Total ionization cross sections for Sr, Y, Ru, Pd and Ag atoms by electron impact

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Introduction

Theoretical Methods

- Spherical Complex Optical Potential (SCOP)
- Complex Scattering Potential ionization contribution (CSP-ic)

Results

Summary
Electrons: an effective source

Applications of e-atom / e-molecule CS to,
- atmospheric sciences (ozone, climate change etc.)
- plasma etching
- understanding & modeling plasmas in fusion devices
- In radiation physics (medical science) etc.

Difficulty in performing experiments
- Expensive
- Limitation to targets
- Time consuming

Need for reliable calculations
Theoretical Method
(SCOP*)

- **Spherical Complex Optical Potential (SCOP) formalism**

- **Schrödinger eqn is solved by partial wave analysis employing the potentials of the system**

- This would give complex phase shifts for each partial wave through,

\[
\tan \delta_l(k) = \frac{k j'_l(ka) - \gamma_l(k) j_l(ka)}{k \eta'_l(ka) - \gamma_l(k) \eta_l(ka)}
\]

Where, \( j \) and \( \eta \) are the Bessel and Neumann functions respectively obtained from the solution of the radial part of the Schrödinger eqn using the potentials incorporated in the formalism.

*Joachain C J 1983 Quantum Collision Theory (Amsterdam: North-Holland)
The potential employed here is spherical and complex and hence the name Spherical Complex Optical Potential formalism, which is given by,

\[ V_{opt}(r, E_i) = V_R(r) + iV_I(r, E_i) \]

Where the real part is,

\[ V_R(r, E_i) = V_{st}(r) + V_{ex}(r, E_i) + V_p(r, E_i) \]

The inelastic cross section cannot be obtained directly from experiments, whereas ionization cross section is measurable.

*Joachain C J 1983 Quantum Collision Theory (Amsterdam: North-Holland)*
The Q_{ion} is then obtained using a semi-emperical approach “Complex Scattering Potential-ionization contribution” (CSP-ic)* method from Q_{inel} by defining an energy related ratio.

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

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

The parameters are obtained using the conditions,

\[ R(E_i) = 0 \quad \text{for} \quad E_i \leq I \]
\[ = R_P \quad \text{at} \quad E_i = E_P \]
\[ \cong 1 \quad \text{for} \quad E_i >> E_P \]

Results

Fig 1: $Q_{\text{ion}}$ for e – Sr scattering in Å$^2$

Fig 2: $Q_{\text{ion}}$ for e – Y scattering in Å$^2$

Fig 3: $Q_{\text{ion}}$ for e – Ru scattering in Å$^2$

Fig 4: $Q_{\text{ion}}$ for e – Pd scattering in Å$^2$

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Fig 5: $Q_{\text{ion}}$ for $e$ – Ag scattering in Å$^2$

Fig 7: $Q_{\text{ion}}$ for all the targets in Å$^2$

Percentage deviation of Bartlett and Stelbovics from the present data for all the atoms.

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We have performed a series of calculations on electron collisions with atoms.

Accurate measurements are quite tedious to perform. They are not only expensive, but also not viable for many systems where cross sections are required.

Our calculations are based on quantum mechanical approximations with less degree of accuracy compared to fully quantum mechanical theories.
However, the results obtained by present method seems to agree quite well with the experiments and other theories where ever available. They are within the experimental uncertainties otherwise.

Present formalism has been tested for a vast target systems and we have observed that they are quite successful even with radicals and heavier hydrocarbon molecules.

We are hence quite sure that the results obtained by our method is reliable and may be utilized for further modeling.
Thanks

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