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# ELECTRON AND POSITRON IMPACT IONIZATION CROSS SECTIONS FOR $CO_2$ MOLECULE - THEORETICAL INVESTIGATIONS

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## ABSTRACT

**In this paper we have calculated total ionization cross sections of $CO_2$ by electron and positron impact using the complex potential formalism. Our total inelastic ($Q_{inel}$) cross section contains $Q_{ion}$, $Q_{Ps}$, $\Sigma\, Q_{exc}$. Our goal in the paper is to calculate $Q_{ion}$ basically from $Q_{inel}$ for electrons and positrons separately. We have extracted $Q_{ion}$ from $Q_{inel}$ using the method 'Complex Scattering Potential – ionization contribution' (*CSP*- ic), at energies from threshold to 2000 eV. It is of interest to see how the same basic method works out for electron and positron impact ionization on the same target $CO_2$. The results are compared mutually, along with other available data.**

***Keywords***: *Electron and positron impact scattering, complex potential, ionization cross sections*

## INTRODUCTION

Carbon dioxide is an important molecule in view of its occurrence in the atmospheres of Venus and Mars. On the Earth its behavior has to be carefully scrutinized with respect to the global warming process. In laboratory $CO_2$ is widely used in gaseous discharges or in low temperature plasma devices. Various cross sections of electron collisions with this molecule were first compiled by Itikawa and Shimizu [1] and were reviewed later on by Itikawa [2].

Electron impact ionization of atoms and molecules is of fundamental importance in the production of atomic/molecular ions and extensive ion molecular reactions in the atmospheric science. It is also important in modeling plasma processes. To understand the electron impact ionization processes in space and laboratory ionization cross sections are needed. Tawara [3] noticed the role of such process in nuclear fusion devices and also published a review of data on electron impact cross sections of $CO_2$. Also Shirai *et al* [4] evaluated the cross sections for impurity species involved in the electron collision processes and Karwasz *et al* [5] published a review article on the few polyatomic molecules like $CO_2$. Straub *et al* [6] have reported the absolute partial ionization cross sections for $CO_2$ from threshold to 1000 eV by electron impact. On the theoretical front Kim et al [7] have obtained the cross section for $CO_2$ by employing their Binary Encounter Bethe (BEB) model for electron impact. S pal [8] have reported the partial double differential and partial single differential cross sections for $CO_2$ molecule by electron impact at 100 to 500 eV.

Positron as an alternative probe for electron has also been used for the study of atoms, molecules and matter in bulk. Interaction of positron with atoms and molecules differs from electron interactions due to opposite sign of the static potential and absence of exchange potential. Several experimental and theoretical investigations of positron - molecule scattering have been made [9-12]. In the present paper, our aim is to apply an identical theoretical method to electron as well as positron ionization of the title molecule. Thus we have calculated the total cross sections (elastic, inelastic, excitation and total) from the SCOP (Spherical Complex Optical Potential Method) and extracted ionization cross sections through CSP-ic (Complex scattering Potential- ionization contribution) method developed by Sardar Patel University group [12-14]. Some details of the method are outlined in the next section.

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## THEORETICAL METHODOLOGY FOR ELECTRON SCATTERING

The theoretical method (*CSP-ic*) has successfully been in vogue for the past decade or so and has been discussed adequately in our recent papers [12-14]. Briefly the method basically treats elastic and inelastic electron scattering simultaneously in a complex spherical potential $V(r, E_i) = V_R(r, E_i) + iV_I(r, E_i)$, with $r$ as the radial distance from the mass-centre of the target. Further $V_R(r, E_i)$ is the real part and $V_I(r, E_i)$ is imaginary part of the total potential. The real part consists of the sum of static ($V_{st}$), exchange ($V_{ex}$) and polarization ($V_{pol}$) interaction potentials, and the imaginary term is the absorption potential $V_{abs}$. While the static potential is determined directly from the target charge density, the exchange potential is calculated using Hara's free gas exchange model [15] and polarization potential is calculated using Zhang model [16]. The molecular radial charge density is constructed through a single-centre expansion of the atomic charge densities at the molecular mass-centre [17], and is available with the UK R-matrix code Quantemol-N. Detailed expressions of real and absorption potentials can be found in [18-20].

The total (Complete) cross section $Q_T$ obtained from the complex spherical potential is such that,

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

Where $Q_{el}$ is total elastic cross section and $Q_{inel}$ is the total (cumulative) inelastic cross section at incident energy $E_i$. Now, at energies of our interest, the inelastic channels in electron- molecule scattering consist of discrete electronic excitations as well as ionizations, so that we can bifurcate the total inelastic cross section as,

$$Q_{inel}(E_i) = \sum Q_{exc}(E_i) + \sum Q_{ion}(E_i) \qquad (2)$$

The first term on right hand side of equation (2) is the sum over total discrete excitation cross sections for all accessible electronic transitions in the molecule, while the second term indicates the sum of the total cross sections of all allowed (direct, dissociative, single, double etc.) ionization processes. In the present energy range the single ionization dominates, so that we denote the second term simply by $Q_{ion}$, which includes direct as well as dissociative ionization. The first term in equation (2) arises mainly from the electronic excitations having thresholds [21] below the first ionization threshold $I$ *(=13.77eV)*. The corresponding total excitation cross sections become smaller than $Q_{ion}$ progressively above $I$. Hence, as the incident energy increases the second term in equation (2) dominates over the first, and therefore a method has been developed [22, 23] to derive the total ionization cross section $Q_{ion}$ from the inelastic quantity $Q_{inel}$. The imaginary absorption term $V_{abs}$ in the complex potential is an energy dependant potential that accounts collectively for all possible inelastic scattering channels, and has the generic form, first developed by Staszewska *et al.* [24], in atomic units, as follows

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

Here, $v_{loc}$ is the local speed and $T_{loc}$ the local kinetic energy of the external electron, and $\sigma_{ee}$ denotes the average cross section for binary collision of the external electron with a target electron. In equation (3), $p^2 = 2E_i$, $k_F$ is the Fermi wave-vector magnitude and $\Delta$ is an energy parameter. The Heaviside step-function $\theta(x) = 1$ for $x>0$, and is zero otherwise. The dynamic functions $A_1$, $A_2$ and $A_3$ are different functions of the target charge density $\rho(r)$, as also on $\Delta$, $E_i$ *and* $I$. The energy parameter $\Delta$ basically denotes a threshold below which the potential $V_{abs} = 0$. The choice of this parameter is crucial and its role has been emphasized in our recent publications [18-20, 25]. Accordingly we consider the parameter $\Delta$ *as a function of* $E_i$ *over a small range of energy.* The $V_{abs}$ thus modified thorough $\Delta$ is discussed in [22] and introduced into the Schrödinger equation which we solve numerically, to extract the complex partial wave phase-shifts $\delta_l$, for different angular momenta $l$ at different impact energies.

Now, the inelastic cross section $Q_{inel}$ is cumulative in the sense that it is not a directly measurable quantity in a single experiment. Therefore in view of the equation (2), we have,

$$Q_{inel}(E_i) \geq Q_{ion}(E_i) \quad (4)$$

At incident energies above $I$, the ionization processes begin to play a dominant role due to the availability of infinitely many open channels of scattering. There is no rigorous way of projecting out $Q_{ion}$ from the theoretical quantity $Q_{inel}$. Hence, in our recent publications we have introduced an approximation by defining a ratio,

$$R(E_i) = \frac{Q_{ion}(E_i)}{Q_{inel}(E_i)} \quad (5)$$

## THEORETICAL METHODOLOGY FOR POSITRON SCATTERING

For positrons, our theoretical method CSP-ic has been discussed in detail in [26] and is well explained for electrons in [25, 26] also as above. Therefore, only essential details of the calculations are given here. The method basically starts with positron scattering in complex potential as follows: $V(r, E_i) = V_R(r, E_i) + iV_I(r, E_i)$. Here the real part consists of static potential $V_{st}(r)$ and polarization potential $V_{pol}(r)$ and imaginary part consists of absorption potential $V_{abs}(r)$ as described in [27]. The polarization potential we have used is described in [28]. The imaginary absorption term Vabs in the complex potential is an energy-dependent potential that accounts for all possible inelastic scattering channels cumulatively, and has the generic form, developed by [25, 28, 29]. Presently, for $CO_2$ we have vary the energy gap $\Delta$ from $E_{PS}$ to its average $\Delta_{max} = (E_{PS} + IE)/2$ excitation threshold [26], also mentioned in table 1 along with other parameters. Energy gap $\Delta$ varies as following manner in electron and positron scattering, $\Delta = \Delta_{min} + \beta(E_i - \Delta_{max})$

The detail explanation of above expression is explained in previous paper [26].

**Table 1:** Parameters of $e^-$- $e^+$ $CO_2$

| Target | Ionization potential($I_p$)[a] | Energy at the peak $E_p$ (eV) | Energy gap $\Delta_{min}$ (eV) | Energy gap $\Delta_{max}$ (eV) |
|---|---|---|---|---|
| $e^-$ - $co_2$ | 13.77 | 75 | 11.016 | 13.77 |
| $e^+$ - $co_2$ | | 70 | 6.97 | 10.37 |

After generating the full complex potential of eq. (7) for a given positron–molecule system, we treat it exactly in a partial wave analysis by solving the first-order differential equations for the real ($\delta R$) and imaginary ($\delta_I$) parts of the complex phase shifts function. This is done same as we have done in electron scattering (equation 1).

In case of positron scattering the total inelastic cross-section results from contributions of positronium formation, excitations and ionizations of the target atom, so that [26]

$$Q_{inel}(Ei) = Q_{Ps} + Q_{exc} + Q_{ion} \quad (6)$$

The first term on the right-hand side of eq. (6) is positronium formation cross-section, second term is the sum over total discrete-excitation cross-sections for all accessible transitions in the atom, while the third term indicates the sum of the total cross-sections of all allowed (single, double etc.) ionization processes. Presently the last term will be simply denoted by Qion.

Now, we introduce the quantity

$$Q_{in}(Ei) = Q_{inel} - Q_{Ps} \quad (7)$$

This is such that $V_{abs} = 0$, for $Ei \leq \Delta$. The cross-section $Q_{inel}$ as calculated from our complex potential contains $Q_{Ps}$, $Q_{exc}$ and $Q_{ion}$ as in eq. (6). To ascertain the contribution of $Q$ion, first we have to subtract $Q_{Ps}$ from the calculated $Q$inel in order to obtain $Q_{in}$, i.e. ($Q_{ion} + \Sigma Q_{exc}$). It is possible to extend the usual complex potential formulation by a method called complex scattering potential-ionization contribution (CSP-ic) to deduce $Q$ion from the $Q$in.

To employ the method presently for electrons and positrons, let us introduce a break-up ratio function,

$$R(E_i) = \frac{Q_{ion}(E_i)}{Q_{in}(E_i)} \quad (8)$$

The further process of calculation of ionization cross sections of electron and positron scattering remain same as discussed below

## CSP- *ic* METHOD FOR ELECTRON AND POSITRON

The ratio $R = 0$ when $E_i \leq I$. For a number of stable atomic – molecular targets like Ne, Ar, $O_2$, $CH_4$, $H_2O$, etc., for which several experimental ionization cross section data-sets are known accurately, the energy-dependent quantity $R$ is seen to be rising steadily as the energy increases above the threshold, and approaching unity at high energies. Thus,

$$R(E_i) = 0, \quad \text{for } E_i \leq I \quad (9a)$$

$$R(E_i) = R_p, \quad \text{for } E_i = E_p \quad (9b)$$

$$R(E_i) \lesssim 1, \quad \text{for } E_i >> E_p \quad (9c)$$

In equation 9(b) $R_p$ stands for the value of $R$ at $E_i = E_p$. *Generally the value of $R_p$ lies between 0.7 and 0.8.* This can be understood from the fact that, the peak position $E_p$ of the cross section $Q_{inel}$ occurs at incident energy where the discrete excitation cross section term is decreasing while $Q_{ion}$ is rising fast, suggesting the $R_p$ value to be between 0.5 and 1. An approximate determination of $R_p$ [29] based on simple arguments also points to the same conclusion. The value of $R_p$ has a bearing on the strength of electronic excitations in relation to ionization. There isn't much information available about the electron impact electronic excitations for the present targets. In the present work *we have carried out* calculations with *approximate input i.e. $R_p = 0.75$ as in equation (9b).*

Now, for the actual calculation of $Q_{ion}$ from $Q_{inel}$ we need $R$ as a continuous function of energy $E_i$ above $I$. Hence, we represent the ratio $R(E_i)$ in the following manner.

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

$$with \quad U = \frac{E_i}{I} \quad (11)$$

Justification for adopting a particular functional form of $f(U)$ i.e. second term of the right –hand-side of equation (10) is explained in [18-20]. Equation (10) involves dimensionless parameters $C_1$, $C_2$, and $a$, that depend on the target properties. The three conditions stated in equation (9a-c) are used to determine these three parameters, in an iterative manner as in [17]. Having thus obtained the parameters we calculate $Q_{ion}$ from equation (8), and therefore generate $R_p$ value from these $Q_{ion}$. The resulting $R_p$ value is used next as an input to the equation (9b) iteratively to finally calculate $Q_{ion}$.

## RESULTS AND DISCUSSION

### $e^-$-$CO_2$

In present work we have calculated ionization cross sections of $CO_2$ molecule by electron impact. We have compared our results with measurements of Straub et al [6] as well as with Kim [7], and Itikawa et al [2]. Our present results well matched with [2 and 6] at low as well as at high energies. Our result has little conflict at peak energies of Qion where as results of Kim [7] shows good agreement at peak energies.

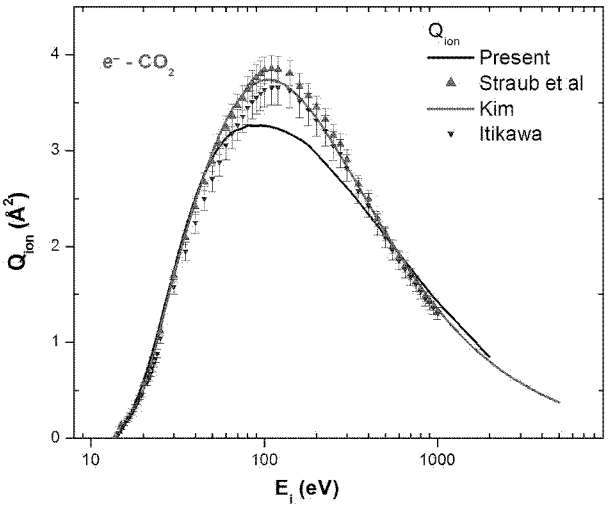


Figure 1: Total ionization cross section for $e^-$ $CO_2$ scattering. Black solid line: present Qion, red triangle: Straub *et al* [6], green solid line: Kim et al [7] and brown triangle: Itikawa [2]

### $e^+$ - $CO_2$

In positron scattering we have calculated and compared present ionization cross sections with electron impact ionization cross sections. In this comparative study we have seen that ionization cross sections of

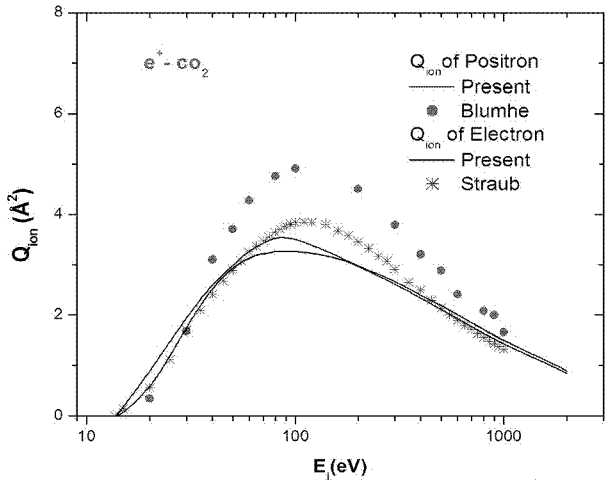


**Figure 2:** Total ionization cross section for $e^-$- $e^+$ $CO_2$ scattering. Blue solid line: present Qion by positron impact, red circle: Blumhe *et al* [30], black solid line: present Qion by electron impact and brown strike: Straub *et al* [6]

Positron impact with measurements of Bluhme *et al* [30] shows good agreement at low energies, around less than 60 eV. We have compared ionization of positron impact with our calculation of electron impact ionization of $CO_2$ molecule. We note that at high energies our $e^+$ - $CO_2$ ionization cross sections merge with present $e^-$ - $CO_2$ ionization cross section as well as with Straub *et al* [6] which is true by theoretical background. The measurements of Bluhme *et al* [30] are higher than present electron impact ionization cross sections. Present positron impact ionizations as well as results of Bluhme *et al* [30] are higher than electron impact ionization cross sections at low energy and at peak energy. At high energy the electron impact ionization cross sections of Bluhme *et al* [30] are not clearly merged with $e^-$ impact

## CONCLUSION

In conclusion we can say that on the basis of complex optical potential formalism total ionization scattering cross sections through different projectiles can be calculated. The main difference in both calculations is that polarities of the projectiles are different and electron exchange is not there in $e^+$ scattering. Also new inelastic channel of positronium formation is introduced in $e^+$ - $CO_2$ scattering. We have compared our result of both $e^-$ - $CO_2$ and $e^+$ - $CO_2$ with experimental results and it shows good agreement at low as well as higher energy region. Also we have compared total ionization cross sections for $CO_2$ by both electron and positron impact, which shows that $Q_{ion}$ by positron impact is higher than electron impact at low and intermediate energies and both are merged at higher energies.

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