ELECTRON IMPACT ATOMIC-MOLECULAR COLLISION PROCESSES RELEVANT IN PLANETARY AND ASTROPHYSICAL SYSTEMS - A THEORETICAL STUDY

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Research Field: THEORETICAL ATOMIC & MOLECULAR PHYSICS
Research Topic: CROSS SECTIONS OF ATOMS, MOLECULES & CLUSTERS
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Outline of the Talk

- Why this work?
- Theoretical Methods Employed
  - SCOP & CSP-ic
    - Theory
    - Results
- Summary & Conclusion
- Merits & Demerits
Applications

- Electron is an effective source for ionization
- Applications of e-atom / molecule CS to,
  - Atmospheric Sciences (Ozone, Climate change etc.)
  - Astrochemistry (Auroral phenom., Electro Glow, UV emissions, etc)
  - Astrophysics (Comets, molecular processes in stellar formation, interpreting new spectral measurement, etc)
  - Plasma Physics (Plasma etching, Semiconductor Physics)
  - Understanding & modeling plasmas in fusion devices
  - In Bio-physics (medical science) etc, Radiation therapy.
Current scenario

- **Experimental methods**
  - Different research groups work on different regions of $E_i$
  - Problems of reactive targets, e.g. radicals (CH, NH, OH, NO etc)
  - Ionization measurements are generally uncertain by 10-15%
  - Neutral dissociation e.g. CH$_4$ fragmentation
    (experimental uncertainty 30 - 35% (Nakano et al. 1991))
  - Bio-molecular targets and condensed matter experiments

- **Accurate theoretical methods**
  - Slow calculations
  - Limitation to energy range
  - Limitation to targets

- **Need for simple, reliable and fast calculations**
Present Theoretical Method

Total elastic cross sections $Q_{el}$

Total inelastic cross sections $Q_{inel}$

Total (complete) cross sections $Q_T$

Total ionization cross sections $Q_{ion}$

Summed total excitation cross sections $\Sigma Q_{exc}$

Grand total cross section $Q_{TOT}$

Total non spherical cross sections $Q_{rot}$

Rate Coefficients, Macroscopic cross sections ($\Sigma_{inel}$, $\Sigma_{ion}$, $\Sigma_{el}$), Collision Frequency ($\nu$), Mean Free Path ($\Lambda_{el}$, $\Lambda_{inel}$, $\Lambda_{el}$).

Rotational cross sections Polar molecule e.g. H$_2$O

Present energy range $\rightarrow$ From ionization threshold to 2 keV
Spherical Complex Optical Potential (SCOP)

- **Spherical Complex Optical Potential**, \( V_{opt} = V_R + i V_I \)

- **Final Form of the Complex Optical Potential**

\[
V_{opt} = V_{st} + V_{ex} + V_{pol} + i V_{abs}
\]

Variable Phase Method

The PHASE EQUATION given by Calogero is of the form

\[
\delta'_l(kr) = -\frac{2}{k} V(r)[\cos \delta_l(r) \cdot \hat{j}_l(kr) - \sin \delta_l(r) \cdot \hat{n}_l(kr)]^2
\]

The function \(\delta_l(kr)\) is the phase function.

- It vanishes at the origin
- It yields asymptotically directly the value of scattering phase shift

Using Spherical Complex Optical Potential and complex phase shift,

\[
\delta_l(kr) = \delta_R(kr) + i \delta_I(kr) \quad \text{and} \quad V(r) = V_R(r) + i V_I(r)
\]

We get a set of first order coupled differential equations for real \((\delta_R)\) and imaginary \((\delta_I)\) parts of the complex phase shift function under the VPA.

\[
\delta_R'(kr) = -\frac{2}{k} [V_R(r) \cdot (X^2 - Y^2) + 2V_{abs}(r) \cdot XY]
\]

\[
\delta_I'(kr) = -\frac{2}{k} [-2V_R(r) \cdot XY + V_{abs}(r) \cdot (X^2 - Y^2)]
\]

**where**

\[
X = \cosh \delta_I(kr)[\cos \delta_R(kr) \cdot \hat{j}_l(kr) - \sin \delta_R(kr) \cdot \hat{\eta}_l(kr)]
\]

\[
Y = \sinh \delta_I(kr)[\sin \delta_R(kr) \cdot \hat{j}_l(kr) + \cos \delta_R(kr) \cdot \hat{\eta}_l(kr)]
\]

We solve these set of coupled equation by fourth order Runge Kutta - Method and obtain the complex phase shift.
For $l = 0$, at 100 eV
Scattering Calculations

- **Calculate the S - matrix**

\[ S_l(k) = \exp(-2\delta_l) \exp(i2\delta_R) \]

- **Finally the cross sections**

\[ Q_{inel} = \frac{\pi}{k^2} \sum_{l=0}^{l_{max}} (2l + 1) [1 - |S_l(k)|^2] \]

\[ Q_{el} = \frac{\pi}{k^2} \sum_{l=0}^{l_{max}} (2l + 1) |1 - S_l(k)|^2 \]

\[ Q_T = \frac{2\pi}{k^2} \sum_{l=0}^{l_{max}} (2l + 1) [1 - \Re S_l(k)] \]
Scattering Calculations continued...

The total (complete) cross section is given by

\[ Q_T(E_i) = Q_{el}(E_i) + Q_{inel}(E_i) \]

\[ Q_{inel}(E_i) = \sum Q_{ion}(A^{+n}) + \sum Q_{exc} \]

Where \( \Sigma Q_{ion}(E_i) = \) The total of all total ionization cross-sections for all energetically allowed states with \( A^{+n} \) as the charge state of the ion.

\( \Sigma Q_{exc}(E_i) = \) Summed total electronic excitation cross section

The quantity \( Q_{inel} \) is not measurable directly in experiments. \( Q_{el} \) is obtained by integrating measured elastic DCS. \( Q_T \) (or \( Q_{TOT} \) for polar molecules) is separately determined in total transmission experiments.
The Complex Scattering Potential-ionization contribution, CSP-ic method for $Q_{ion}$

The CSP-ic originates from the inequality,

$$Q_{inel}(E_i) \geq Q_{ion}(E_i)$$

The $Q_{inel}$ contains $Q_{ion}$, but how to extract it?

It is reasonable to define a ratio

$$R(E_i) = \frac{Q_{ion}(E_i)}{Q_{inel}(E_i)}$$

First ever estimate of ionization in relation to excitation processes was made by Turner et al for $e - H_2O$ scattering near 100 eV.

$$\frac{\sigma_{ion}}{(\sigma_{ion} + \sigma_{exc})} \approx 0.75$$

The ratio $R$ is proposed to be of the form, $1 - f(U)$

$$U = \frac{E_i}{I}$$

$\Rightarrow$ Target specific

$$f(U) = C_1 \left[ \frac{C_2}{U + a} + \frac{\ln U}{U} \right]$$

$$R(E_i) = 1 - C_1 \left[ \frac{C_2}{U + a} + \frac{\ln U}{U} \right]$$

Above ratio has three conditions to satisfy:

$$R(E_i) = \begin{cases} 
0, & \text{at } E_i \leq I \\
R_p, & \text{at } E_i = E_p \\
\sim 1, & \text{for } E_i \gg E_p
\end{cases}$$

This is the method of CSP-ic.

• At $E_p$, $R_p$ is found to be between 70 – 80 %.

• 80% observed in the case of higher IP like Ne (21.56 eV).

• Most of the target studied here have their IP varying from 9 - 15 eV.

• Thus we have selected the lower $R_p$ limit.

For polar targets we add rotational dipole cross sections (non-spherical contribution) to the $Q_T$ and calculate grand total cross section $Q_{TOT}$
**Targets studied in present work**

<table>
<thead>
<tr>
<th>Atoms</th>
<th>Atmospheric molecules</th>
<th>Radicals and parent molecules</th>
<th>Compounds of Silicon</th>
<th>Oxides of Sulfur</th>
<th>Exotic atomic-molecular systems</th>
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<tbody>
<tr>
<td>C</td>
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<td>SO</td>
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<td>SO₂ClF</td>
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<td>NF₁,NF₂</td>
<td>Si(CH₃)₄</td>
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<td>H₂O (Liquid)</td>
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<td>SF₃</td>
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<td>H₂O (Free)</td>
<td>SF₄</td>
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<td></td>
<td></td>
<td>SF₅</td>
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<td></td>
<td></td>
<td>SF₆</td>
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Results

e - H₂O

Q_{\text{ion}}

Present \Delta = IE

Present \Delta = IE+1

Kim

Starub

Prsent \Sigma Q_{\text{exc}}
The diagram shows the total cross sections for electron-NO$_2$ interactions as a function of electronic energy ($E_i$). The graph plots the cross sections in Angstrom$^2$ ($\AA^2$) on the y-axis against the electronic energy ($E_i$) in electron volts (eV) on the x-axis.

The different sets of data are represented by various symbols and lines:
- $Q_T$: Present
- $Q_{el}$: Present
- $Q_{ion}$: Present
- Zecca
- Szmytkowski
- Kim
- Lindsay
- Lopez
- Lukic

Each set of data is distinguished by a different color and symbol, allowing for a clear comparison of the cross sections across different models and data sets.
Summary & Conclusions

- The present calculations that the SCOP along with CSP-ic method is a useful theoretical tool for determining all the major cross sections within the framework of a common general formulation.

- The well known Complex Optical Method formalism is modified by us to include single & multi-centre molecules using the ‘single centre’ and ‘group additivity methods’.

- Under the same umbrella of the present method, we are capable of producing reliable various total cross sections for targets from small atoms to complex polyatomic molecules.

- We have successfully done a first initiation to obtain $Q_{\text{ion}}$ from $Q_{\text{inel}}$ using our method called CSP-ic.

- Results on most of the targets studied shows satisfactory agreement with the previous investigations where ever available.
Merits & Demerits

**Merits of the theory:**

- Quantum mechanical approach
- Calculating different CS under the same formalism
- Can investigate large/reactive molecules
- Simple and fast method
- First initiation to extract $Q_{ion}$ from $Q_{inel}$

**Limitations of the theory:**

- Spherical approximation
- Lower energy limit
- Semi-empirical method to find $Q_{ion}$
## Recent publications

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<tr>
<td>5</td>
<td>H₂O (Ice) and H₂O (Liquid)</td>
<td>J. Phys: Conf. Series 80 (2007) 012008</td>
<td>K N Joshipura, Sumona Gangopadhyay, CGL and MV</td>
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</table>
Thank you

Prof. K N Joshipura
Minaxi Mam, Bobby, Chetanbhai, Bhushitbhai
Prof. P C Vinodkumar
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My Friends

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