Known and unknown in electron-atom and molecule scattering

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Outline:

1. Rationale: what is needed
2. Experimental methods for electron-molecule cross sections
4. Case study: recommended CSs for $e^- + CH_4$
5. Semiempirical estimations: C, Be, W – like species
6. Theoretical progress (ligth targets)
7. State of art.: C, Be, W, ...
8. Conclusions: how to proceed

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) $e + H_2 \rightarrow 2e + H_2^+$
(5) $e + H_2 \rightarrow e + 2H^0$	(replacing (4))
(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[a] for (4), (5) and (6)	CRM[a] for (11), (5) and (6)

[a] Collisional Radiative Model.

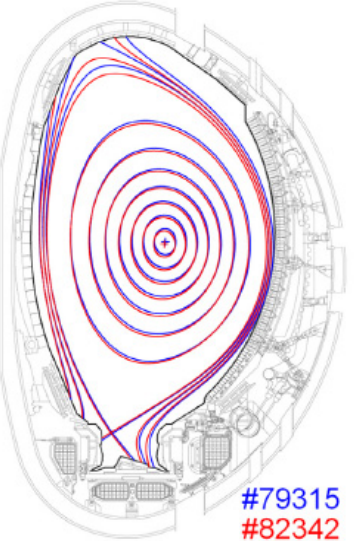
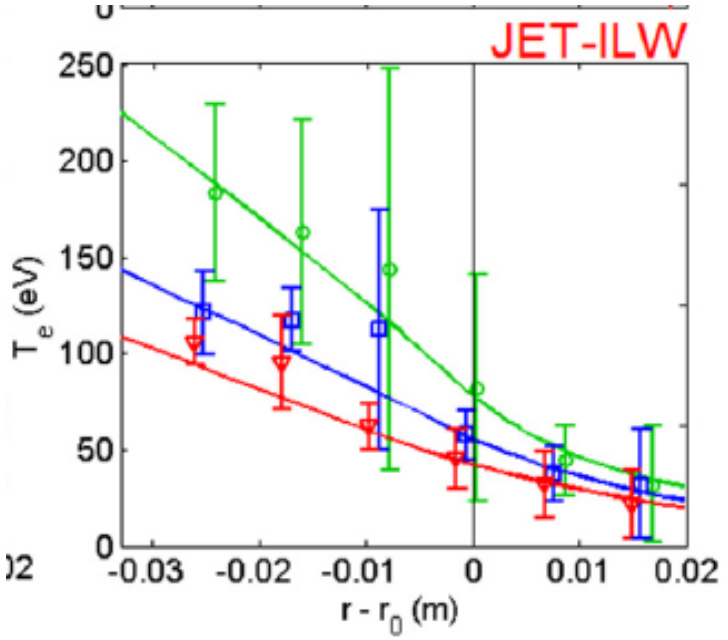


Figure 1. Magnetic equilibria for the shots #79315 and #82342 at 20 s and 13 s, respectively.

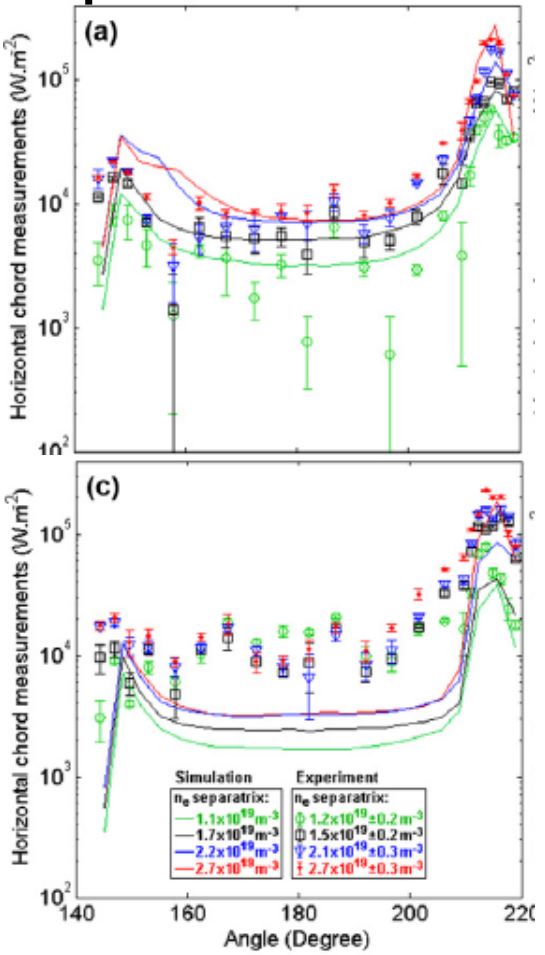
Guillemaut et al. Nucl.Fusion **54** (2014) 093012

Rationale: electron T and power irradiated



Electron temperature (and density) during three points of density ramp

Guillemaut et al. Nucl.Fusion (2014)

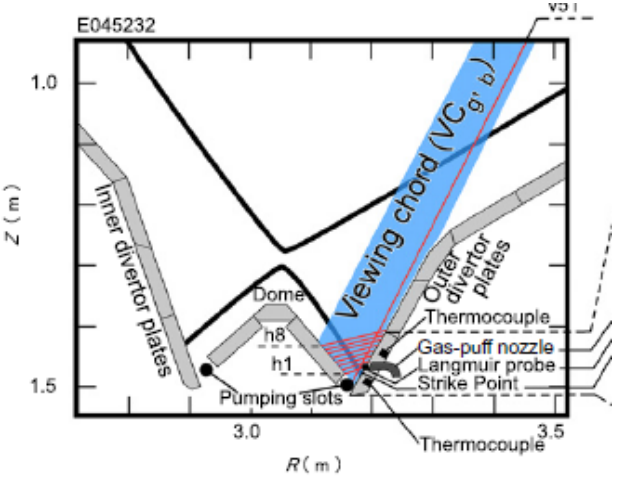


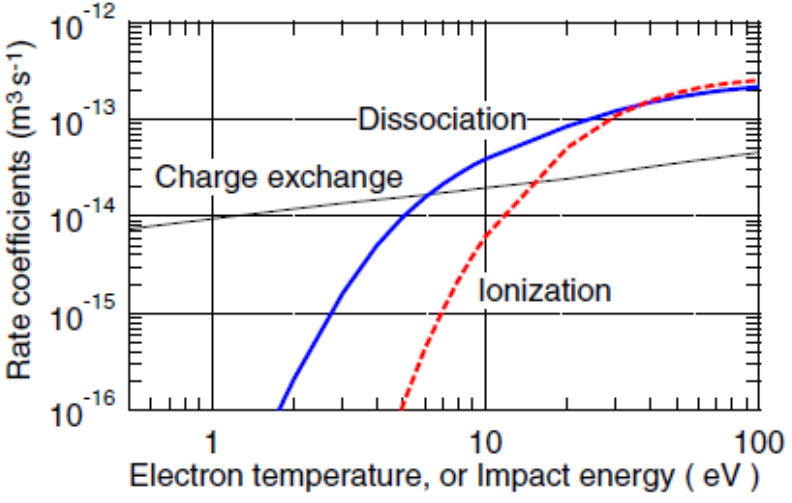
Power irradiated (0.5-1.5 MW) simulation:

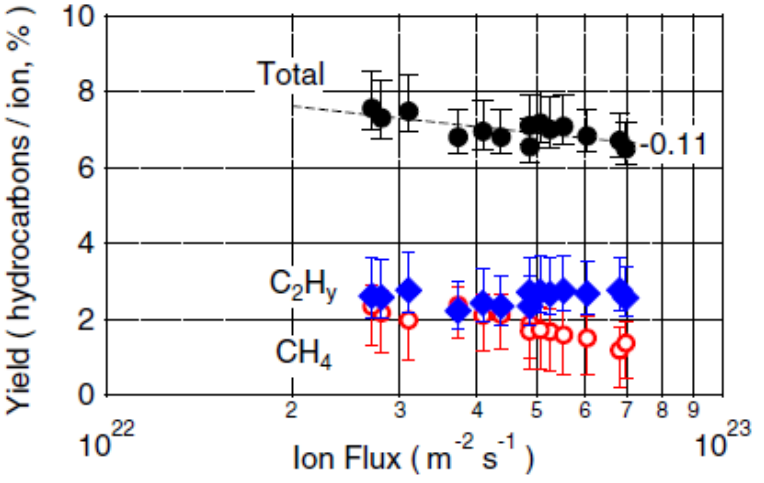
JET-C <10% JET-ILW factor 3!

Carbon sputtering by CH_4 and C_2H_y ions

The emission rates of CH, CD and C_2 spectral bands and a re-evaluation of th chemical sputtering yield of the JT-60U carbon divertor plates







Nakano et al. Nucl.Fusion **54** (2014) 043004

Data needed:

I Neutrals (H, C, C_2, Be, BeH_2, CH_4)

1. Total cross section

2. Partial cross sections:

elastic scattering e+A →e+A

rotational excitation e+CH_4 (J=0) → e+CH_4 (J=2)

vibrational excitation e+AB(v=0) → e+AB(v>0)

electron attachment (dissociative) e+AB → A^- + B

electronic excitation e+A →e+A^*

emission lines: A^* → A + *hv*

neutral dissociation e+AB → A + B + e

emisison from dissociation e + AB → A^* + B + e + *hv*

ionization e+A →A^++2e

dissociative ionization e+AB → A + B^+ + 2°

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

Data needed: II Positive ions (BeH^+)

1.Recombination: $A^+ + e \rightarrow A$

1a. dissociative recombination: $AB^+ + e \rightarrow A^* + B$

2. Partial cross sections:

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

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

double ionization $e+A^+ \rightarrow A^{2+} + 2e$

Databases

OPEN-ADAS
Atomic Data and Analysis Structure

Eu I (5130.1Å)

Freeform Wavelength Ion

DATA CLASSES

FUNDAMENTAL

ADF01
ADF04
ADF07
ADF08
ADF09
ADF38
ADF39
ADF48

DERIVED

ADF11
ADF12
ADF13
ADF15
ADF21

ADF 07

Electron impact ionisation coefficients

The data sets are collections of Maxwell averaged electron impact ionisation rate coefficients represented by the reactions

$$X_i^{z+} + \mathrm{e}^- \rightarrow X_\rho^{(z+1)+} + \mathrm{e}^- + \mathrm{e}^-,$$
$$X_i^{z+} + \mathrm{e}^- \rightarrow X^{*(z)+} + \mathrm{e}^- \rightarrow X_\rho^{(z+1)+} + \mathrm{e}^- + \mathrm{e}^-.$$

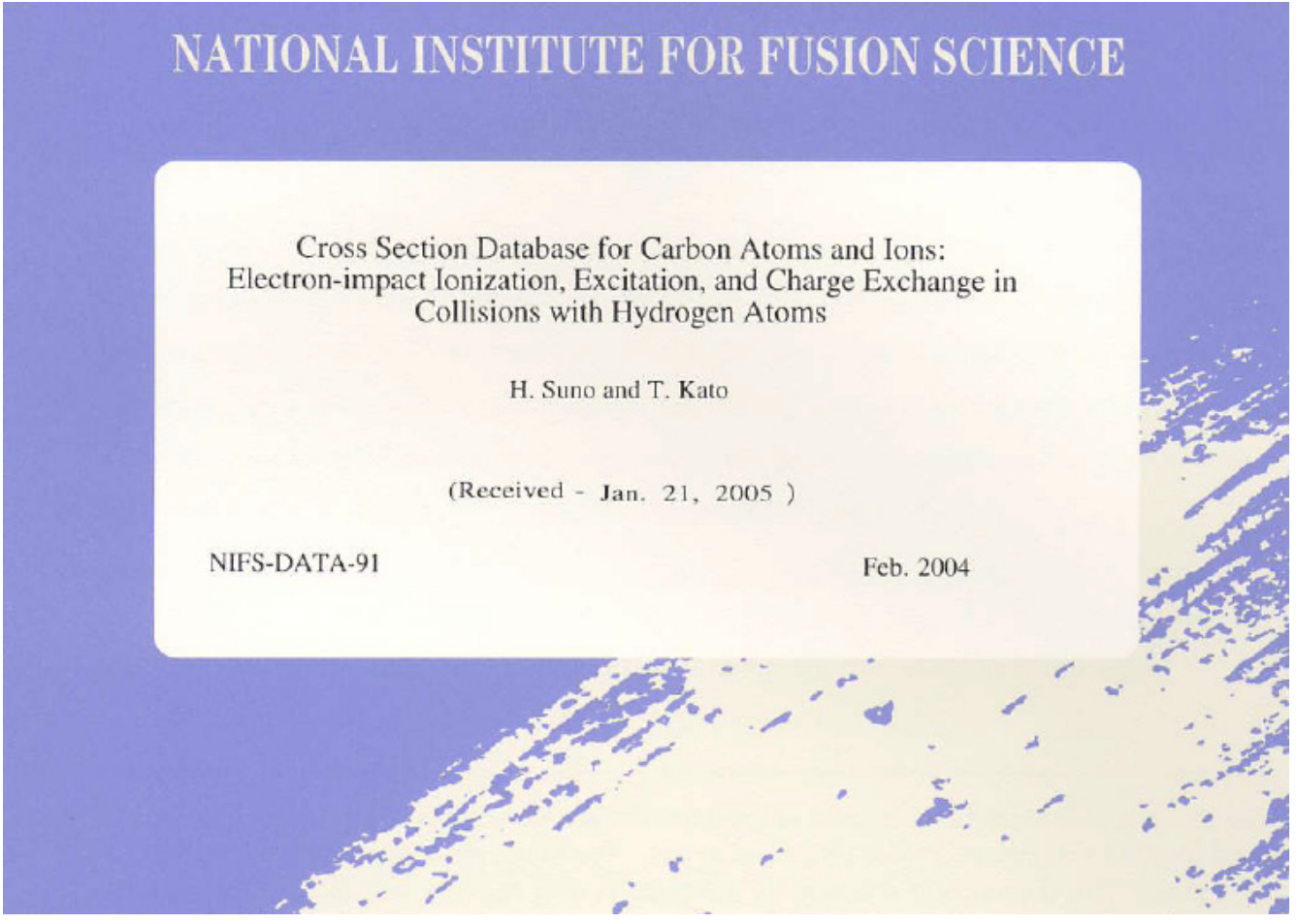
That is the coefficients combine both direct ionisation and excitation/autoionisation. The tabulations are resolved by initial state i and final metastable ρ, with the initial state also mostly spanning just metastables. The rate coefficients are tabulated as a function of electron temperature. The data sets are typically grouped in sub-directories for a particular element. ADF07 is a fundamental data format. It should be noted that it does not include step-wise ionisation via multiple sequential excitations and then a final ionising collision. Effective ionisation coefficients, including step-wise ionisation, occur as a derived data output from collisional–radiative modelling and such data are archived as a sub-class of data format ADF11.

Search ADF07 files

Ion

Element Atomic number of symbol Charge Ion charge

Databases


NATIONAL INSTITUTE FOR FUSION SCIENCE
Cross Section Database for Carbon Atoms and Ions:
Electron-impact Ionization, Excitation, and Charge Exchange in
Collisions with Hydrogen Atoms
H. Suno and T. Kato
(Received - Jan. 21, 2005)
NIFS-DATA-91
Feb. 2004

Databases

Forschungszentrum Jülich
in der Helmholtz-Gemeinschaft

Institut für Plasmaphysik
EURATOM Association, Trilateral Euregio Cluster

Collision Processes in Low-Temperature Hydrogen Plasmas

Jül-4105
Dezember 2003
ISSN 0944-2952

Ratko K. Janev, Detlev Reiter, Ulrich Samm

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N J Mason, Open University, UK

*https://www-amdis.iaea.org/meetings/.../**Mason**-**VAMDC**-2012-09-06.pdf*

The Open University CEPSAR
Centre for Earth, Planetary, Space & Astronomical Research

Data Center for Plasma Properties

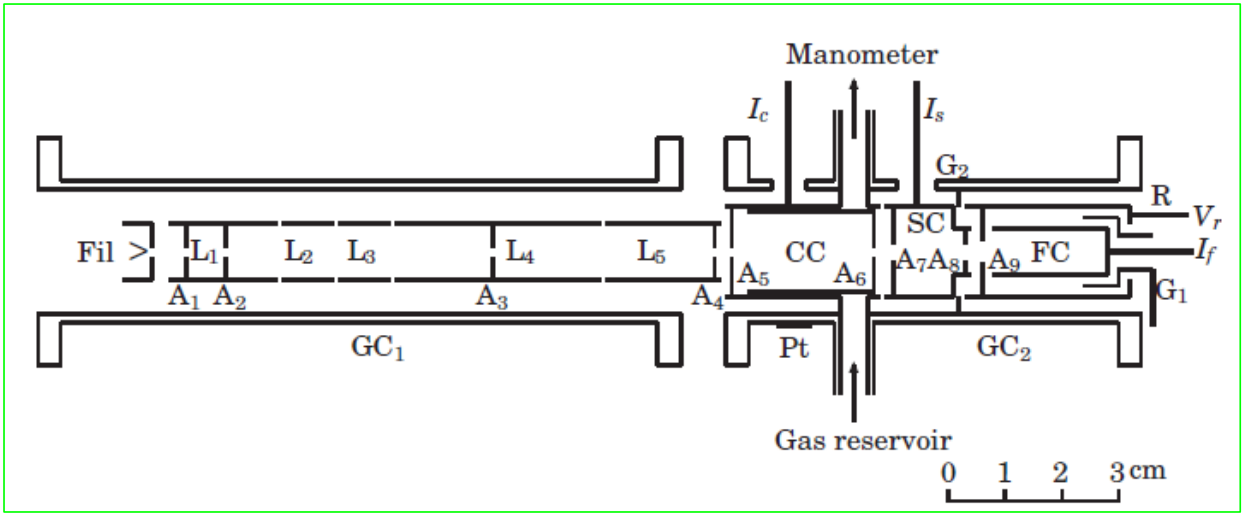
Group Research on Procedures for Evaluation of CH4 Collision Processes

Mi-Young Song

NFRI National Fusion Research institute

Experimental methods: total

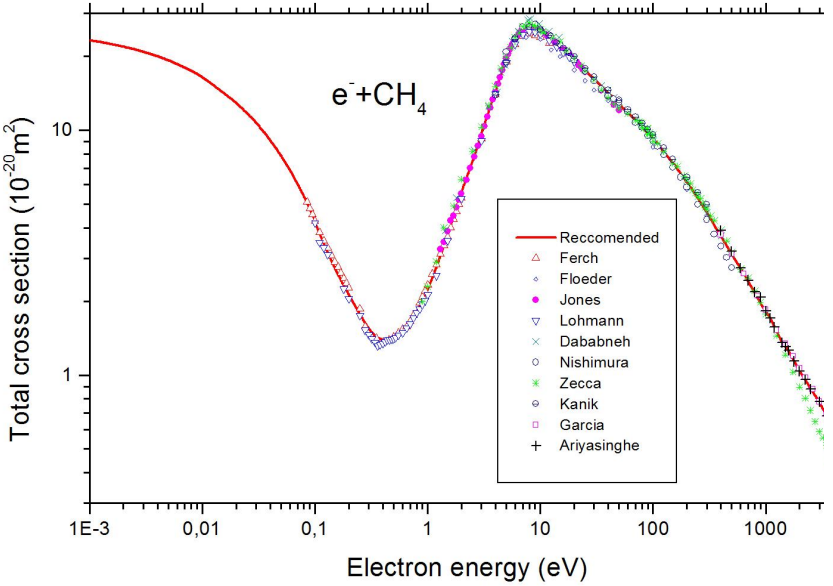
attenuation method $I = I_0 \exp(-\sigma n L)$
precision <5%

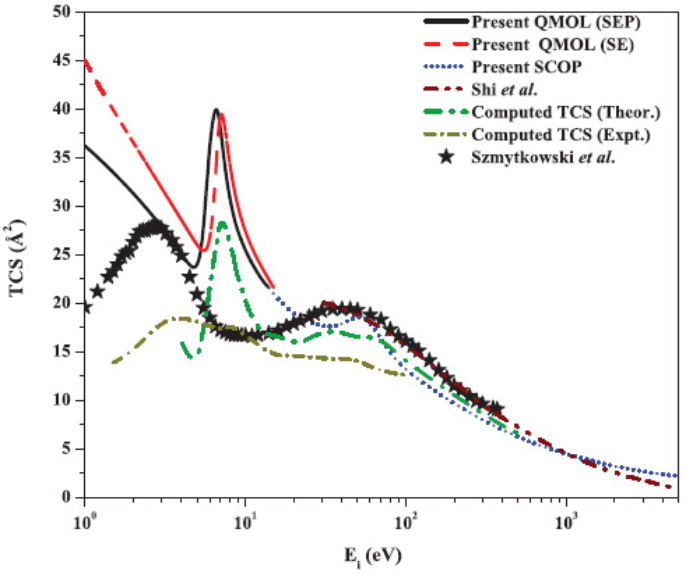


H. Nishimura et al., J.Phys. Soc. Japan **72** (2003) 1080
M.-Y. Song et al., to be published
B. Goswami et al. PRA **88** (2013) 032707 (NF_3)

NF_3

Experimental methods: total

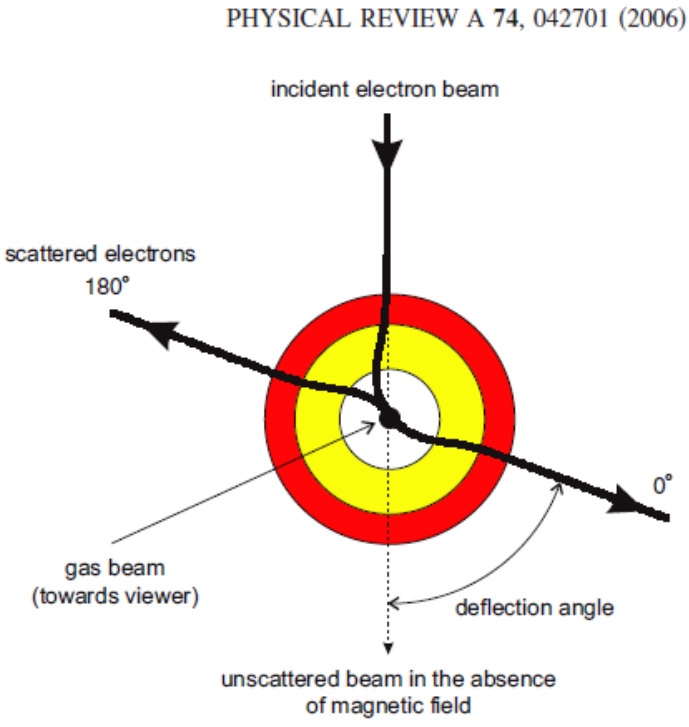


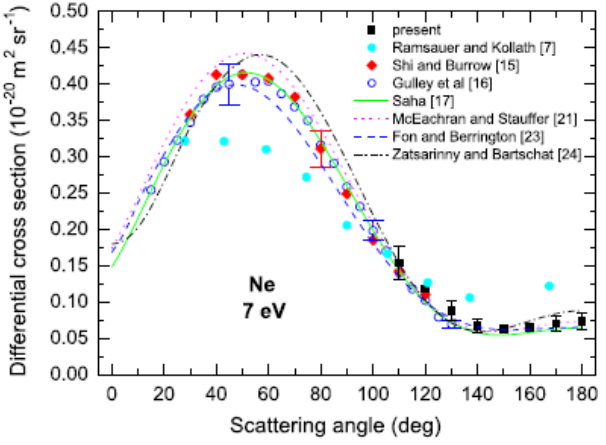


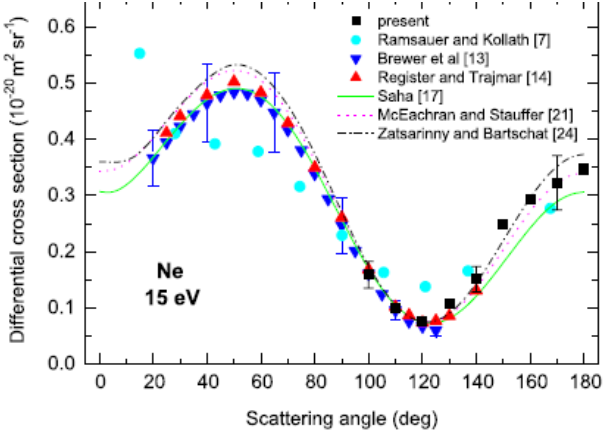
H. Nishimura et al., J.Phys. Soc. Japan **72** (2003) 1080
M.-Y. Song et al., to be published
B. Goswami et al. PRA **88** (2013) 032707 (NF_3)

NF_3

Experimental methods: elastic

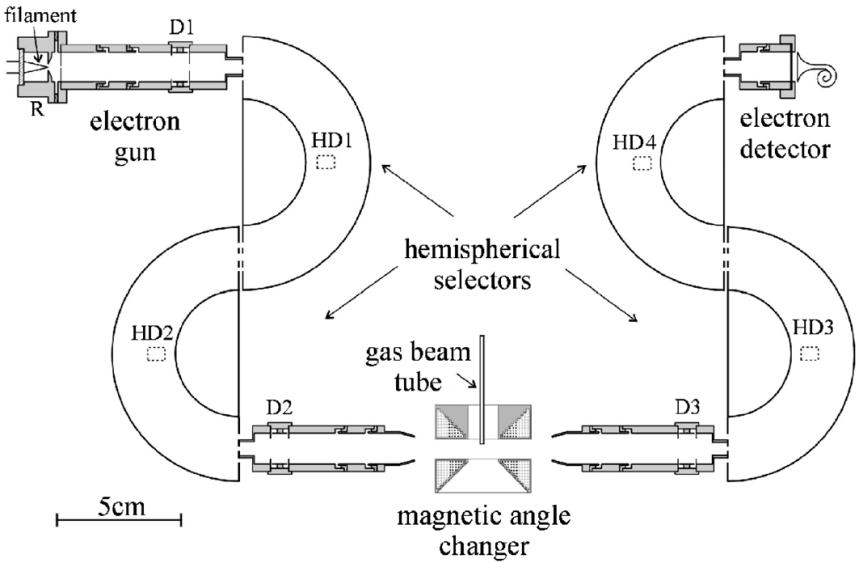


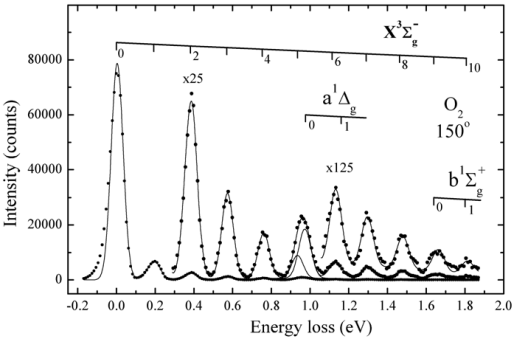


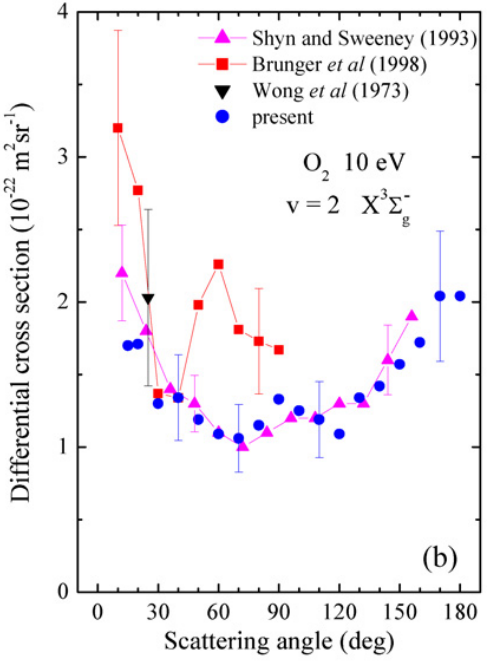


I. Linert, B. Mielewska, G. King, and M. Zubek, PRA (2006)

Experimental methods: excitation (electronic, vibrational)







$e^- + O_2$ (v=0) – $e^- + O_2$ (v=0, 1, 2, etc.)

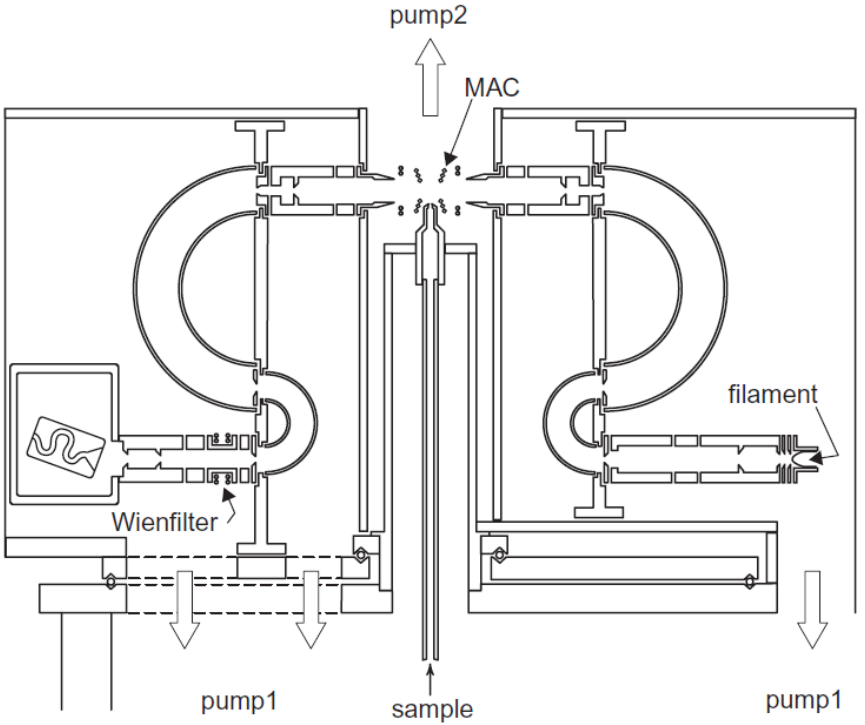
Experiments by:

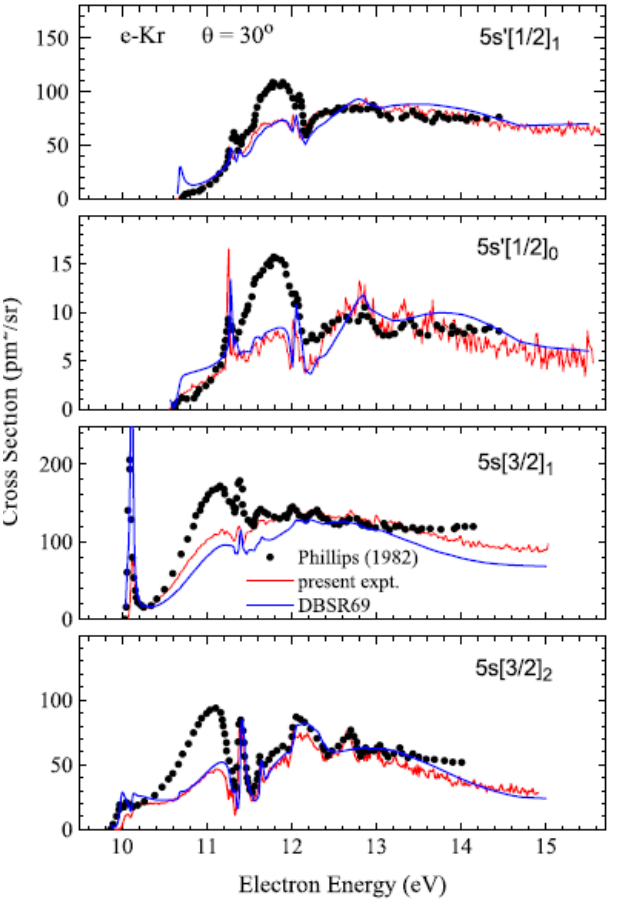
I. Linert, M. Zubek (Gdansk) J. Phys. B **39** (2006)

M. Khakoo et al. (Fullerton California)

M. Allan (Freiburg University)

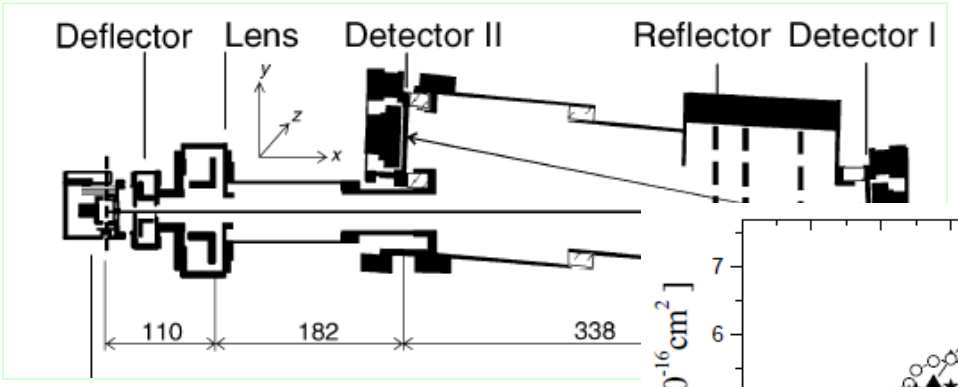
Experimental methods: electronic, vibrational, DA





M. Allan, O. Zatsarinny. K. Bartschat, PRA (2011**) Kr: experiment and Dirac R-matrix**

Experimental methods: ionization (1)

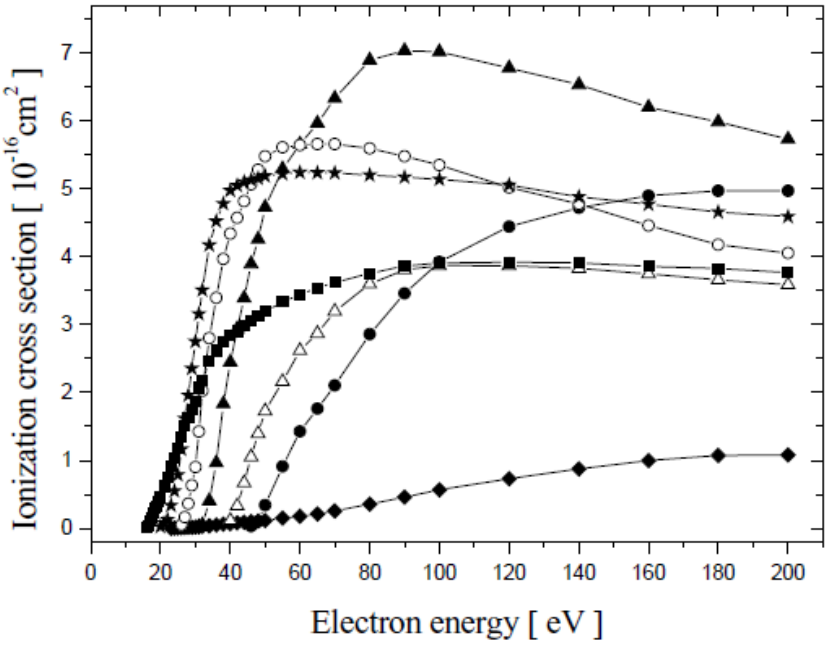


$WF_6 \rightarrow$

$WF_5^+ > WF_2^+ >$

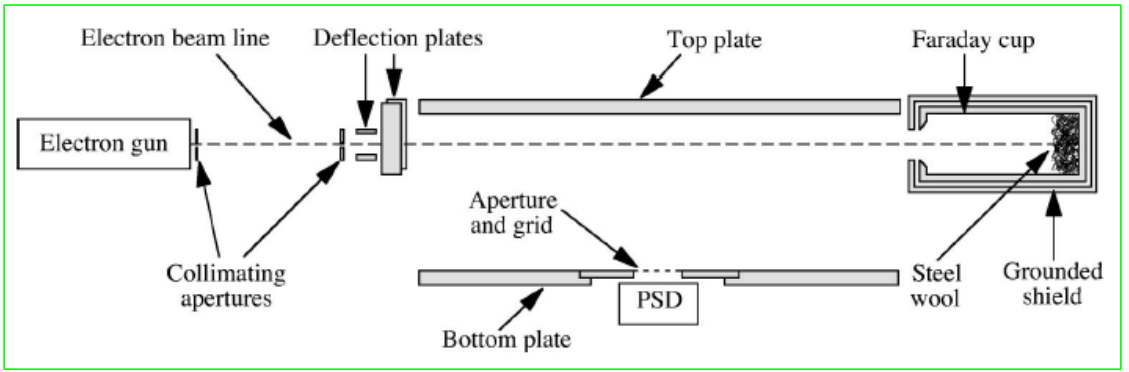
$WF_3^+ \approx WF_4^+$

Accuracy: ±15%

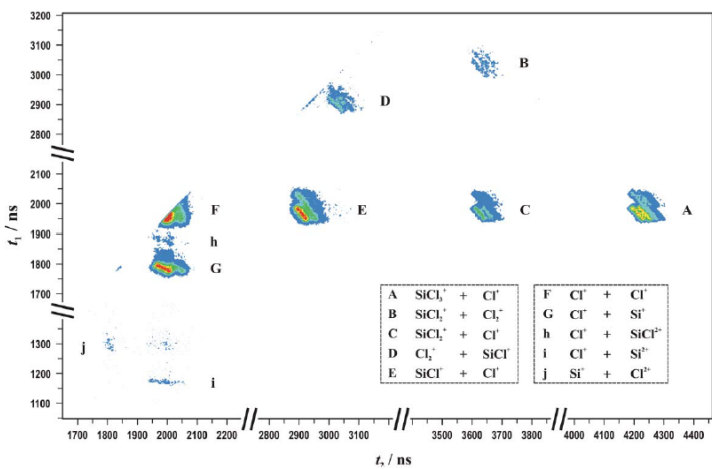


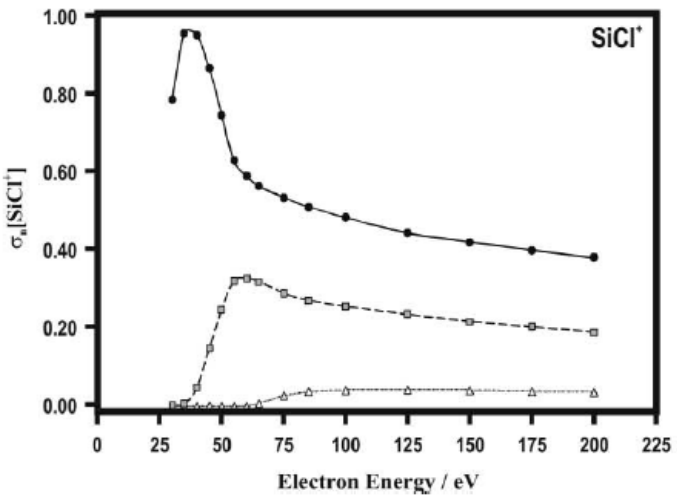
R. Basner, M. Schmidt, K. Becker, Int. J. Mass Spectr. 233 (2004) 25

Experimental methods: ionization (2)



$SiCl^+$ from single, double, triple ionization of $SiCl_4$





B. G. Lindsay et al., JCP **129** (2004), S J King nad S D Price, JCP**134** (2011) 074311

Dissociation into neutrals (CF_4, CH_3F...)

volatile organotellurides

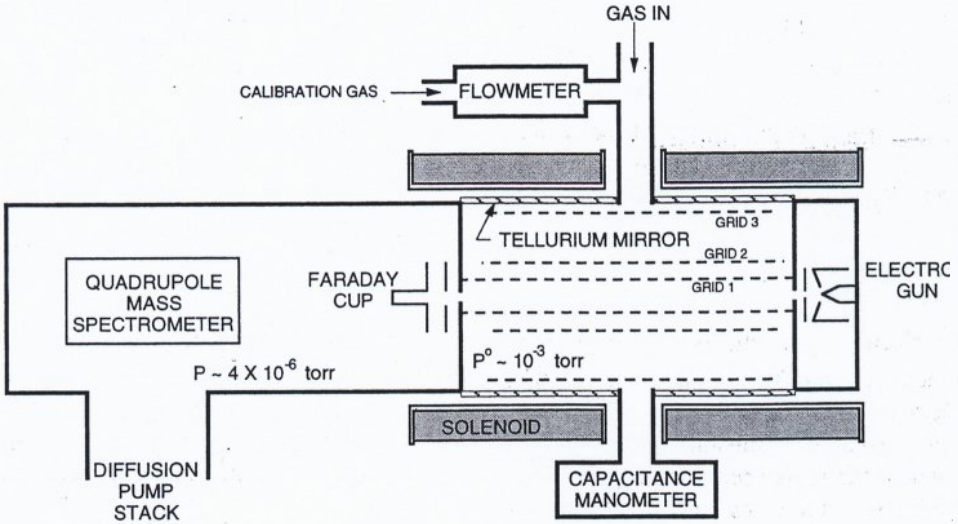


FIG. 1. Schematic diagram of the apparatus.

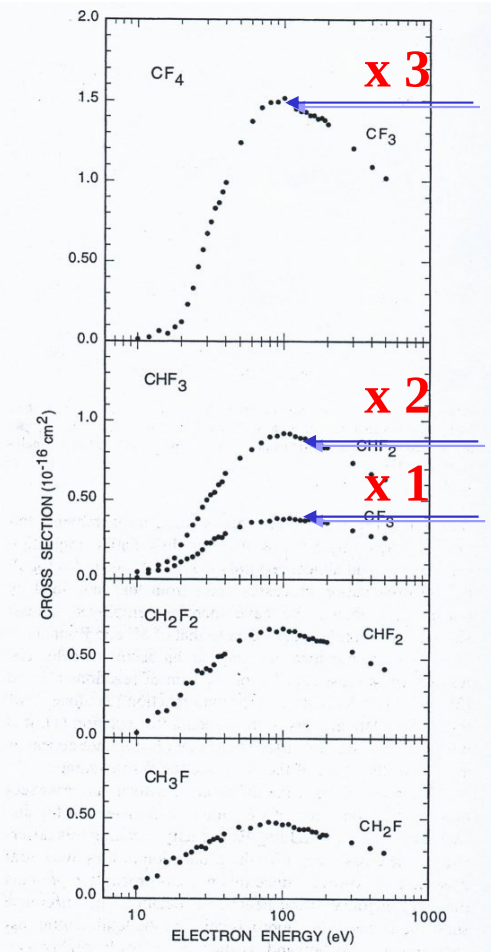


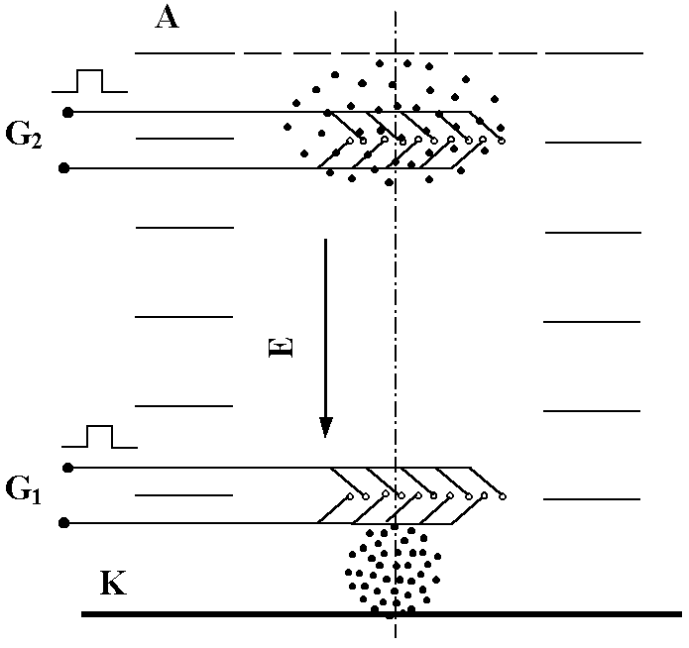
FIG. 5. Cross sections for the production of fluoromethyl radicals by neutral dissociation (n.d.) and dissociative ionization (d.i.) from electron impact on fluoromethanes.

Additivity rule:
cross section = sum of paths

Motlagh and Moore, JCP**109** (1988) 432

Diffusion coefficients → electronic distribution function $n_e(\boldsymbol{r}, \boldsymbol{v}, t)$

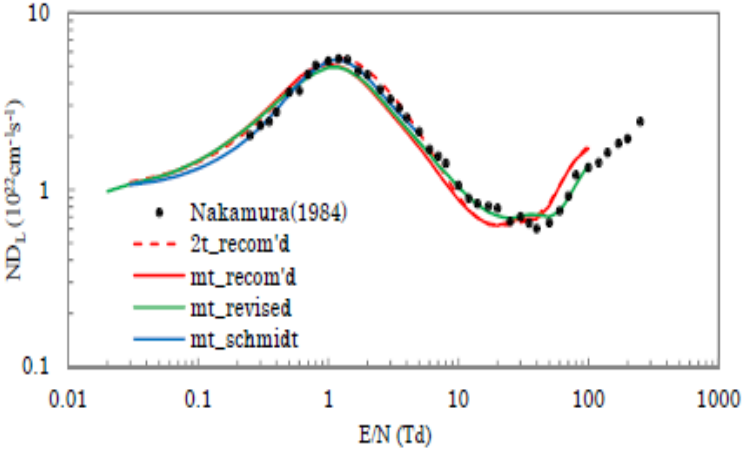
$$\frac{\partial}{\partial t} n_e(\mathbf{r},t) = -w \frac{\partial}{\partial z} n_e(\mathbf{r},t) + D_T \left[\frac{\partial^2}{\partial x^2} n_e(\mathbf{r},t) + \frac{\partial^2}{\partial y^2} n_e(\mathbf{r},t) \right] + D_L \frac{\partial^2}{\partial z^2} n_e(\mathbf{r},t)$$

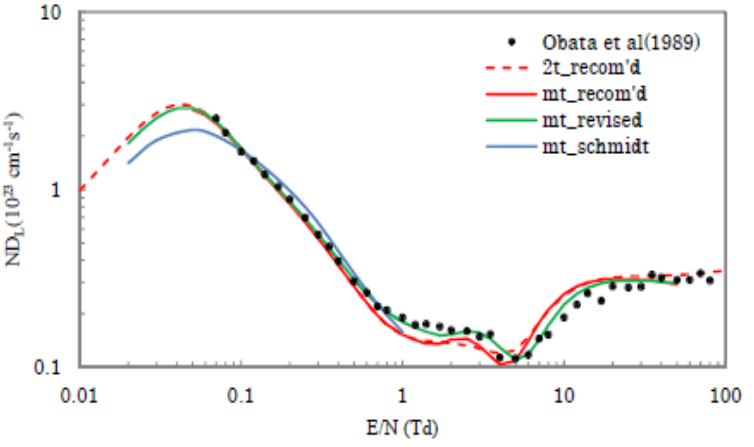


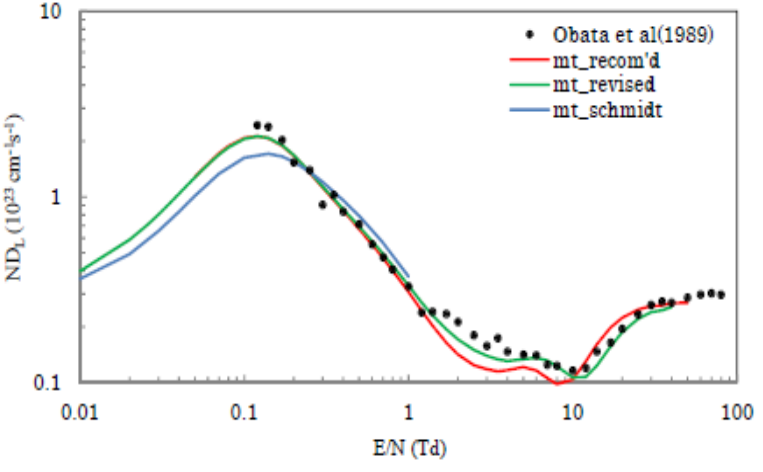
$$w = -\left(\frac{2}{m}\right)^{1/2} \frac{eF}{3N} \int_0^\infty \frac{E}{\sigma_m(E)} \frac{df_0(E)}{dE} dE$$

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

Methane: swarm in mixtures



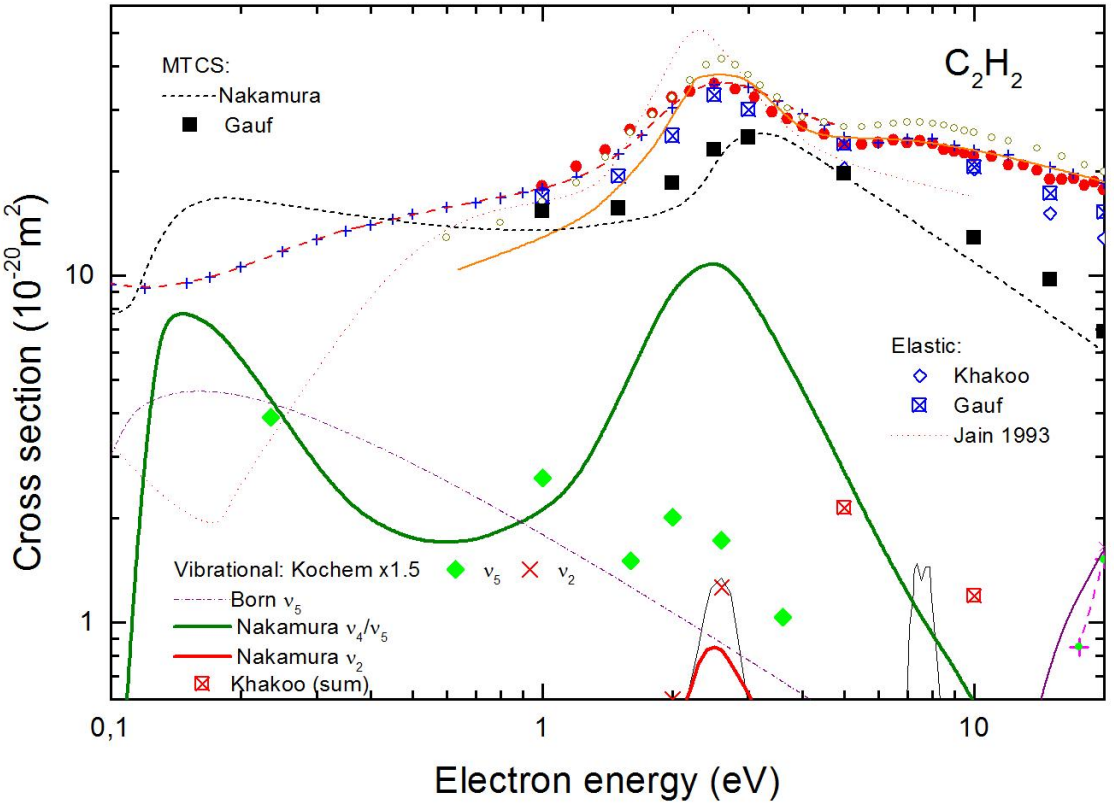




0%, 1.03%, 5.13% Ar

Y. Nakamura, in M.-Y.Song et al..

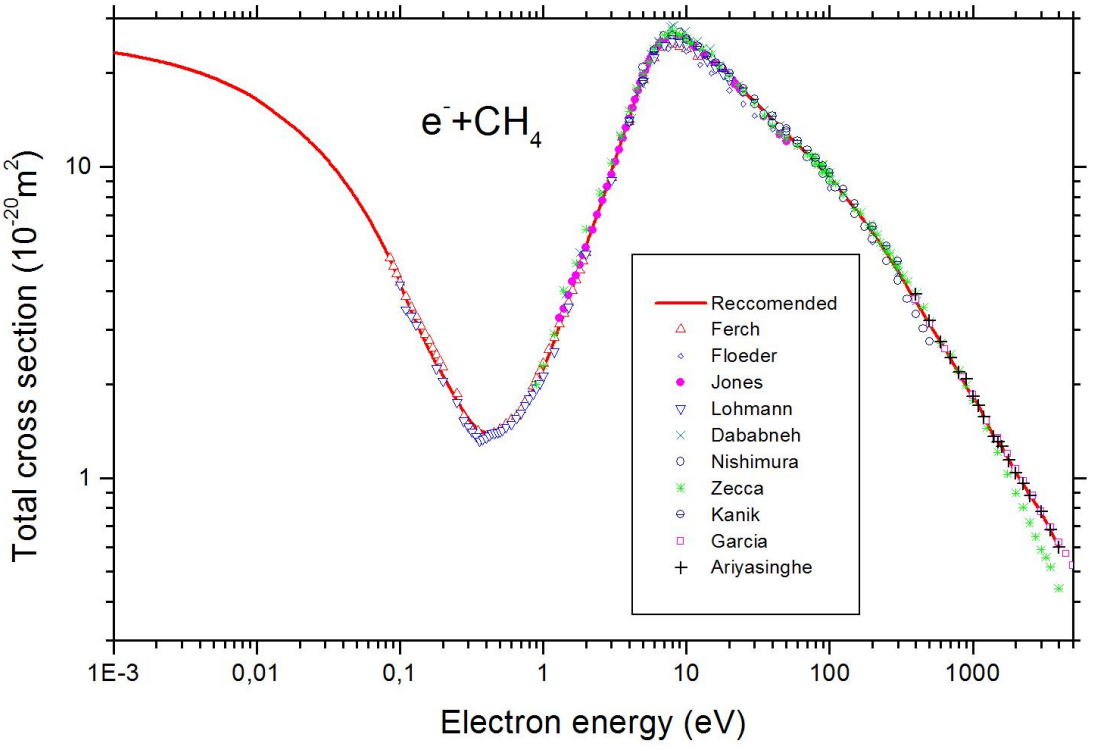
Acetylene: swarm ↔ beam: vibrational, MTCS



Swarm MTCS and vibrational (Nakamura, 2010) seem better than beam (Kochem, 1986)

Review case study: CH_4

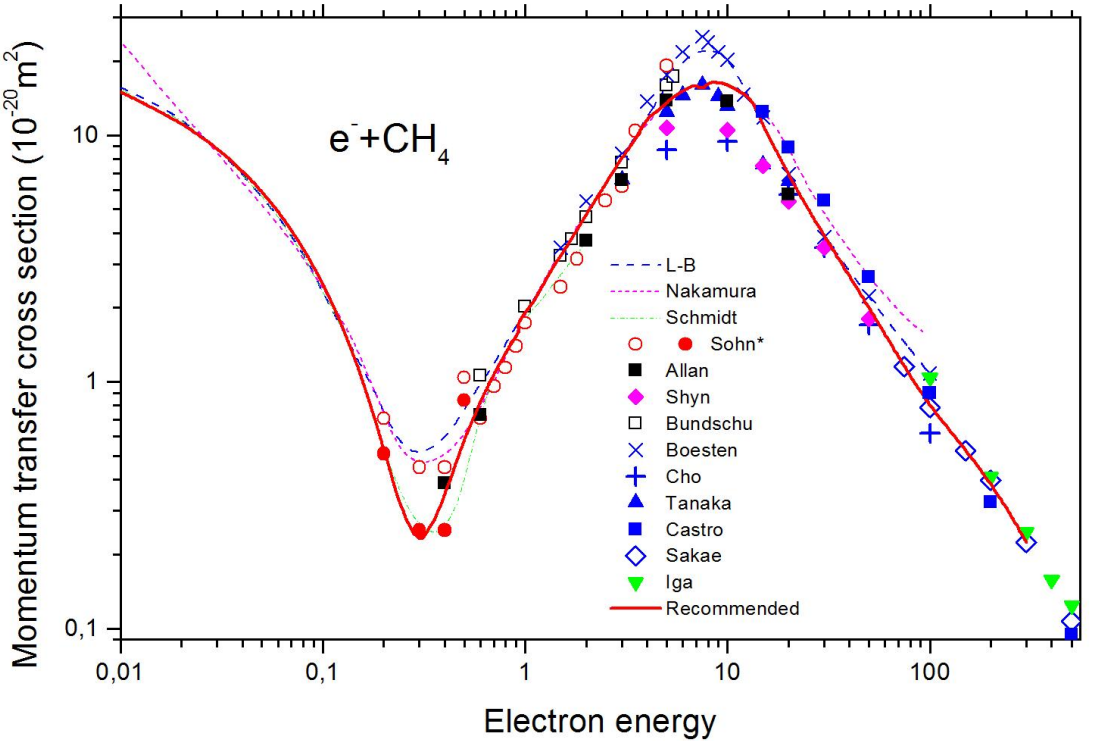
1. Total cross section: ±5%



M.-Y. Song, J. S. Yoon, H. Cho, Y. Itikawa, G. Karwasz, V. Kukooulin, Y. Nakamura, J. Tennyson, to be published

Review case study: CH_4

2. Momentum transfer (and elastic) cross sections: ±15%



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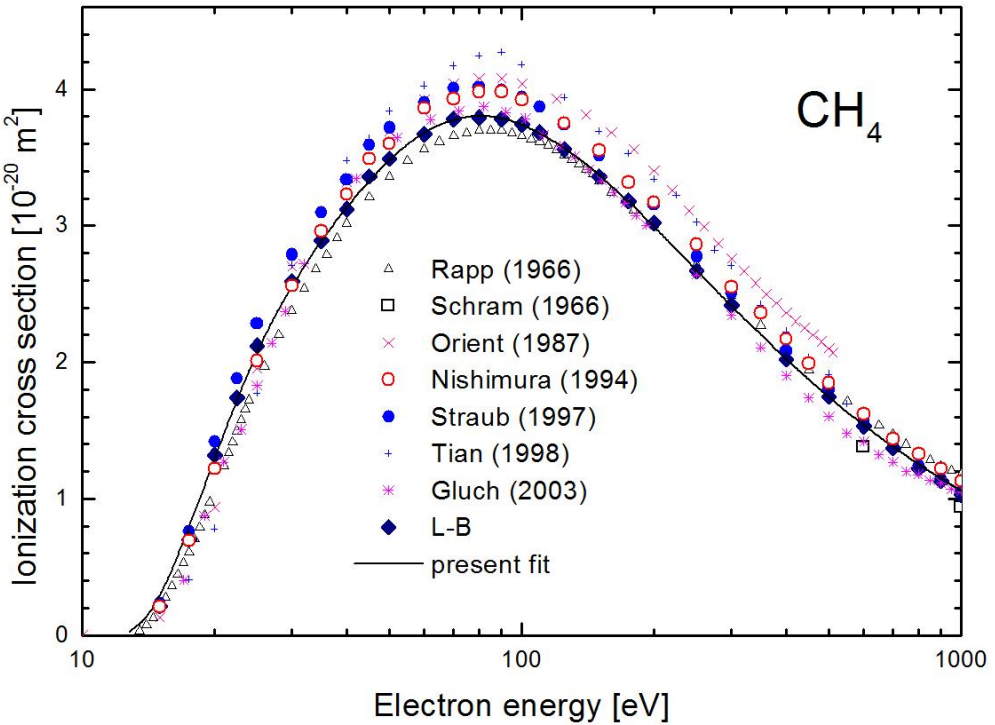
Review case study: CH_4

3. Ionization total: ±10%



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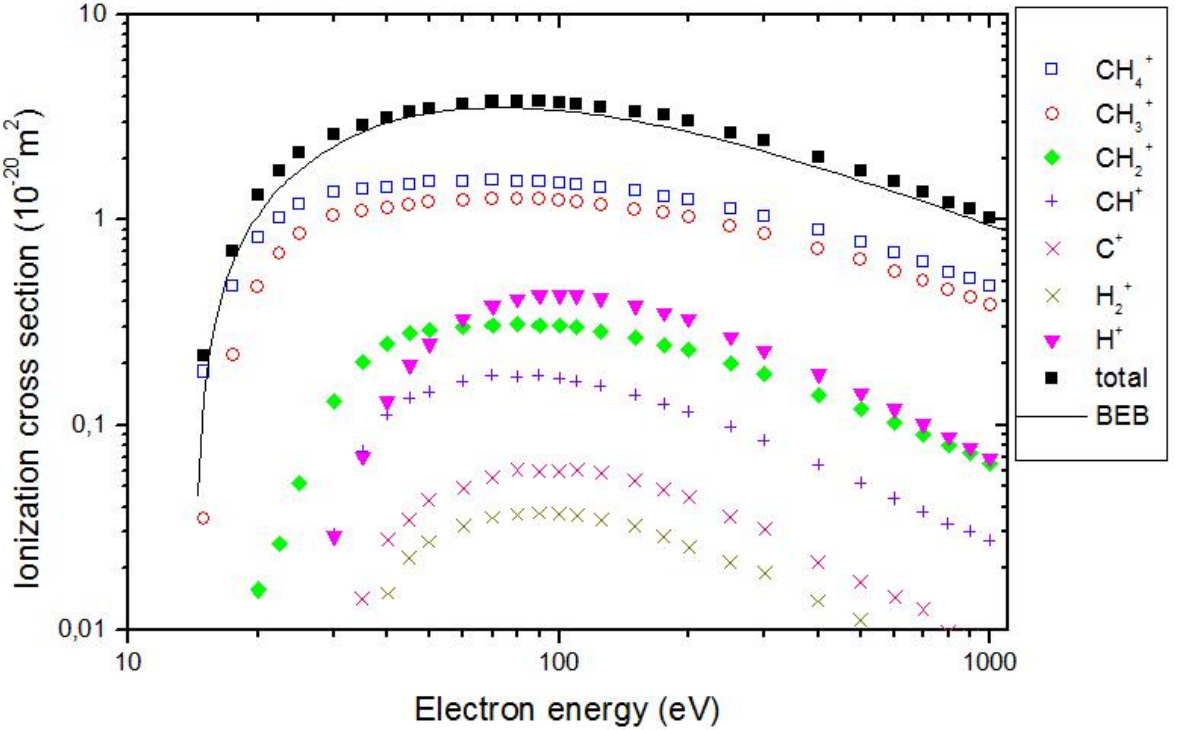
Review case study: CH_4

3a. Ionization partial: ±10%



M.-Y. Song, J. S. Yoon, H. Cho, Y. Itikawa, G. Karwasz, V. Kukooulin, Y. Nakamura, J. Tennyson, to be published

Review case study: CH_4

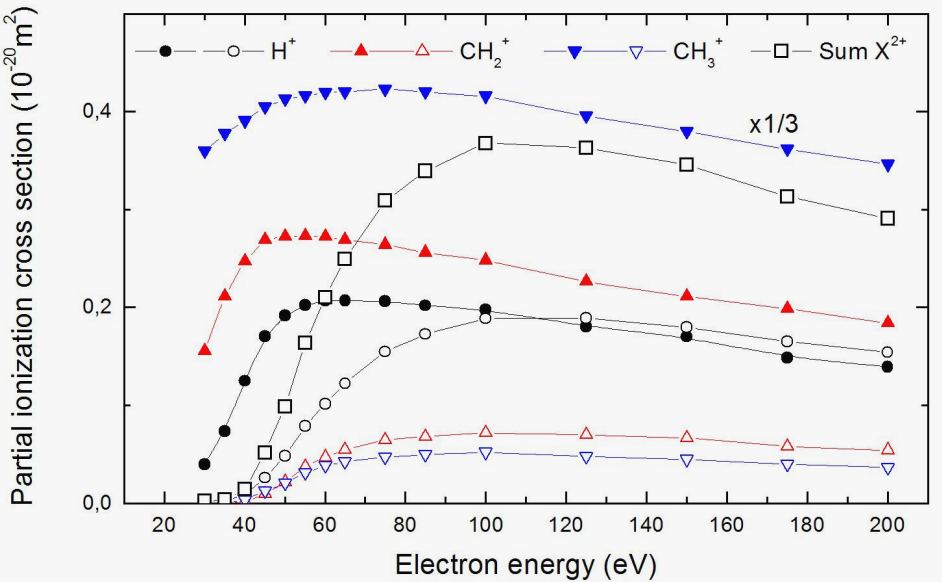
3a. **Ionization partial**: channel resolved

e.g. $e + CH_4 \rightarrow CH_3^+ + H^+ + 2e$

or $e + CH_4 \rightarrow (CH_4^+)^* + e \rightarrow CH_3^+ + H^+ + 2e$

or $e + CH_4 \rightarrow CH_3 + H^+ + e$

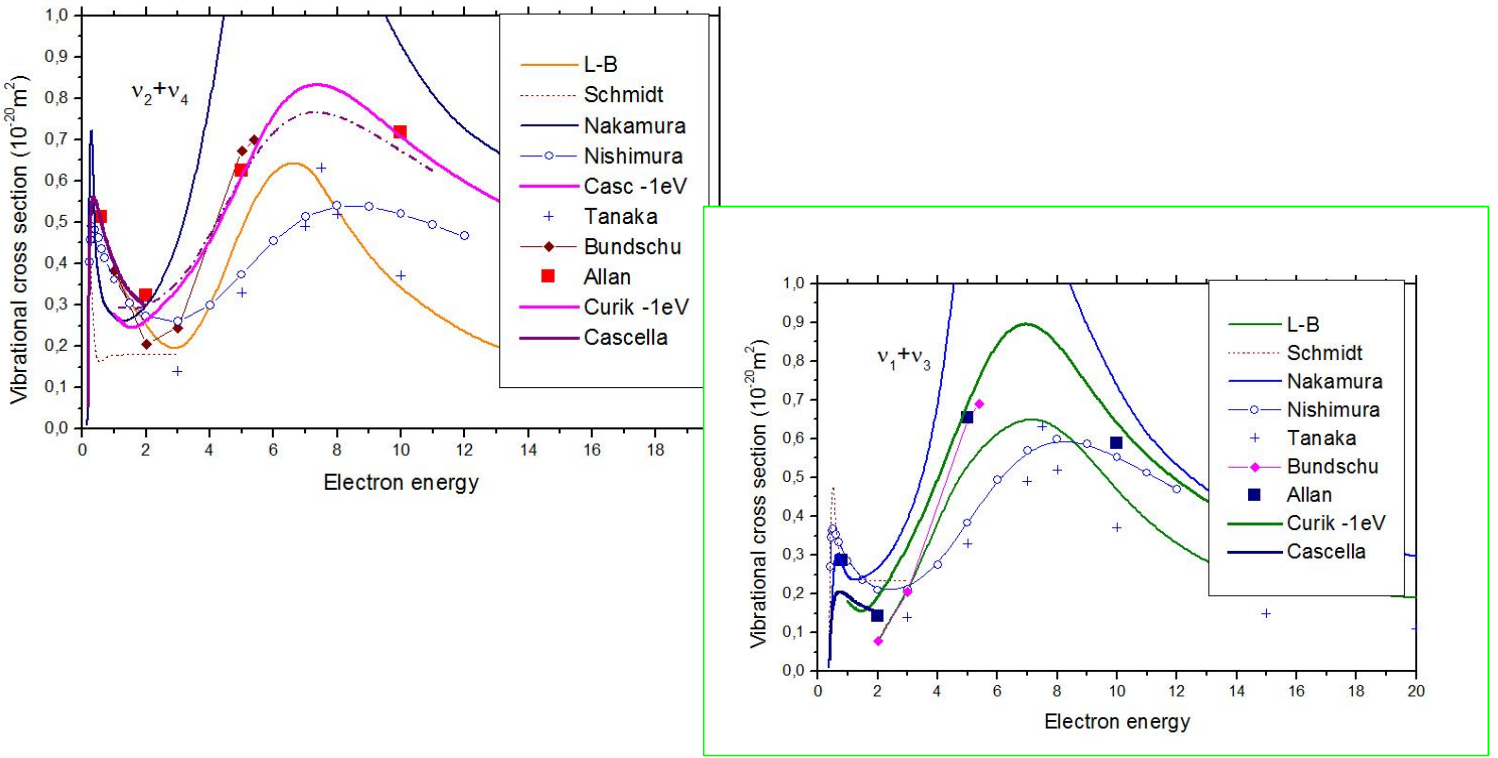
Experimental data (coincidence measurements): Ward et al.. 2011



to be **done...**

Review case study: CH_4

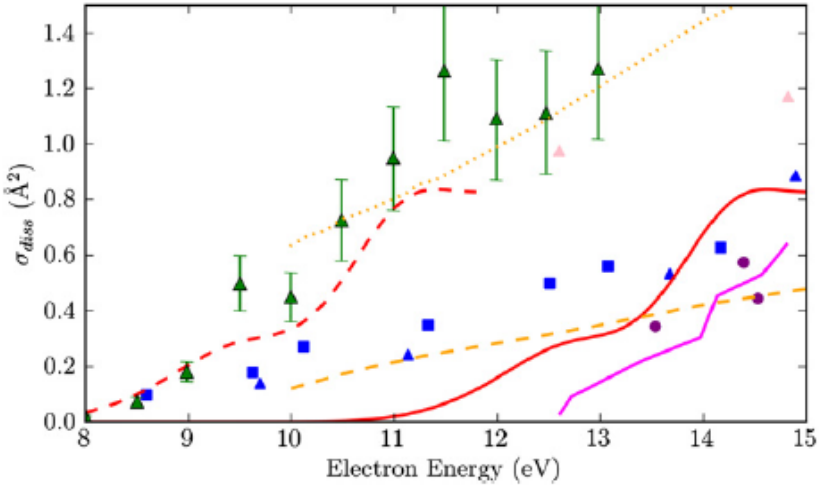
4. Vibrational: „we are in troubles”



M.-Y. Song, J. S. Yoon, H. Cho, Y. Itikawa, G. Karwasz, V. Kukooulin, Y. Nakamura, J. Tennyson, to be published

Review case study: CH_4

5. Electronic excitation: „we *were* in troubles”

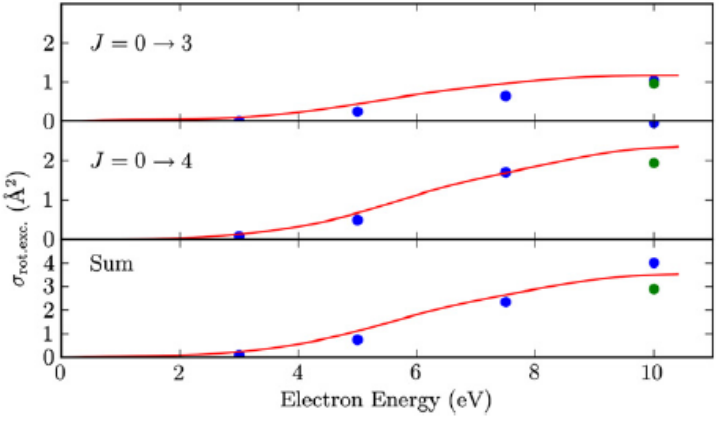


W. J. Brigg, J. Tennyson, M. Plummer
J. Phys. B **47** (2014) 185203
R-Matrix

Figure 13. Electron impact dissociation cross section. Theory: red solid line: present work; red dashed line: present work, shifted to lower energy by 3.2 eV; purple solid line: Hayashi (1991); orange dashed line: CH_2 of Ziółlkowski *et al* (2012); orange dotted line: CH_3 of Ziółlkowski *et al* (2012). Experiment: blue squares: CH_2 of Nakano *et al* (1991); blue triangles: CH_3 of Nakano *et al* (1991); green triangles: CH_3 of Makochekanwa *et al* (2006); pink triangles: CH_3 of Motlagh and Moore (1998); purple circles: Winters (1975).

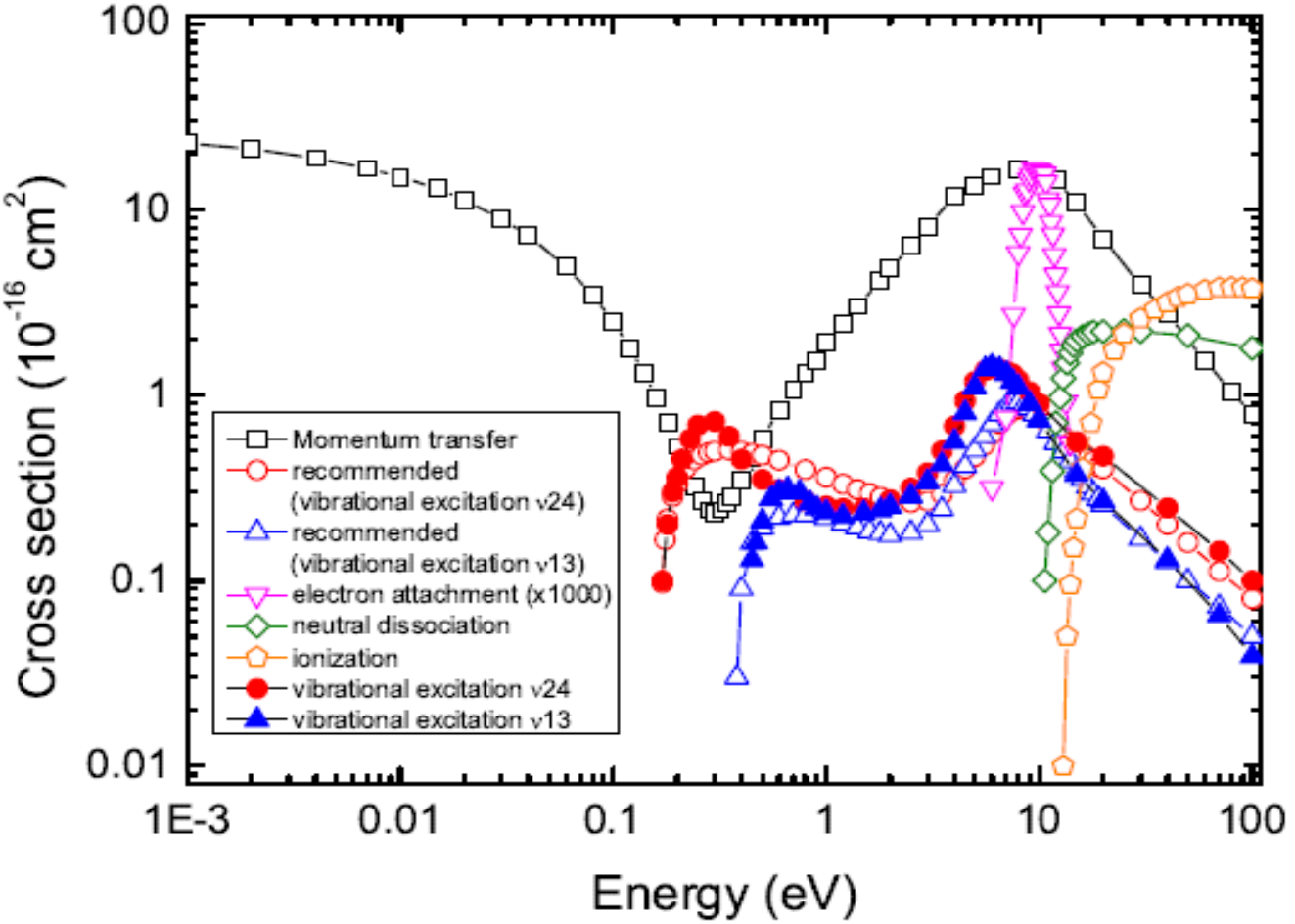
Review case study: CH_4

6. Rotational excitation: „we *were* in troubles”



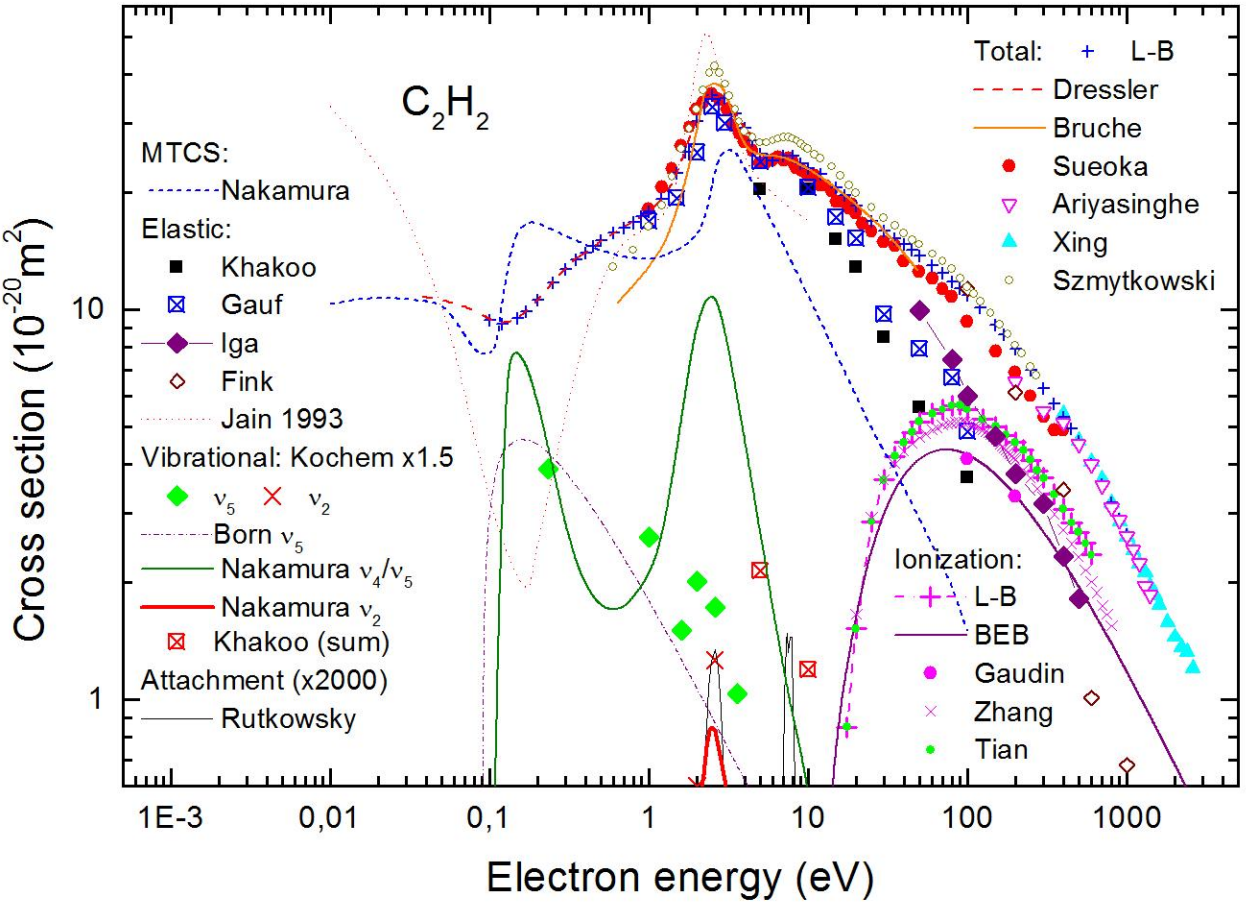
W. J. Brigg, J. Tennyson, M. Plummer, J. Phys. B **47** (2014) 185203
R-Matrix

CH_4 - overview



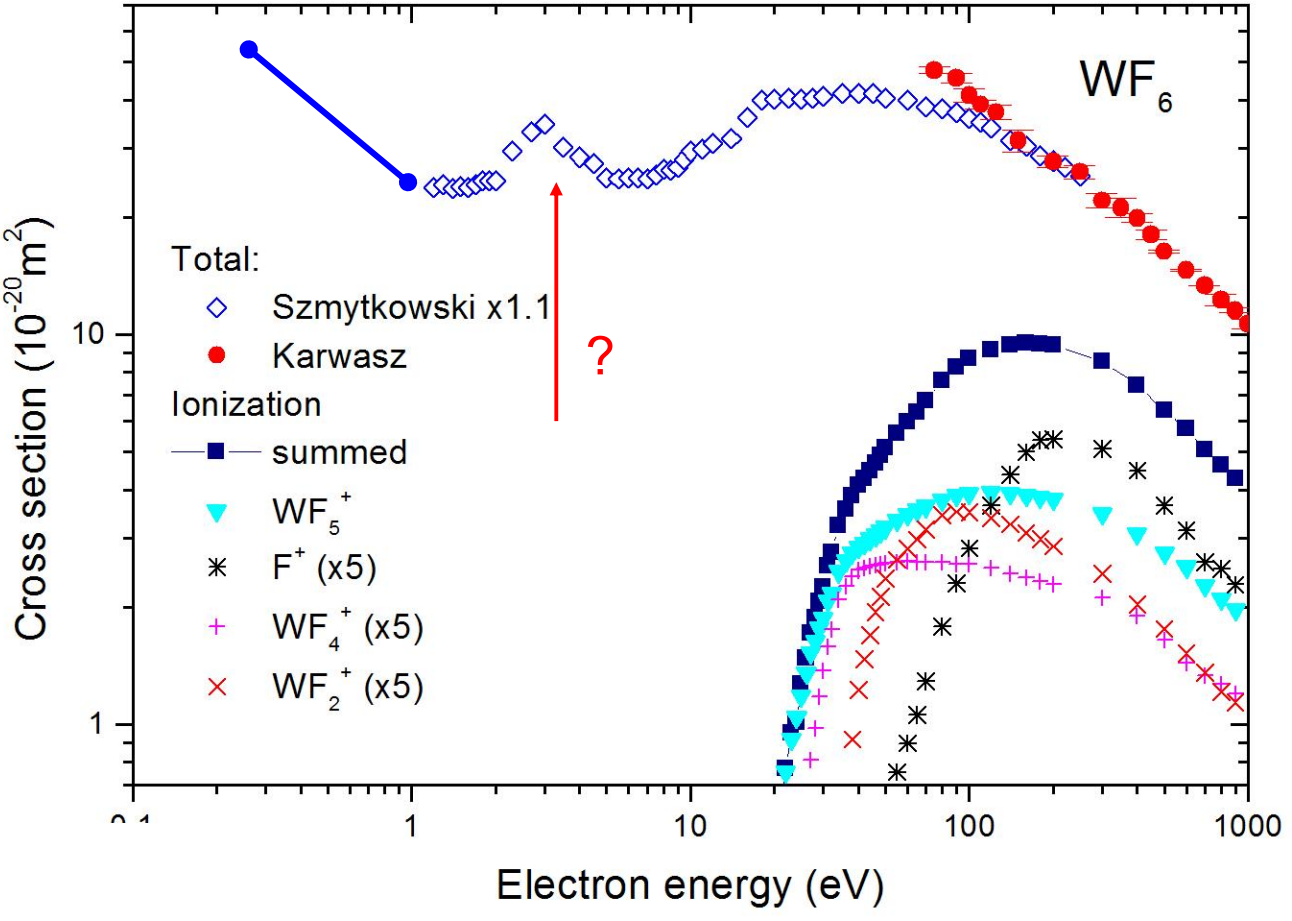
M.-Y. Song, J. S. Yoon, H. Cho, Y. Itikawa, G. Karwasz, V. Kukooulin, Y. Nakamura, J. Tennyson, to be published

C_2H_2 - preliminary



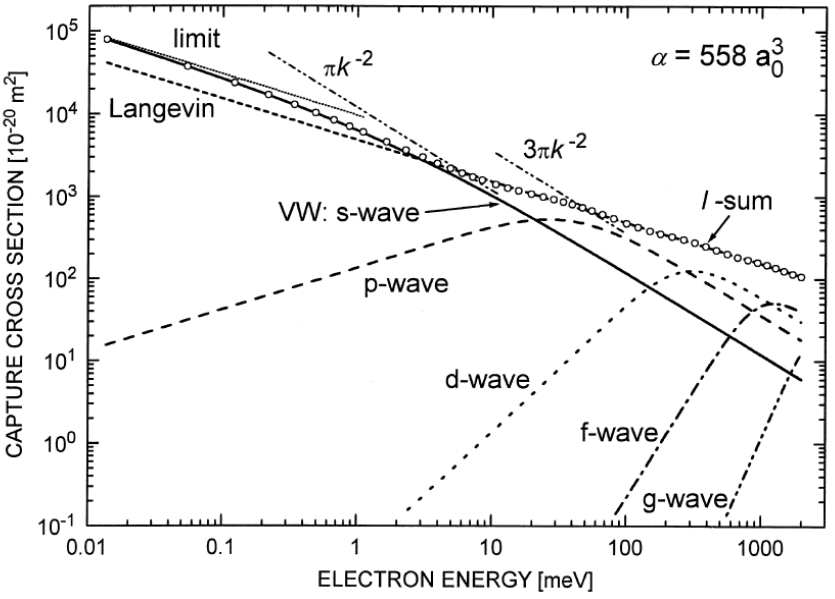
M.-Y. Song, J. S. Yoon, H. Cho, Y. Itikawa, G. Karwasz, V. Kukooulin, Y. Nakamura, J. Tennyson, to be published

WF_6 - few data



GK, work in progress

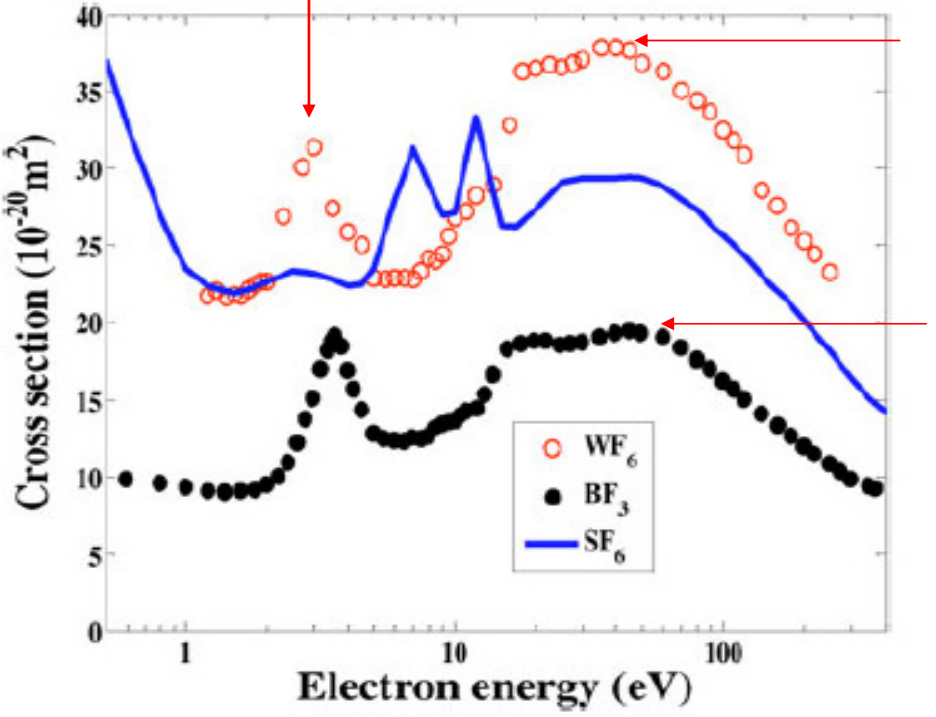
Semi-empirical methods - zero-energy cross section: Langevin, Voigth-Wannier



Allan et al., Advances At. Mol. Phys. (2004)

Searching analogies (2):

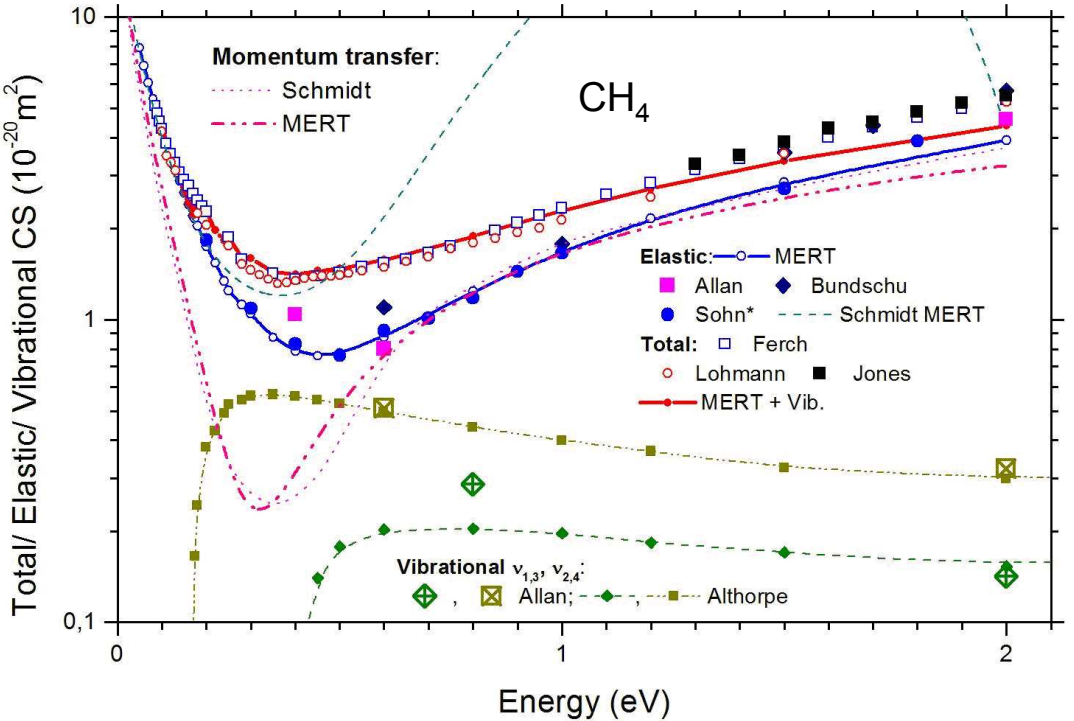
„resonances” in total cross sections



G. Karwasz, K. Fedus, FS&T (2013), experimental data: Szmytkowski and collaborators

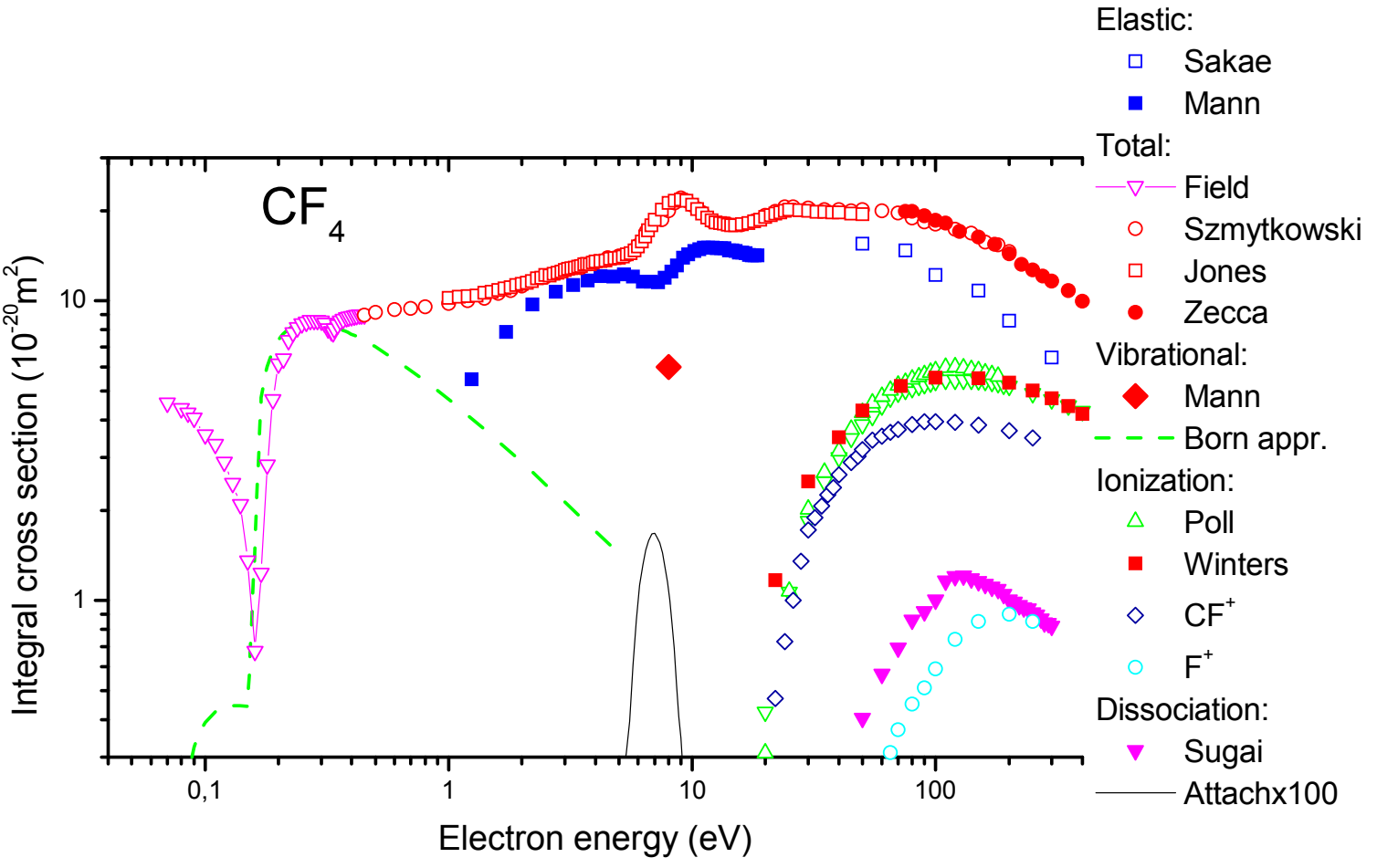
Semi-empirical methods: elastic (MERT)

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



K. Fedus, G. Karwasz, Eur. J. Phys. D (2014)

Semi-empirical methods: vibrational (Born)



Vibrational (Born):
transition dipole moments can be calculated

Journal of Molecular Spectroscopy 298 (2014) 1–6

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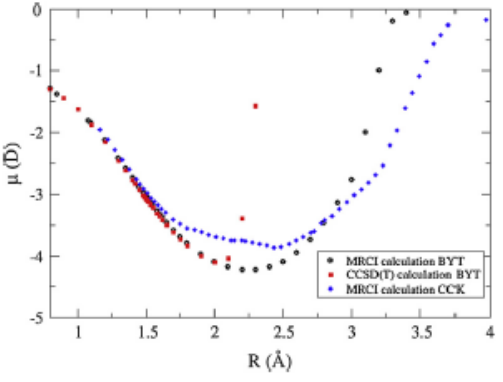
journal homepage: www.elsevier.com/locate/jms

Vibration–rotation transition dipoles from first principles

Jonathan Tennyson



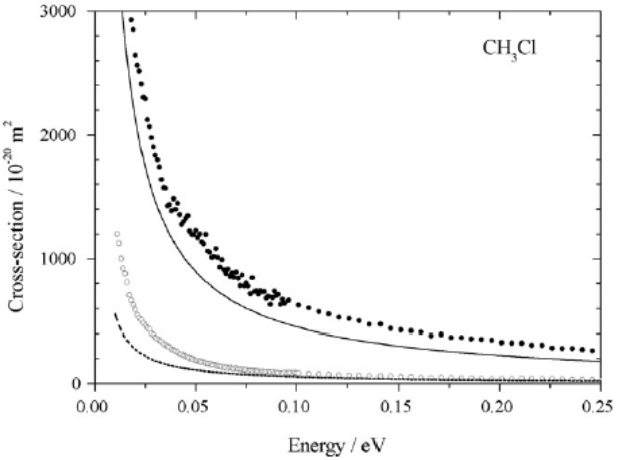
SiO

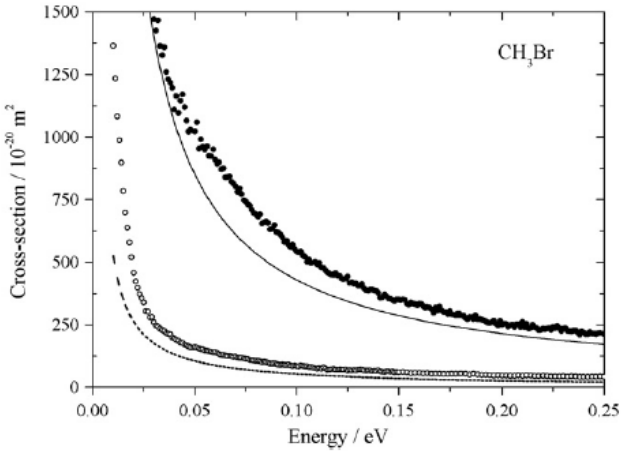
Rotational, very low energy limit (Born):

Polar molecules:

$$\sigma(J,K;J',K') = \xi(2J+1)\begin{pmatrix} J & J' & 1 \\ K & -K' & 0 \end{pmatrix}^2 \times \ln\left[\left|\frac{k^2+k'^2-2kk'\cos\theta_2}{k^2+k'^2-2kk'\cos\theta_1}\right|^{1/2}\right]$$

$$\xi = (4\pi/3k^2)(\mu^2/[ea_0]^2).$$

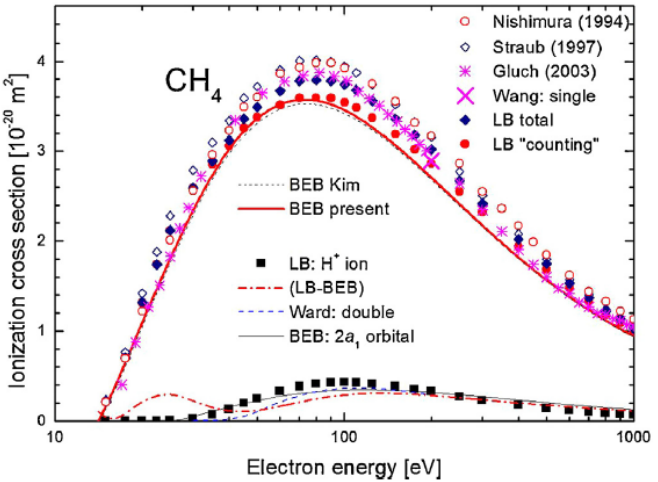




N C Jones et al. Intr. J. Mass Spectr. 277 (2008) 91

Ionization: semiempirical formulae

$$\sigma[\mathrm{cm}^2] = \frac{10^{-13}}{IE}\left\{A_1 \ln(E/I) + \sum_{i=2}^{N} A_i \left(1 - \frac{I}{E}\right)^{i-1}\right\},$$



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

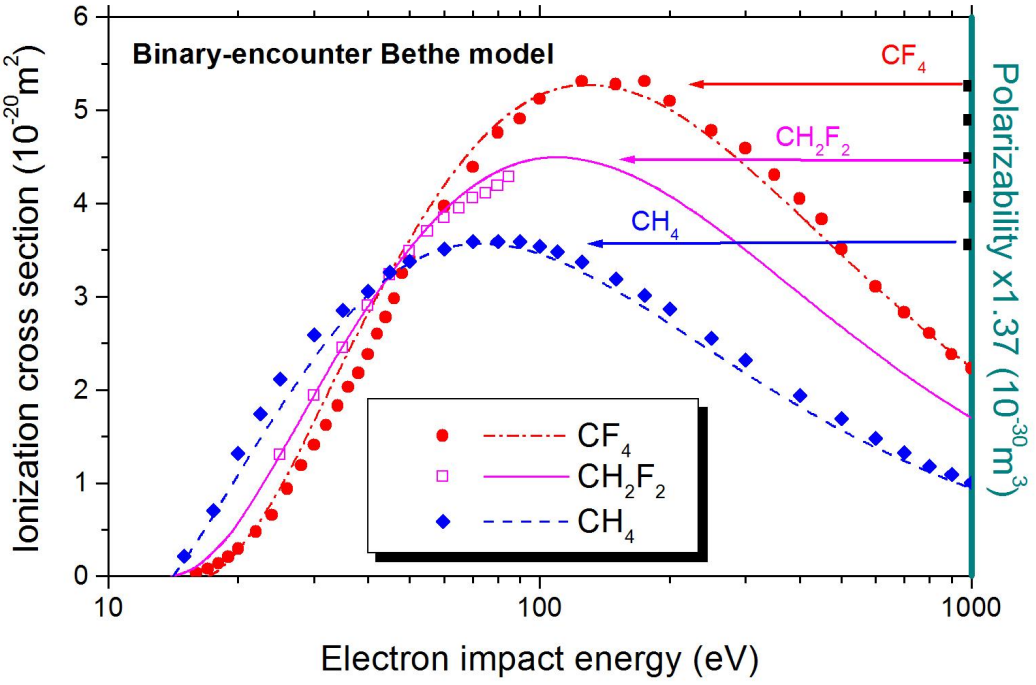
Normalized energies: $t = E/I_n$, $u_n = E_{kin}/I_n$ Only two values needed from QCh

Y.-K. Kim and M. E. Rudd, Phys. Rev. A 50 (1994) 3954

G. Karwasz, P. Mozejko, M.-Y. Song, Int. J. Mass Spectrometry (2014)

Ionization (BEB): CH_4, CH_3F, ... CF_4

Born-Bethe binary-encounter model (i.e. classical collisions)



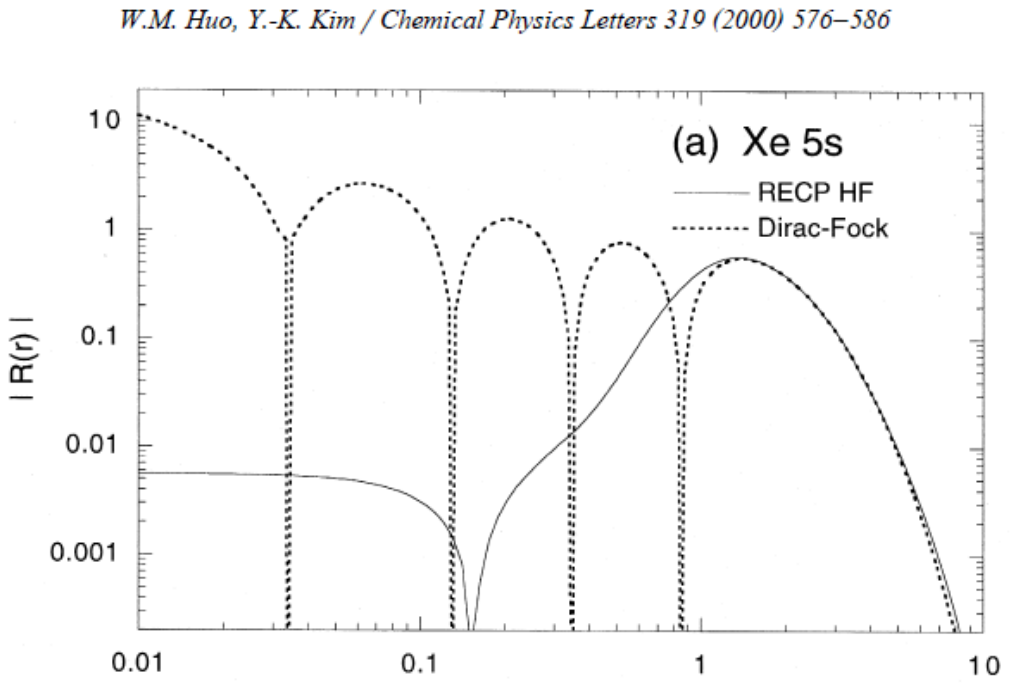
It holds also SF_6 and WF_6!

Why important?

G. Karwasz, P. Mozejko, M.-Y. Song, Int. J. Mass Spectrometry (2014)

Ionization (BEB): CH_4, CH_3F, ... CF_4

Born-Bethe binary-encounter model (i.e. classical collisions)



It holds also SF_6 and WF_6!

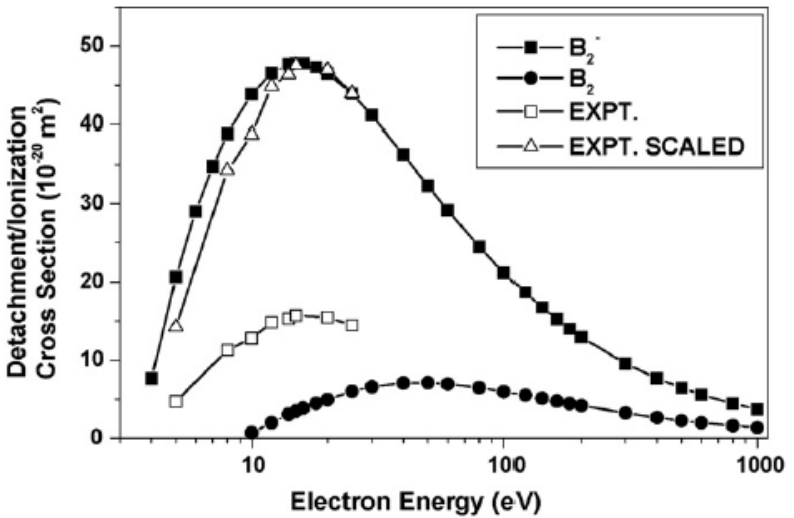
Why important?

G. Karwasz, P. Mozejko, M.-Y. Song, Int. J. Mass Spectrometry (2014)

Electron detachment(D-M): B_2^-, BO^-, O_2^-, CN^-)

Deutsche-Mark formalism

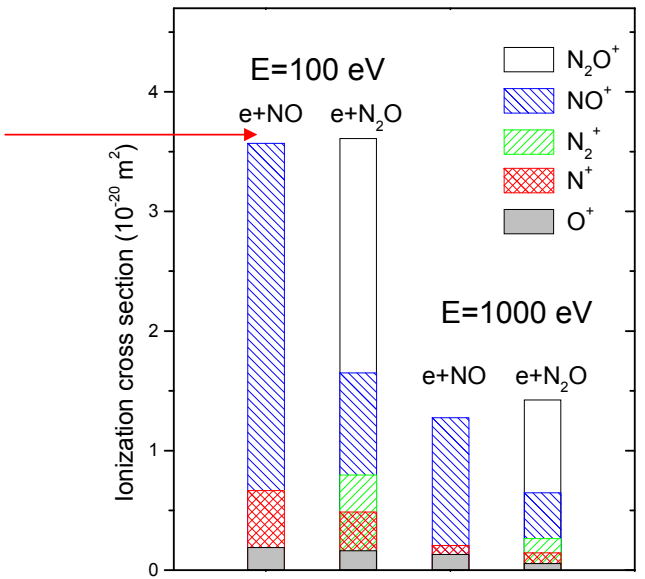
$$\sigma(u) = \sum_{n,l} g_{nl} \pi r_{nl}^2 \xi_{nl} b_{nl}^{(q)}(u) \left[\frac{\ln(c_{nl} u)}{u} \right] \qquad b_{nl}^{(q)} = \frac{A_1 - A_2}{1 + (u/A_3)^p} + A_2$$

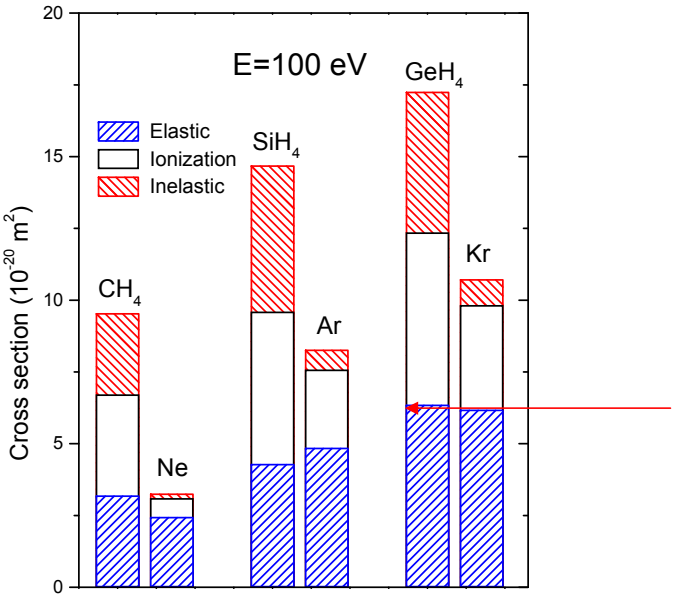


H. Deutsch et al. Int. J. Mass Spectr. **277** (2008) 151

Searching analogies (1):

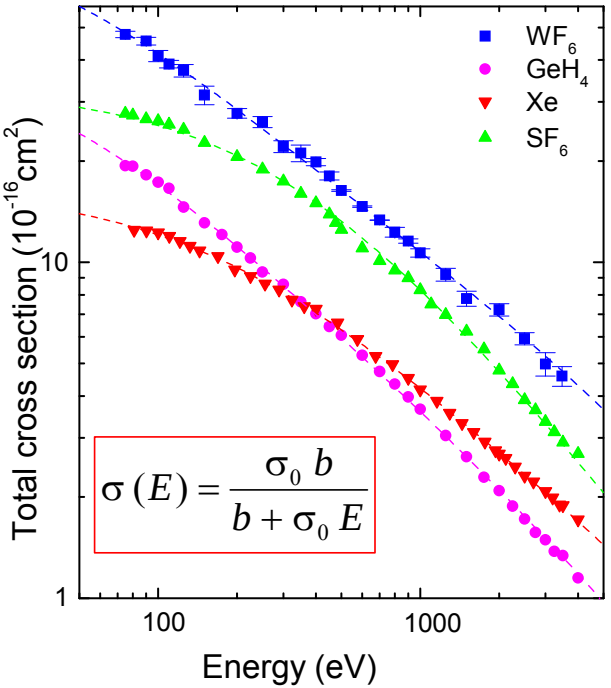
partitioning into elastic & ionization

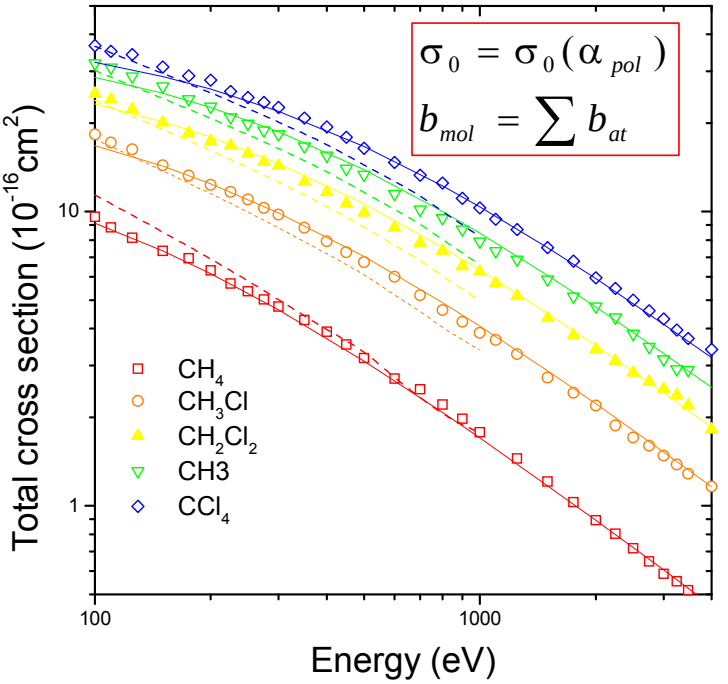




High energies: in search for additivity rule

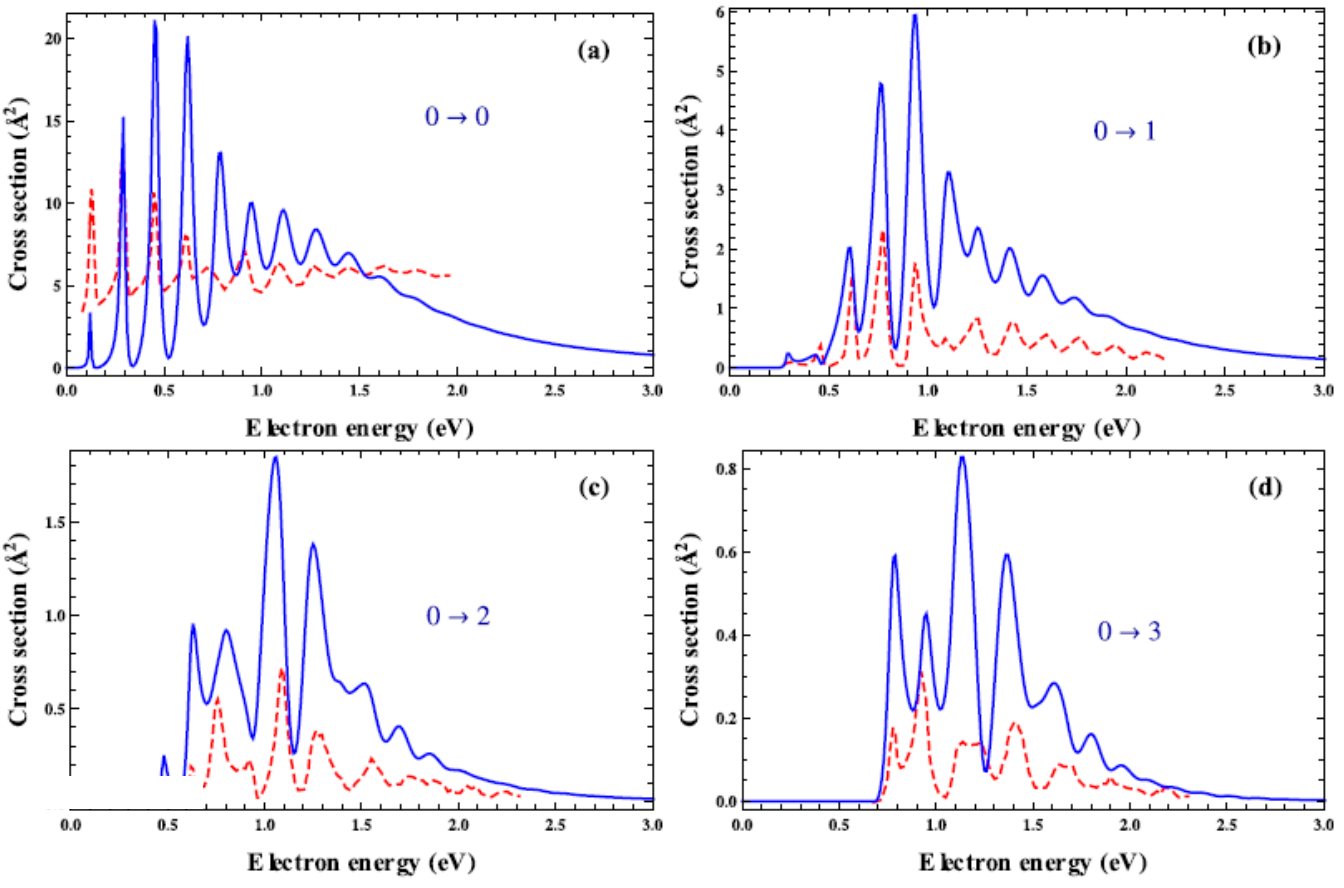
CH_4, CF_4, SiH_4, ... WF_6 → CH_2F_2, SiF_4 ...
→ H, C, Si, ... W





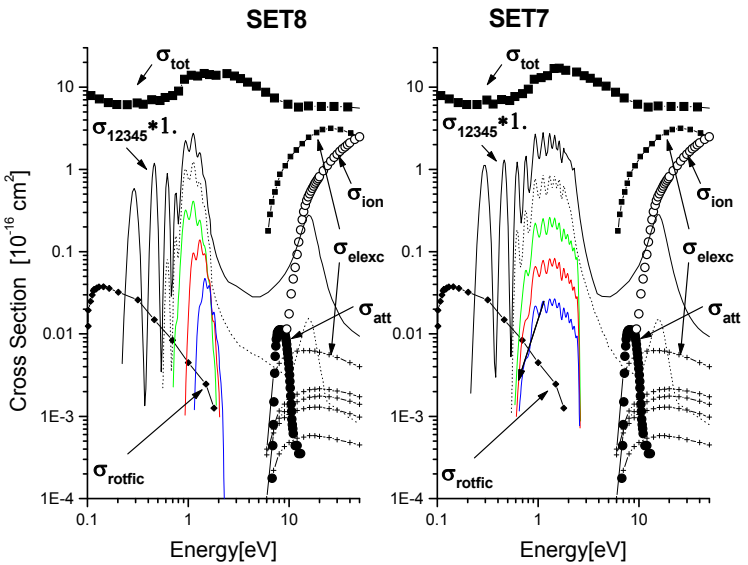
G. Karwasz et al., PRA (2000)

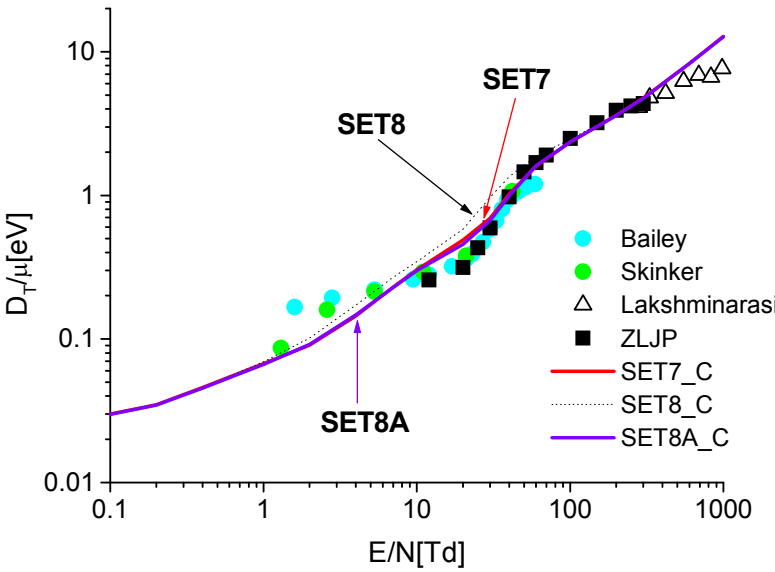
Theoretical progress: resonances in NO (R-matrix)



Laporta, ... J Tennyson, Plasma Sources Sci. Technol. 21 (2012) 055018

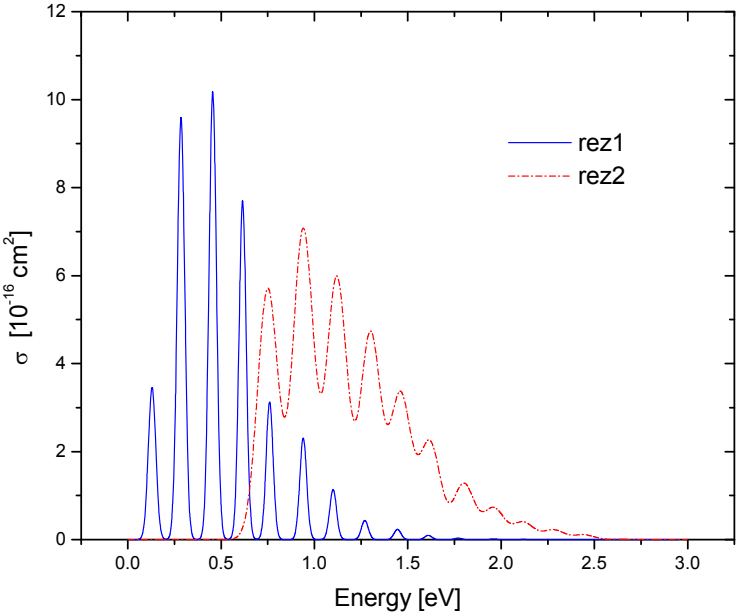
Swarm analysis: resonances in NO

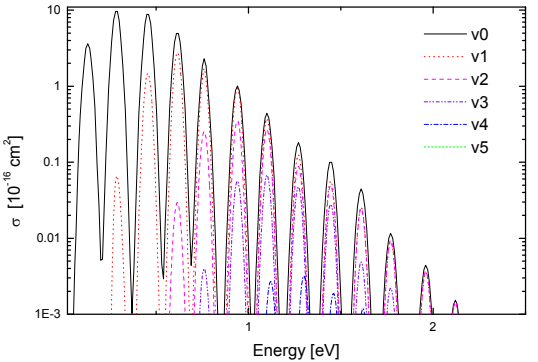


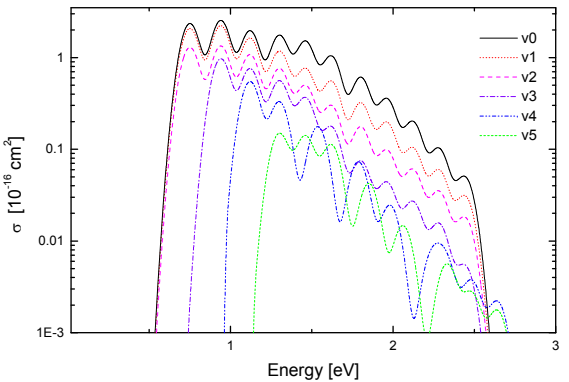


M. Josic, J. Mechlińska-Drewko, Z. Petrovic, G. Karwasz, Chem. Phys. Lett. (2003)

Overlapping resonances: NO (swarm guess)

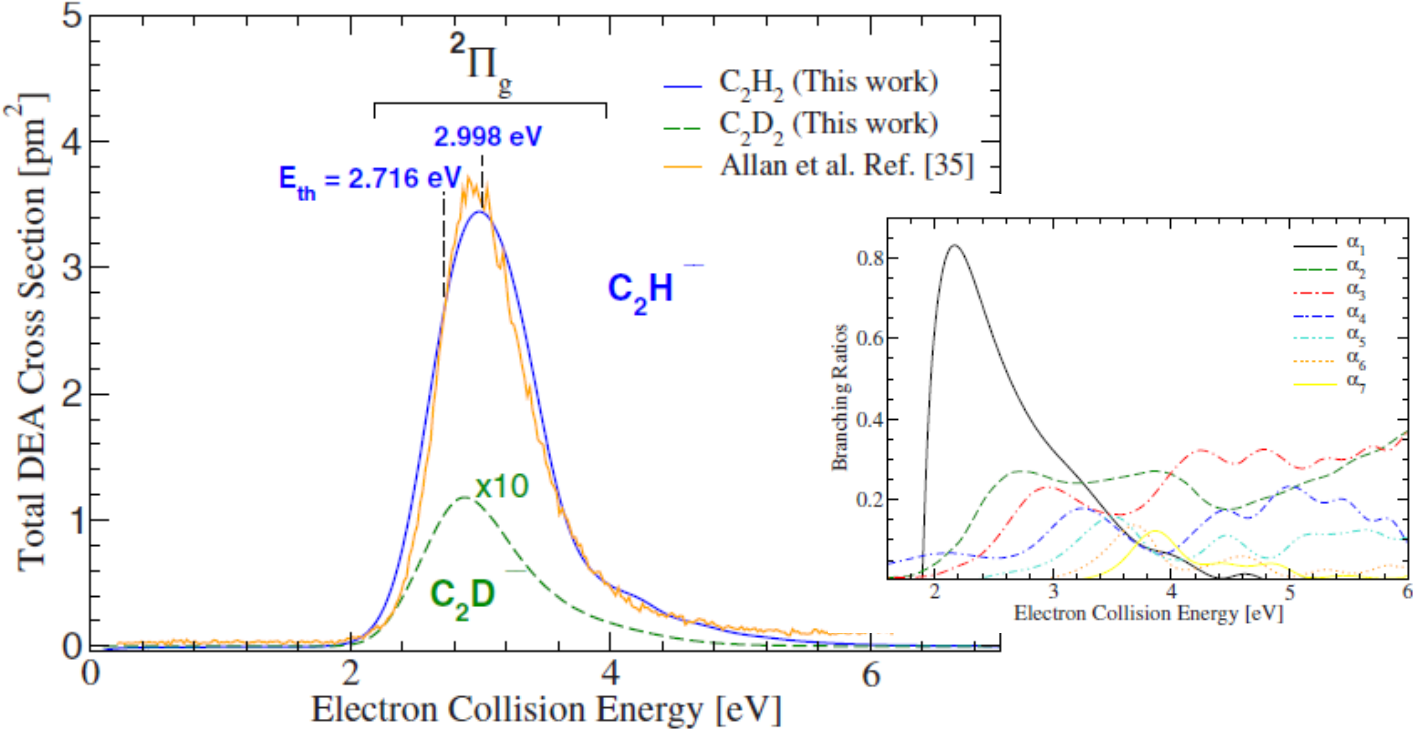






M. Josic, J. Mechlińska-Drewko, Z. Petrovic, G. Karwasz, Chem. Phys. Lett. (2003)

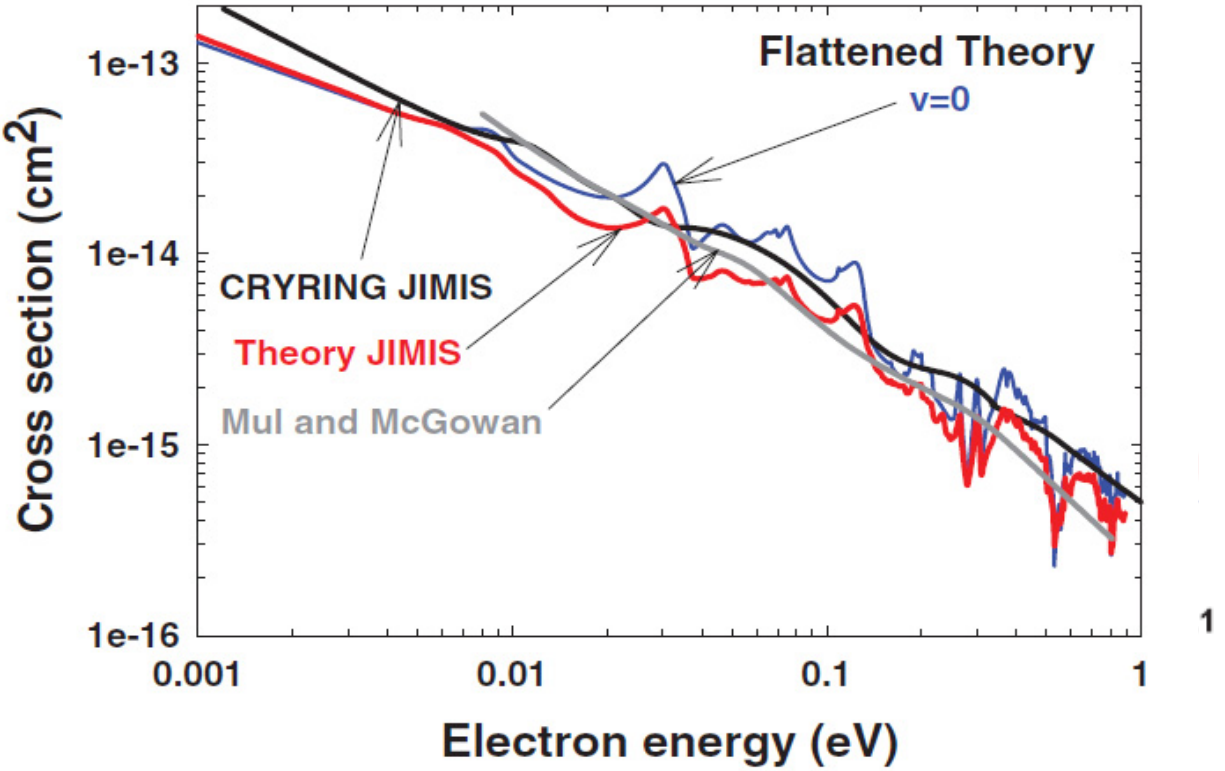
Theoretical progress - Kohn variational: dissociative attachment (C_2H_2)



S. T. Chorou and A. E. Orel, Phys. Rev. A. **77** (2009) 042079

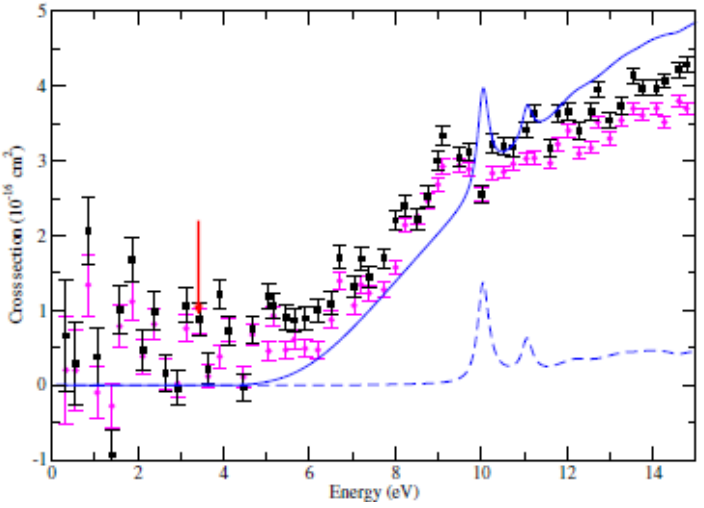
Theoretical progress:

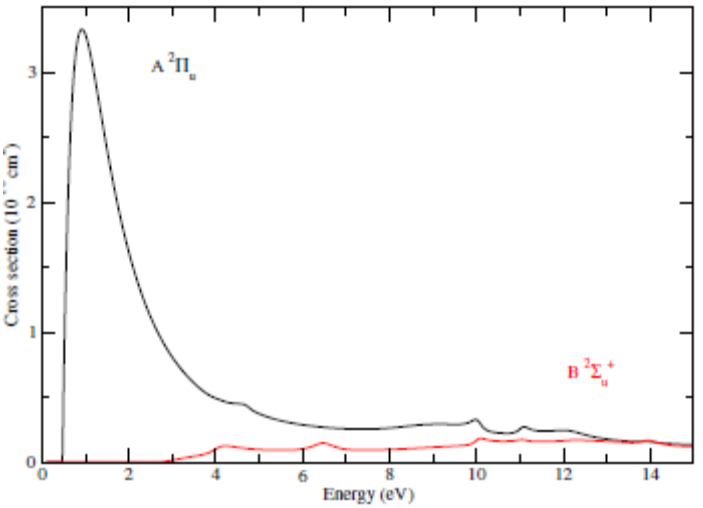
dissociative recombination ($N_2^+ + e^- \rightarrow N^* + N^*$)



S. L. Guberman, J. Chem. Phys. 139 (2013) 124318
Also Tennyson and collaborators, PRA (2014)

C_2^- – electron detachment, electronic excitation

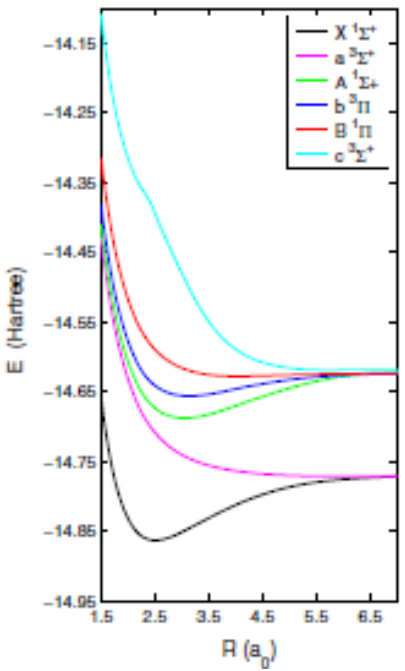


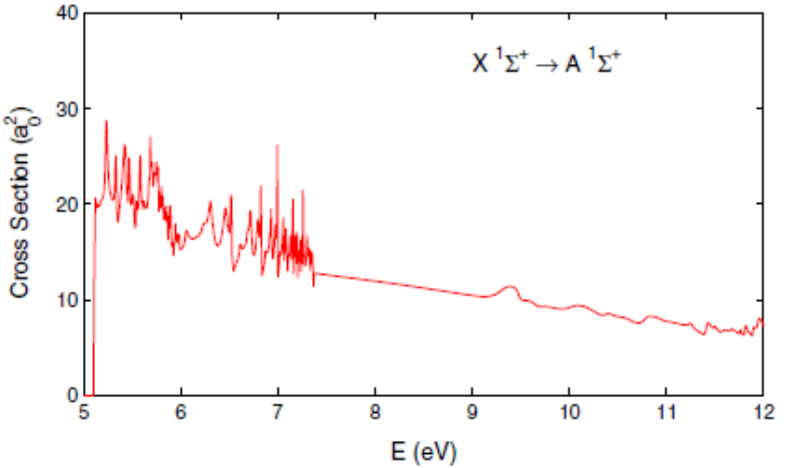


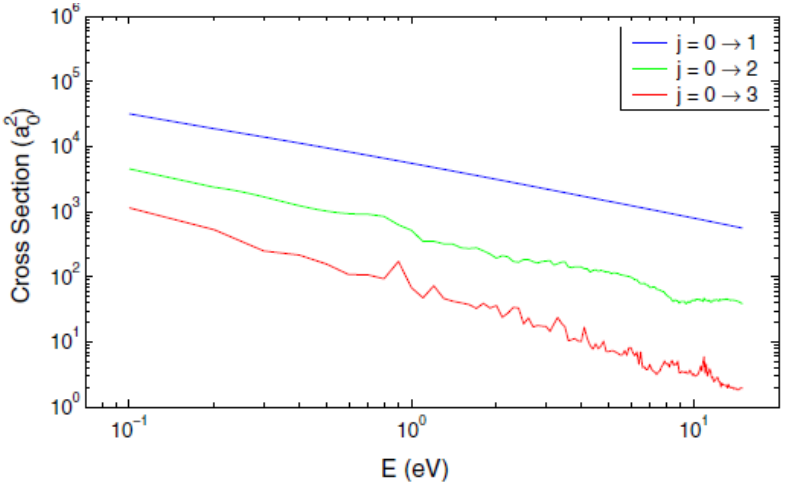
solid line – with Born correction
broken – without Born correction

Halnova, Gorkenfield, J Tennyson, JPB 41 (2008)
UK Molecular R-matrix code: electronic, rotational

BeH^+ – electronic and rotational excitation



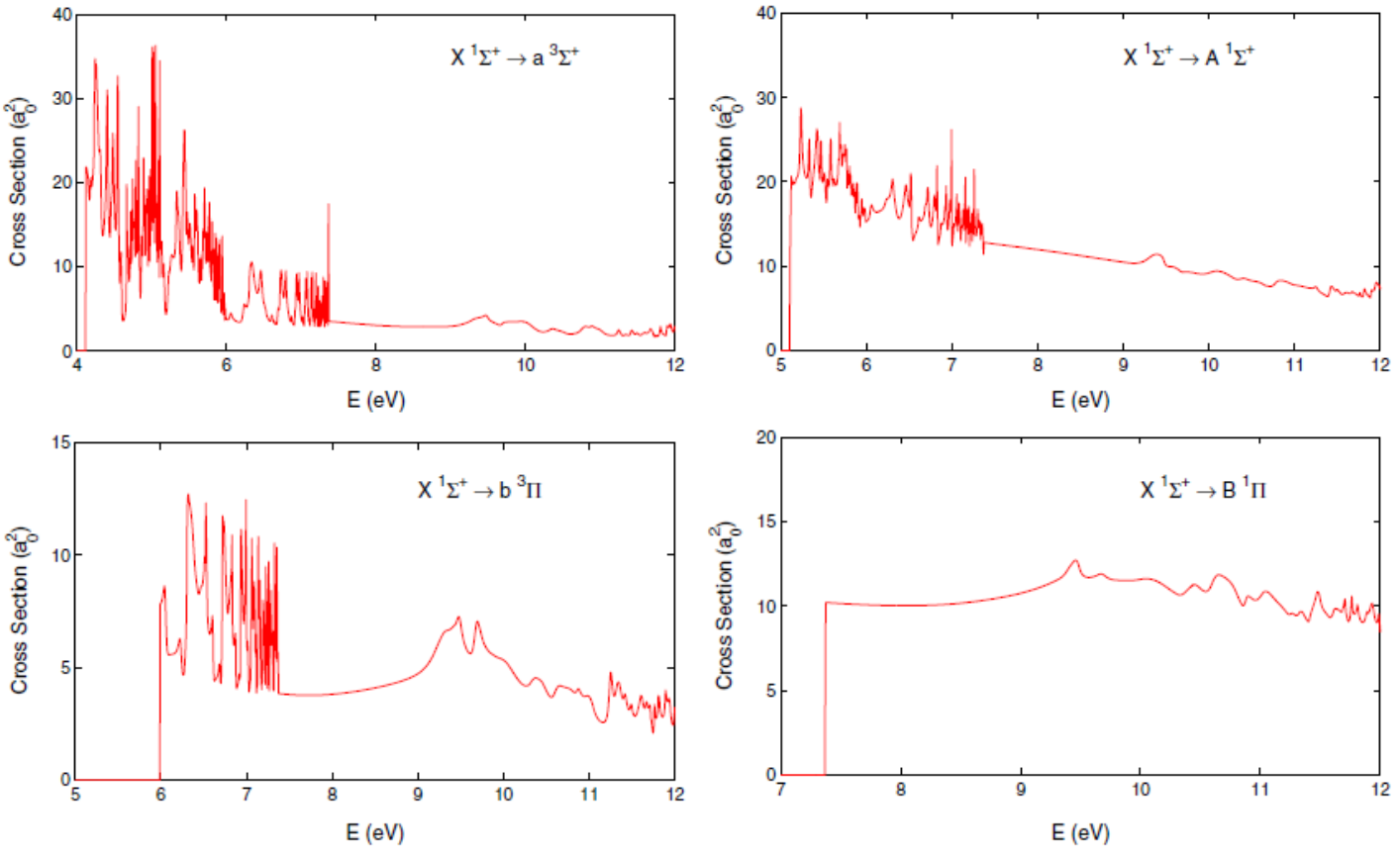




K Chakrabarti and J Tennyson, Eur. Phys. J. D 66 (2012) 31

UK Molecular R-matrix code: electronic, rotational

BeH^+ – electronic excitation



K Chakrabarti and J Tennyson, Eur. Phys. J. D 66 (2012) 31

UK Molecular R-matrix code: electronic, rotational

BeH^+ dissociative recombination

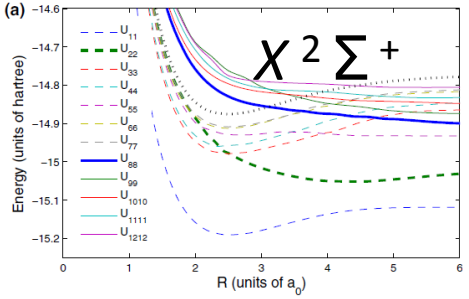
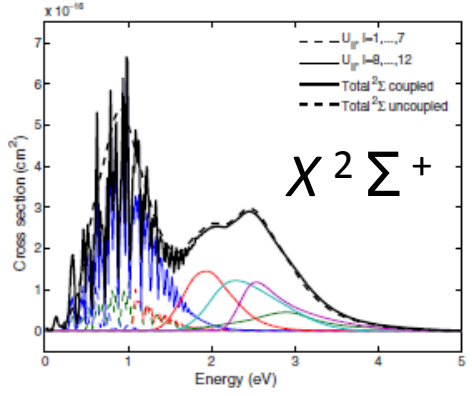


FIG. 2. (Color online) Quasidiabatic potentials of BeH of (a) $^2\Sigma^+$, (b) $^2\Pi$, and (c) $^2\Delta$ symmetries. The solid curves are the resonant states while the electronically bound states are dashed curves. Also the electronic ground state of the BeH^+ is displayed with the dotted curve.



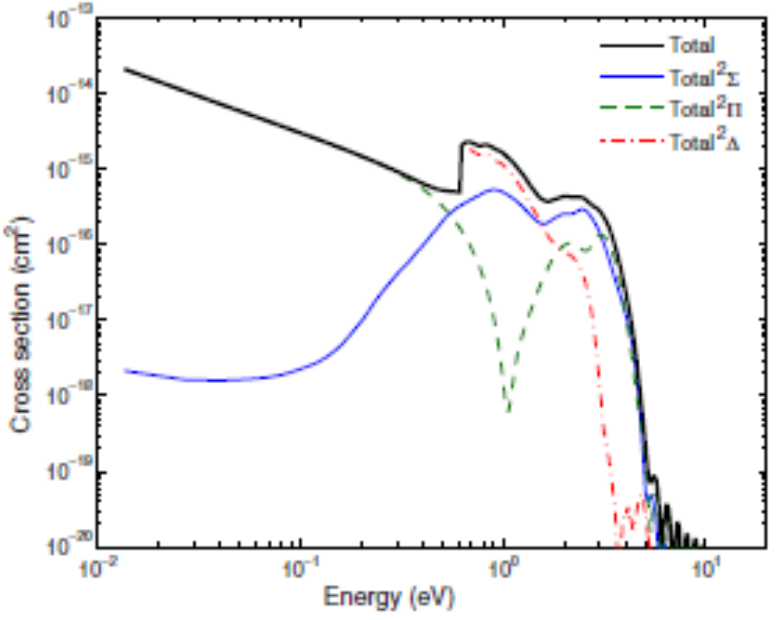


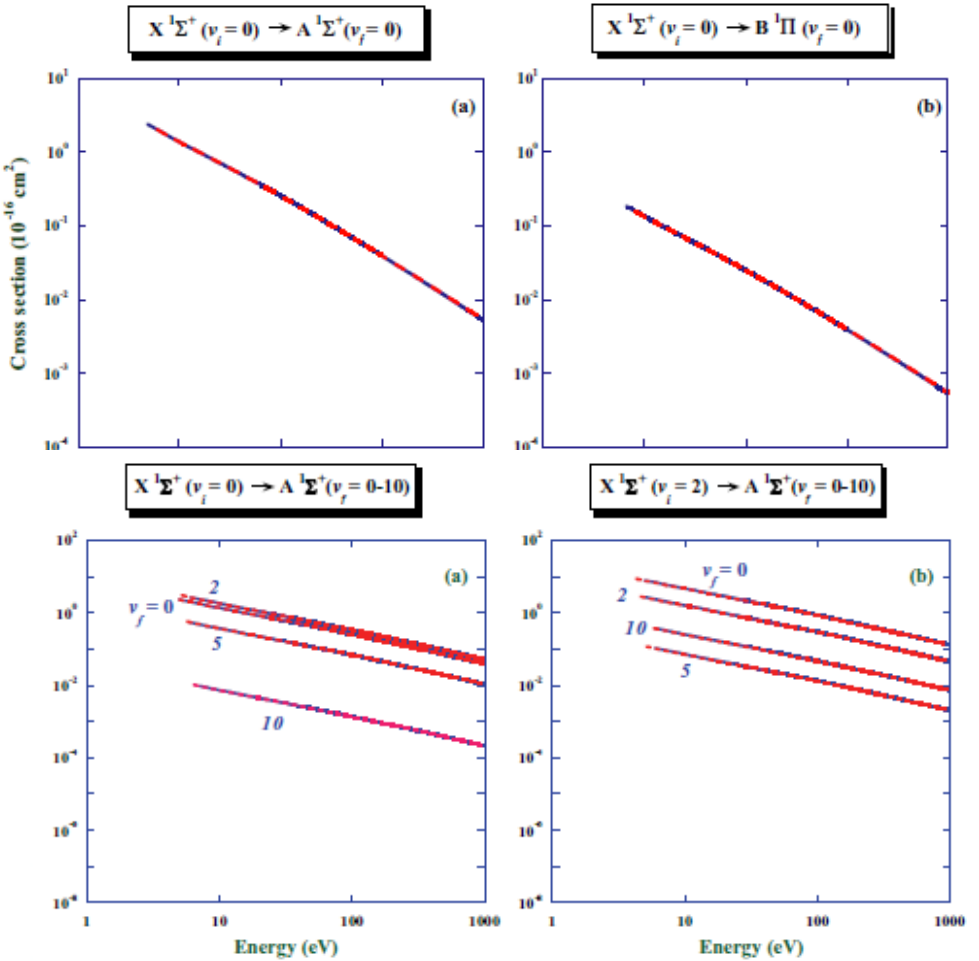
TABLE I. Parameters for the fitted form of the dissociative recombination cross sections at low collision energies.

Ion	Vibrational level	σ_0 (10^{-16}cm^2 eV^b)	b
BeH^+	$v=0$	3.10	0.99
BeH^+	$v=1$	6.90	0.93
BeD^+	$v=0$	3.32	1.02
BeD^+	$v=1$	4.72	1.05

Roos,..Orel, PRA 80 (2009) 012501
Variational Kohn method

σ/E^b

BeH^+ – electronic and vibrational excitation

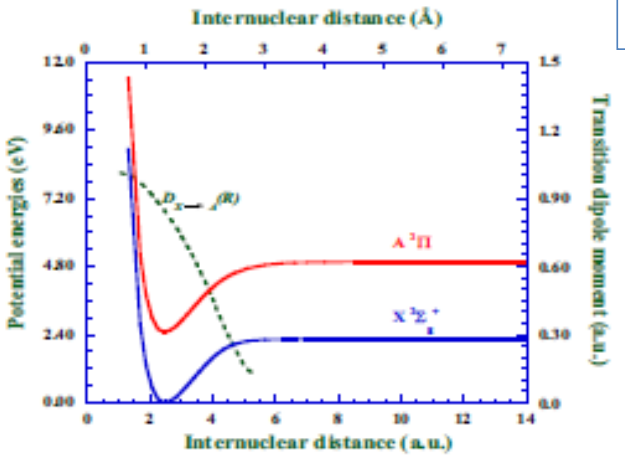


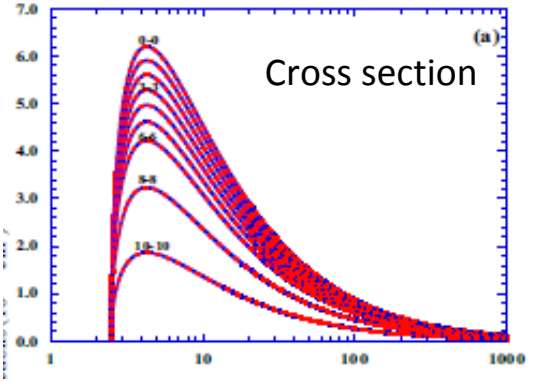
R Celiberto, R K Janev, D Reiter, Plasma Phys. Control. Fusion **54** (2012) 035012

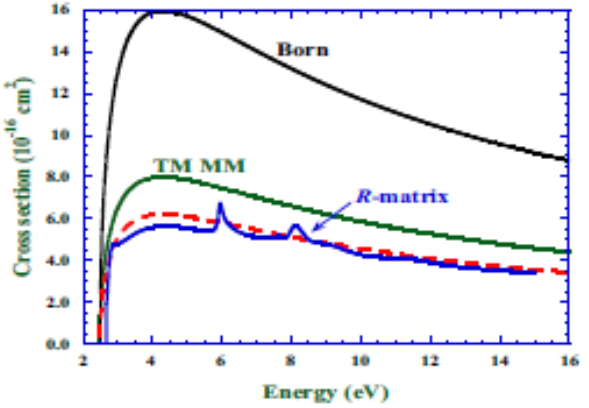
Coulomb-Born approximation: cross sections, excitation rates T=0.1-10,000 eV)

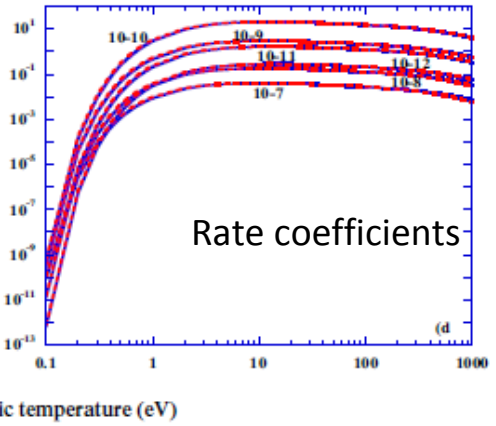
BeH: electronic and vibrational excitation

$X\,^2\Sigma^+ (v=0) \longrightarrow A\,^2\Pi (v')$





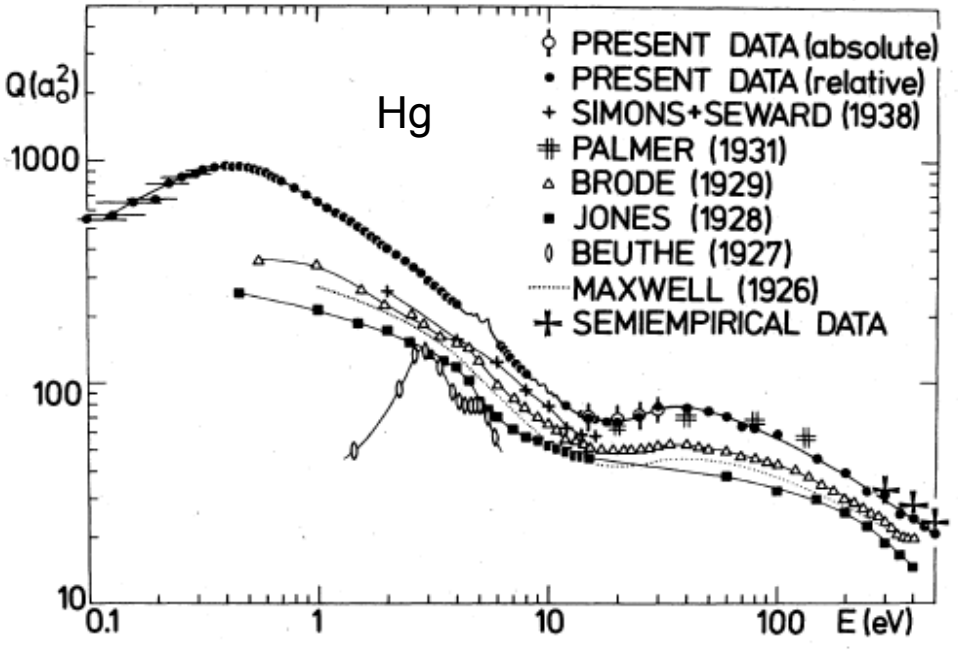


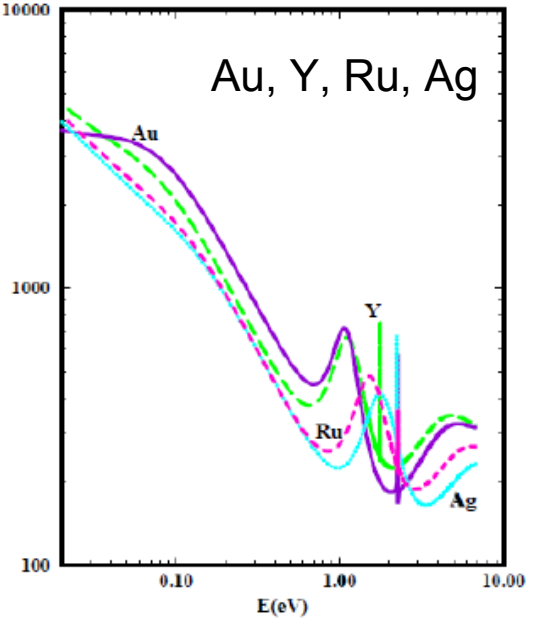


R Celiberto, K L Baluja and R K Janev, Plasma Sources Sci. Technol. **22** (2013) 015008

Mott-Massey Schr. eq.

Metals: Hg, Au, Ru



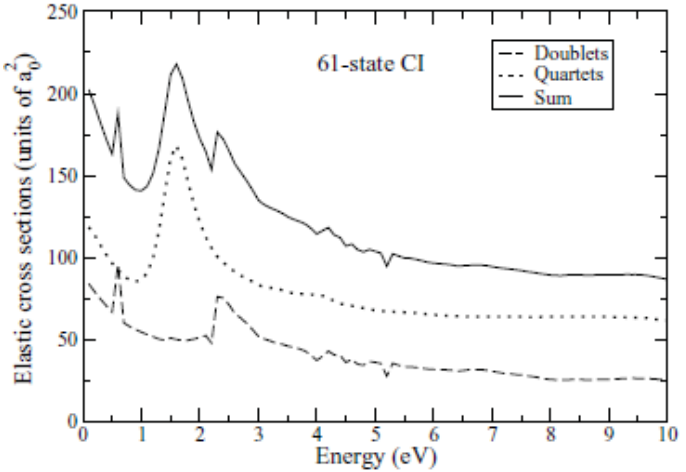


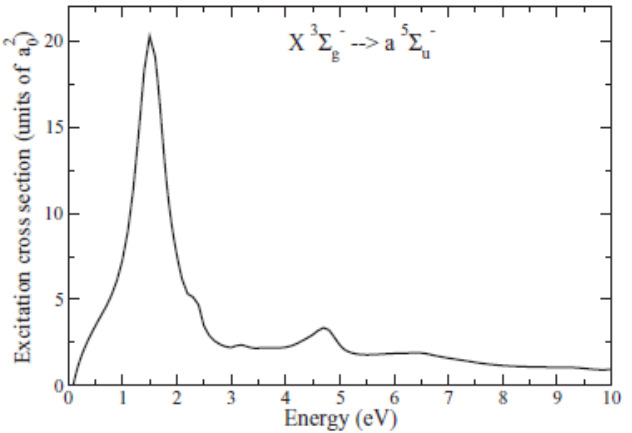
ure 1 Electron elastic TCSs for Au, Y, Ru and
in the region of negative ion formation

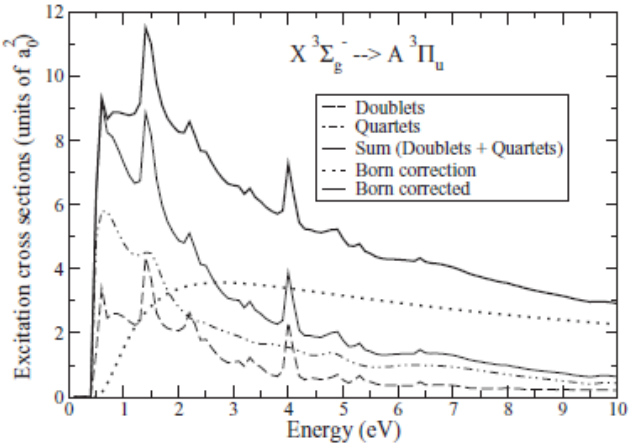
K. Jost and B. Ohnemus, Phys. Rev. A **19** (1979) 641

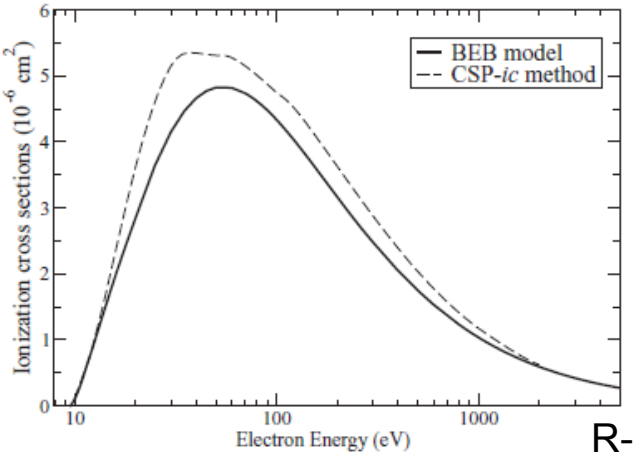
A. Z. Msezane, Z. Felfli, D Sokolovski
J. Phys.: Conf Series, **388** (2012) 042002
Thomas-Fermi potential

Metal molecules (B_2): electronic excitation









R-Matrix

Conclusions – state of art

1. Total cross sections (for “easy” molecules) OK
2. Elastic (and therefore total also): theory OK
3. Vibrational: theory on a promising way
4. Ionization: abundant data and models
5. Dissociative attachment (and dissociative neutralization) – theory proves OK, work needed
6. Electronic excitation (and dissociation) – remains most challenging

Conclusions (2) - perspectives:

1. „Physical” cross sections still needed
2. „Chemical” cross sections even more
3. Reviews for new targets: Be, BeH_2, W ?
4. Simple theories and scalling laws useful
5. Advanced theories „at reach”
6. Lab experiments still needed
7. and ITER-like experiment even more

→ **constructing cooperative networks**

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Data Center for Plasma Properties