



## CALCULATION OF TOTAL ELECTRON-SCATTERING CROSS SECTION FOR TETRAHYDROPYRAN, (CH<sub>2</sub>)<sub>5</sub>O MOLECULE

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### ABSTRACT

We report electron impact total cross sections for tetrahydropyran, (CH<sub>2</sub>)<sub>5</sub>O, molecule from threshold of the target to 2000 eV. We employed Spherical Complex Optical Potential (SCOP) to compute total inelastic ( $Q_{inel}$ ) and elastic ( $Q_{el}$ ) cross sections. Total cross sections is sum of these two calculated cross sections (i.e  $Q_{inel}$  &  $Q_{el}$ ). The only experimental data reported by Szymtkowski and Denga, [J. Phys. B: At. Mol. Opt. Phys. 44 (2011) 015203] on absolute total cross section (TCS) for electron scattering from tetrahydropyran (THP:(CH<sub>2</sub>)<sub>5</sub>O) molecules measured from 1 to 400 eV, using a linear electron transmission technique revealed a good agreement with the present calculations. In paucity of the data, present work is important and will fill the void of the data needed in applications of electron-assisted processes in the complex DNA (RNA) Compounds.

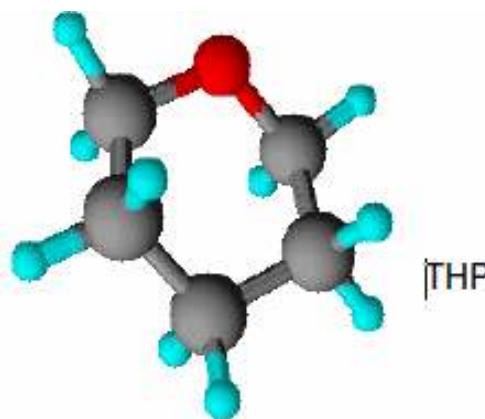
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### INTRODUCTION

The discovery that slow electrons can induce strand breaks in the DNA [1] stimulated increasing interest in experimental and theoretical studies concerning electron interactions with living-cell constituents [2,3]. To overcome difficulties in investigations of electron-induced reactions in vivo state, the studies are focused on the basic DNA components as well as on molecules which may serve as simple models of building blocks for living matter, like furan's structured molecules: tetrahydrofuran (THF: (CH<sub>2</sub>)<sub>4</sub>O) 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 [4]. Tetrahydropyran (THP: (CH<sub>2</sub>)<sub>5</sub>O), with O atom embedded in the six-membered ring, is a homologue of the THF molecule (see figure 1). The THP ring is the core of pyranose sugars and is a structural base for numerous molecules important in the synthesis of biologically active and pharmaceutically effective compounds [5]. The THP moiety has also been identified as a highly advantageous component of liquid crystal mixtures for LCD devices [6]. In contrast to THF, for which extensive studies on the electron impact have been performed, the THP has received much less attention in electron-scattering research. For THP, until now, only the core excitation spectra taken at 2.5 keV electron energy [7] and recent calculations of elastic and ionization cross sections at intermediate energies are available [8]. In the literature, one can also find an experiment concerning the electron diffraction study of the THP molecular structure [9]. Present study aims to provide calculated values of total cross sections (TCSs) for electron-THP scattering from ionization threshold to (2000 eV). The results are then compared with experimental TCS for THP.

**Fig.1:** Schematic of the tetrahydropyran - THP (CH<sub>2</sub>)<sub>5</sub>O



### THEORETICAL METHODOLOGY

The present theory is based on a quantum mechanical calculation solved by the method of partial waves, giving complex phase shifts as the output. The unique phase shifts thus obtained are the key ingredients and they carry the signature of the interaction of the incoming projectile and the target. These complex phase shifts are further used to evaluate the total elastic cross sections ( $Q_{el}$ ) and its inelastic counterpart ( $Q_{inel}$ ) [10, 11] given as.

$$Q_{el}(k) = \frac{\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) |\eta_l \exp(2i \text{Re} \delta_l) - 1|^2 \quad (1)$$

$$Q_{inel}(k) = \frac{\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) (1 - \eta_l)^2 \quad (2)$$

Where  $k$  is the wave vector,  $l$  is the angular momentum,

$$Q_T(E_i) = Q_{el}(E_i) + Q_{inel}(E_i) \quad (3)$$

We represent the electron-atom/molecule system by a complex potential comprising of real and imaginary potentials as,

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$$V(r, E_i) = V_R(r, E_i) + iV_I(r, E_i) \quad (4)$$

Such that

$$V_R(r, E_i) = V_{st}(r) + V_{ex}(r, E_i) + V_p(r, E_i) \quad (5)$$

Where,  $E_i$  is the incident energy. The three terms on the RHS of the eqn. (5) are real potentials arising from the electron target interaction namely; static, exchange and the polarization potentials, respectively. The static potential is Columbian in nature and arises due to static charge distribution between target and incoming electron. The exchange potential takes care of exchange of the incoming electron with one of the target electrons since they are undistinguishable particles. The polarization potential takes in account the momentarily redistribution of target charge cloud arising due to incoming electron which in turn gives rise to temporary dipole and quadrupole moments. Basically all effects of the incoming electron onto the target are taken into account through these potentials that is beyond the scope of present theoretical computations. Hence we consider various model potentials which are accurate enough to describe the phenomenon. The basic input for evaluating all these model potentials is the electronic charge density of the target. For atoms the charge density is derived from the parameterized Hartree-Fock wave functions given by Bunge and Barrientos[12]. The e - molecule system is more complex in comparison to e - atom system. In case of tetrahydropyran,  $(CH_2)_5O$  our attempt is to reduce the system in five group of  $CH_2$  and one O atom. For each group, we introduced centre of mass method by taking into consideration properties of whole target. This is possible as C-C bond length is quiet large 1.531 Å (more than De-Broglie wave length of incoming electrons for threshold to 2000 eV energy) and similarly C-O bond length 1.420 Å is also large. The molecular charge density  $\rho(r)$  so obtained is renormalized to incorporate the covalent bonding. This has been employed earlier for many targets and is found successful in better representation of the target and hence predicting relevant cross sections[13,14]. We have employed parameter free Hara's 'free electron gas exchange model'[15] for the exchange ( $V_{ex}$ ) potential. All the target parameters, namely ionization potential, bond length and dipole polarizability of the target used in the calculation are available elsewhere [16, 17] and are listed in Table 1.

**Table 1 :** Target properties

Target	IP(eV)	Polarizability (Å <sup>3</sup> )	Bond length(Å)
(CH <sub>2</sub> ) <sub>5</sub> O	9.25	9.8	1.116 (C - H) 1.420 (C - O) 1.531 (C - C)

The imaginary part in  $V_{opt}$ , also called the absorption potential  $V_{abs}$ , accounts for the total loss of scattered flux into all the allowed *electronic* channels of excitation and ionization. Here we have neglected the non-spherical terms arising from the vibrational and rotational excitation in the full expansion of the optical potential. This is due to the fact that anisotropic contribution from vibrational excitation will be

significant at very low impact energies while it will be negligible at the energies of present interest.

Finally, for the absorption potential we have employed a well-known quasi-free model of Staszewska *et. al.*[18] given by,

$$V_{abs}(r, E_i) = -\rho(r) \sqrt{\frac{T_{loc}}{2}} \cdot \left( \frac{8\pi}{10k_f^3 E_i} \right) \theta(p^2 - k_f^2 - 2\Delta) \cdot (A_1 + A_2 + A_3) \quad (6)$$

The local kinetic energy of the incident electron is

$$T_{loc} = E_i - (V_{st} + V_{ex}) \quad (7)$$

The parameters  $A_1$ ,  $A_2$  and  $A_3$  are defined as

$$A_1 = 5 \frac{k_f^3}{2\Delta}; \quad A_2 = \frac{k_f^3(5p^2 - 3k_f^2)}{(p^2 - k_f^2)^2};$$

and

$$A_3 = \frac{20(2k_f^2 + 2\Delta - p^2)(2k_f^2 + 2\Delta - p^2)^{5/2}}{(p^2 - k_f^2)^2} \quad (8)$$

The absorption potential is not sensitive to long range potentials like  $V_{pol}$ . Hence it is not included in the representation of  $T_{loc}$  as shown in eqn. (7). In equation (6),  $p^2 = 2E_i$ ,  $k_f = [3\pi^2 \rho(r)]^{1/3}$  is the Fermi wave vector and  $\Delta$  is an energy parameter. Further  $\theta(x)$  is the Heaviside unit step-function, such that  $\theta(x) = 1$  for  $x \geq 0$ , and is zero otherwise. The dynamic functions  $A_1$ ,  $A_2$  and  $A_3$  occurring in the equation (6) depend apparently on  $\rho(r)$ ,  $I$ ,  $\Delta$  and  $E_i$  as evident from eqn. (8). The energy parameter  $\Delta$  determines a threshold below which  $V_{abs} = 0$ , and the ionization or excitation is prevented energetically. In fact  $\Delta$  is the governing factor which decides the values of total inelastic cross section, is also a characteristics of Staszewska model [18]. The original model of Staszewska *et. al.*[18] has been modified by us considering  $\Delta$  as a slowly varying function of  $E_i$  around  $I$ . Briefly, a preliminary calculation for  $Q_{inel}$  is done with a fixed value  $\Delta = I$ . From this the value of incident energy at which our  $Q_{inel}$  reaches its peak, named as  $E_p$  is obtained. This is meaningful since  $\Delta$  fixed at  $I$  would not allow excitation at incident energies  $E_i \leq I$ . On the other hand, if the parameter  $\Delta$  is much less than the ionization threshold, then  $V_{abs}$  becomes unexpectedly high near the peak position. The modification introduced in our paper has been assigned a reasonable minimum value 0.8I to  $\Delta$  and express this parameter as a function of  $E_i$  around  $I$  follows as.

$$\Delta(E_i) = 0.8I + \beta(E_i - I) \quad (9)$$

The consideration of 0.8I is discussed elaborately in our earlier publication [19]. Here the value of the parameter  $\beta$  is obtained by requiring  $\Delta = I$  (eV) at  $E_i = E_p$ , beyond which  $\Delta$  is held constant and equal to  $I$ . The above expression for  $\Delta(E_i)$  is meaningful since  $\Delta$  fixed at  $I$  would not allow excitation at incident energy  $E_i \leq I$ . On the other hand, if parameter  $\Delta$  is much less than the ionization threshold, then  $V_{abs}$  becomes substantially

high near the peak position. After generating the full complex potential given in equation (4) for a given electron - molecule system, we solve the Schrödinger equation numerically using partial wave analysis. At low energies only few partial waves are significant, e.g. at ionization threshold of the target around 5 to 6 partial waves are sufficient but as the incident energy increases more partial waves are needed. Using these partial waves the complex phase shifts are obtained which are employed to find the relevant cross sections vide equation (1)& (2)[20].

## RESULTS AND DISCUSSION:

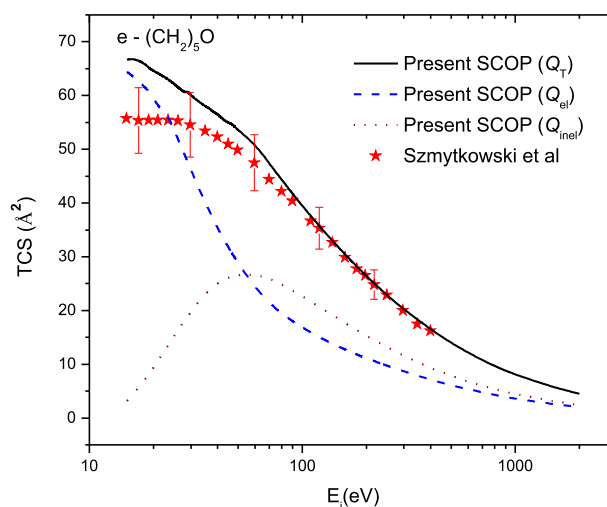
The theoretical approach of SCOP [21-22] is used to calculate the total cross section for studied target. Present numerical data of total cross sections for tetrahydropyran-(CH<sub>2</sub>)<sub>5</sub>O is tabulated in Table 2. The numerical result is also plotted graphically along with the available comparisons in Figure 2.

**Table 2 :** Total cross sections for (CH<sub>2</sub>)<sub>5</sub>O studied in Å<sup>2</sup>.

E <sub>i</sub> (eV)	TCS (Å <sup>2</sup> )	E <sub>i</sub> (eV)	TCS (Å <sup>2</sup> )	E <sub>i</sub> (eV)	TCS (Å <sup>2</sup> )
15	66.67	40	56.53	150	31.48
16	66.81	42	55.76	160	30.29
17	66.49	44	55.02	170	29.21
18	66.05	46	54.90	180	28.20
19	65.19	48	54.23	190	27.27
20	64.54	50	53.56	200	26.42
21	64.14	55	52.19	225	24.50
22	63.68	60	50.70	250	22.87
23	63.19	65	49.08	275	21.45
24	62.68	70	47.35	300	20.22
25	62.15	75	45.77	400	16.49
26	61.59	80	44.31	500	13.98
27	61.05	85	42.98	600	12.16
28	60.50	90	41.74	700	10.78
29	60.82	95	40.58	800	9.69
30	59.96	100	39.49	900	8.81
32	59.13	110	37.52	1000	8.09
34	58.31	120	35.77	1500	5.77
36	57.80	130	34.19	2000	4.52
38	56.99	140	32.77		

In Figure 2, presently calculated results shows overall a good agreement with measured data of Szmytkowski *et al.*[16] throughout the energy range except at the peak where present data is slightly higher but well within the experimental uncertainty of 10% given by Szmytkowski *et al.*[16]. Absolute total cross section (TCS) for electron scattering from tetrahydropyran (THP: (CH<sub>2</sub>)<sub>5</sub>O) molecules was measured from 1 to 400 eV, using a linear electron transmission technique [16].

**Fig. 2.** Total cross sections for e-(CH<sub>2</sub>)<sub>5</sub>O scattering



Solid line, Present SCOP ( $Q_T$ ); Dash line, Present SCOP ( $Q_{el}$ ); Dot line, Present SCOP ( $Q_{inel}$ ); Filled Star, Szmytkowski *et al.*[16].

## CONCLUSIONS

We have employed well-known spherical complex optical potential method to calculate electron impact total cross sections for (CH<sub>2</sub>)<sub>5</sub>O. The advantages of this method are as follows: first, it is valid for the entire range of energy from threshold of the target to 5 keV; secondly, it can be applied to a large variety of targets with ease and has been successfully tested, as can be seen from the literature [10,13,14,19], for more than three dozen targets; thirdly, it does not require any fitting parameters, requires only basic characteristics of the target such as ionization threshold, geometry of the molecule, Polarizability etc. We note that, in view of the result presented here, by and large our calculated results fall within the experimental error limit of available measured data. In paucity of the data on studied target, present calculated data is important to fill the void of needed data in biological and other applications of present target.

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