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Computation of total electron scattering cross sections for molecules of astrophysical relevance

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Abstract. In this paper we report calculations of various total cross sections namely total elastic \((Q_{el})\), total ionization \((Q_{ion})\), total (complete) cross sections \((Q_T)\) and grand total cross sections \((Q_{TOT})\) for the impact of electrons on methyl compounds namely, methanol, methylamine and total ionization cross sections on reactive diatomic radical SO and SO₂ molecule at energies from circa threshold to 2000 eV. We have employed the ‘Spherical Complex Optical Potential’ (SCOP) formalism to evaluate \(Q_{el}, Q_{inel}, Q_T\) and \(Q_{TOT}\) and used our semi-empirical, ‘Complex Spherical Potential – ionization contribution’ (CSP-ic) method to derive \(Q_{ion}\). These results are compared with available experimental and other theoretical data and overall good agreement is observed.

1. Introduction

The list of astrophysically relevant molecules is long and growing. The study of dynamics and cross sections of electron molecule collisions forms the essential basis for understanding the characteristics of a target molecule. Moreover relations between electron scattering and physio-chemical properties of target molecules have been investigated since the earliest systematic measurements of these cross sections. These correlations indicate the role of target properties in the scattering process, while the semi-empirical formulae describing these correlations will help to estimate total cross sections of targets that are still lacking the experimental data or calculations.

The total cross sections including elastic plus all energetically possible inelastic channels for electron molecule systems are important in many applied sciences. Here we are interested in the intermediate and high-energy region (from ionization threshold up to 2 KeV) where almost all inelastic channels (rotational, vibrational and electronic excitation, ionization, dissociative processes etc) are open. Moreover, in order to develop understanding of the basic chemical behavior of above listed molecules of astrophysical relevance, the data on the total elastic, inelastic and ionization cross sections would prove crucial and therefore such study has attracted theoreticians and experimentalists in the last few decades.
Among the targets considered in this paper dipolar SO molecule is an example of a reactive diatomic radical. The SO radical is an abundant constituent of plasma containing sulfur dioxide. SO is readily produced by electron impact and ion impact dissociation and by photo dissociation of the parent SO\(_2\) molecule [1-3]. Electron collisions with SO, in particular the electron-impact induced ionization and dissociation of SO, play an important role in a quantitative understanding of the fundamental collision processes and the plasma chemistry in SO\(_2\) containing plasma. Electron collisions with the SO\(_2\) molecule are important in many areas of application ranging from the SO\(_2\) containing plasma torus around Jupiter and its satellite to diffuse-discharge switches to the plasma assisted treatment of biocompatible materials and biomedical surfaces [4].

Molecules involving carbon, hydrogen and oxygen have received much scientific interest in the field of molecular physics as prototypes of polyatomic molecules. Discovery of simple alcohols like methanol and methylamine in the interstellar space and in the atmosphere of planets in our own solar system has prompted the theoreticians and experimentalists to investigate electron impact cross sections in particular ionization cross sections. Further for In order to understand the behavior of these molecules in natural systems and in the laboratory, various reliable absolute cross sections are needed. Understanding of the formation of molecules containing carbon, nitrogen and hydrogen in Interstellar medium (ISM) is important because these are the building blocks of proteins and DNA [5].

In spite of the importance of these molecules, the information available for them is very scarce. Tarnovsky et al [1] have reported measurements of absolute partial ionization cross sections for the formation of parent and fragment ions resulting from the electron-impact ionization and dissociative ionization of SO free radical from threshold to 200 eV. Deustch et al [6] have calculated total single ionization cross sections using a modified additivity rule. Except these results there is no other data available in the literature for SO to the best of our knowledge. Hence the study of this molecule becomes important. Compared to SO molecule, SO\(_2\) is studied more intensively. There are numerous experimental investigations compared to theoretical data [4]. The measurement of total cross section is reported by Szymkowsk and Maciag [7] while total ionization cross sections are reported by Basner et al [4] and Cadez et al [8].

Szymkowsk and Krzysztofowicz [9] have reported the total cross sections for methanol and methyl amine in the range 1 to 250 eV. Sueoka et al [10] have also reported the total cross sections for methanol. But no data either theoretical or experimental are available for total elastic cross sections for methanol. Duric et al [11] and Srivastava et al [12] have reported ionization cross sections for methanol. Very recently Rejoub et al [13] have determined the total and partial ionization cross sections for simple alcohols. For methyl amine the total cross sections are reported by Szymkowsk and Krzysztofowicz [9] and Schmieder [14]. Despite the importance of electron scattering from methylamine, not much is known about any theoretical calculations or experimental data for total elastic and total ionization cross sections. The total elastic cross sections for methanol is also not seen in the literature and hence probably reported here for the first time perhaps.

2. Theoretical Methodology

We briefly describe the theoretical formalism employed here to determine various total cross sections (TCS) for the impact of electrons on the targets studied. A more detailed discussion can be found in our earlier papers [15 -21]. Our aim in this paper is to calculate \(Q_{el} \), \(Q_{tot} \) and \(Q_T \).
and to study their relative contributions to the total (complete) cross sections, $Q_T$ for the chosen targets. Towards this goal, we have employed the well-known ‘spherical complex optical potential’ (SCOP) formalism, through which the total elastic cross sections $Q_{el}$ and its inelastic counterpart, $Q_{inel}$ are obtained such that,

$$Q_T(E_i) = Q_{el}(E_i) + Q_{inel}(E_i)$$  \hfill (1)$$

For the polar molecules like CH$_3$OH and CH$_3$NH$_2$, we have also determined the dipole rotational excitation cross section $Q_{rot}(D, E_i)$. We can then define the grand total cross section by

$$Q_{TOT}(E_i) = Q_T(E_i) + Q_{rot}(D, E_i)$$  \hfill (2)$$

The dipole rotational excitation cross section $Q_{rot}(D, E_i)$ is calculated using the first Born approximation for a molecular dipole of strength ‘$D$’ [15].

In the present range of electron energy (threshold to 2 keV), many scattering channels that lead to discrete as well as continuum transitions in the target are open. Therefore we represent the electron-molecule system by a complex potential,

$$V(r, E_i) = V_r(r, E_i) + i V_i(r, E_i), \text{ such that}$$  \hfill (3)$$

$$V_r(r, E_i) = V_{tr}(r) + V_{ex}(r, E_i) + V_{pol}(r, E_i)$$  \hfill (4)$$

The three terms on the RHS of the equation (4) represent the various real potentials arising from the electron target interaction namely, static, the exchange and the polarization potentials respectively. The most important basic input for evaluating all these potentials is the charge density of the target. This is obtained from the spherically averaged molecular charge-density $\rho(r)$, which is determined from the constituent atomic charge densities derived from the wave functions of Bunge and Barrientos [22]. The molecular $\rho(r)$ is renormalized to incorporate the covalent bonding as in our earlier papers [15-21].

For the exchange potential, we have used Hara’s ‘free electron gas exchange model’ [23]. And for the polarization potential $V_{pol}$, Zhang et al [24] has given a smooth form at all $r$, which has a correct asymptotic form $(-\alpha / 2r^4)$ at large ‘$r$’ and approaches free electron-gas correlation energy $V_{co}(r)$ proposed by Perdew and Zunger [25] in the near target region as

$$V_p(r) = -\frac{\alpha}{2(r^2 + r_{CO}^2)}$$  \hfill (5)$$

where the constant $r_{CO}$ can be determined by letting $V_p(0) = -\alpha / 2r_{CO}^4 = V_{co}(r = 0)$ and $\alpha$ is the average dipole polarizability. This potential model has been proved fairly successful to TCS for electron atom scattering [25].

Finally, the imaginary part $V_i$ of the complex potential is the absorption potential which represents approximately the combined effects of all inelastic channels. Here we have employed a well-known non-empirical quasi-free model form given by Staszeweska et al [26], see also Fujimoto and Lee [27]. Thus,
The local kinetic energy of the incident electron is

\[ T_{\text{loc}} = E_i - (V_{\text{in}} + V_{\text{ex}}) \]  

The absorption potential is not sensitive to long range potentials like \( V_{\text{pol}} \). In equation (6), \( p^2 = 2E_i \), \( k_F = \left( \frac{3\pi^2 \rho(r)}{10} \right)^{1/3} \) 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 \( A_0, A_2, A_3 \) occurring in the equation (6) depend differently on \( \rho(r), \Delta, E_i \) and \( I \) (Ionization threshold of target). Detailed expressions of these functions are given in Staszeweska et al [26] and also in Fujimoto and Lee [27]. The energy parameter \( \Delta \) determines a threshold below which \( V_{\text{abs}} = 0 \), and the ionization or excitation is prevented energetically. We have modified the original model, by considering \( \Delta \) as a slowly varying function of \( E_i \) around \( I \). A preliminary calculation is done with a fixed value \( \Delta = I \), but \( \Delta \) as a variable accounts for the screening of the absorption potential in the target charge-cloud region (Blanco & Garcia [28]), and also yields better agreement with experimental and other data in many cases. The modification introduced in our paper has been to assign a reasonable minimum value \( 0.8I \) to \( \Delta \) and expressing this parameter as a function of \( E_i \) around \( I \), as follows;

\[ \Delta(E_i) = 0.8I + \beta(E_i - I) \]  

Now let us say that \( E_p \) is the value of \( E_i \) at which our \( Q_{\text{inel}} \) attains maximum. In equation (8) \( \beta \) is then obtained by requiring that \( \Delta = I + 1 \) (eV) at \( E_i = E_p \), beyond which \( \Delta \) is held constant. The expression for \( \Delta(E_i) \), equation (8), is meaningful since \( \Delta \) fixed at \( I \) would not allow even excitation at incident energy \( E_i \leq I \). On the other hand, if parameter \( \Delta \) is much less than the ionization threshold, then \( V_{\text{abs}} \) becomes unduly high near the peak position. In short the present form of \( \Delta(E_i) \), equation (8) balances all these aspects and allows us to obtain satisfactory values of \( Q_{\text{inel}} \) for a given target. After generating the full complex potential given in Equation (3) for a given electron-target system, we solve the Schrödinger equation to get complex phase shifts which are used to find the cross sections given in Equation 1.

The total inelastic cross section, \( Q_{\text{inel}} \), cannot be measured directly and this restricts the scope of the traditional calculations. The total inelastic cross section, \( Q_{\text{inel}} \), can not be measured directly, but the experimental quantity is total ionization cross section, \( Q_{\text{ion}} \), which is contained in \( Q_{\text{inel}} \). \( Q_{\text{inel}} \) can be partitioned into two main contributions viz.

\[ Q_{\text{inel}}(E_i) = \sum Q_{\text{exc}}(E_i) + Q_{\text{ion}}(E_i) \]  

where the first term is the sum over total excitation cross sections for all accessible electronic transitions. The second term is the total cross section of all allowed ionization processes induced by the incident electrons. The first term arises mainly from the low-lying dipole allowed transitions for which the cross section decreases rapidly at higher energies. Now, the second term in equation (9), electron impact ionization corresponds to infinitely many open channels, as against the electronic excitation, which comes from a small number of discrete scattering channels. The second term in equation (9), corresponds to transition to continuum state.
Therefore, ionization contribution in $Q_{\text{inel}}$ increases as the incident energy increases, thereby making $Q_{\text{ion}}$ to dominate in $Q_{\text{inel}}$. Thus from equation (9),

$$Q_{\text{inel}}(E_i) \geq Q_{\text{ion}}(E_i)$$

(10)

There is no rigorous way to project out $Q_{\text{ion}}$ from $Q_{\text{inel}}$. But in order to achieve this, a reasonable approximation can be evolved by starting with a ratio function,

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

(11)

Perhaps a first ever estimate of ionization in relation to excitation processes was made by Turner et al [29]. They concluded from semi-empirical calculations that in gaseous water (H$_2$O), ionization was more probable than excitation above $\approx$30 eV. If $\sigma_{\text{ion}}$ and $\sigma_{\text{exc}}$ are the cross sections of ionization and excitation respectively, then above 100 eV [29],

$$\sigma_{\text{ion}}/(\sigma_{\text{ion}} + \sigma_{\text{exc}}) \approx 0.75$$

(12)

Since the usual complex potential calculations do not help in determining ionization contribution from the inelastic cross section, we have introduced a method based on the equation (11). In Complex Scattering Potential – ionization contribution (CSP-ic) method, the energy dependence of $R(E_i)$ is given by the following relation [12-15]

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

(13)

where the incident energy is scaled to the ionization potential $I$ through a dimensionless variable,

$$U = \frac{E_i}{I}$$

(14)

Equation (13) involves dimensionless parameters $C_1$, $C_2$, and ‘$a$’, which are determined by imposing three conditions on the function $R(E_i)$ as discussed in earlier papers [15-21]. Specifically, we have $0 \leq R \leq 1$, such that

$$R(E_i) = 0 \quad \text{for} \quad E_i \leq I$$

(15-a)

$$R(E_i) = R_p \quad \text{for} \quad E_i = E_p$$

(15-b)

$$R(E_i) \equiv 1 \quad \text{for} \quad E_i > E_p$$

(15-c)

Here, $R_p \approx 0.7$ stands for the value of the ratio $R$ at $E_i = E_p$. The choice of this value is approximate but physically justified. The peak position $E_p$ (typically around 50 eV) occurs at an incident energy where the discrete excitation cross sections are on the wane, while the ionization cross section is rising fast, suggesting that the $R_p$ value should be above 0.5 but still below 1. We follow the general trend observed in well known targets like Ne, Ar, O$_2$, N$_2$, CH$_4$ etc. Joshipura et al [18-19], Vinodkumar et al [15-17], Turner et al [29] and Karwasz et al [30], that near the peak of ionization, the contribution of the cross section $Q_{\text{ion}}$ is about 70-80% in the total inelastic cross section $Q_{\text{inel}}$ and the same increases with energy. The choice of $R_p$ follows from the general
observation that at energies close to peak of ionization, the contribution of molecular $Q_{\text{mol}}$ is about 70 – 80% in the total inelastic cross sections $Q_{\text{inel}}$. For a number of stable molecules like O$_2$, H$_2$O, CH$_4$, SiH$_4$ etc for which the experimental cross sections $Q_{\text{ion}}$ are known accurately, the ratio rises steadily as the energy increases above threshold. [17-19, 29, 30] This behavior is attributed to the faster fall of the first term $\sum Q_{\text{exc}}$ in equation (1). However the choice of $R_p$ in equation (15) is not rigorous and it introduces uncertainty in the final results. For about two dozen atomic and molecular targets examined by us so far, the said uncertainty is found to be within the experimental errors ~10-15% generally involved in most of the ionization measurements.

3. Results and discussion

Here we have used the well known SCOP formalism to calculate the total elastic and total inelastic cross sections. They are added coherently to give us the total (complete) cross sections $Q_T$. Further, for the polar molecule, the rotational excitation cross section, $Q_{\text{rot}}$, is calculated separately using the first Born approximation and then added incoherently to the total cross section to evaluate the grand total cross section $Q_{\text{TOT}}$. Finally we applied our CSP-ic method to extract the total ionization cross sections from total inelastic cross sections. The summed total excitation cross sections are obtained as a byproduct vide Equation (9).

Total ionization cross sections, $Q_{\text{ion}}$, for e- SO, SO$_2$, CH$_3$OH and CH$_3$NH$_2$ and grand total cross section $Q_{\text{TOT}}$ (this is not in table 1!!), complete cross sections $Q_T$ for CH$_3$OH and CH$_3$NH$_2$ are exhibited in Table 1 in ($\text{Å}^2$). Also, the presently calculated $Q_{\text{TOT}}, Q_T, Q_{\text{el}}$ and $Q_{\text{ion}}$ for all the listed targets are plotted along with available other theoretical and experimental data. Low energy behavior of these cross sections is of much scientific interest because various elastic and inelastic phenomena occur around the threshold of the target. The sum total (complete) cross sections provide a useful sum-check of the different investigations. The CSP-ic method defined through the equations (8-15) has already been employed successfully to obtain total ionization cross sections of a number of atomic–molecular targets as demonstrated in Joshipura et al [19,21] and Vinodkumar et al [15-17].

Table 1: Various total cross sections for e-SO, SO$_2$, CH$_3$OH and CH$_3$NH$_2$ in ($\text{Å}^2$)

| $E_i$ (eV) | SO | SO$_2$ | CH$_3$OH | CH$_3$NH$_2$ |
|-----------|----|--------|----------|-------------|
|           | $Q_{\text{ion}}$ | $Q_T$ | $Q_{\text{TOT}}$ | $Q_{\text{ion}}$ | $Q_T$ | $Q_{\text{TOT}}$ | $Q_{\text{ion}}$ | $Q_T$ | $Q_{\text{TOT}}$|
| 15        | 0.88 | 0.27  | 0.21  | 25.15 | 25.65 | 37.58 | 1.15 | 13.78 | 16.99 | 25.50 |
| 20        | 2.28 | 1.37  | 1.04  | 21.5  | 22.65 | 31.78 | 3.08 | 13.59 | 18.72 | 24.28 |
| 25        | 3.36 | 2.17  | 1.98  | 18.00 | 20.79 | 28.23 | 4.46 | 13.03 | 19.36 | 23.55 |
| 30        | 4.02 | 2.62  | 2.78  | 15.4  | 19.28 | 25.56 | 5.31 | 12.19 | 19.24 | 22.63 |
| 35        | 4.40 | 3.19  | 3.41  | 13.28 | 18.04 | 23.50 | 5.79 | 11.28 | 18.71 | 21.61 |
| 40        | 4.64 | 3.70  | 3.89  | 11.49 | 16.83 | 21.65 | 6.04 | 10.41 | 18.03 | 20.55 |
| 50        | 4.95 | 4.33  | 4.42  | 8.89  | 14.84 | 18.75 | 6.12 | 9.02  | 16.62 | 18.84 |
| 60        | 5.06 | 4.84  | 4.55  | 7.34  | 13.51 | 16.82 | 6.03 | 7.98  | 15.43 | 17.40 |
| 70        | 5.02 | 5.11  | 4.50  | 6.43  | 12.48 | 15.34 | 5.90 | 7.19  | 14.47 | 16.18 |
| 80        | 4.97 | 5.36  | 4.37  | 5.88  | 11.72 | 14.23 | 5.73 | 6.6   | 13.65 | 15.16 |
| 90        | 4.91 | 5.47  | 4.30  | 5.51  | 11.08 | 13.35 | 5.55 | 6.14  | 12.94 | 14.29 |
| 100       | 4.85 | 5.60  | 4.14  | 5.22  | 10.55 | 12.59 | 5.38 | 5.77  | 12.33 | 13.55 |


Consider first the exotic free SO radical. In Fig.1, we have plotted total ionization cross sections for SO and compared with the available results of Tarnovsky et al [1]. Very good agreement is observed between the measured values of Tarnovsky et al and present results from threshold to 100 eV, but above 100 eV the values of Tarnovsky et al [1] are lower than our values. The calculated total single ionization cross sections [1] using the modified additivity rule for (SO+) are shown by the dashed curve in Figure 1.

| Temperature (eV) | Cross Section (10^-16 cm²) |
|------------------|-----------------------------|
| 200              | 4.15 5.22 3.04 3.86 7.51 8.58 4.13 4.01 9.17 9.81 |
| 300              | 3.60 4.63 2.43 3.23 6.02 6.74 3.43 3.31 7.58 8.02 |
| 400              | 3.18 4.11 2.05 2.82 5.10 5.65 2.95 2.88 6.73 7.07 |
| 500              | 2.86 3.68 1.77 2.52 4.46 4.91 2.60 2.58 5.87 6.09 |
| 600              | 2.60 3.33 1.56 2.29 3.98 4.35 2.33 2.35 5.15 5.38 |
| 700              | 2.39 3.04 1.41 2.09 3.59 3.92 2.11 2.16 4.65 4.84 |
| 800              | 2.21 2.79 1.27 1.94 3.29 3.29 1.93 2.01 4.24 4.41 |
| 900              | 2.06 2.58 1.16 1.81 3.04 3.04 1.78 1.88 3.91 4.06 |
| 1000             | 1.93 2.40 1.09 1.69 2.82 2.82 1.65 1.77 3.63 3.77 |
| 2000             | 1.16 1.36 0.64 0.97 1.63 1.63 0.97 1.15 2.40 2.47 |
Fig. 1: Total ionization cross sections for $e^{-}$ – SO scattering

Fig. 2 shows the comparison of total ionization cross sections of SO$_2$ molecule on electron impact. From threshold to 50 eV there is very good agreement of present results with theoretical values of Kim et al [31] and the experimental values of Cadez et al [8] and Basner et al [4]. But above 50 eV, present results are in good accord with experimental values of Cadez et al but they are lower compared to theoretical values of Kim et al [30] and experimental values of Basner et al [4]. Basner et al have reported 18 – 25% error in their measurements and our results fall within their experimental uncertainties.
Consider next methanol which is more widely studied molecule compared to other targets investigated here. Fig 3 shows the comparison of grand total cross section $Q_{TOT}$, total (complete) cross sections $Q_T$ and total ionization cross sections $Q_{ion}$ for e- CH$_3$OH scattering. The present $Q_{TOT}$ is found to be in good agreement with the experimental values of Szmytkowski and Krzysztofowicz [9] and Sueoka et al [10] between the energies 50 -200 eV while at lower energies the experimental values are quite lower than our $Q_{TOT}$ values. This discrepancy especially at lower energies can be attributed as mentioned by Itikawa and Mason [32] in connection with e- H$_2$O scattering, to the dipolar nature of the target that affects measurements of complete total cross sections $Q_{TOT}$. The present total ionization cross sections are in excellent agreement with available experimental data [11] upto 100 eV beyond which their values are slightly higher than our values. There is no data either theoretical or experimental for total elastic cross sections in the literature to the best of our knowledge.

Fig 2 : Total ionization cross sections for e – SO$_2$ scattering
Finally Fig 4 shows the dependence of various total cross sections as function of incident energy for $e-CH_3NH_2$ scattering. $CH_3NH_2$ is a polar molecule with permanent dipole moment of 1.31 Deybe ‘D’ [6]. Hence it gives rise to rotational excitation and the rotational cross sections are significant at lower energies below 100 eV which can be noted in the figure. At low energies there is clear distinction between $Q_T$ and $Q_{TOT}$ curve while at high energies both curves match reflecting the fact that at very high energy there is negligible contribution to the total cross section from the rotational excitation. Despite the importance of methylamine there is not much work found in the literature. However for $Q_T$, there are experimental results of Szmytkowski and Krzysztofowicz [6] from low energy to 250 eV. There is good agreement between present $Q_{TOT}$ and experimental values of Szmytkowski and Krzysztofowicz between 50 eV to 250 eV. Below 50 eV there is a discrepancy between the two results. There is no comparison either theoretical or experimental for total elastic as well as total ionization cross sections to best of our knowledge. There is probably no theoretical or experimental data for total elastic and total ionization cross sections found in the literature.

Fig 3 : Various total cross sections for $e-CH_3OH$ scattering
4. Conclusion

In conclusion, this paper presents our calculations on electron impact cross sections $Q_{TOT}$, $Q_{el}$, $Q_{inel}$ and $Q_{ion}$ for the methyl compounds and total ionization cross sections $Q_{ion}$ for diatomic radical SO and SO$_2$ molecule. The resulting $Q_{TOT}$ values are reliable and agree in general. The CSP-ic method adopted here though not rigorous is capable of yielding reasonable total ionization cross section as a fraction of total inelastic cross section at a given incident energy. The present comparison can help in obtaining a recommended data set for listed molecules. Besides this, we can also conclude about the relative importance of various collision processes like elastic scattering, ionization etc, induced by electrons. As for the lesser known SO radical and CH$_3$NH$_2$ molecule, it is hoped that the present work will stimulate experimental and further theoretical research on electron scattering and ionization.

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