Elastic electron scattering by atomic particles and cross section representation in the Belgrade Electron-Atom/Molecule Database - BEAMDB

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IAEA Tech.meeting, 27.11.2019
**Data providers**
(Atomic physicists)
* theory
* experiment

**Data users in various application fields**
* fusion science
* astrophysics
* industrial plasmas
* environmental physics
* medical (radiotherapy) etc.

**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.

Views from Database assessed data on electron collision cross sections

By courtesy of Prof. Hiroshi Tanaka
The parameters which characterize collision processes are the cross sections. Electron collision cross sections depend on impact energy $E_0$ and scattering polar angles $\vartheta$ and $\varphi$. The differential cross section, for a specific well-defined excitation process indicated by the index $n$ is defined as:

$$\frac{d\sigma_n(E_0 \Omega)}{d\Omega} = \frac{k_f}{k_i} |f_n(E_0 \Omega)|^2$$

where $\Omega$ is the polar angle of detection, $k_i$ and $k_f$ are the initial and final electron momenta, and $f_n$ is the complex scattering amplitude ($n = 0$ refers to elastic scattering).

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

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

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

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

Electron spectrometer ESMA at IP Belgrade

UNITS

\frac{m^2}{sr}

m^2/sr

m^2/sr

m^2/sr

m^{(2)}s^{(-1)}
Intensity measurements and DCS

\[ I(E_0, \theta) = \text{DCS}(E_0, \theta) \eta (E_0) V_{\text{eff}}(\theta) \]

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, \( \eta \) – response function of the detector detecting electrons of the energy \( E_0 \), \( V_{\text{eff}} \) – effective scattering volume:

\[ V_{\text{eff}}(\theta) = \int r \rho(r) f(r) \Delta \Omega(r) G[\theta(r)] \, dr \]

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 \( r \), \( G[\theta(r)] \) – the assumed angular dependence in the region of interest.
Effective Path Length Correction

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

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.

\[
DCS_x(E, \theta) = DCS_{\text{ref}}(E, \theta) \frac{N_x F_x}{N_{\text{ref}} F_{\text{ref}}} \frac{M_{\text{ref}}}{M_x}
\]

\[
PV_0 = nkT_0
\]

\[
\frac{dP}{dt} = \frac{kT_0}{V_0} \frac{dn}{dt} = cF
\]
Normalization of DCS

• \( f(K,E_o) = \omega/2 \cdot k_i/k_f \cdot K^2 \cdot \text{DCS}(E_o, \Theta) \)

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

\[
K^2 = 2 \cdot E \left[ 2 - \omega/E_o - 2 \left( 1 - \frac{\omega}{E_o} \right)^{1/2} \cos(\Theta) \right]
\]

• **E. Lassettre** – (1959) extrapolation procedure
  \[ \lim f = \text{OOS as } K^2 \to 0 \]

• FSF = 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


Summary of the recommended electron collision cross sections for H2O. Cross sections smaller than 10E-18 cm² are not shown.

Absolute cross sections for electron-impact simple ionization of CN⁺
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
IPB : BEAMDB & MoID

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<tr>
<th>Species</th>
<th>InChI</th>
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<th>Node</th>
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<tr>
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<tr>
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<tr>
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<td>1S/C3H7NO2/c1-2(4)/3(5)/6/h2H,4H2,1H3,(H,5,6)/t2-/m1/s1</td>
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<tr>
<td>NNO Nitrous oxide</td>
<td>1S/N2O/c1-2-3</td>
<td>4</td>
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</table>

https://portal.vamdc.eu/vamdc_portal/nodes.seam
https://species.vamdc.eu/
LCAP@IPB e/Mol database - BEAMDB

- Elastic el. scatt.
- DCS($E_o, \theta$) surface
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