sub>	C	V	V	D	Q	Q			Q		V	Q	Q
2	O <sub>2</sub>	Q	Q	Q	D	Q	V	Q		V	Q		V	
3	N <sub>2</sub>	Q	Q	V	D	Q	V	Q			Q	Q	Q	Q
4	Ar	V	Q	Q	D	V	V							
5	Xe	V	Q	Q	D	V	V							
6	CF <sub>4</sub>	V	V	V	V	V	Q	Q	Q	Q				
7	C <sub>2</sub> F <sub>6</sub>	V	Q	Q	V	V	V	Q		Q				
8	C <sub>3</sub> F <sub>8</sub> -2013	V	Q	Q	V	V	Q	Q		Q				
9	C <sub>4</sub> F <sub>8</sub> -2013	V	V	V	V	Q	Q	Q		Q				
10	CF <sub>3</sub> I-2013	V			D	Q	Q							
11	CHF <sub>3</sub>		V	V	D	V	Q	Q						
12	CCl <sub>2</sub> F <sub>2</sub>	Q	Q		D	V	Q							
13	SF <sub>6</sub>	V	Q	Q	D	Q	Q							
14	CCl <sub>4</sub>	V			D	V	V							
15	SiF <sub>4</sub>	V			D	Q	Q		Q					
16	SiF <sub>3</sub>					Q	Q							
17	SiF <sub>2</sub>					Q	Q							
18	SiF					Q	Q							
19	Si					Q	Q							
20	SiH <sub>4</sub>	V	Q	Q	D	V	V	Q						
21	Si <sub>2</sub> H <sub>6</sub>	Q	Q	Q	D			Q						
22	NF <sub>3</sub>	Q	Q	Q	D	Q	Q			Q				
23	NH <sub>3</sub>	V	Q	Q	D	Q	Q							
24	N <sub>2</sub> O					V	Q			Q	Q			
25	NO <sub>2</sub>					Q	Q							
26	NO	Q				Q	Q			Q				
27	C					Q	Q							
28	O					Q	Q							
29	N					Q	Q							
30	F					Q	Q							
31	Cl					Q	Q							
32	Br					Q	Q							



## Cross Sections for Electron Collisions with Methane

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(Received 18 December 2014; accepted 8 April 2015; published online 28 May 2015)

Cross section data are compiled from the literature for electron collision ( $\text{CH}_4$ ) molecules. Cross sections are collected and reviewed for total scattering, momentum transfer, excitations of rotational and vibrational state ionization, and dissociative attachment. The data derived from swarm experiments are also considered. For each of these processes, the recommended values of the cross sections are presented. The literature has been surveyed through early 2014. © 2015 AIP Publishing LLC [doi:10.1063/1.4918670]

## Cross Sections for Electron Collisions with Acetylene

Mi-Young Song<sup>1,2</sup>, Jung-Sik Yoon,<sup>2</sup> Hyuck Cho,<sup>2</sup> Grzegorz P. Karwasz,<sup>3</sup> Vlatcheslav Kokouline,<sup>4</sup> Yoshiharu Nakamura,<sup>5</sup> and Jonathan Tennyson<sup>6</sup>

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(Revised 18 November 2015)

Cross section data are compiled from the literature for electron collisions with acetylene ( $\text{HCCH}$ ) molecules. Cross sections are collected and reviewed for total scattering, elastic scattering, momentum transfer, excitations of rotational and vibrational states, dissociation, ionization, and dissociative attachment. The data derived from swarm experiments are also considered. For each of these processes, the recommended values of the cross sections are presented. The literature has been surveyed through early 2016.

PACS numbers: 34.80.Bm, 52.20.Fs

Keywords: electron collisions, total cross sections, ionization, dissociation, attachment, evaluation

### I. INTRODUCTION

Acetylene ( $\text{HCCH}$ ) is the

The accuracy for the measured cross section data for processes involving ground state species is

### II. TOTAL SCATTERING CROSS SECTION

### III. ELASTIC SCATTERING CROSS SECTION

Since the last review of electron-acetylene collisions by Nakamura<sup>1</sup>, theoretical cross sections for excitation of

### IV. MOMENTUM TRANSFER CROSS SECTION

The momentum-transfer cross-section for electron-acetylene collisions has been determined in several recent studies in which elastic differential cross sections were measured or calculated. Similarly to the recommended data for differential elastic cross sections discussed above, the recommended momentum-transfer cross section is from the recent study by Gaaf et al.<sup>3</sup>. The agreement of the data by Gaaf with a previous experimental work by Iga et al.<sup>4</sup> is very good. Theoretical cross sections determined in the same work by Gaaf et al.<sup>3</sup>, and also by Jain<sup>5</sup>, and Giantureco and Stoecklin<sup>6</sup> agree with each other within 5–10% above 1 eV. However, they are larger than experimental data by about 30% over the whole



# Nitrogen oxides (2019)

Journal of Physical and  
Chemical Reference Data

ARTICLE

[scitation.org/journal/jpr](https://scitation.org/journal/jpr)

## Cross Sections for Electron Collisions with NO, N<sub>2</sub>O, and NO<sub>2</sub>

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Yoshiharu Nakamura,<sup>5</sup> and Jonathan Tennyson<sup>6</sup> 

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# Nitrogen oxides (2019)

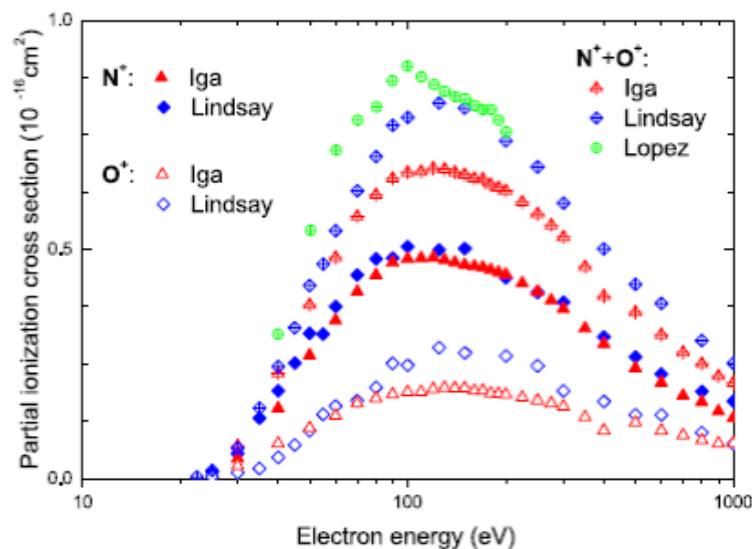
recommended total and partial cross sections in NO are shown in Fig. 17 and given in Table 7, respectively.

**TABLE 7.** Recommended total and partial cross sections for electron-impaction ionization of nitric oxide, NO in  $10^{-16} \text{ cm}^2$ . Energy in eV

Energy	$\text{NO}^+$	$\text{N}^+$	$\text{O}^+$	$\text{NO}^{2+}$	Total
12.5	0.048				0.048
15	0.21				0.21
17.5	0.48				0.48
20	0.59				0.59
22.5	0.75				0.76
25	0.98	0.014	0.004		0.99
30	1.20	0.054	0.013		1.27
35	1.37	0.132	0.022		1.53
40	1.51	0.191	0.046	0.000 17	1.75
45	1.67	0.252	0.073	0.001 5	2.00
50	1.74	0.317	0.104	0.004 2	2.16
55	1.84	0.315	0.140	0.007 6	2.31
60	1.89	0.375	0.158	0.011 3	2.43
70	1.92	0.444	0.170	0.015 8	2.55
80	1.96	0.479	0.199	0.025 0	2.67
90	1.97	0.481	0.251	0.029 5	2.74
100	1.97	0.506	0.247	0.029 5	2.75
125	1.92	0.499	0.286	0.032 1	2.73
150	1.84	0.502	0.274	0.029 5	2.65
200	1.69	0.438	0.267	0.030 6	2.43
250	1.55	0.406	0.246	0.028 4	2.23
300	1.40	0.385	0.191	0.023 3	2.00
400	1.24	0.309	0.168	0.023 2	1.74
500	1.11	0.265	0.139	0.020 3	1.53
600	0.98	0.228	0.139	0.014 7	1.36
800	0.81	0.190	0.100	0.013 2	1.11
1000	0.70	0.169	0.076	0.006 9	0.95

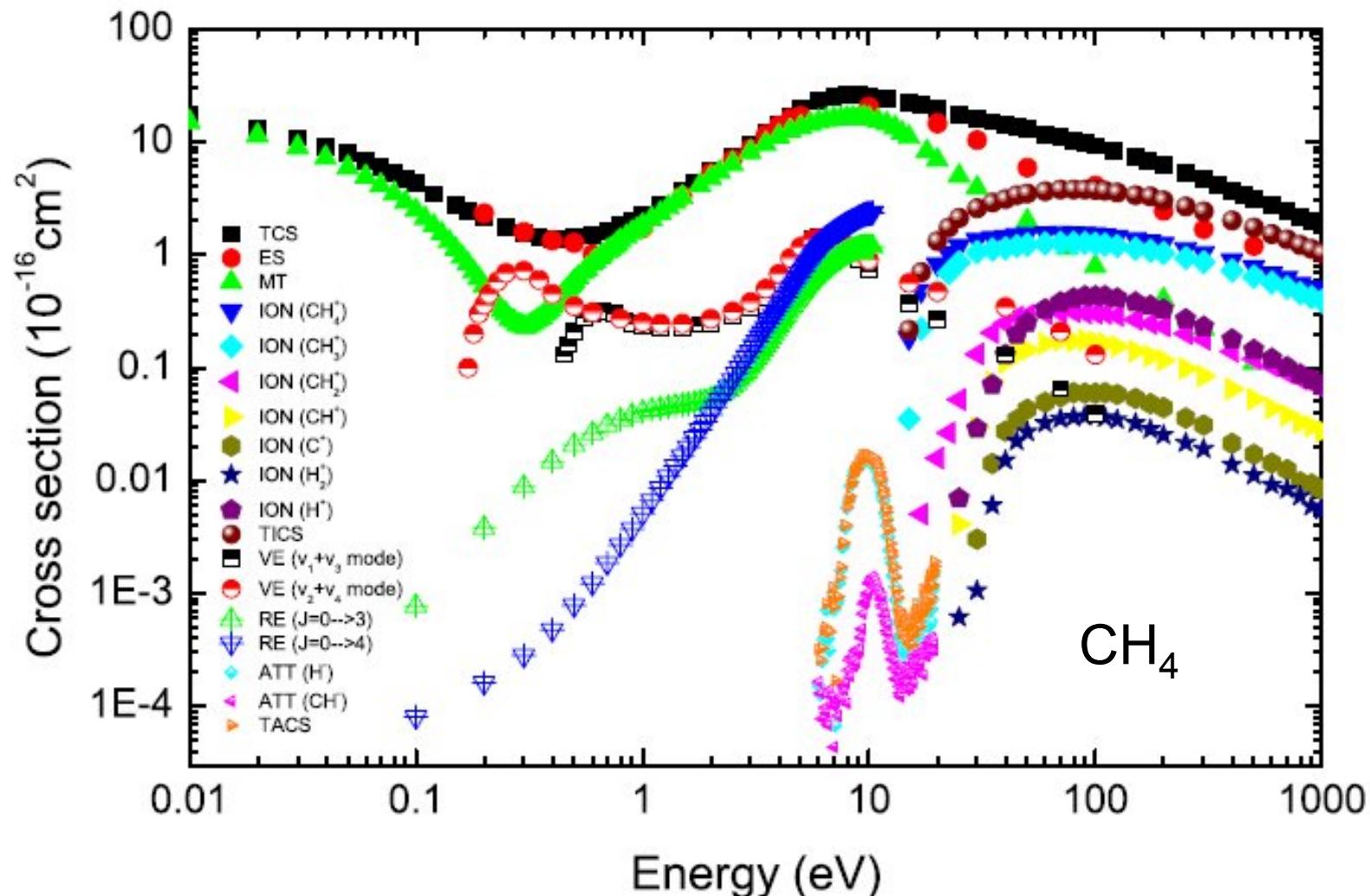
## 2.10. Electron attachment (DEA) cross section

Rapp and Briglia<sup>70</sup> measured the absolute TCS's for negative-ion formation in NO by electron impact in a total ionization tube. The dissociative electron attachment (DEA) channel forming this negative ion is  $\text{O}^-$  from NO. Orient and Chutjian<sup>71</sup> identified three channels forming  $\text{O}^-({}^2\text{P})$ , but did not present the absolute cross sections. Rapp and Briglia<sup>70</sup> is the only available measured DEA cross sections and



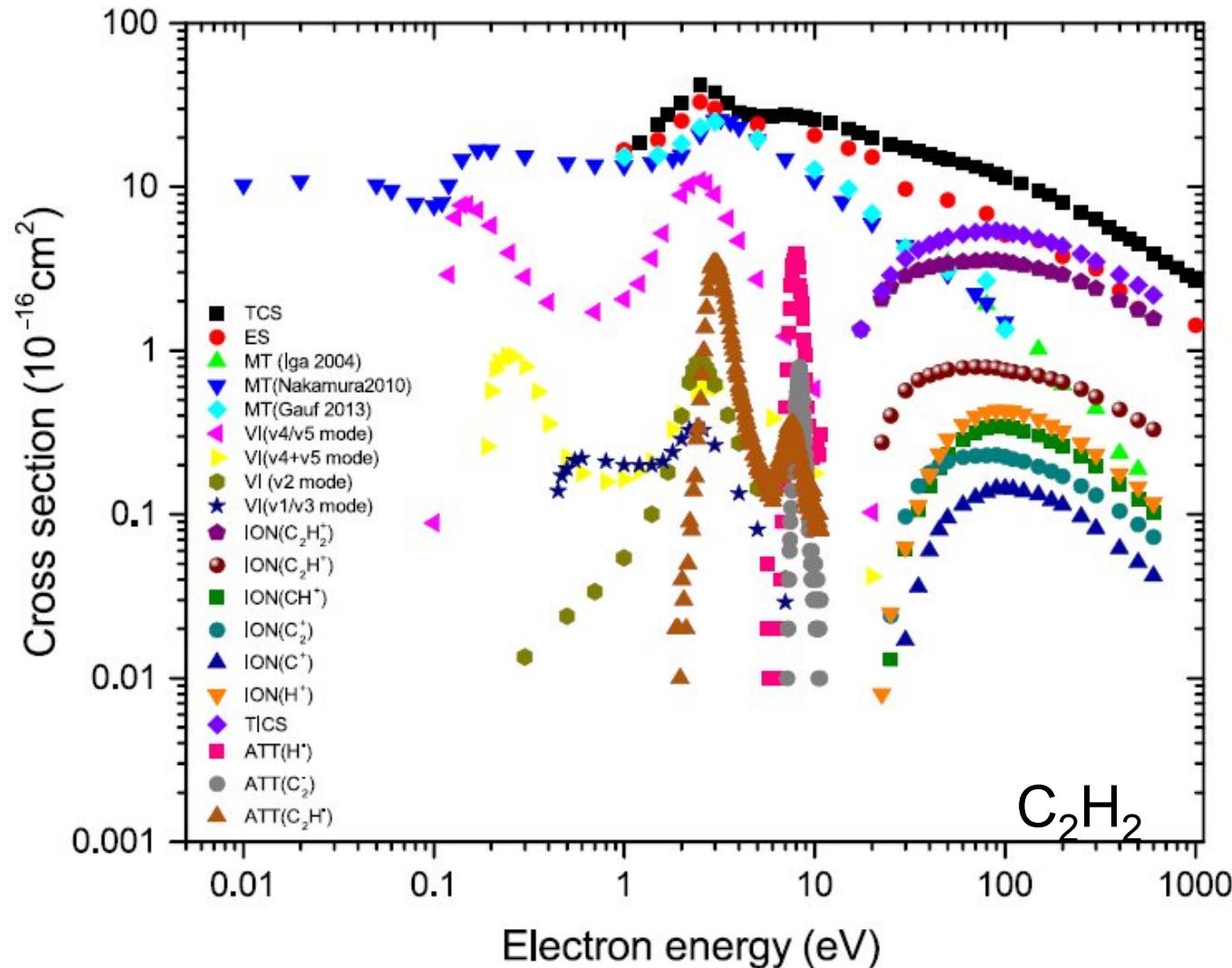
**FIG. 16.** Partial ionization cross sections for ionization of NO by electron impact: fragment  $\text{N}^+$  and  $\text{O}^+$  ions and the summed  $(\text{N}^+ + \text{O}^+ + \text{NO}^{2+})$  ion signal unresolved in measurements of Lopez *et al.*<sup>31</sup>). Experimental data are from Iga *et al.*<sup>30</sup>, Lindsay *et al.*<sup>29</sup>, and Lopez *et al.*<sup>31</sup>.

# „Recommended” cross-sections: $\text{CH}_4$

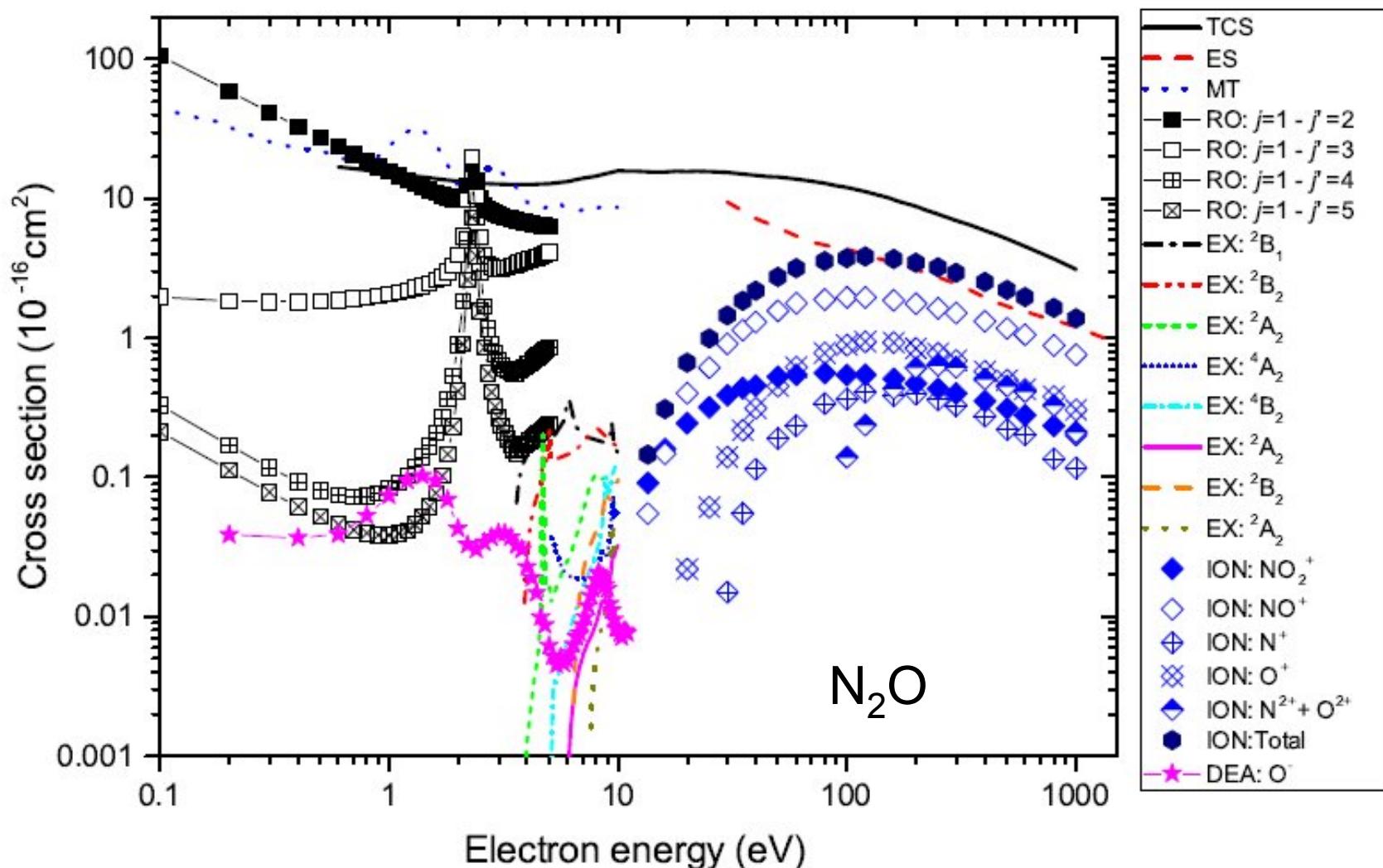


M.-Y. Song, J.-S Yoon, H. Cho, Y. Itikawa, G.P. Karwasz, V. Kokououline, Y. Nakamura, and J. Tennyson,  
Cross Sections for Electron Collisions with Methane, J. Phys. Chem. Ref. Data, 44 (2015) 023101.

# „Recommended” cross-sections: C<sub>2</sub>H<sub>2</sub>



# „Recommended” cross-sections: N<sub>2</sub>O



# Acknowledgments:



Thank you for the attention!

