

Total Electron Scattering Cross Section Calculations for Tetrahydropyran (CH₂)₅O and Tetrahydrofurfuryl Alcohol (C₅H₁₀O₂) Bio-Molecules

Jayantilal. G. Raiyani¹Associate Professor, Department of Physics, Shri M. M. Science College, Morbi, Gujarat, India¹

ABSTRACT: The rotational excitation total cross section (TCS) for electron scattering from tetrahydropyran (CH₂)₅O and tetrahydrofurfuryl alcohol (C₅H₁₀O₂), bio-molecules have been calculated from 1 to 80 eV, using the Born Eikonal Series (BES) Approximation method. In present calculations, the hard sphere dipole interaction potential model is employed for electron-molecule interaction. The TCS energy function for electron-tetrahydropyran (THP: (CH₂)₅O and tetrahydrofurfuryl alcohol (THFA: C₅H₁₀O₂) bio-molecule collisions is significantly show the sharp decrement at low energy from 1 to 20 eV and above it's decreases smoothly. Comparison is also made between the present results for (CH₂)₅O and C₅H₁₀O₂ bio-molecules with earlier TCS experiment measurements data and theoretical results available in the literature.

KEYWORDS: Hard sphere dipole potential, Born Eikonal Series method, Total cross section.

I. INTRODUCTION

The discovery that slow electron can induce strand breaks in the DNA (Boudaffa et al[1] 2000) stimulated increasing interest in experimental and theoretical studies concerning electron interaction with living-cell constituents[2] To overcome difficulties in investigations on the basic DNA components as well as on molecules which may serve as simple models of building blocks for living matter, like structured molecules: tetrahydropyran (THP:(CH₂)₅O) and tetrahydrofurfuryl alcohol (THFA:C₅H₁₀O₂), bio-molecule and its derivatives. It is believed that the comprehensive and reliable electron-scattering data for such isolated subunits may help to understand and model the electron-assisted processes occurring within the cell in the complex DNA (RNA) compound [3]. Tetrahydropyran (CH₂)₅O molecule with O atom embedded in the six-member ring. The THP ring is the core of pyranose sugars and is a structural base for numerous molecules important in the synthesis of biological active and pharmaceutically effective compounds[4] The THP has also been identified as a highly advantageous component of liquid crystal mixture for LCD devices[5]

The main goal this work is to provide absolute values of total cross section (TCS) describing electron-THP and THFA molecule scattering over impact energies from low (1eV) to intermediates (80 eV) The Born Eikonal Series (BES) Approximation method and hard sphere dipole interaction potential model is employed for present calculations. The hard sphere cut-off parameter "a" is considered as "D/2", where "D" is dipole moment of molecule[6-7]. The present TCS results are compared with experimental results of Szmytkowski Cz et al[9] 2011 for THP molecule and the results of Mozejko P et al[10] 2006 for THFA molecule. In general the present TCS results for tetrahydropyran (THP: (CH₂)₅O) and tetrahydrofurfuryl alcohol (THFA: C₅H₁₀O₂) bio-molecule at the energy range from 1 eV. to 80 eV. are found in good agreement.

International Journal of Innovative Research in Science, Engineering and Technology

(An ISO 3297: 2007 Certified Organization)

Vol. 4, Issue 6, June 2015

II. METHODOLOGY

BORN EIKONAL SERIES METHOD (BES)

In order to take into account somewhat higher terms of Born series, one can use Eikonal approximation. Ashihara et al[8] (1975) employed Glauber formulation in Eikonal approximation for electron dipole collisions. They calculated cross section for strongly polar molecules. Although this approximation is originally a high energy approximation, it has been applied successfully to the low energy electron atom collisions (Gerjuoy; 1971). In the present investigations an attempt is made to employ Born Eikonal Series method for the cross sectional calculations for the electron- THP and THFA bio-molecule collision.

The interaction potential $V(r)$ can be expressed in following form⁷,

$$V(\underline{r}) = -2eq \sum_{n=odd} \frac{r_{<}^n}{r_{>}^{n+1}} P_n(\hat{r}, \hat{s}) \quad \text{--- (1)}$$

Where $r_{>}$ and $r_{<}$ are the larger and the smaller of r and $P_n(\hat{r}, \hat{s})$ is the Legendre polynomial of the order n . "a" is the parameter which indicates finiteness of the dipole and related to the dipole moment by the relation $D=2aq$. Taking $n = 1$ only one can get the expression for electron finite dipole interaction potential and it is employed in cylindrical polar co-ordinate, one can name a linear dipole model[7].

$$V(\underline{r}, \hat{s}) = V(\underline{b}, z) = 0 \quad \text{for } z < a \quad \text{--- (2)}$$

$$V(\underline{r}, \hat{s}) = V(\underline{b}, \hat{z}) = - \frac{D}{b^2 + z^2} P_1(\underline{r}, \hat{s}) \quad \text{for } z > a \quad \text{--- (3)}$$

Where, "a"- is the hard sphere parameter (cut-off parameter).

The formula for the Eikonal phase shift function $\chi(b)$ is given by,

$$\chi(b) = - \frac{2D\gamma}{ki} \int_a^\infty \frac{z dz}{(b^2 + z^2)^{3/2}} \quad \text{--- (4)}$$

' γ ' is the direction cosine of the dipole axis with respect to the polar axis.

A series expansion of scattering amplitude as give by,

$$f_{E1} = \frac{2D\gamma}{\Delta \exp(a\Delta)} \quad \text{--- (5)}$$

$$f_{E2} = \frac{2iD^2\gamma^2}{ki} k_o(a\Delta) \quad \text{--- (6)}$$

International Journal of Innovative Research in Science, Engineering and Technology

(An ISO 3297: 2007 Certified Organization)

Vol. 4, Issue 6, June 2015

$$f_{E3} = \frac{4}{3} \frac{D^3 \gamma^3}{ki} \frac{e^{-a\Delta}}{a} \quad \text{--- (7)}$$

Where $K_0(a\Delta)$ - is a Bessel function, $\Delta=|ki-kf|$ is momentum transferred. The differential cross section (DCS) for three terms in Born Eikonal Series Approximation can be expressed as follow,

$$\frac{d\sigma}{d\Omega}(j_0 m_{j_0} \rightarrow j m_j; \theta) = \frac{kf}{ki} |f_{E1} + f_{E2} + f_{E3}|^2 \quad \text{--- (8)}$$

Summing over m_j and averaging over m_{j_0} , one gets the DCS for the rotational transition $j_0 \rightarrow j_0 + 1$. Therefore using the standard formula, one can calculate the expression for the TCS which will be as follows

$$\begin{aligned} Q_{j_0, j_0+1} &= \frac{2D^2}{ki^2} \left\{ \frac{4(j_0 + 1)}{3(2j_0 + 1)} \right\} \int_{|ki-kf|}^{|ki+kf|} \frac{e^{-2a\Delta}}{\Delta} d\Delta \\ &+ \frac{32D^6}{9ki^6 a^2} \left\{ \frac{6(j_0 + 2)(j_0 + 1)j_0}{175(2j_0 + 5)(2j_0 - 1)(2j_0 + 1)} \right. \\ &+ \left. \frac{3(j_0 + 1)}{25(2j_0 + 1)} \right\} \left[\frac{\exp[-2|ki+kf|a]}{4a^2} \{-2a(ki+kf)-1\} \right. \\ &- \left. \frac{\exp[-2|ki-kf|a]}{4a^2} \{-2a|ki-kf|-1\} \right] \\ &+ \frac{16D^4}{3ki^4 a^4} \left\{ \frac{j_0 + 1}{5(2j_0 + 1)} \right\} \left[\exp[-2|ki+kf|a] - \exp[-2|ki-kf|a] \right] \quad \text{--- (9)} \end{aligned}$$

III. RESULTS AND DISCUSSION

Aim of the present study is to obtain theoretical the rotational excitation total cross sections (TCS) are calculated for electron scattering by bio-molecules like as tetrahydropyran (THP: $(CH_2)_5O$) and tetrahydrofurfuryl alcohol (THFA: $C_5H_{10}O_2$) at the energy from 1 eV. to 80 eV. The Born Eikonal Series (BES) Approximation method and hard sphere dipole interaction potential model is employed for present calculation. The hard sphere cut-off parameter "a" is considered as $D/2$, D-is the dipole moment of molecule.

Figure.1 show the rotational excitation total cross sections (TCS) results for $e-(CH_2)_5O$ scattering in the energy from 1 eV. to 80 eV. The present calculated energy dependence TCS results are compared with experimental measured results of Szmytkowski Cz et al[9] As shown in fig.-1, it is found that present TCS results are sharply decreases at low energy 1 eV to 20 eV. But at higher energy range 20 eV to 80eV, it decreases slowly. The distinctive feature of the calculated $e-(CH_2)_5O$ TCS results are relatively large magnitude at the low energy range as compared with the results of Szmytkowski Cz et al[9] Such high cross section values can be related, at least in part, to the larger interaction time, geometrical size and dipole moment of the THP molecule. Present TCS results at higher energy are relatively smaller magnitude as compared with the results of Szmytkowski Cz et al[9] Present energy dependence TCS results are in good agreement in shape of curves, but differ in magnitude with results of Szmytkowski Cz et al[9] In general the present results are shown in the agreement with the results of Szmytkowski Cz et al[9]

International Journal of Innovative Research in Science, Engineering and Technology

(An ISO 3297: 2007 Certified Organization)

Vol. 4, Issue 6, June 2015

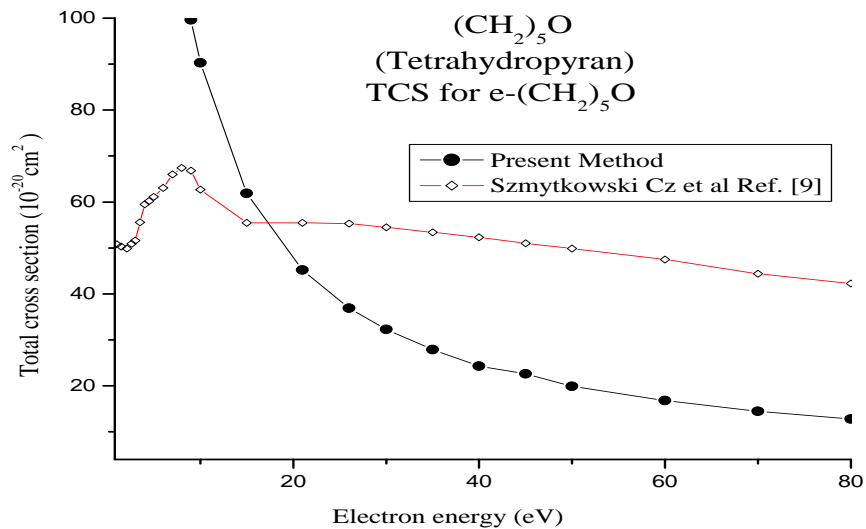


Figure 1. Total cross section (TCS) for e-(CH₂)₅O molecule scattering

Figure. 2 show the rotational excitation total cross sections (TCS) results for e- C₅H₁₀O₂ scattering in the energy from 1 eV. to 80 eV. using the present method. The present calculated TCS results are compared with the experimental results of Mozejko P et al[10]. The present TCS results are found with sharp decrement at low energy (1 to 20 eV.) region. At higher energy it decreases slowly. The present TCS results for C₅H₁₀O₂ at energy range from 1 eV to 80 eV. are found better than results of Mozejko P et al[10]. In general the present TCS results for (CH₂)₅O and C₅H₁₀O₂ at the energy from 1 eV. to 80 eV. are found in good agreement with those of compared results.

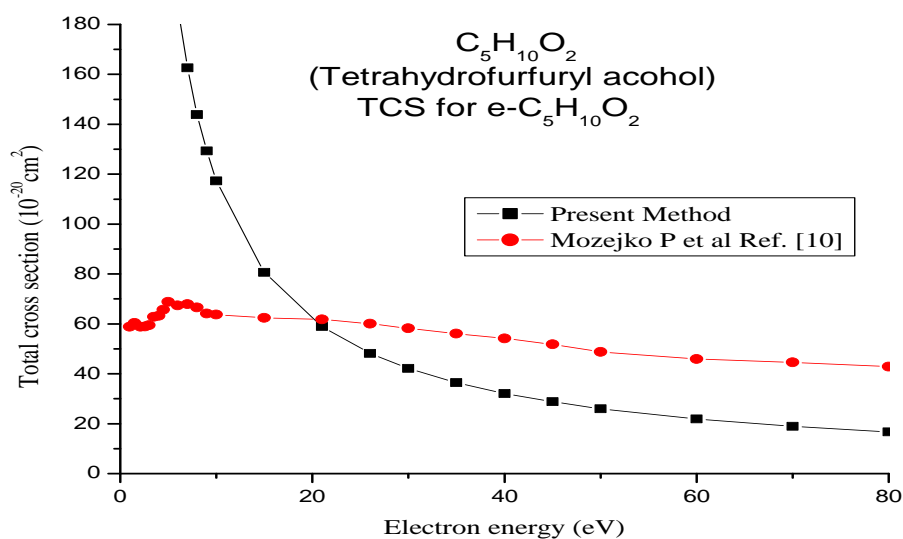


Figure 2. Total cross section (TCS) for e-C₅H₁₀O₂ molecule scattering

International Journal of Innovative Research in Science, Engineering and Technology

(An ISO 3297: 2007 Certified Organization)

Vol. 4, Issue 6, June 2015

IV. CONCLUSION

This paper provides theoretical study of TCS for electron scattering from $(\text{CH}_2)_5\text{O}$ and $\text{C}_5\text{H}_{10}\text{O}_2$ bio-molecules over impact energies from 1 to 80 eV. using BES method and hard sphere dipole potential model. The rotational excitation total cross section (TCS) results are presented in comparison with some existing experimental results[9,10] The results are in general good agreement with the measured data. This good agreement supports the description of the interaction dynamic considered in the present methods used for solving the scattering equations. Hence it will be worthwhile to use hard sphere dipole potential model in Born Eikonal Series (BES) for better to study of electron- $(\text{CH}_2)_5\text{O}$ and $\text{C}_5\text{H}_{10}\text{O}_2$ bio-molecules collision process in low and intermediate energy region. The present results may be improved to consider higher terms in present method.

REFERENCES

- [1] Boudaiffa B, Cloutier P, Hunting D and Sanche L, Science **287** 1658-601, 2000
- [2] Sanche L, Eur. J. Phys. D **35** 367-90, 2005
- [3] Sanche L, Chem. Phys.Lett. **474** 1-6, 2009
- [4] Smith A, Mesaros E and Meeyar E, J. Am. Chem. Soc. **128** 5292-99, 2006
- [5] Kirsch P and Maillard D, Eur.J. Chem. **2006** 3326-31, 2006
- [6] Saha S, Ray S, Bhattacharya B & Barua A.K, Phys Rev (USA), **23** 2926, 1981
- [7] Desai H S and Chhaya V M, Ind. J. Pure & Appl. Phys, **7** 180, 1979
- [8] Ashihara I and Takayanagi K, J. Phys. Soc. **38** 1732, 1975
- [9] Szymtkowski Cz, Ptasinska-Denga E, J Phy. B: At. Mol. Opt. Phys. **44** 15203, 2011
- [10] Mozejko P, Domaracka A, Ptasinska-Denga E and Szymtkowski Cz , Chem. Phys. Lett. **429** 378-81, 2006b