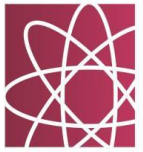


Laboratory for Atomic Collision Processes

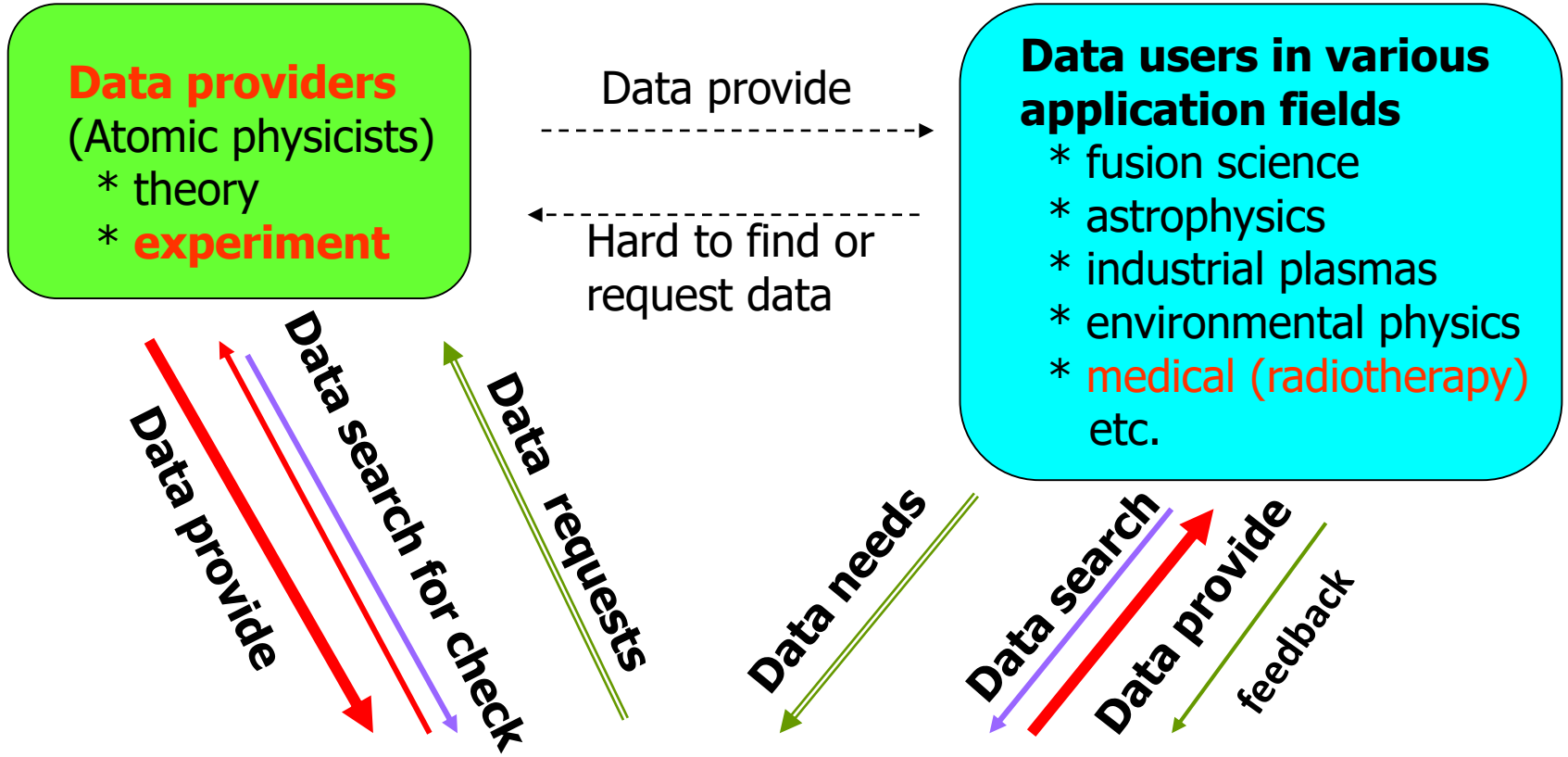
Elastic electron scattering by atomic particles and cross section representation in the **B**elgrade **E**lectron-**A**tom/**M**olecule **D**ata**B**ase -BEAMDB

Bratislav Marinković

Institute of Physics Belgrade

IAEA Tech.meeting, 27.11.2019

Views from Database *assessed data on electron collision cross sections*



Data centers
data compilation
data evaluation (important but not easy)
dissemination and updating of database
retrievable online database
= easy to access, use, find data

International A&M data center network
IAEA, NIFS, A-PAN, KAERI, NIST, ORNL, GAPHIOR, VAMDC, etc.

By courtesy of Prof. Hiroshi Tanaka

The parameters which characterize collision processes are the cross sections. Electron collision cross sections depend on impact energy *E*o and scattering polar angles ϑ and φ. The differential cross section, for a specific well-defined excitation process indicated by the index *n* is defined as:

$$\frac{d\sigma_n(E_o\Omega)}{d\Omega} = \frac{k_f}{k_i}|f_n(E_o\Omega)|^2$$

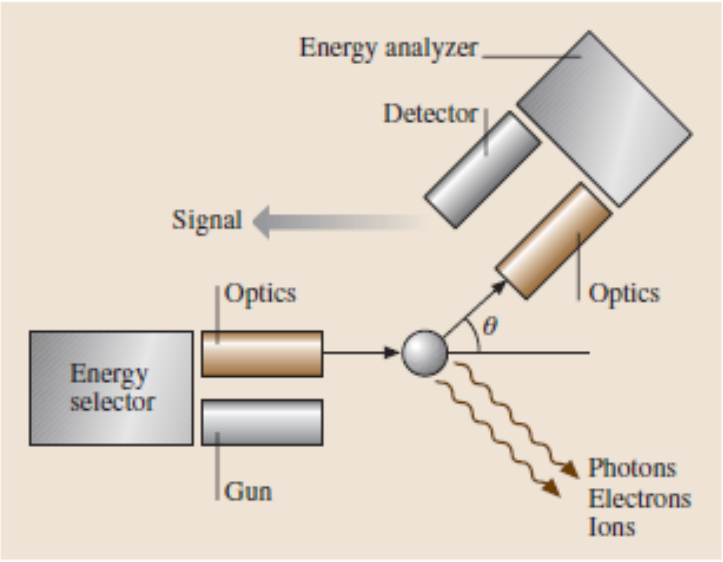
where Ω is the polar angle of detection, *ki* and *kf* are the initial and final electron momenta, and *fn* is the complex scattering amplitude (*n* = 0 refers to elastic scattering).

Integration over all scattering angles yields the integral and momentum transfer cross sections:

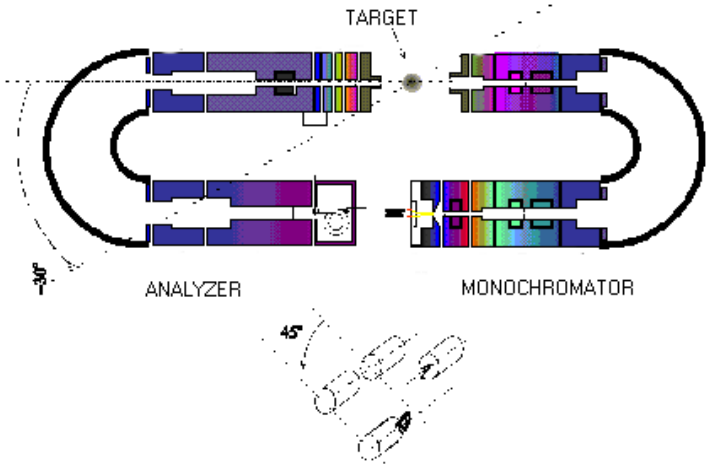
$$\sigma_n(E_0) = \int_0^{2\pi}\int_0^{\pi} \frac{\mathrm{d}\sigma_n(E_0, \Omega)}{\mathrm{d}\Omega} \sin\theta \, \mathrm{d}\theta \, \mathrm{d}\phi$$

$$\sigma_0^{\mathrm{M}}(E_0) = \int_0^{2\pi}\int_0^{\pi} \frac{\mathrm{d}\sigma_0(E_0, \Omega)}{\mathrm{d}\Omega}(1-\cos\theta) \sin\theta \, \mathrm{d}\theta \, \mathrm{d}\phi$$

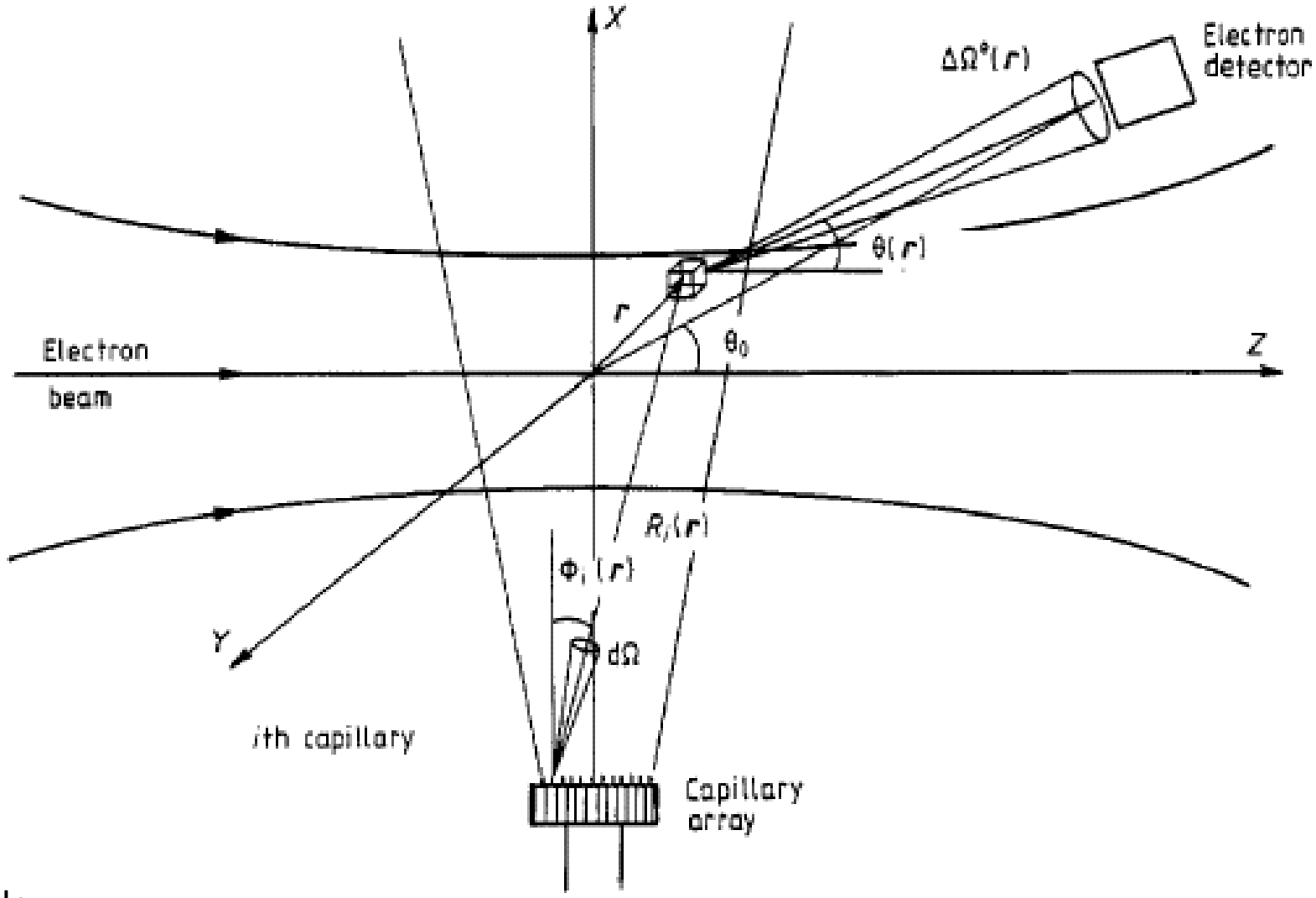
Effective interaction volume



Springer Handbook of Atomic, Molecular, and Optical Physics
Gordon W. F. Drake (Ed.)



Electron spectrometer ESMA at IP Belgrade
Panajotović et al. *IJMS,* **233** (2004) 253-257



Brinkmann and Trajmar, *J.Phys.E* **14** (1981) 245-255

UNITS

$$\frac{m^2}{sr}\P$$

$$m^2/sr\P$$

m2/sr¶

m^2/sr¶

m^{2}sr^{-1}¶

Intensity measurements and DCS

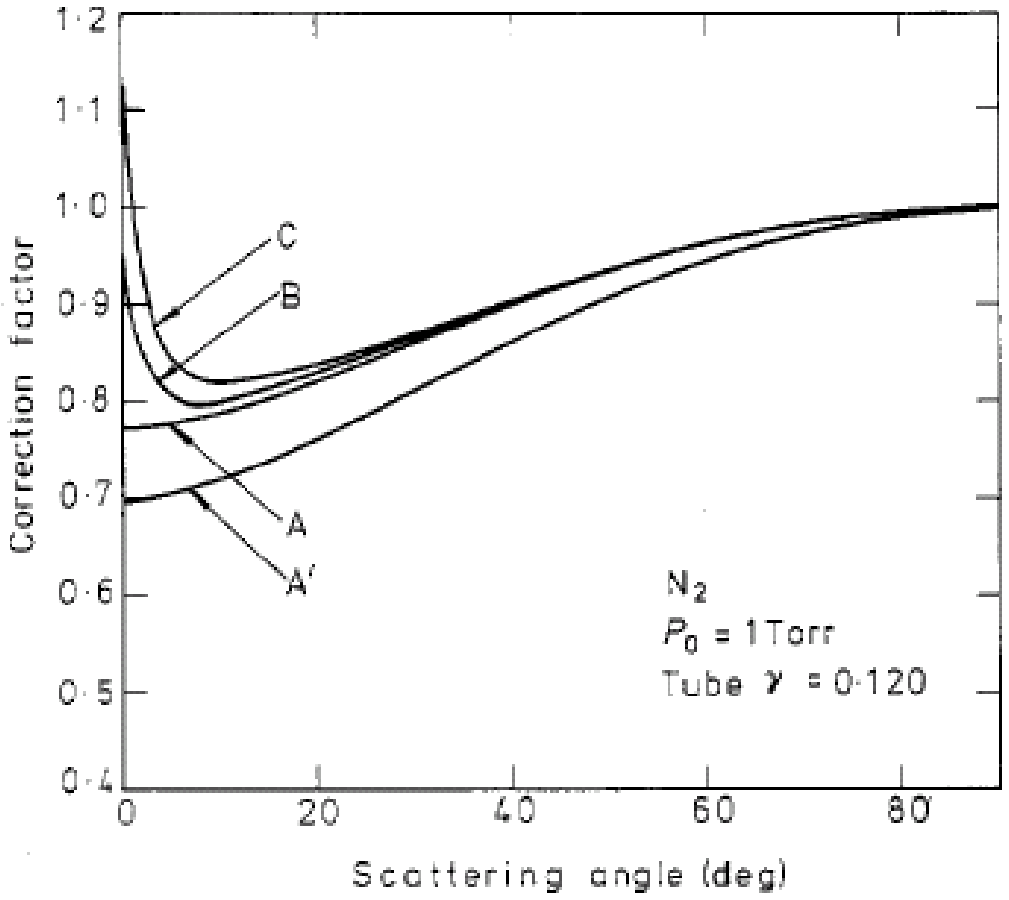
- $I(E_o,\vartheta)=\mathrm{DCS}(E_o,\vartheta)\eta(E_o)V_{eff}(\vartheta)$

Where are: DCS – differential cross section at the nominal angle and scattering angle averaged over the incident electron energy distribution and the detector energy and angle distributions, η – response function of the detector detecting electrons of the energy E_o, V_{eff} – effective scattering volume:

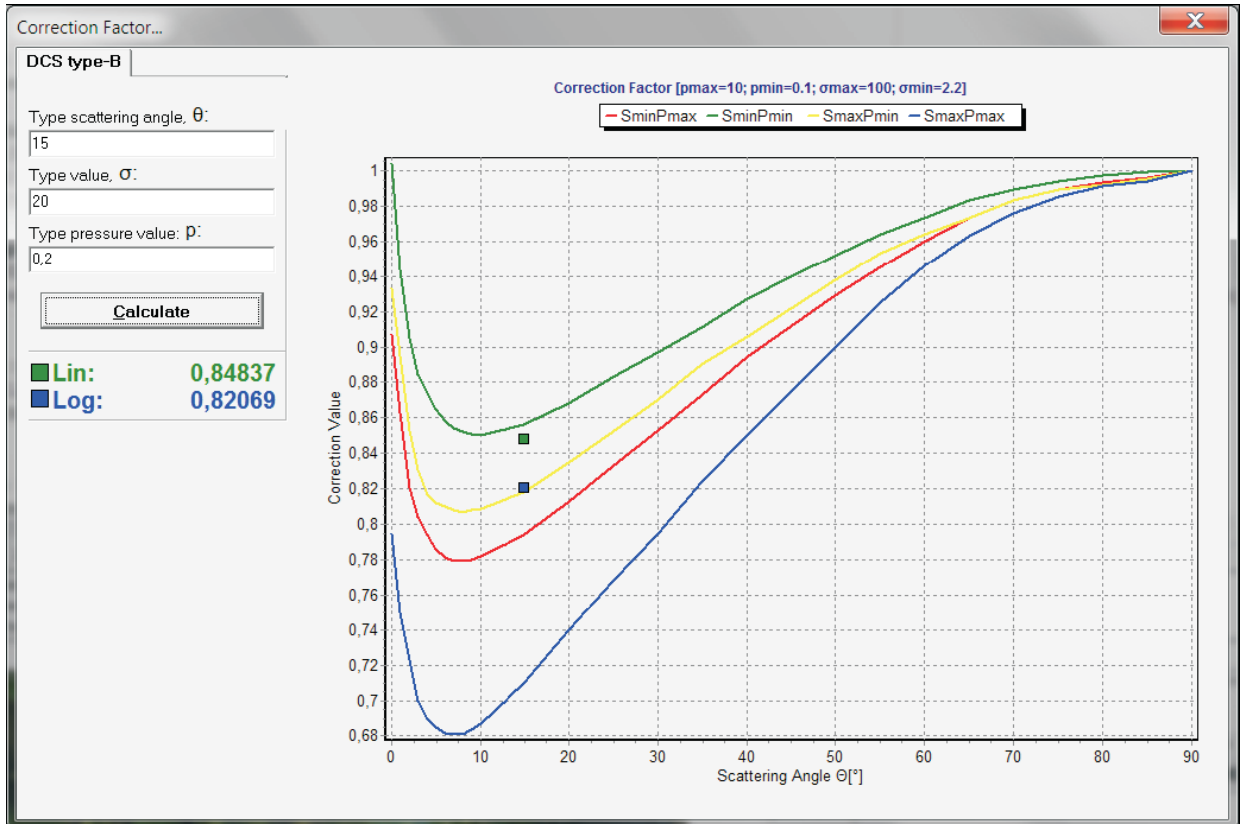
- $V_{eff}(\vartheta)=\int_r \rho(r)f(r)\Delta\Omega(r)G[\vartheta(r)]\mathrm{d}r$

Where are: $\rho(r)$ – the spatial distribution of the target beam, $f(r)$ – the spatial distribution function of the incident electron flux, $\Delta\Omega(r)$ – the solid angle subtended by the electron detector at the scattering point r, $G[\vartheta(r)]$ – the assumed angular dependence in the region of interest.

Effective Path Length Correction

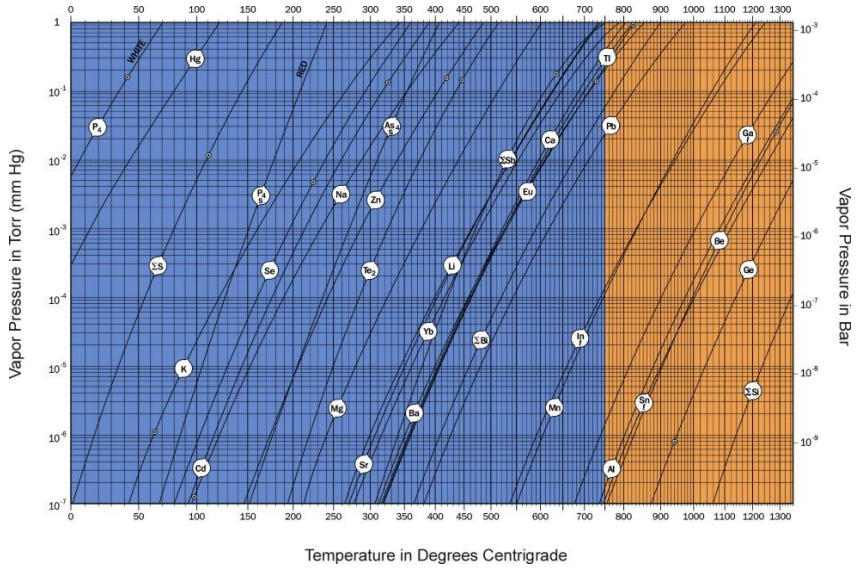


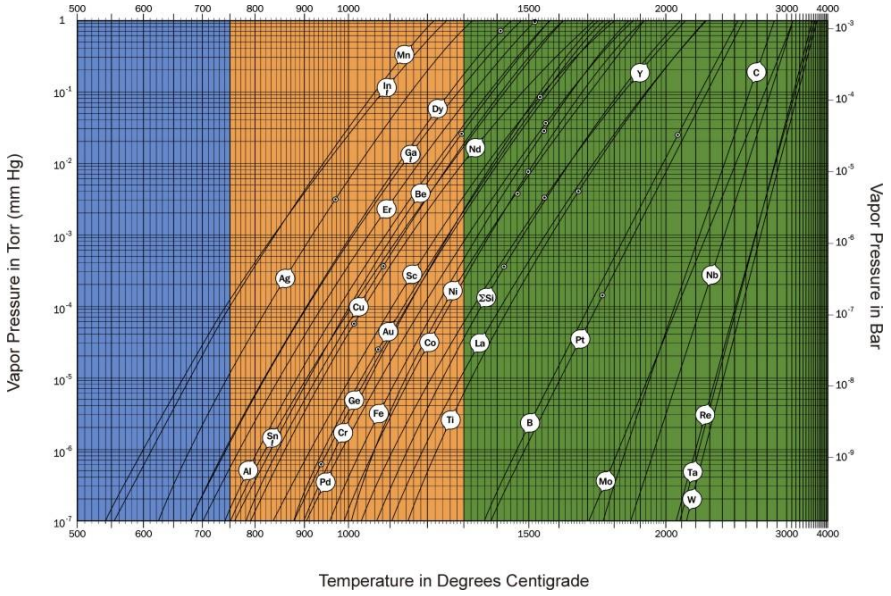
R. Brinkmann and S. Trajmar 1981 *J.Phys.E: Sci. Instrum.* **14** 245



User-friendly software for resolving some of the parameters in electron spectrometry experiments: scattering volume correction factor

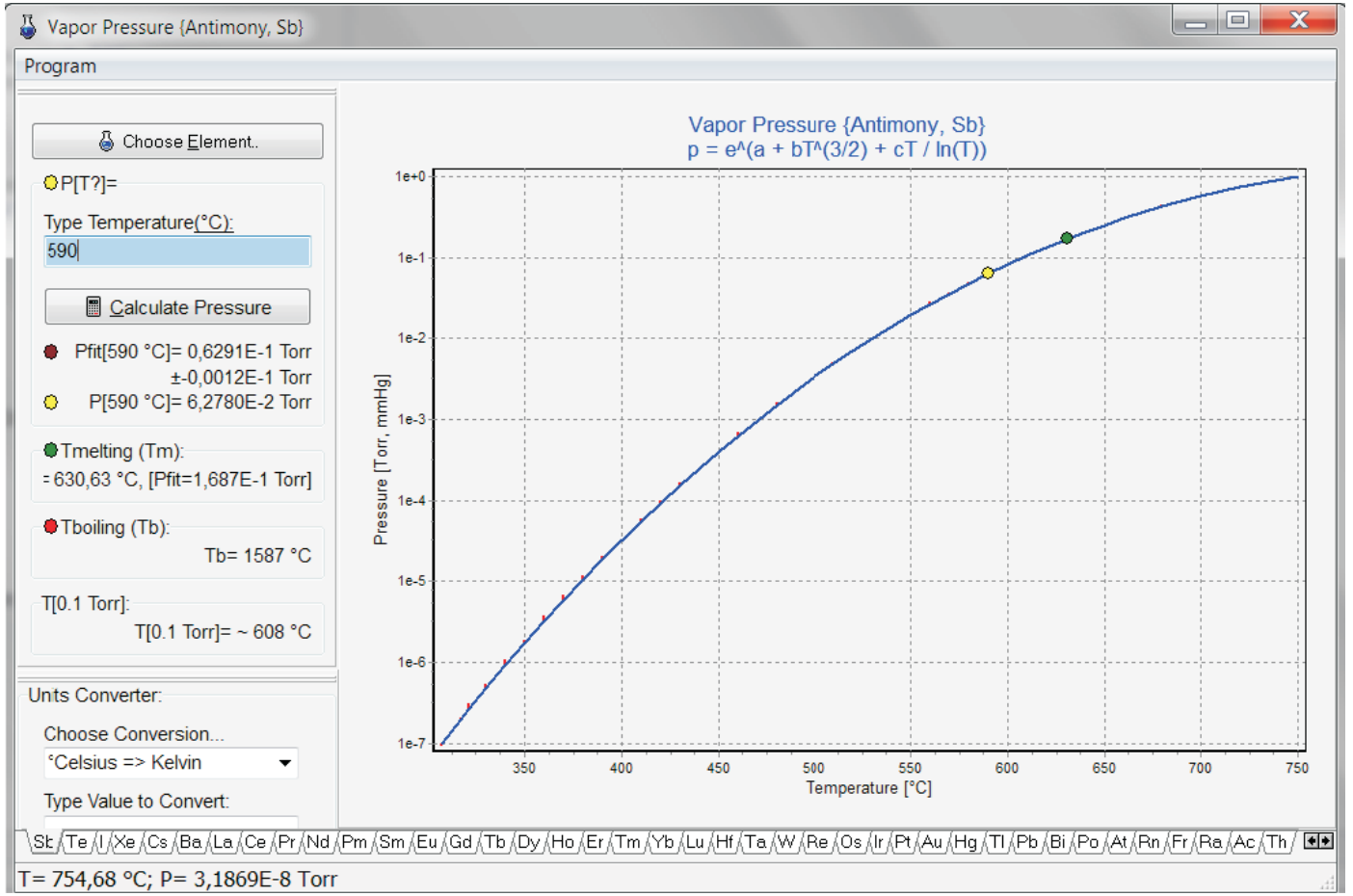
NIST data tables



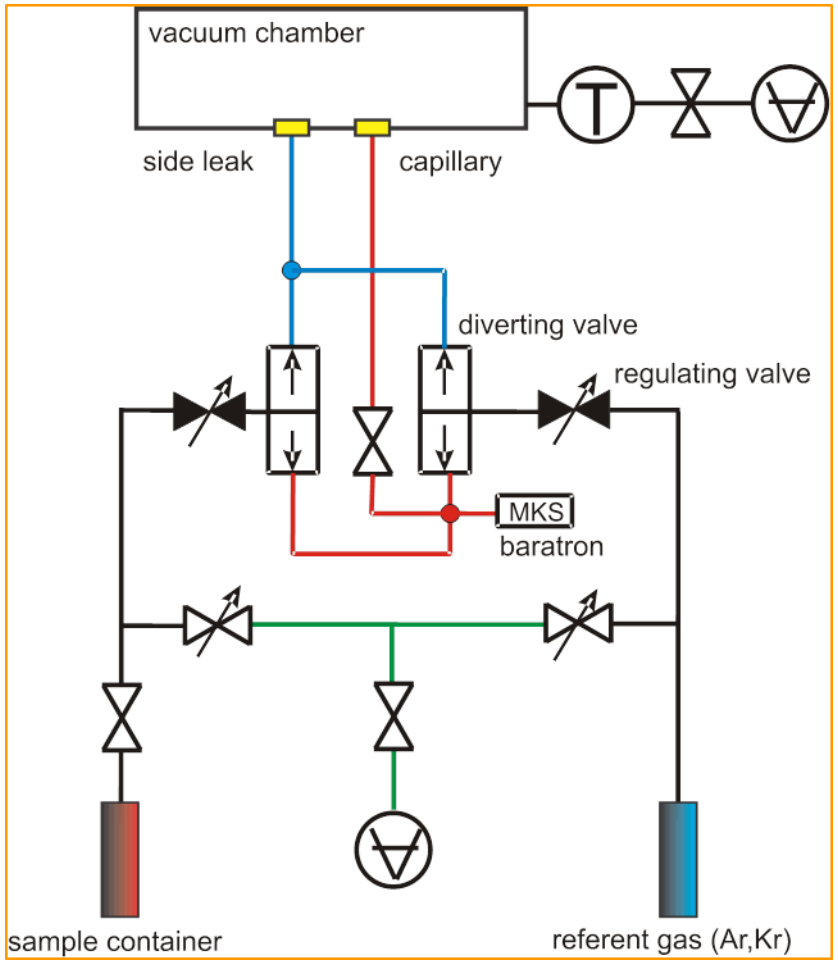


User-friendly software for resolving some of the parameters in electron spectrometry experiments: scattering volume correction factor and

metal vapour pressure curves



Relative flow technique - measuring absolute DCSs



- In the relative flow method, the DCSs for scattering of unknown gas is determined by comparing scattering signals from the standard target with its known differential cross sections, at a given incident electron energy and scattering angle under identical collision geometry conditions

- To obtain the same profiles for both gas beams, the gases must be operated at pressures behind the needle so that their mean free paths are the same.

$$DCSx(E,\theta) = DCSref(E,\theta)\frac{NxFref}{NrefFx}\sqrt{\frac{Mref}{Mx}}$$

$$PV_0 = nkT_0$$

$$\frac{dP}{dt} = \frac{kT_0}{V_0}\frac{dn}{dt} = cF$$

- S. K. Srivastava, Chutjian A and Trajmar S J. Chem. Phys. 63 2659 (1975)
- J. C. Nickel, J.Phys.B: at. Mol. Opt. Phys. 21,1867 (1988)
  M. Rankovic et al. EPJD 72, 30 (2018)

Normalization of DCS

- $f(K,E_o)=\omega/2\cdot k_i/k_f\cdot K^2\cdot DCS(E_o,\vartheta)$

Where are: $f(K,E_o)$ – generalized oscillator strength k_i and k_f - incident and final electron momenta, K^2 – momentum transfer, ω – excitation energy

$$K^2=2E\,[2-\omega/E_o-2(1-\omega/E_o)^{1/2}\cos(\vartheta)]$$

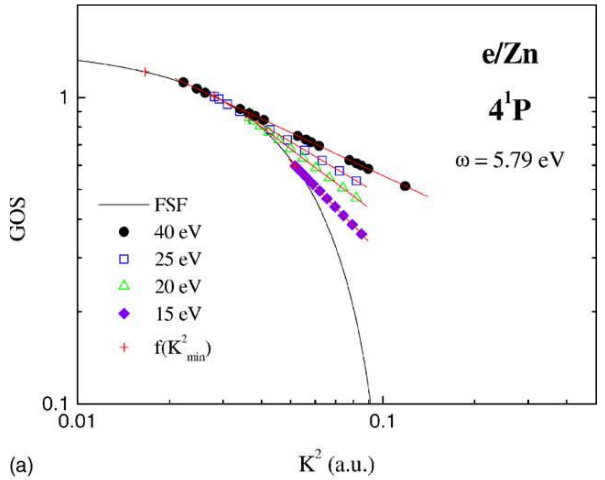
- ***E. Lassettre*** – (1959) extrapolation procedure

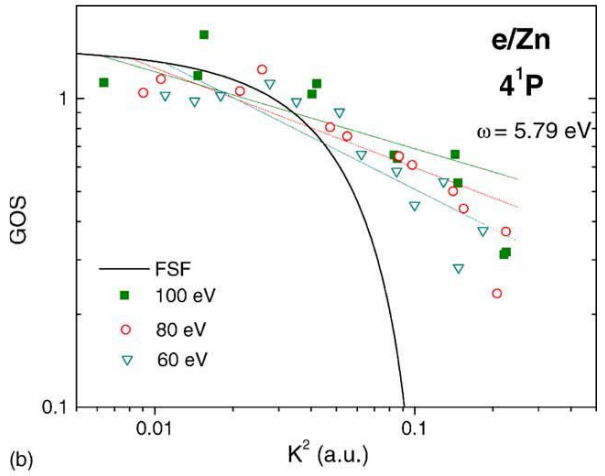
$$\lim f = \text{OOS} \text{ as } K^2\to 0$$

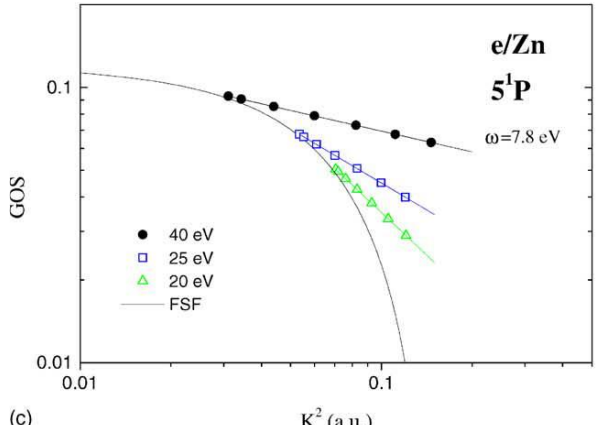
- $\text{FSF}= \text{OOS}(1-x/x_{max})\exp[-(x/x_{max})^2]$

Where are: $x = K^2/2\omega$ and $x_{max}=0.25$ as defined in

Avdonoina *et al. J.Phys.B* **30** (1997) 2591.



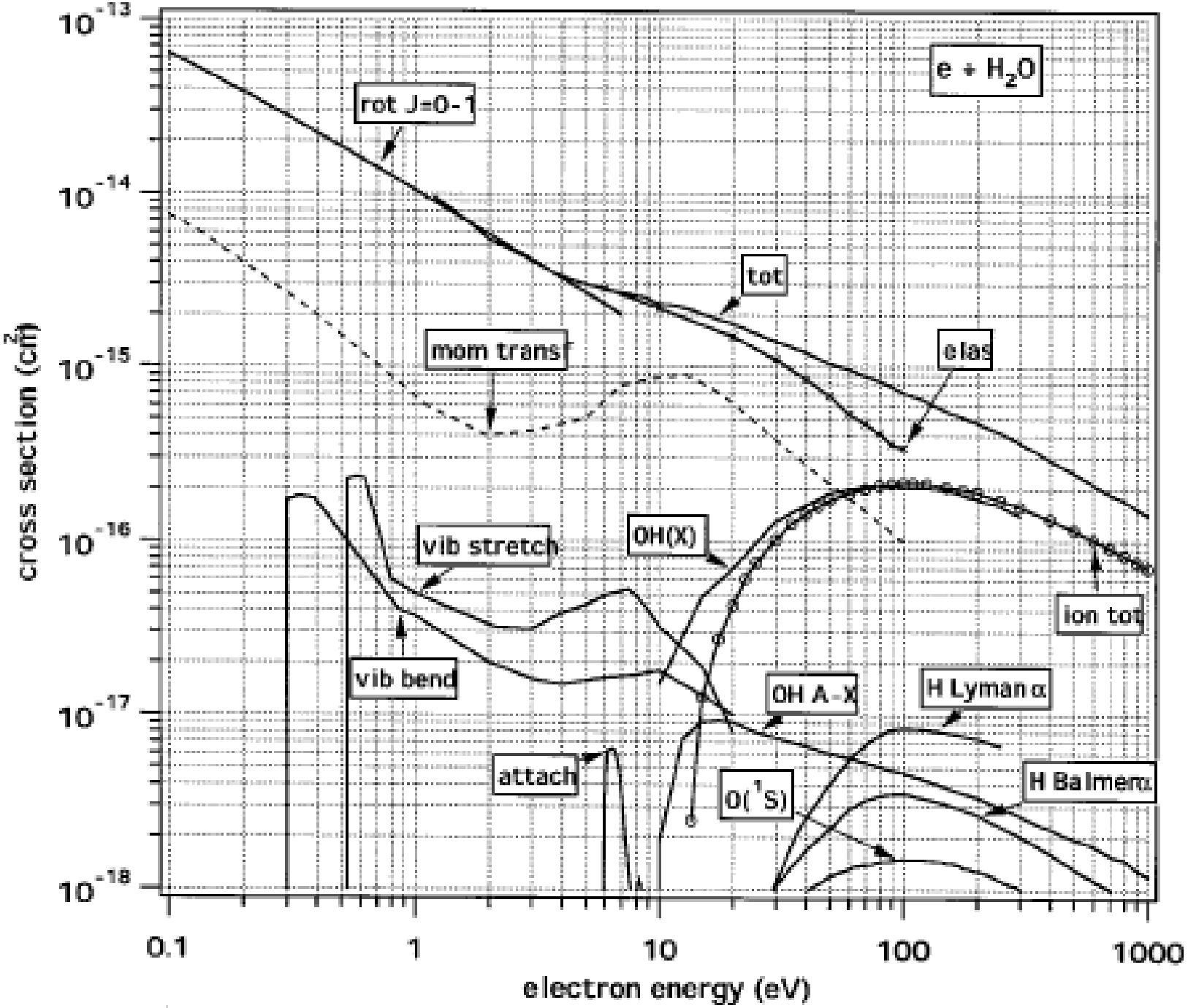




R. Panajotović, D. Ševic, V. Pejčev, D.M. Filipovic, B.P. Marinković, "The $^1S–^1P$ electron excitations of Zn at small scattering angles" *Int. J. of Mass Spectrom*. **233** (2004) 253–257

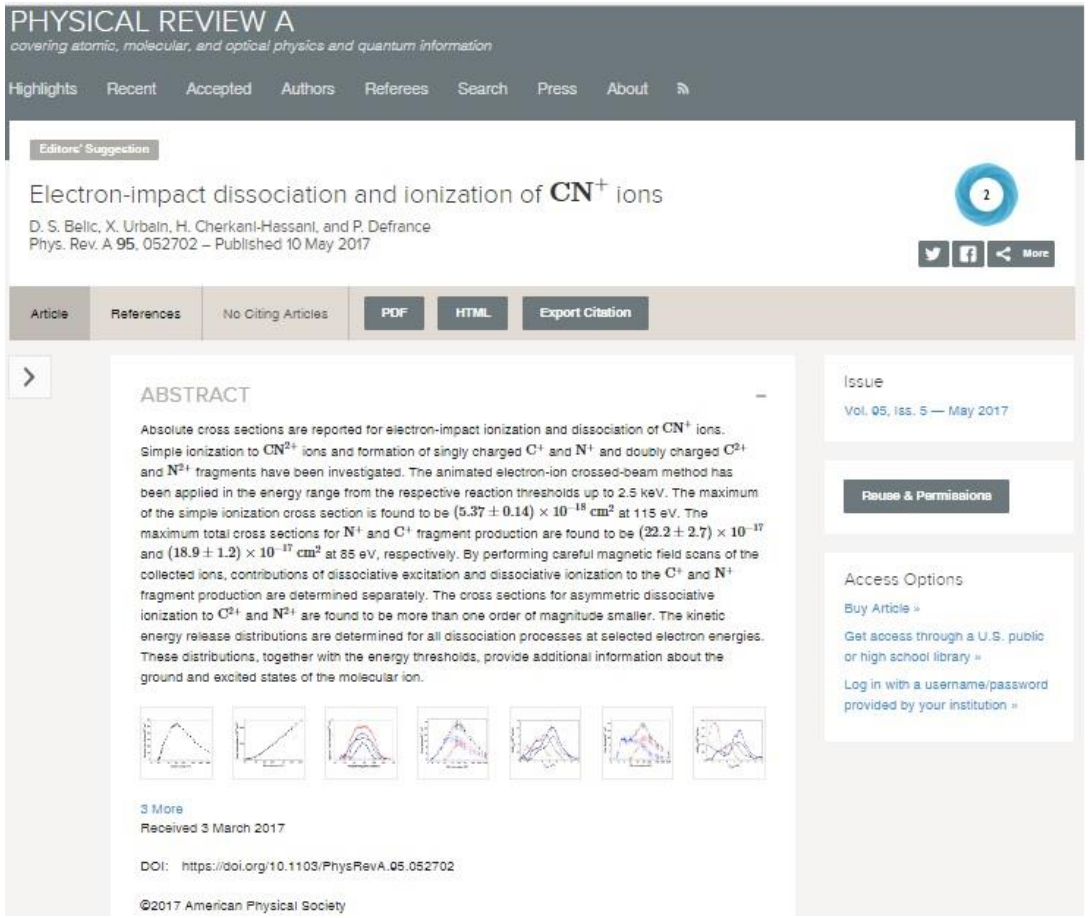
e/H_2O

Summary of the recommended electron collision cross sections for H2O. Cross sections smaller than 10E-18 cm^2 are not shown.



Itikawa and Mason, J. Phys. Chem. Ref. Data, **34**, (2005) 1-22.

e/CN^+ Belić et al. PRA **95**, 052702 (2017).



PHYSICAL REVIEW A

covering atomic, molecular, and optical physics and quantum information

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Editors' Suggestion

Electron-impact dissociation and ionization of CN^+ ions

D. S. Belic, X. Urbain, H. Cherkani-Hassani, and P. Defrance
Phys. Rev. A 95, 052702 – Published 10 May 2017

Article References No Citing Articles PDF HTML Export Citation

ABSTRACT

Absolute cross sections are reported for electron-impact ionization and dissociation of CN^+ ions. Simple ionization to CN^{2+} ions and formation of singly charged C^+ and N^+ and doubly charged C^{2+} and N^{2+} fragments have been investigated. The animated electron-ion crossed-beam method has been applied in the energy range from the respective reaction thresholds up to 2.5 keV. The maximum of the simple ionization cross section is found to be $(5.37 \pm 0.14) \times 10^{-18}$ cm^2 at 115 eV. The maximum total cross sections for N^+ and C^+ fragment production are found to be $(22.2 \pm 2.7) \times 10^{-17}$ and $(18.9 \pm 1.2) \times 10^{-17}$ cm^2 at 85 eV, respectively. By performing careful magnetic field scans of the collected ions, contributions of dissociative excitation and dissociative ionization to the C^+ and N^+ fragment production are determined separately. The cross sections for asymmetric dissociative ionization to C^{2+} and N^{2+} are found to be more than one order of magnitude smaller. The kinetic energy release distributions are determined for all dissociation processes at selected electron energies. These distributions, together with the energy thresholds, provide additional information about the ground and excited states of the molecular ion.

3 More

Received 3 March 2017

DOI: https://doi.org/10.1103/PhysRevA.95.052702

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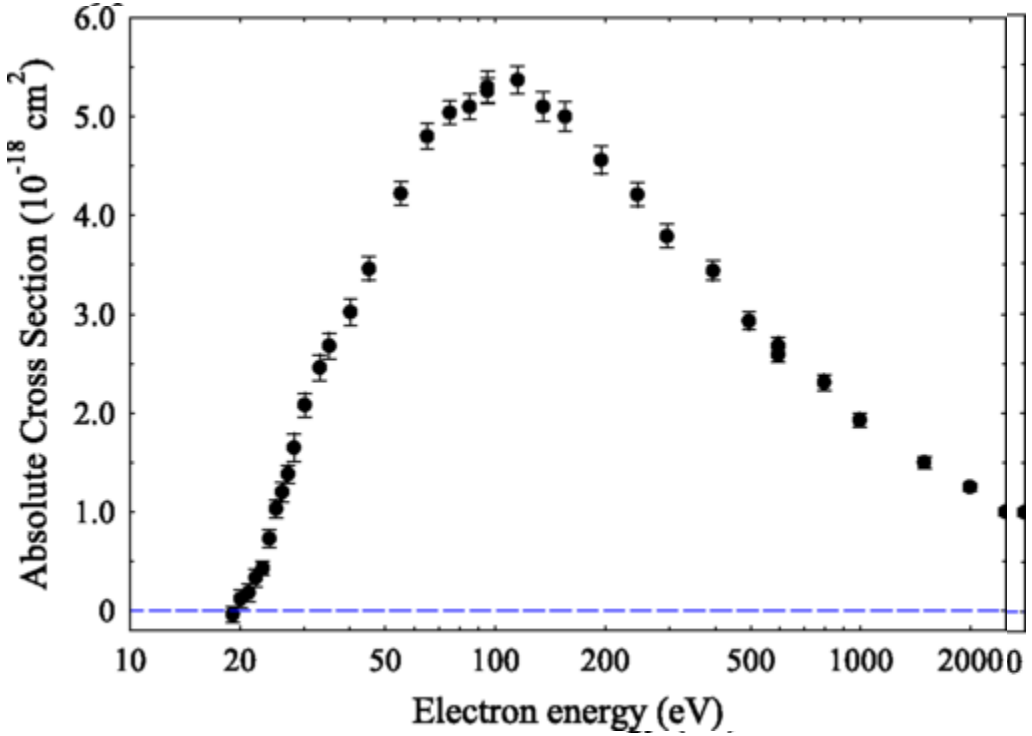
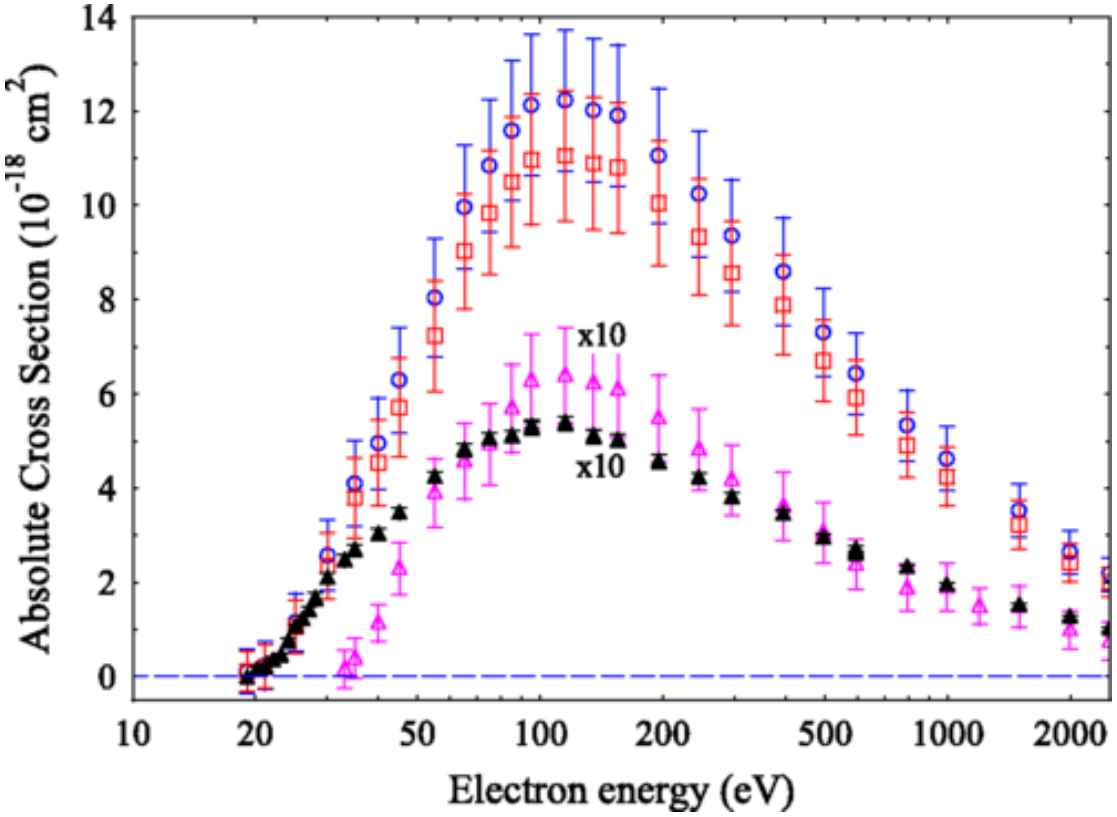
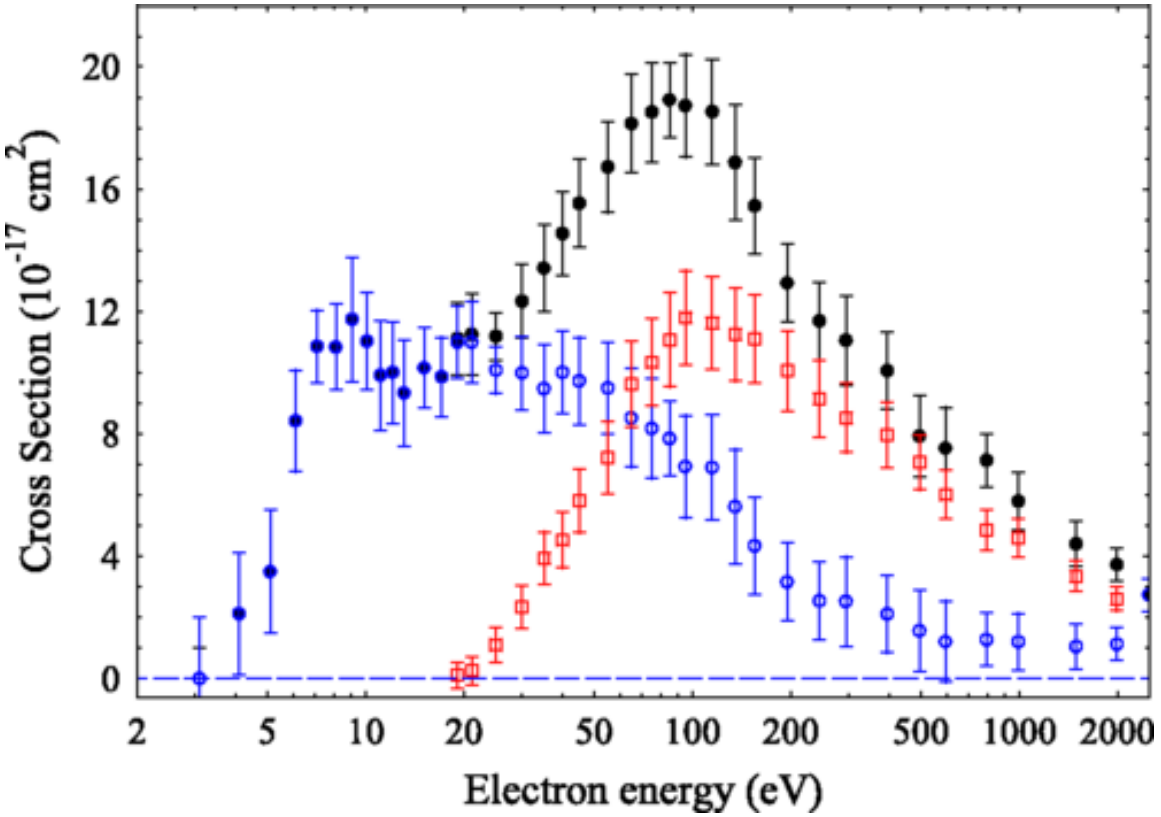


Absolute cross sections for electron-impact simple ionization of CN^+

e/CN^+ Belić et al. PRA **95**, 052702 (2017).



Absolute cross sections for CN^+ fragment production versus electron energy: total cross sections (solid circles), dissociative excitation contribution (open circles), and dissociative ionization (squares)



Absolute cross sections for C^+ fragment production versus electron energy: total cross sections (solid circles), dissociative excitation contribution (open circles), and dissociative ionization (squares)

LCAP@IPB e/Mol database - BEAMDB

B.P. Marinković *et al*. *NIMB* **354** (2015) 90-95; M L Dubernet *et al*. *J.Phys.B* **49** (2016) 074003;
B.P. Marinković *et al*. *EPJD* **71** (2017) 158; B.P. Marinković *et al*. *Atoms* **7** (2019) 11.

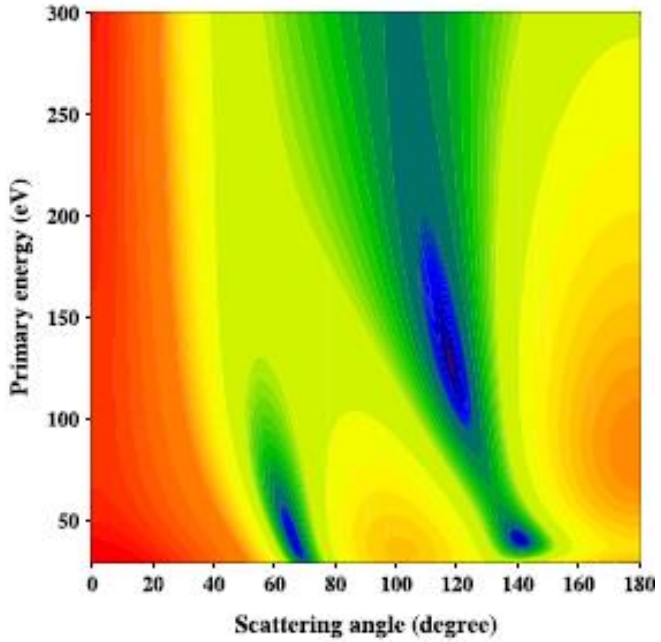
IPB : BEAMDB & MoID

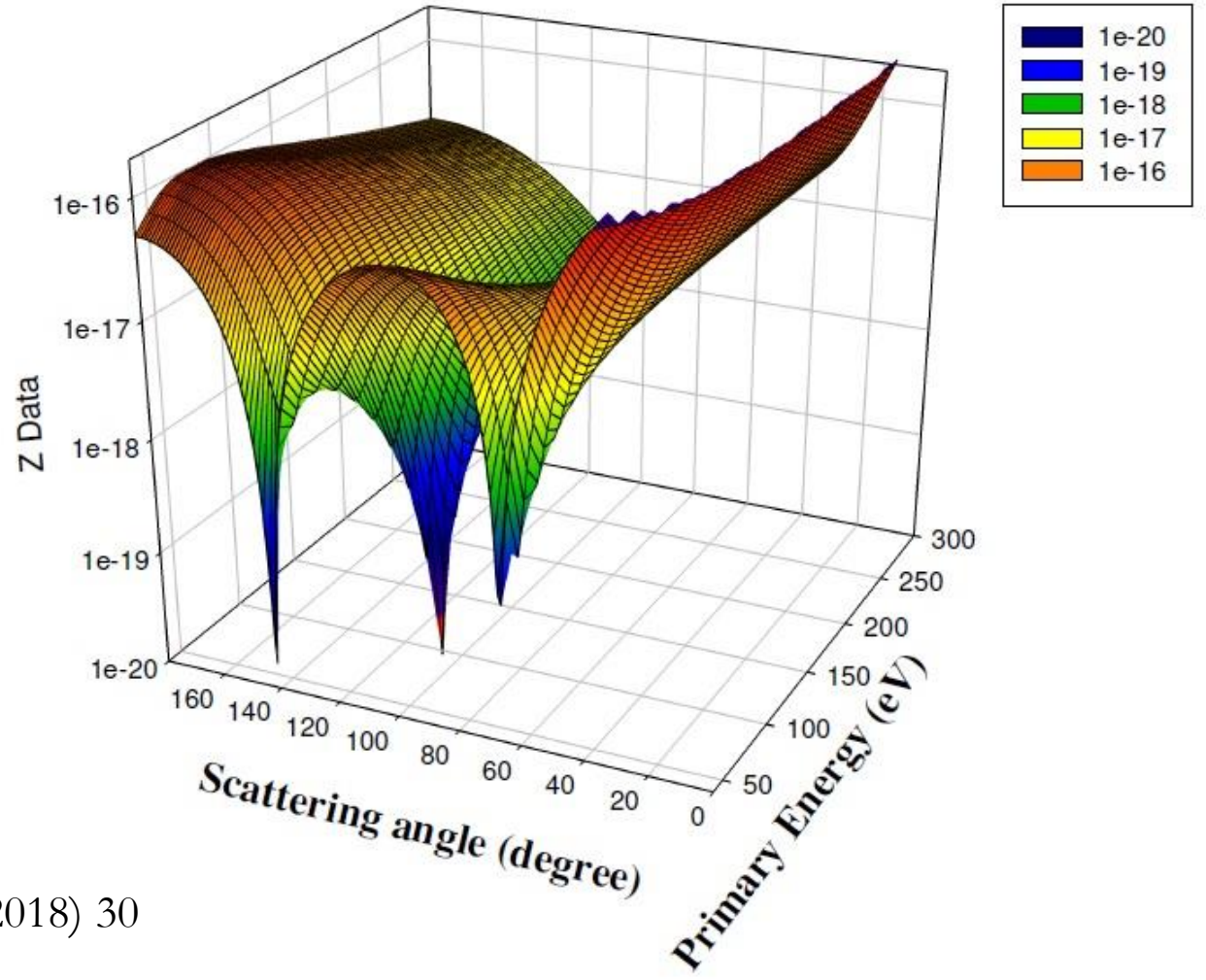
Species	InChI	States	Node
Ag	1S/Ag	2	BEAMDB
Ar	1S/Ar	1	BEAMDB
Ca	1S/Ca	1	BEAMDB
Cd	1S/Cd	1	BEAMDB
Hg	1S/Hg	5	BEAMDB
Kr	1S/Kr	3	BEAMDB
Mg	1S/Mg	3	BEAMDB
Na	1S/Na	1	BEAMDB
Yb	1S/Yb	1	BEAMDB
He_2^+	1S/He2/c1-2/q+1	834	MolD
H_2^+	1S/H2/h1H/q+1	424	MolD
LiH^+	1S/Li.H/q+1	60	MolD
MgH^+	1S/Mg.H/q+1	600	MolD
NaH^+	1S/Na.H/q+1	50	MolD
C2H5NO N-methylformamide	1S/C2H5NO/c1-3-2-4/h2H,1H3,(H,3,4)	3	BEAMDB
C3H7NO2 alanine	1S/C3H7NO2/c1-2(4)3(5)6/h2H,4H2,1H3,(H,5,6)/t2-/m1/s1	2	BEAMDB
C4H4N2 pyrimidine	1S/C4H4N2/c1-2-5-4-6-3-1/h1-4H	1	BEAMDB
C4H4O furan	1S/C4H4O/c1-2-4-5-3-1/h1-4H	1	BEAMDB
C4H8O tetrahydrofuran	1S/C4H8O/c1-2-4-5-3-1/h1-4H2	1	BEAMDB
CH3NO formamide	1S/CH3NO/c2-1-3/h1H,(H2,2,3)	1	BEAMDB
H2O water	1S/H2O/h1H2	4	BEAMDB
NNO Nitrous oxide	1S/N2O/c1-2-3	4	BEAMDB

https://portal.vamdc.eu/vamdc_portal/nodes.seam
https://species.vamdc.eu/

LCAP@IPB e/Mol database - BEAMDB

- Elastic el. scatt.
- DCS(E_o,θ) surface

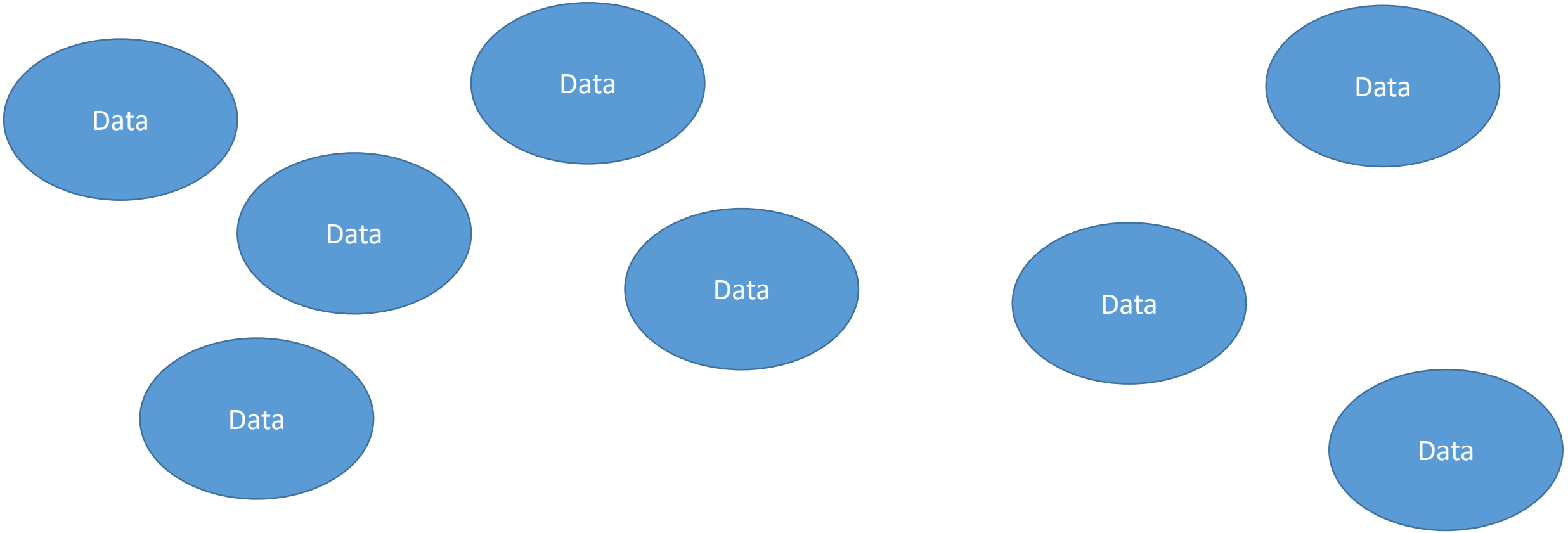




M. Rankovic *et al. EPJD* **72** (2018) 30

Conclusions

- Electron and particle scattering data (not only photo-processes data) are needed to better understand processes in astrophysical observations;
- VAMDC as a distributed databases with a common portal is a powerful aid;
- Settling the *Information System* in a specific field of research (like the field of Atomic Collision Physics) could be very useful for each Lab or research group;
- Need for improved accuracy of cross section measurements and smaller uncertainties – consistency of data:
- Still we need refinements in theoretical approaches to the electron scattering problem;
- Work with more complex systems (larger biomolecules, molecules being precursors for FEBID-focused electron beam induced deposition, radio-sensitizers, drugs, chelators, bio-chemically active compounds…) is challenging task ahead;
- Urgent need for settling the panel for critical assessment of e/Mol data and normalization procedures!



DATA REPOSITORY submissions welcome