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Total ionization cross sections of NO_2, CO and CS molecules due to electron impact

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Abstract. The total cross sections for NO_2, CO and CS have been calculated by Binary-Encounter-Bethe [BEB] method of Khare from threshold energy to 10 MeV due to electron impact. This model has been developed by combining the useful features of Plane Wave Born Approximation (PWBA) and BEB model of Kim. It is shown that Bethe and Mott cross section terms differ from those of the Kim [BEB] method but their sums are very close to other. Results are presented with the help of graphs. Adequate comparisons of collisional parameter have been made with other available experimental values. The calculated cross-sections are compared extensively with a number of all possible experimental data and theoretical results.

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Key words: ionization cross section, molecules, electron impact

1 Introduction

Total ionization cross-sections of molecules by electron impact are required in the study of plasma diagnostics, astrophysical and fusion applications, radiation physics, mass spectrometry, ionization in gas discharge, modeling of fusion plasmas, modeling of radiation effects for both materials and medical research, and astronomy [1], etc. NO_2 is an atmospheric pollutant, founds in troposphere and stratosphere. Nitrogen dioxide plays a role in atmospheric chemistry, including the formation of troposphere ozone. In plasma physics, ionization of NO_2 plays important role [2]. CO plays a major role in modern technology, in industrial processes such as iron smelting and as a precursor to myriad

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products. CS is also present in atmosphere. These molecules are important constituents that found at different altitudes of the atmosphere [3].

For these molecules experimentally the total ionization cross sections have been measured by various groups Lindsay *et al.* [4], Lukic *et al.* [5], Lopez *et al.* [6], Freund *et al.* [7], Hudson *et al.* [8] and theoretically calculated by Kim *et al.* [9] and Joshipura *et al.* [10]. Total cross sections for NO_2 are measured by Lindsay *et al.* [4], Lukic *et al.* [5] for energy range threshold to 1 keV whereas Lopez *et al.* [6] measured it for energy range threshold to 2000 eV. Kim *et al.* [11] used Binary-Encounter-Bethe [BEB] model to calculate total ionization cross section. Total cross sections for CO are measured by Mangan *et al.* [12], Hudson *et al.* [8], for energy from threshold ionization energy to 250 eV. However Rieke and Prepejchal [13] have measured the total cross section in the energy range 0.1 MeV to 2.7 MeV. Freund *et al.* [7] have measured the partial ionization cross sections for CS for threshold to 200 eV. According to best of our knowledge for NO_2 and CS there are no experimental data and theoretical cross sections available for high energy range. Kim *et al.* [9] have used Binary Encounter Bethe theory with the vertical ionization potential to calculate the total cross section. Joshipura *et al.* [10] have calculated the total ionization cross sections by using 'complex scattering potential-ionization contribution' method.

In 1997 Saksena *et al.* [14] proposed a model for the molecular ionization cross sections by using the plane wave born approximation (PWBA) which includes transverse as well as longitudinal interactions. They have employed the exchange and relativistic corrections. In PWBA continuum generalized oscillator strengths (CGOS) are required, which are very difficult to evaluate. Hence, they employed a semi-phenomenological relation of Mayol and Salvet [15] which expresses CGOS in terms of the continuum optical oscillator strengths (COOS). The use of the above relation breaks the expression of the ionization cross section σ_j for the j^{th} molecular orbital into two terms one representing the Bethe term (Soft collision) and other one the Mott term (hard collision). Later on this model was modified by Khare *et al.* [16] for CH_4 molecule, where $(1-\omega/E')$ was replaced by $E'/(E'+I+U)$, where ω is the energy lose suffered by incident electron in the ionizing collision, E' is the relativistic kinetic energy of incident electron, I is the ionization energy, U is the average kinetic energy of bound electron. Here $I+U$ represent the increase in kinetic energy of the incident electron due to its acceleration by the field of the target nucleus. Furthermore, they have employed the useful features of the Binary Encounter Bethe models of Kim and Rudd [11]. Following Kim *et al.* they have used the COOS $df/d\omega = NI/\omega^2$ and dropped the contribution of exchange to Bethe term. They have also shown that Bethe and Mott cross-section terms obtained by Kim *et al.* are the approximate forms of their model. Although Bethe and Mott cross-sections in Khare *et al.* model are different corresponding cross-sections of Kim [BEB] model but the total ionization cross sections obtained in both model are very close to other. In Khare *et al.* [BEB] method calculated cross sections were in better agreement with the experimental data over a wide energy range varying from threshold to several MeV.

2 Theory

Kim and his associates have carried out numbers of calculation in Binary Encounter-Bethe (BEB) model. For the j^{th} molecular orbital their total ionization cross-section, for incident energy E, is given by

$$\sigma_{jT} = \sigma_{jKBB} + \sigma_{jKMB} \tag{1}$$

where

$$\sigma_{jKBB} = \frac{AN_j}{2I_j^2(t+u_j+1)}\left[1-\frac{1}{t^2}\right]\ln t, \tag{2}$$

$$\sigma_{jKMB} = \frac{AN_j}{I_j^2(t+u_j+1)}\left[\frac{t-1}{t}-\frac{\ln t}{1+t}\right], \tag{3}$$

σ_{jKBB} and σ_{jKMB} are the Bethe's and Mott's cross–section, respectively with the following values of t and u_j

$$t = \frac{E}{I_j}, \quad u_j = \frac{U_j}{I_j}.$$

Here U_j is the average kinetic energy of the bound electron, N_j is the occupation number for the j^{th} molecular orbital, I_j is the ionization potential and $A = 4\pi a_0^2 R^2$, with R and a_0 are the Rydberg energy and first Bohr radius, respectively.

In Khare model [16] the present total ionization cross- section is

$$\sigma_{jt} = \sigma_{jpBB} + \sigma_{jpMB} + \sigma_{jjt}, \tag{4}$$

$$\sigma_{jpBB} = \frac{AN_jI_j}{(E'+U_j+I_j)}\int_{I_j}^{E}\frac{1}{\omega^3}\ln\left[\frac{\omega}{Q_-}\right]d\omega, \tag{5}$$

$$\sigma_{jpMB} = \left[\frac{AN_j}{(E'+U_j+I_j)}\right]\times\left[\left(1-\frac{2}{t+1}+fract-12t^2\right)\right.$$
$$\left.+\left(\frac{S-t^2}{2(t+1)^2}-\frac{1}{t(t+1)}\right)-\left(\frac{(t+1)}{t^2}\ln(\frac{t+1}{2})\right)\right], \tag{6}$$

$$\sigma_{jjt} = -\frac{A}{RE}M_j^2[\ln(1-\beta^2)+\beta^2]. \tag{7}$$

In Eq. (5), $Q_- = 0.5mc^2\left[\left(E(E-\omega)\right)^{0.5} - \left((E-\omega)(E-\omega_2 mc^2)\right)^{0.5}\right]^2$, where m is the rest mass of the electron, Q_- is the recoil energy, M_j^2 is equal to the total dipole matrix squared and $\beta = \frac{v}{c}$, where $v =$ incident velocity, $c =$ velocity of light.

From Eq. (4), the ionization cross-sections σ_{jt} is calculated for each orbit of the molecules for incident energy E varying from threshold ionization energy to 10 MeV. The cross-sections for each orbital are added to obtain the total cross section for the whole molecule. Eq. (5) can be evaluated numerically.

Table 1: Molecular orbital constants [17], where I denotes binding energy, U the average kinetic energy, and N the electron occupation number.

Molecules	Mol. orbital	I(eV)	U(eV)	N
NO_2	$1b_1$	562.48	794.45	2
	$1a_1$	562.48	794.46	2
	$2a_1$	431.59	602.08	2
	$3a_1$	46.11	73.41	2
	$2b_1$	41.06	79.40	2
	$4a_1$	25.00	78.97	2
	$5a_1$	21.60	56.73	2
	$3b_1$	21.46	73.27	2
	$1b_2$	21.19	51.57	2
	$4b_1$	14.95	69.09	2
	$1a_2$	14.40	65.23	2
	$6a_1$	11.23	76.20	1
CS	$2a_1$	308.84	436.58	2
	$1b_1$	245.09	509.11	2
	$3a_1$	182.00	478.18	2
	$1b_2$	181.94	478.41	4
	$4a_1$	30.24	59.97	2
	$2b_1$	18.75	58.81	2
	$5a_1$	12.76	44.37	2
	$2b_2$	11.33	41.13	4
CO	3σ	41.92	79.63	2
	4σ	21.92	73.18	2
	1π	17.66	54.30	4
	5σ	14.01	42.26	2

Rieke and Prepejchal [13] have measured the molecular cross-section in the energy range 0.1 to 2.7 MeV in terms of two collision parameters and C. Their cross sections are given by

$$\sigma_{jjt} = \frac{A}{RE}\left[M_j^2\left(\ln(\frac{\beta^2}{1-\beta^2})-1\right)+C\right].$$

3 Results and discussion

In the present paper, the total ionization cross–sections have been calculated for nitrogen dioxide (NO_2), carbon monoxide (CO) and carbon monosulfide (CS). Table 1 presents

Table 2: Collision parameters; C and M_j^2

Molecules	Calculated		Experimental[13]	
	C	M_j^2	C	M_j^2
NO_2	68.1	5.62	—-	—
CS	61.24	4.97	—-	—-
CO	42.2	3.46	35.14	3.7

the values of binding energy (I), average kinetic energy (U), electron occupation number (N) of each orbit of molecules [17] under consideration. Table 2 presents the calculated and experimental [13] values of collision parameters C and M_j^2 for the three molecules presently investigated. These values are obtained at 1 MeV.

In the Figs. 1-3 the Mott, Bethe and total cross sections are indicated separately obtained in present method and Kim *et al.* for all three molecules. These figures show that the contribution of Mott and Bethe cross sections are different in both models but their sums are very close to each other. In the Kim [BEB] model the two curves (Mott & Bethe) intersect to each other at 35 eV in the case of CO and NO_2. At low energies Mott cross sections are higher than the Bethe cross sections in Kim [BEB] method. Same thing is observed for CS at 25.5 eV. However in the Khare [BEB] method at low energies Bethe cross sections are very high in comparison of the Mott cross sections and the ratio PBB/

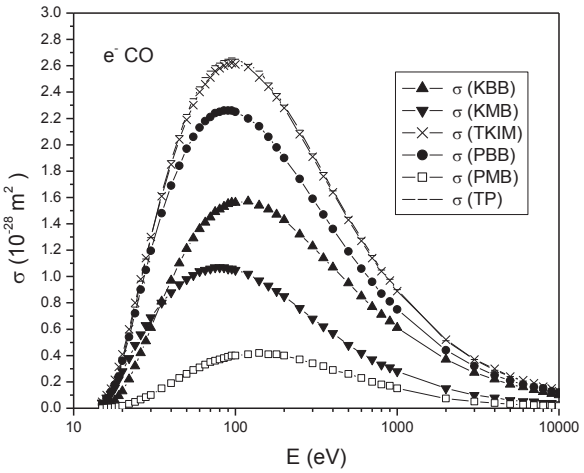

Figure 1: The present theoretical electron impact ionization cross section, compared with the electron impact ionization cross section of NO_2 by Kim *et al.*[9, 11]. Triangles ▲, Kim Bethe cross sections (KBB); inverted triangles ▼, Kim Mott cross sections (KMB); dash —, Kim total cross sections (TKIM); Circle •, present Bethe cross sections (PBB); square □, present Mott cross sections (PMB); cross -X-, and present total cross sections (TP).

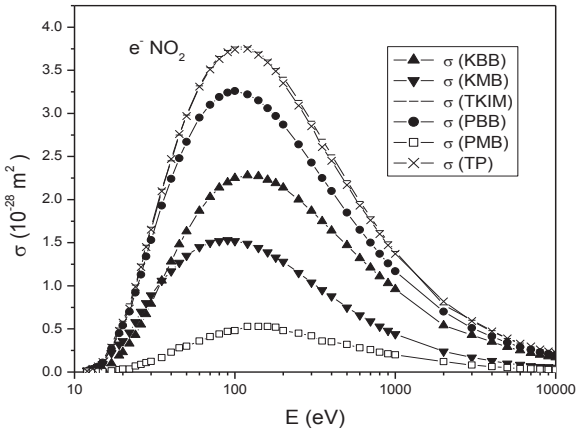

Figure 2: The present theoretical electron impact ionization cross section, compared with the electron impact ionization cross section of CO by Kim *et al.* [9,11]. Triangles ▲, Kim Bethe cross sections (KBB); inverted triangles ▼, Kim Mott cross sections (KMB); cross -X-, Kim total cross sections (TKIM); Circle •, present Bethe cross sections (PBB); square □, present Mott cross sections (PMB); dash —, and present total cross sections (TP).

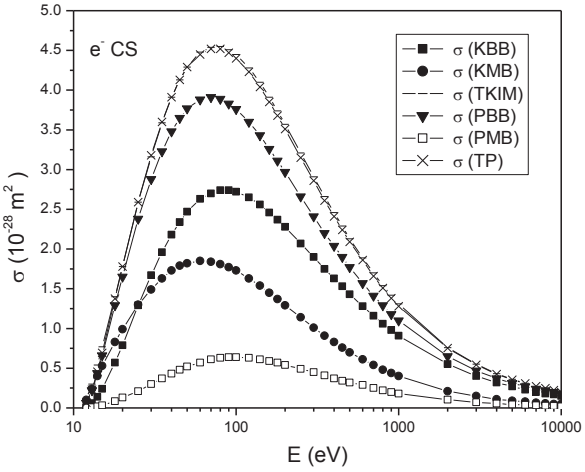

Figure 3: The present theoretical electron impact ionization cross section, compared with the electron impact ionization cross section of CS by Kim *et al.* [9,11]. Squares ■, Kim Bethe cross sections (KBB); Circle •, Kim Mott cross sections (KMB); dash —, Kim total cross sections (TKIM); inverted triangles ▼, present Bethe cross sections (PBB); square □, present Mott cross sections (PMB); and cross -X-, present total cross sections (TP).

PMB remain greater than one for whole energy range.

In the Figs. 4-6 the present results compared with other theoretical and experimental values. In Fig. 4 the present cross sections for nitrogen dioxide NO_2 are compared with the experimental data of Lindsay *et al.* [4], Lopez *et al.* [6], Lukic *et al.* [5] and two the-

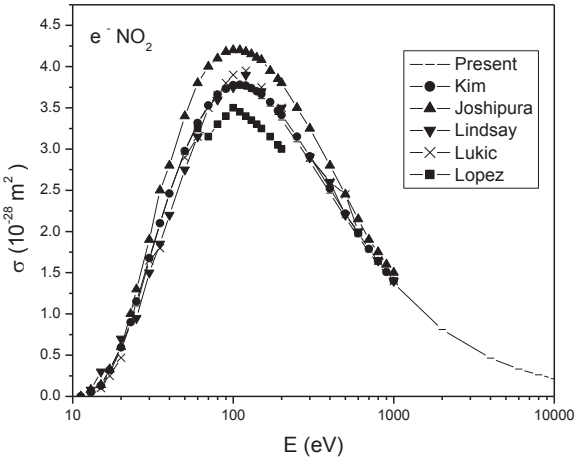

Figure 4: The present theoretical electron impact ionization cross section, compared with other experimental and theoretical electron impact ionization cross sections of NO_2. Dash —, the present work; Circle •, theoretical data by Kim *et al.* [9]; triangles ▲, theoretical data by Joshipura *et al.* [10]; inverted triangles ▼, experimental data by Lindsay *et al.* [4]; cross -X-, experimental data by Lukic *et al.* [5]; squares ■, experimental data by Lopez *et al.* [6].

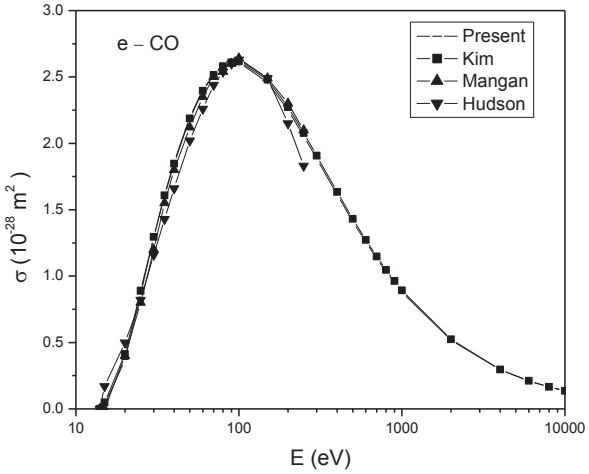

Figure 5: The present theoretical electron impact ionization cross section, compared with other experimental and theoretical electron impact ionization cross sections of CO. Dash —, the present work; Squares ■ theoretical data by Kim *et al.* [11]; triangles ▲, experimental data by Mangan *et al.* [12]; inverted triangles ▼, experimental data by Hudson *et al.* [8].

oretical cross sections Kim *et al.* [9] and Joshipura *et al.* [10]. The present cross-section underestimates the cross-section obtained by Joshipura *et al.* [10] for $E > 20$ eV. The experimental data and the present results are in good agreement with each other.

Fig. 5 shows the present total cross section for CO, it exactly matches with that of Kim *et al.* [11]. Experimental data are taken from Mangan *et al.* [12] and Hudson *et al.* [8].

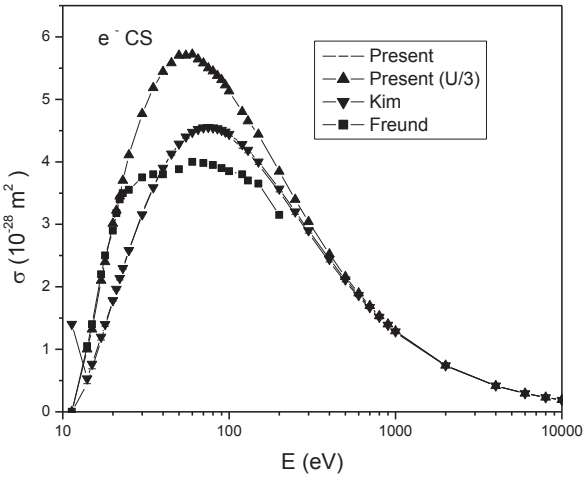

Figure 6: The present theoretical electron impact ionization cross section, compared with other experimental and theoretical electron impact ionization cross sections for CS. Dash —, the present work; triangles ▲, present work (U/3); inverted triangles ▼, theoretical data by Kim *et al.* [9]; squares ■, experimental data by Freund *et al.* [7].

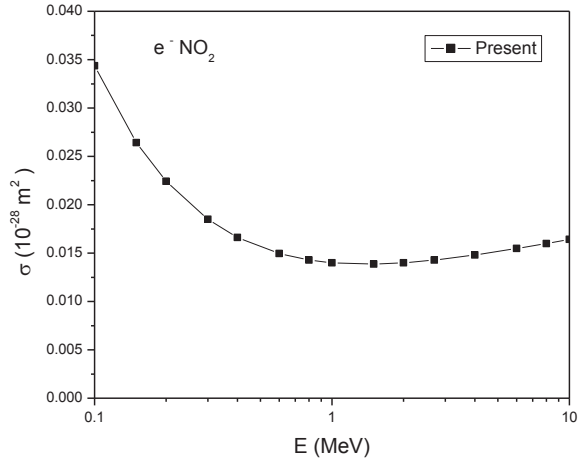

Figure 7: The present theoretical electron impact ionization cross section of NO_2.

Present calculations are agreed within 9 % of the experimental data of Hudson *et al.* [8].

Fig. 6 shows the total cross-section for carbon monosulfide (CS), compared with experimental cross–section by Freund *et al.* [7] and the theoretical cross-section by Kim *et al.* [9]. Experimental data are partial cross-section of the production of CS^+ ions only. So it should be lower than present cross-section. Following Kim *et al.* we have modified the Khare *et al.* [16] cross–section in this case. When a molecular orbital is dominated by an atomic orbital with high principal quantum number, its kinetic energy is high and makes

the cross section low because the expression of the cross sections have average kinetic energy U. To correct this U has been divided by principal quantum number ($n = 3$) of the dominant atomic orbital ($3p$ orbital of S). It is noted that the present cross-section are very close to the cross-section obtained by Kim *et al.* [9], while the expression for both cross-sections are different.

Figs. 7, 8 and 9 show the total cross sections for NO_2, CO and CS respectively from 0.1 MeV to 10 MeV. From Eq. (8) only for CO the total cross sections could be obtained by the fitting of the experimental data [13]. They are in good agreement with the present values. The calculated value of C is 16.73% higher and the value of M_j^2 is about 6% lower than the

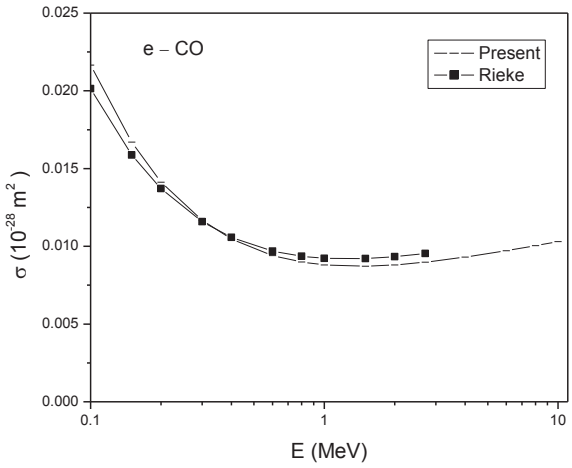

Figure 8: The present electron impact ionization cross section, compared with the experimental data of CO. Dash —, the present work; Squares ■, experimental data by Rieke and Prepejchal [13].

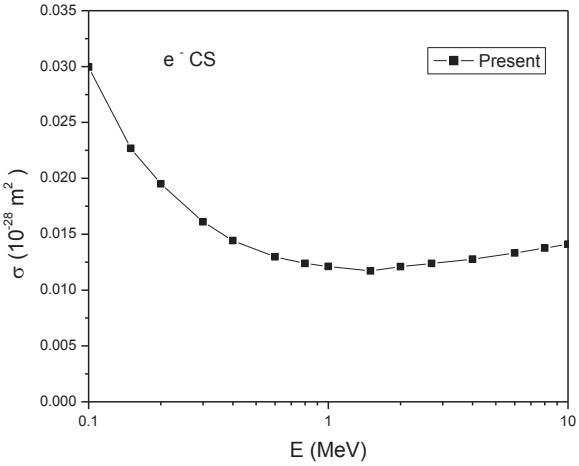

Figure 9: The present theoretical electron impact ionization cross section of CS.

corresponding experimental values of Rieke and Prepejchal [13]. The agreement between the experimental and theory is good, although theory has a tendency to underestimate the cross sections. All these values of the collision parameter do not change with the increase of E. For NO_2 and CS there are no experimental and theoretical data available to compare it with present calculation.

4 Conclusion

From the present study it is concluded that the theoretical predictions and measured value of the total cross sections for NO_2, CO and CS molecules are in good concurrence. Present method has been successfully tested for a number of molecular targets [18, 19]. Furthermore we concluded that a combination of useful features of Kim *et al.* [9] model with Saksena *et al.* [16] model have considerably improved the agreement between the experimental and theoretical data at low energy. At higher values of energy, there is hardly any difference between the present and data measured by Rieke and Prepejchal [13]. The present value of collisional parameters seems to be in reasonable agreement with the experimental data by Rieke and Prepejchal [13]. Thus the experimental data is in good agreement with the present data over a wide energy range.

As far as we know there is no other single model to apply for such a wide range of energies and seems to be very use full for applications. The application of the present model to the ionization of other molecules and atoms, including inner-shell and dissociative ionizations is of interest.

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