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ELECTRON IMPACT TOTAL CROSS SECTIONS FOR ETHYLENE OXIDE

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ABSTRACT

Present paper reports various total cross sections viz. total elastic, total inelastic, total ionization and total cross sections for ethylene oxide on electron impact from ionization threshold to 2 keV. We have employed the well established Spherical Complex Optical Potential (SCOP) formalism to compute total elastic and total inelastic cross sections. While total (complete) and total ionization cross sections are derived from these cross sections. There is only one measurement for total (complete) cross sections and a BEB (Binary - encounter Bethe) calculation by the same group for total ionization cross sections. In the present case, both cross sections are derived from the same formalism and hence we are quite confident that these results are consistent. Also, the results give an overall good agreement with other data in both cases.

Key worlds : *ethylene oxide; Total cross section; Spherical Complex Optical Potential; Complex Optical Potential ionization contribution*

INTRODUCTION

Ethylene oxide (C_2H_4O) is an organic compound composed of two alkyl groups attached to an oxygen atom in a cyclic shape. Because of its special molecular structure, ethylene oxide easily participates in the addition reaction, opening its cycle, and thus forming polymers [1,2]. Electron impact studies on these molecules are very important since they find applications in varied fields [3-5]. Its principle use lies in the manufacture of ethylene glycol and higher alcohols which find important applications in automotive antifreeze, explosives, cellophane, polyester resins, synthetic fibers and rubbers, and hydraulic fluids. Moreover ethylene oxide in mixture with carbon dioxide and halogenated propellants find utility as a fumigant, fungicide and sterilizing agent [6]. The local chemistry in all these cases is dependent on the reactive nature of these chemicals and their radicals formed by the scattering by electrons. Hence, electron impact scattering and ionization is very important to characterize the nature of reactions possible in such cases.

Electron impact studies with organic targets gained prominence after the study of Boudaiffa et al [7]. They pointed out that secondary electrons produced by energetic radiations are responsible for single and double strand breaks in DNA. Moreover systematic and detailed knowledge of cross sections resulting from electron collisions with simple organic systems can help us to understand the behavior of more complex biomolecules. Despite its importance very little attempts were made in this direction. The only measurement of electron impact total cross sections is performed by Szmytkowski et al [8]. They have also reported total ionization cross section using BEB formalism. To the best of our knowledge, no other experimental and/or theoretical cross section data is available for this molecule in the present energy range.

THEORETICAL METHODOLOGY

In our Spherical Complex Optical Potential (SCOP) formalism [9], the electron-molecule system is represented by a complex potential given by,

$$V(r,E_i) = V_R(r,E_i) + i\,V_I(r,E_i) \qquad (1)$$

such that

$$V_R(r,E_i) = V_{st}(r) + V_{ex}(r,E_i) + V_p(r,E_i) \qquad (2)$$

represents various real potentials arising from the electron target interaction namely, static, exchange and polarization respectively. To evaluate these potentials we use spherically averaged molecular charge-density ρ(r), determined from the constituent atomic charge densities given by Cox and Bonham [10]. Since the molecule dealt here is quite large, we have adopted a group additivity method to represent the charge density. In this method the molecular charge density is partitioned depending on the bond length and various groups associated with the molecule. For ethylene oxide, the C_2H_2- and O were treated as separate groups and then the charge density is formulated by expanding it at the centre of mass of each group in the molecule [11]. Later the charge densities corresponding to these groups are added together and renormalized incorporating the covalent bonding to get the complete picture. The exchange potential may be derived from the static potential thus obtained employing Hara's parameter free and energy dependent 'free electron gas exchange model' [12]. The polarization potential is of Zhang et al [13]. Finally, the imaginary part VI of the complex potential is derived from the well-known non-empirical quasi-free model form given by Staszeweska et al. [14],

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

The local kinetic energy of the incident electron is given by,

$$T_{loc} = E_i - (V_{st} + V_{ex} + V_{pol}) \qquad (4)$$

Where, A_1, A_2 and A_3 are dynamic functions (defined in ref [14]) depends differently on $\theta(x)$, I, Δ and E_i, where I is the ionization threshold of the target. $p^2 = 2E_i$ and $k_F = [3\pi^2\rho(r)]^{1/3}$ is the Fermi wave vector. Further, $\theta(x)$ is the Heaviside unit step-function and Δ is the energy parameter which determines a threshold below which $V_{abs} = 0$, where the ionization or excitation is prevented energetically. We have modified the original model by considering Δ as a slowly varying function of E_i around I as,

$$\Delta(E_i) = 0.8\,I + \beta\,(E_i - I) \qquad (5)$$

β is obtained by requiring that $\Delta = I$ (eV) at $E_i = E_p$, and also beyond E_p it is held constant equal to I. This is done to include excitations at low energies and inner shell ionization at high

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energies. After generating the full complex potential given in Eq. (2), we solve the Schrödinger equation numerically using partial wave analysis to obtain complex phase shifts which are then used to find cross sections Q_{inel} and Q_{el} [15]. Using these cross sections, the total cross section is obtained through,

$$Q_t = Q_{inel} + Q_{el} \tag{6}$$

Since Q_{inel} cannot be measured directly and the measurable Q_{ion} is of more practical importance, we extract Q_{ion} contained in the Q_{inel}. Hence, to obtain Q_{ion}, Q_{inel} is partitioned as,

$$Q_{inel}(E_i) = \Sigma\, Q_{exc}(E_i) + Q_{ion}(E_i) \tag{7}$$

Where, the first term is the sum over total excitation cross sections for all accessible electronic transitions. The second term is the total cross sections of all allowed ionization processes induced by the incident electrons. In order to extract Qion from Qinel, a reasonable approximation can be evoked by using a dynamic ratio function,

$$R(E_i) = \frac{Q_{ion}(E_i)}{Q_{inel}(E_i)} \tag{8}$$

Such that, $0 < R \le 1$. We assign three physical conditions to this ratio. It is apparent that when the incident energy is less than or equal to the ionization threshold of the target, this ratio is zero as the ionization process has not started. Also, at very high energy, the only dominant process is the ionization and hence the ration approaches almost 1. Thus,

$$\begin{aligned} R(E_i) &= 0 \text{ for } E_i \le I \\ &= R_p \text{ at } E_i = E_p \\ &\approx 1 \text{ for } E_i >> E_p \end{aligned} \tag{9}$$

R_p is the value of R at $E_i = E_p$. The general observation is that, at energies close to peak of ionization, the contribution of Q_{ion} is about 70–80% of the total inelastic cross sections Q_{inel}. This behavior is attributed to the smaller values of $\sum Q_{exc}$ compared to Q_{ion} with the increase in energy beyond E_p value. However the choice of R_p in Eq. (9) is not rigorous and introduces uncertainty in the final results. It has been by now tested for large number of atoms and molecules and it is observed that the proposed uncertainty is found to be less than 10% [9]. For calculating the Q_{ion} from Q_{inel} we use the following analytical form.

$$R(E_i) = 1 - C_1\left(\frac{C_2}{U+a} + \frac{\ln(U)}{U}\right) \tag{10}$$

Here, $U = E_i / I$. At low and intermediate energies the first term dominates and gives reasonable energy dependence at this range. However, when the energy increases further, the second term catches up and defines the ratio quite adequately here. The reason for such variation is due to the fact that initially the contribution to electron excitation is high, the contribution to the ionization channel is just picking up. However, as the energy is increased further, ionization contribution rises and the discrete excitation decreases rapidly. Consequently, we need to use the above functional form to attribute this behavior. It is quite evident that the conditions (as shown in Eq. 9) to find the parameters C_1, C_2, and a used in Eq. (10) will depend on the properties of the target under investigation [9,16,17]. The method given above to extract Q_{ion} from Q_{inel} is called the Complex Scattering Potential–ionization contribution (CSP-ic) [9]. Once Q_{ion} is obtained, $\sum Q_{exc}$ can easily be evaluated by eqn (7).

The values of Q_{el}, Q_{inel} and $\sum Q_{exc}$ for ethylene oxide are not reported here, but are available with the authors. We note that in view of the approximations made here, no definitive values are claimed, but by and large our results fall within the experimental error limits in most of the cases

RESULTS AND DISCUSSION

The theoretical approach of SCOP along with CSP-ic method discussed above offers the determination of the total cross sections Q_T, Q_{el} and Q_{ion} along with a useful estimation of electronic excitations in terms of the summed total cross section $\Sigma\, Q_{exc}$. Various important target parameters used for the present calculation are the best available from the literature [18].

The main advantage of the present work is that it covers all the major TCSs on electron impact of Ethylene oxide under the same formalism of SCOP along with CSP-ic. The present values of the total elastic, total inelastic, total ionization and total cross sections for C_2H_4O for the impact of electrons from threshold to 2 keV are tabulated in Table 1.

Table 1 Numerical values of ionization cross section (Q_{ion}) and total cross section (Q_T) in $Å^2$ for C_2H_4O

E_i (eV)	Q_{ion}	Q_T	E_i (eV)	Q_{ion}	Q_T
11	0.024	43.456	65	6.338	18.282
12	0.121	42.969	70	6.405	17.559
13	0.274	42.269	75	6.437	16.912
14	0.472	41.423	80	6.472	16.367
15	0.701	40.523	85	6.486	15.878
16	0.951	39.590	90	6.484	15.430
17	1.215	38.654	95	6.468	15.013
18	1.484	37.746	100	6.442	14.630
19	1.752	36.828	110	6.363	13.932
20	2.017	35.965	120	6.262	13.293
21	2.276	35.132	130	6.151	12.729
22	2.528	34.346	140	6.034	12.214
23	2.768	33.579	150	5.912	11.738
24	2.999	32.842	160	5.790	11.297
25	3.219	32.136	170	5.667	10.884
26	3.427	31.458	180	5.547	10.884
27	3.625	30.809	190	5.429	10.504
28	3.813	30.186	200	5.315	9.806
30	4.157	29.032	225	5.047	9.064
32	4.463	27.958	250	4.803	8.428
34	4.736	26.970	275	4.578	7.877
36	4.976	26.069	300	4.374	7.391
38	5.189	25.225	400	3.713	5.955
40	5.377	24.446	500	3.229	4.999
42	5.541	23.734	600	2.860	4.321
44	5.684	23.067	700	2.568	3.805
46	5.805	22.446	800	2.334	3.410
48	5.909	21.877	900	2.139	3.090
50	5.994	21.340	1000	1.977	2.830
55	6.145	20.142	1500	1.437	1.997
60	6.226	19.105	2000	1.128	1.545

Present results are also shown graphically along with available comparison in Figures 1 and 2. We have also presented the mutual comparison of various total cross sections using bar chart in Figure 3.

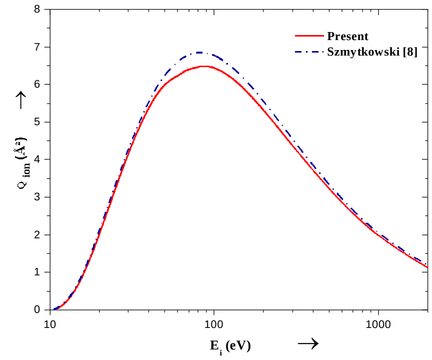

Figure 1: Total ionization cross section of C_2H_4O. Solid line represents present data and dash dot line represents the BEB

Figure 1 shows comparison of electron impact total ionization cross section for e – C_2H_4O scattering. Present results are in excellent agreement with theoretical results of Szmytkowski et al [8]. They have employed BEB method for computation of total ionization cross section. There is no other theoretical or experimental data available in the literature for this molecule.

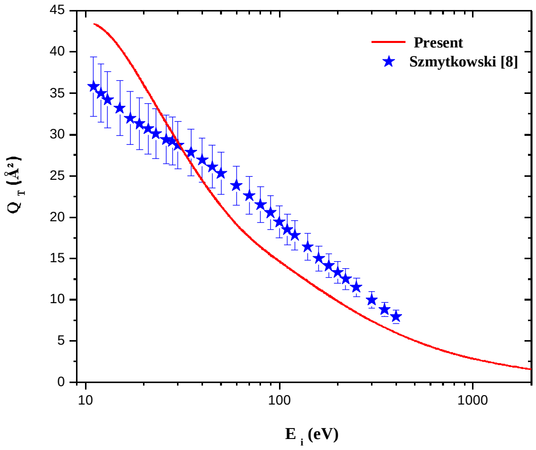

Fig. 2 Total cross section of e- C_2H_4O. Solid line represents present data and stars gives the experimental values from Szmytkowski et al [8].

Figure 2 shows comparison of total cross section for e – C_2H_4O scattering. Present results are in overall agreement with measured values of Szmytkowski et al [8]. At low energies present results are slightly higher than Szmytkowski et al [8]. This may be due to the fact that we have employed group addititvity approach which will overestimate at low energies. There are no other theoretical or experimental results available to best of our knowledge.

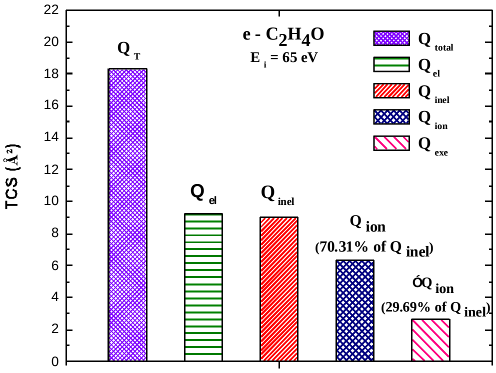

Fig. 3 Bar Chart of various total cross sections at incident energy E_i=65 eV.

Figure 3 shows bar chart for various total cross sections for e – C_2H_4O scattering at 65 eV. Bar chart gives us pictorial comparison of mutual contribution of various cross sections to total cross section. At 65 eV, total elastic and total inelastic cross sections are almost 50%. Also total ionization cross section is 70% of total inelastic cross section while total ionization cross section is 30% of total inelastic cross section.

CONCLUSION

We have calculated total and ionization cross section for ethylene oxide molecule within the 11 - 2000 eV incident energy range. The method employed here is the Spherical Complex Optical Potential method and Complex Scattering Potential – ionization contribution method. These methods are well established for obtaining cross section with reasonable accuracy. The present total ionization cross section obtained shows a maximum centred near 85eV which is very well replication by the theoretical values of Szmytkowski et al [8]. The comparison is quite good throughout the energy range. We have also calculated the total cross section and at the intermediate and high impact energies up to 2 keV. This is in reasonable agreement with the experimental cross section by Szmytkowski et al [8]. The slight variation in the cross section may be due to the fact the group additivity method adopted here might overestimate the cross section at low energies. Further, the inconsistencies present in the total cross section may be rectified once more theoretical and experimental works will be available in the future. We are quite sure that present work will inspire other researchers to look into this less studied, but very important molecule, ethylene oxide.

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