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

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Outline

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

Results

- Summary

Introduction

Why e-atom/molecule collision calculations?

- **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**
- **Schrodinger eqn is solved by partial wave analysis employing the potentials of the system**
- **This would give complex phase shifts for each partial wave through,**

$$\tan\delta_l(k) = \frac{kj_l^{'}(ka) - \gamma_l(k)j_l(ka)}{k\eta_l^{'}(ka) - \gamma_l(k)\eta_l(ka)}$$

Where, *j and* η 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)

Theoretical Method continued...

- **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.**

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

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

- **The parameters are obtained using the conditions,**

$$\begin{aligned} R(E_i) &= 0 \quad && for \quad E_i \le I \\ &= R_P \quad && at \quad E_i = E_P \\ &\cong 1 \quad && for \quad E_i >> E_P \end{aligned}$$

*Joshipura K N, Vinodkumar M, Limbachiya C G, Antony B K 2004 Phys. Rev. A 69 022705.

Results*

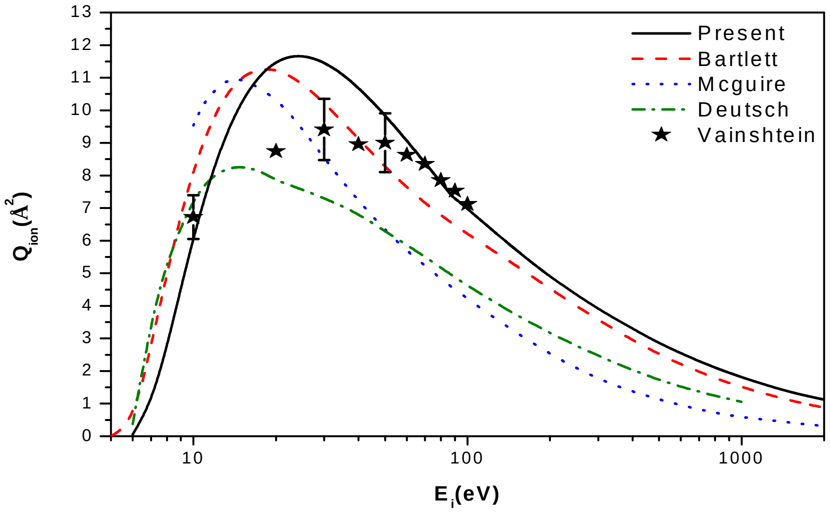

Fig 1: Q_{ion} for e – Sr scattering in $Á^2$

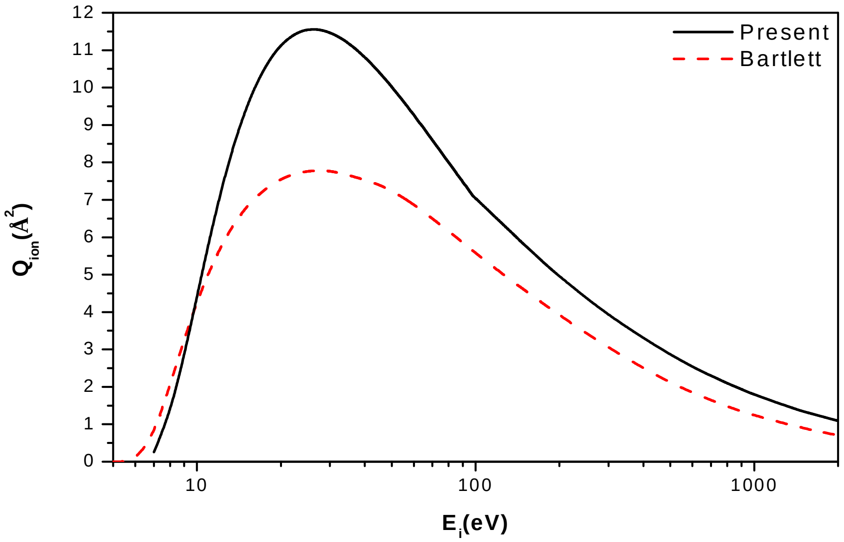

Fig 2: Q_{ion} for e – Y scattering in $Á^2$

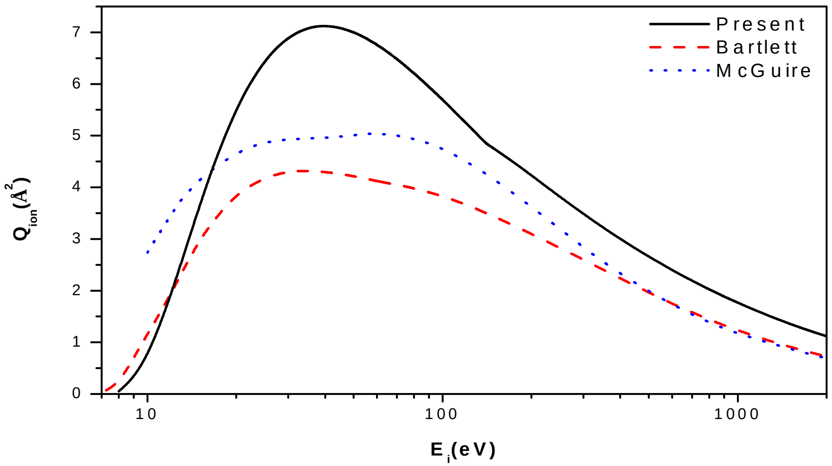

Fig 3: Q_{ion} for e – Ru scattering in $Á^2$

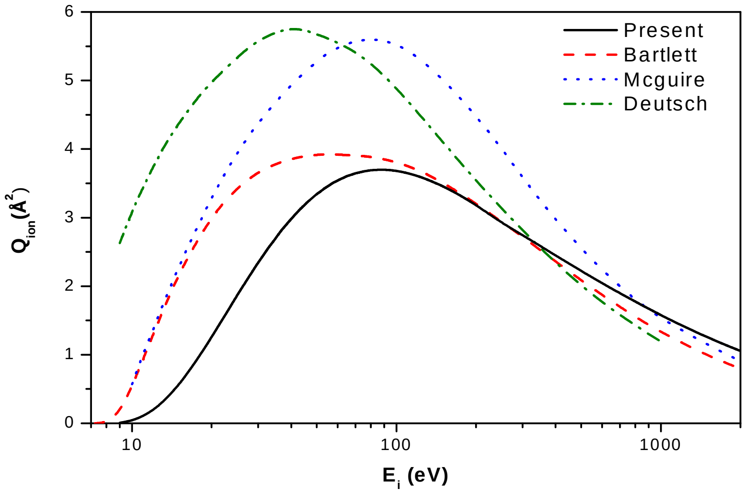

Fig 4: Q_{ion} for e – Pd scattering in $Á^2$

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Results continued...

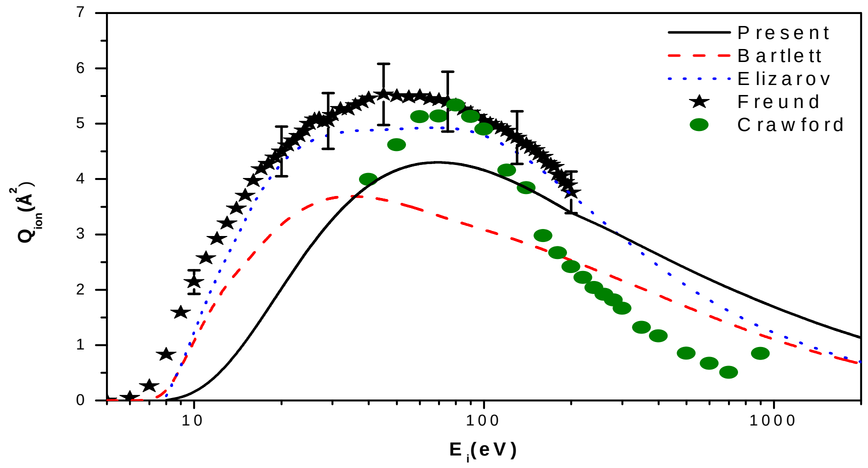


Fig 5: Q_{ion} for e – Ag scattering in Á²

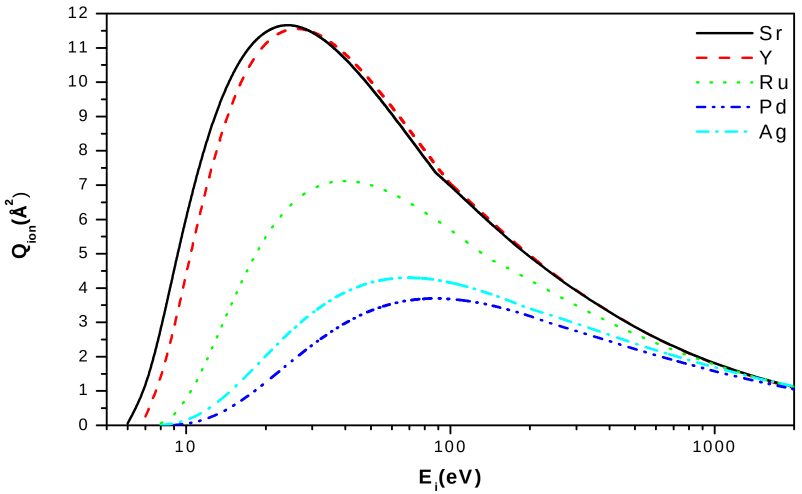
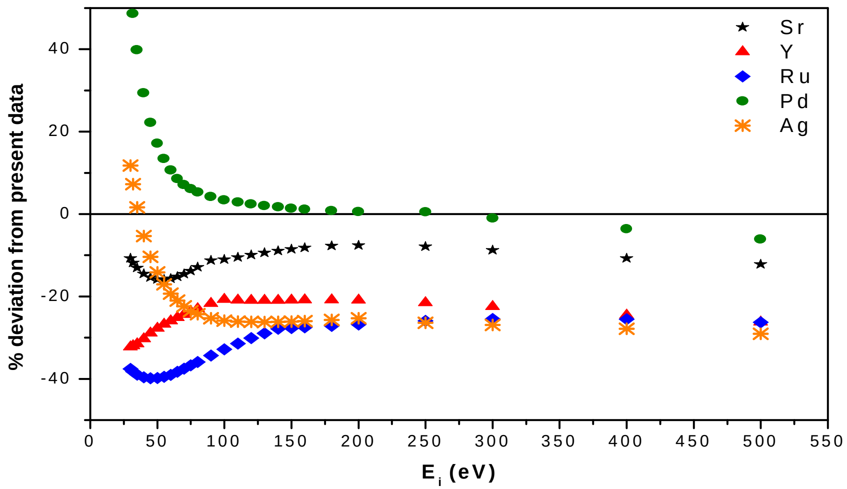


Fig 7: Q_{ion} for all the targets in Á²



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

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Summary

- 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 moleclues.

➨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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