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Total Ionization Cross Sections Due to Electron Impact of Carbon Tetrachloride

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ABSTRACT

In present article, we have employed modified Khare-BEB model to calculate the electron impact ionization cross section for carbon tetrachloride (CCl_4) from ionization threshold to 10 MeV. We also calculated the collisional parameters C_{RP} and M^2. At relativistic energies, the present calculations for ionization cross sections of carbon tetracloride are first calculations in the best of our knowledge. The calculated cross sections were compared with available experimental data. A good agreement was found among the present results, other previous calculations, and experimental data.

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Keywords- Ionization cross section, Electron-impact.

I. INTRODUCTION

Among the various variety of inelastic process, the ionization of molecules due to electron impact has an importance in many research fields such as plasma science, astrophysics, biosciences etc. The Carbon tetrachloride is an important member of chlorofluoromethanes family that is used in many industrial applications. It has also been detected in the upper atmosphere where it reacts with some beneficial species and destroys them. It is also used as a reactive etching gas from silicon wafers in micro electro-mechanical systems, microelectronic device fabrication and cleaning surfaces by chemical vapour deposition in semiconductor industries. Due to these applications and naturally created halomethanes are diffused into the upper atmosphere and destroys the beneficial species. There is also an efficient contribution of it to the greenhouse effect. Thus, theoretical electron impact ionization cross sections are needed to understand fundamental process of collision of microscopic particles in model etching and industrial plasmas [1-5].

Sierra et al. [6] have measured the electron impact ionization of present molecule from threshold to 85 eV. They have used double focusing time of flight mass spectrometer. Bart and his associates [7] have measured the cross section experimentally by using the condenser plate ion source from threshold to 220eV. We have an old experimental data set which was reported by Leiter et al. [8]. They had measured the cross section from threshold to 180 eV by using a double-focusing mass spectrometer system in combination with an electron impact ion source. They claimed 10% uncertainty in their experiment. We have also calculated cross sections through Kim-BEB method [9] to compare our results.

II. THEORY

The electron impact ionization cross sections of a molecule for j_{th} molecular orbital in the modified Khare-BEB method [10] are given by

$$\sigma_{jT} = \sigma_{jM} + \sigma_{jB} + \sigma_{tj} \qquad (1)$$

where, Mott term (the ionization cross section due to the hard collision) σ_{jM} is given by

$$\sigma_{jM} = \frac{AN}{[E+I+U]I}\left[1 - \frac{2}{t+1} + \frac{t-1}{2t^2} + \frac{5-t^2}{2(t+1)^2} - \frac{1}{t(t+1)} - \frac{t+1}{t^2} ln\left(\frac{t+1}{2}\right)\right] \qquad (2)$$

where $t = E/I$, $E = \frac{1}{2}mc^2\left[1 - \frac{1}{1+\frac{T}{mc^2}}\right]$, $A = 4\pi a_0^2 R^2$. The notations U, a_0, I, N, T, m, c and R represent the average kinetic energy of bound electron, the first Bohr radius, the ionization energy, the occupation number of molecular orbital, the kinetic energy of the incident electron, rest mass of electron, velocity of light and Rydberg energy, respectively. The Bethe cross-section σ_{jB} is

$$\sigma_{jB} = \frac{AN}{2[E+I+U]I}\left[\frac{1}{2}\left(1 - \frac{1}{t^2}\right) - X\right] \qquad (3)$$

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where the term X is given by $\left(\sqrt{t} - \sqrt{(t-1)}\right) + \frac{1}{2t^2}\left\{1 - \frac{1}{2}\left(\frac{t}{t-\sqrt{t(t-1)}}\right)^2 + \frac{1}{2}\left(\frac{t}{t+\sqrt{t(t-1)}}\right) - \left(\frac{t}{t-\sqrt{t(t-1)}}\right) - \frac{3}{4} ln\left(\frac{t+\sqrt{t(t-1)}}{t-\sqrt{t(t-1)}}\right)\right\}$
and the cross section due to the transverse interaction is

$$\sigma_{tj} = -\frac{4\pi a_0^2 R}{E} M_j^2 [ln\,(1-\beta^2) + \beta^2] \qquad (4)$$

where β is the ratio of the incident velocity v and the velocity of light c, M_j^2 represents the total dipole matrix squared measured in units of a_0^2 and given by

$$M_j^2 = \int_{I_j}^{E} \frac{R}{w} \frac{df_j(w,0)}{dw} dw \qquad (5)$$

where the continuum optical oscillator strength (COOS) per unit energy range $\frac{df_j(w,0)}{dw}$ is

$$\frac{df_j(w,0)}{dw} = \frac{NI_j}{w^2} \qquad (6)$$

The expression of collision parameter for jth molecular orbit C_{jRP} is given by [9]

$$C_{jRP} = \frac{RE}{A} \sum_j (\sigma_{jB} + \sigma_{jM}) - M_j^2 ln\beta^2 \qquad (7)$$

To evaluate total ionization cross section and collision parameters of molecule, the contributions come from all molecular orbital are added.

III. RESULTS AND DISCUSSION

The theoretical method described in above section has been used to calculate the absolute ionization cross sections of carbon tetrachloride. The required molecular parameters binding energies I, kinetic energies of bound electrons U and occupation numbers N are taken from Irikura [3].

The present results along with other previous available data have been shown in figure (1). Our calculations overestimate the experimental results of Bart et al. [7] for E<25eV. However, beyond this value of incident energy, the present cross sections are in excellent agreement with the experimental values. A good agreement is found between present values and experimental results those measured by Sierra et al. [6] except near threshold. At near threshold our calculations are slightly lower than experimental data. The experimental values.

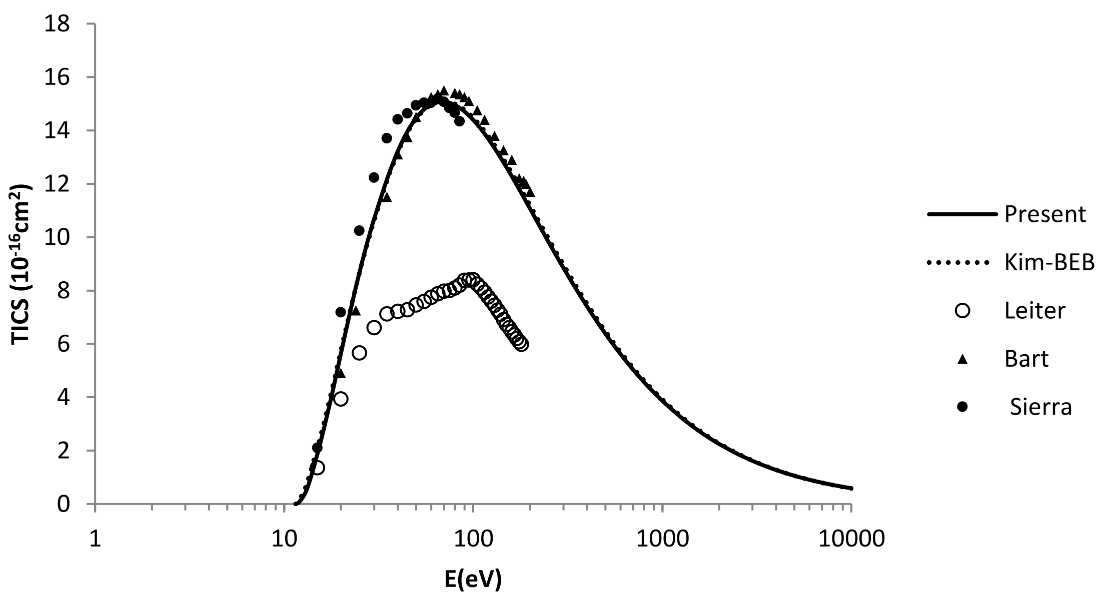

Fig.1 Total ionization cross sections (TICS) for carbon tetracloride in 10^{-16} cm^2. Solid line, and dotted line represent present results, and Kim-BEB calculations , respectively. Open circles, filled tringles, and filled circles represent the experimental results of Leiter et al. [8], Bart et al.[7], and Sierra et al. [6], respectively of Leiter et al. [8] disagree with present calculations as well as all other available data. The reason of this discrepancy is not clear. The present cross sections and other results are higher than experimental data. The two theoretical results, present and Kim-BEB calculations, are very close to each other.

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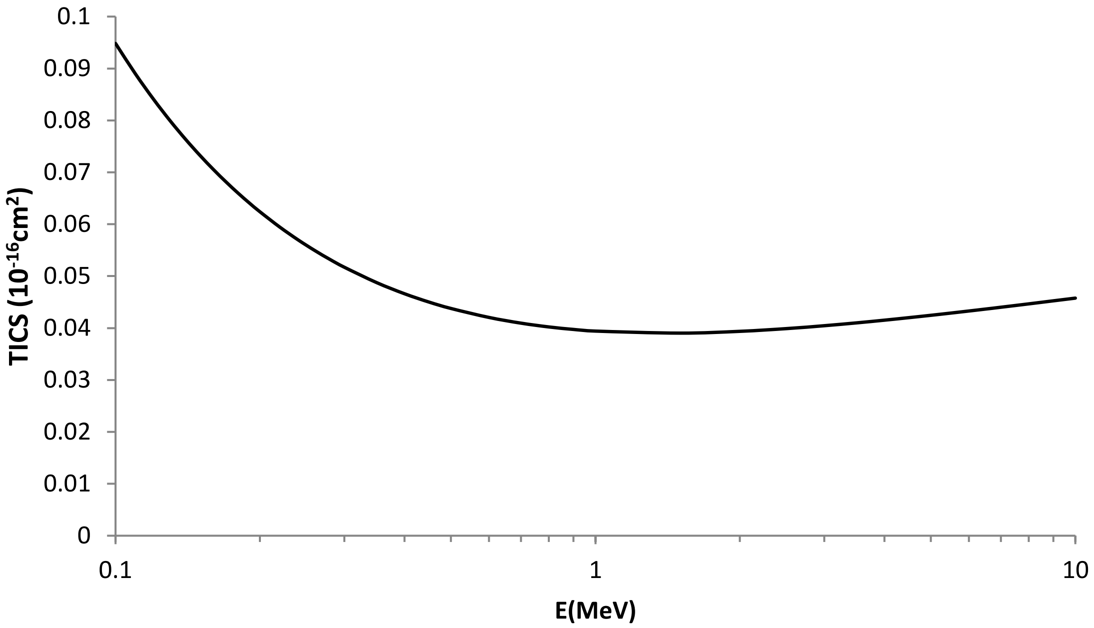

Fig. 2 This figure shows the present total ionization cross sections for carbon tetracloride in energy range (.1-10MeV) in 10^{-16} cm^2

Figure (2) represents the present ionization cross sectionsin energy range .1 MeV to 10 MeV. We have no experimental data to compare our results. However, tendency of curve is similar to other reported earlier [10]. Thus these results will be important in future to compare. These are first calculation in our knowledge for present molecule. The value of collisional parameters C_{RP} and M_i^2 are 168.1 and 14.78, respectively.

IV. CONCLUSION

In present paper,we have presented the theoretical total ionization cross sections of tetrachloride by using modified Khare-BEB method [10] and compared with the available experimental results. The our calculations are found in good agreement with experimental data over a wide energy range. In future work, we hope to measure the total ionization cross sections due to electron impact of carbon tetrachloride at relativistic energies. These measurements will test the present predictions.The application of the present method to calculate the total ionization cross sections of other molecules will be of interest.

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