Study of positron scattering from the acetylene molecule

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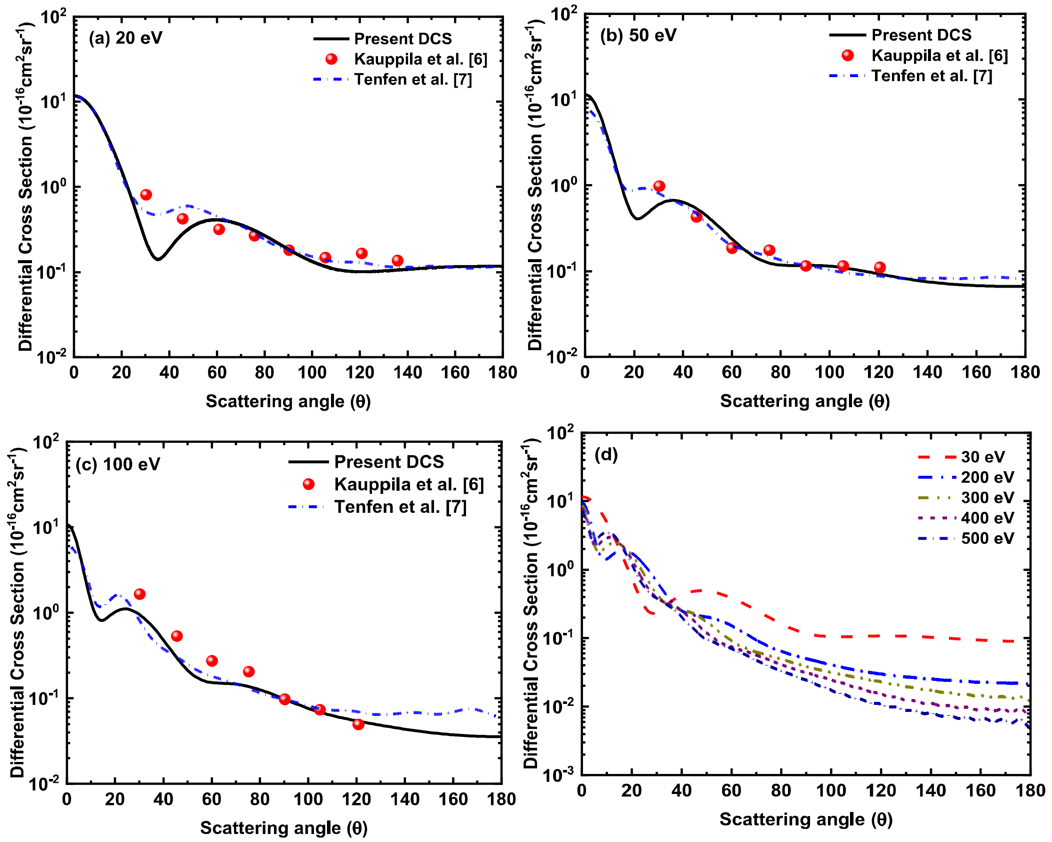
Introductions :

- Acetylene (C_2H_2) is used in various plasma polymerization process and also found in several astronomical environments such as in Saturn and its moon.
- Therefore, the study on electron collision with acetylene is important for the applications in plasma and astronomical environments to understand involved different physical and chemical reactions.
- We study electron scattering from acetylene molecule using optical model potential approach [1-3].
- Static potential (V_{st}) is calculated using Gaussian wavefunction and polarisation (V_{pol}) potentials are added to it, to form the optical model potential (V_{opt}).
- The scattering amplitude and phase shifts are obtained by solving the Schrödinger equation with the model potential.

Differential cross sections of acetylene at (a) 20 eV, (b) 50 eV, (c) 100 eV and (d) 30-500 eV incident positron energy.



Theory :

Optical Model Potential

$$V_{opt} = V_{st} + V_{pol}$$

Spherically Averaged Static Potential

$$V_{st} = V_{ele} + V_{nuc}$$

Electronic Static Potential

$$V_{ele}(r) = \int \frac{\rho(r')}{|r-r'|}dr'; \qquad \rho(r') = \sum_{i=1}^{N} |X_i(r')|^2$$

$$V_{ele}(r) = \sum_{i}\sum_{k,k'} a_{ik}a_{i'k'} \sum_{j,j'} N_{kj}N_{k'j'}c_{kj}c_{k'j'}E_{kj,k'j'}$$

$$\times \int e^{-\alpha|r'-r_p|^2}(x-A_x)^{m^x}(x-A_y)^{m^y}(z-A_z)^{m^z}$$

$$\times (x-A_x)^{m^{x'}}(y-A_y)^{m^{y'}}(z-A_z)^{m^{z'}}\frac{1}{r_>}dr'$$

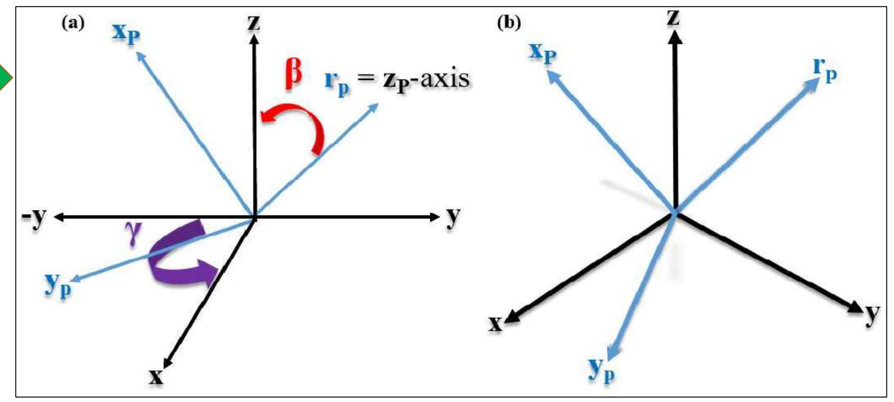
Nuclear Potential

$$V_{nuc}(r) = \begin{cases} -\dfrac{2Z_H}{r} - \dfrac{2Z_C}{r} & for\ r \geq r_H \\ -\dfrac{2Z_H}{r_H} - \dfrac{2Z_C}{r} & for\ r_C < r < r_H \\ -\dfrac{2Z_H}{r_H} - \dfrac{2Z_X}{r_C} & for\ r \leq r_C. \end{cases}$$

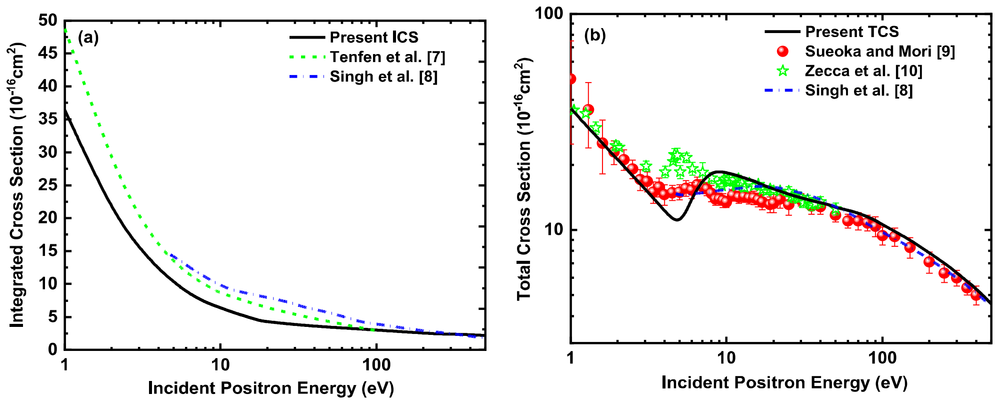
Absorption Potential

Absorption potential formula given by Reid and Wadehra [4] and cut off parameter is taken as [5],

$$\Delta(E) = \Delta - \frac{(\Delta - \Delta_p)}{[1+(E/3I-1)^2]}$$



Integrated and total cross sections for positron-acetylene scattering.



Conclusions :

- A new approach is applied to obtain the static potential analytically by using the Gaussian wavefunction.
- Results for the differential, integrated and total cross sections of positron-acetylene scattering are reported and compared with the experimental and theoretical results.
- We have also reported the differential cross section results at 30, 200, 300, 400 and 500 eV for the first time.

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