International Journal of Engineering and Management Research e-ISSN: 2250-0758 | p-ISSN: 2394-6962
Volume-12, Issue-2 (April 2022)
www.ijemr.net https://doi.org/10.31033/ijemr.12.2.12

Total Ionization Cross Sections due to Electron Impact of Carbon Tetrafluoride from Ionization Threshold to 10 MeV

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ABSTRACT

Modified Khare-BEB model has been used to calculate the electron impact ionization cross section for carbon tetrafluoride (CF_4) from ionization threshold to 10 MeV. The collisional parameters C_{RP} and M^2 also has been calculated. The calculations are compared with available experimental data. A good agreement is found among the present results, other previous calculations, and experimental data.

Keywords-- Ionization, Tetrafluoride, Carbon

I. INTRODUCTION

The electron impact ionization of molecules is one of the fundamental process in the collision physics. It has a number of applications in plasma modelling process, atmospheric science, astrophysics, fusion etc. [1]. Tetrafluoride methane (CF_4) is a gas which is mostly commonly used for plasma etching in semiconductors industries, and plasma processing in the semiconductor manufacturing [2-4]. Therefore, calculations and measurements of the ionization cross section for this molecule have been of the most important . Hence a large number of investigations for the theoretical and experimental evaluation of the total ionization cross section have been carried out in the last few decades.

Bruce and Bonham [5] measured the absolute ionization for carbon tetra fluoride through pulsed-electron-beam time-of-flight method. They have claimed uncertainty 16% (for CF_3^+ cation) in their studies. Torres et al. [6] have measured the ionization cross sections for CF_4 by using time-of-flight mass spectrometer system for electron incident energies up to 100 eV. With uncertainty of 10%. Nishimura and his associates [7] have reported the experimental data of electron impact ionization cross section for present molecule. They have used parallel plate condenser type apparatus. Poll et al. [8] have also measured total ionization cross section due to electron impact. Their experiment was based on the geometry of the ion source and analyses of double focusing mass spectrometer. They have measured cross section for CF_4 up to 180 eV. Sieglaff et al. [9] have reported the ionization cross section for CF_4 incident electron energies from threshold to 1 keV. They have also used time-of-flight mass spectrometer with a position sensitive detector to detect the product ions. These ions are collected with the equal efficiency irrespective of their kinetic energies. We have only one experimental data set for high energy electrons (.1 - 2.7 MeV) those measured by Rieke, and Prepejchal [10]. They have measured the ionization cross sections in terms of two parameters, collisional parameter C_{RP} and dipole matrix squared M^2 (measured in units of a_0^2). Recently, Karwasz and his associates [11] reported review of experimental methods and binary-encounter models and calculated the theoretically total ionization cross section for tetrafluoromethanes by using Kim-BEB method.

II. THEORY

In the modified Khare-BEB model [12], the electron impact ionization cross section of a molecule for j_{th} molecular orbital is 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

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

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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

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

where the term X is given by

$$X = 2ln\left(\sqrt{t}-\sqrt{(t-1)}\right) + \frac{1}{2t^2}\left\{\begin{array}{c} 1-\frac{1}{2}\left(\frac{t}{t-\sqrt{t(t-1)}}\right)^2 \\ +\frac{1}{2}\left(\frac{t}{t+\sqrt{t(t-1)}}\right)-\left(\frac{t}{t-\sqrt{t(t-1)}}\right) \\ -\frac{3}{4}ln\left(\frac{t+\sqrt{t(t-1)}}{t-\sqrt{t(t-1)}}\right) \end{array}\right\}$$

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 methods described in above section are employed to calculate the total ionization cross sections of tetrafluoromethane. The required molecular parameters binding energies I, kinetic energies of bound electrons U and occupation numbers N are taken from reference [13].

The figure 1 shows present total ionization cross sections of carbon tetrachloride (CF_4) due to electron impact from ionization threshold to 10 keV along with available experimental data and calculated theoretical results. A good agreement has been seen between the present calculations and those measured by Bruce and Bonham [5] within 6% between incident range of energy 30 eV<E<300 eV. Beyond this range our results lower than the experimental values while for E>300 eV, the difference between them is not large.

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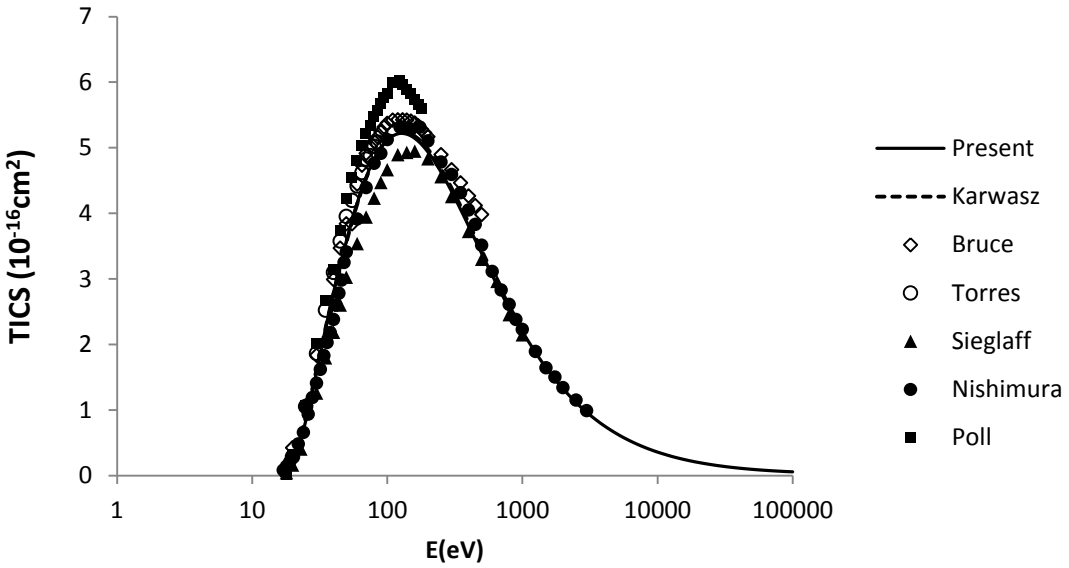

Figure1: Total ionization cross sections (TICS) for carbon tetra fluoride in 10^{-16} cm^2. Solid line, dashed line, long dashed line and dotted line represents present results, and Karwasz et al. [11] calculations, respectively. Open rhombus, open circles, filled tringles filled circles, and filled rectangles represents the experimental results of Bruce and Bonham [5], Torres et al.[6], Seiglaff et al. [9], Nishimura et al. [7], and Poll et al. [8] respectively

A good agreement is found between present cross section and experimental data of Torres et al. [6] within 9% except near threshold energy. At near threshold, the present values are slightly higher than the experimental results. Our results overestimate the experimental data those measured by Sieglaff et al. [9] for E <100 eV, while for E>100eV, our calculations are found in good agreement with experimental values. The present result are in good agreement with the experimental data those measured by Nishimura et al. [7] for most of incident energies studied by them. Our calculations underestimate the experimental results of Poll et al. [8] for whole range of impact energy. However the difference between two data is not large. The present cross sections are very closed to theoretical results of Karwasz et al. [11].

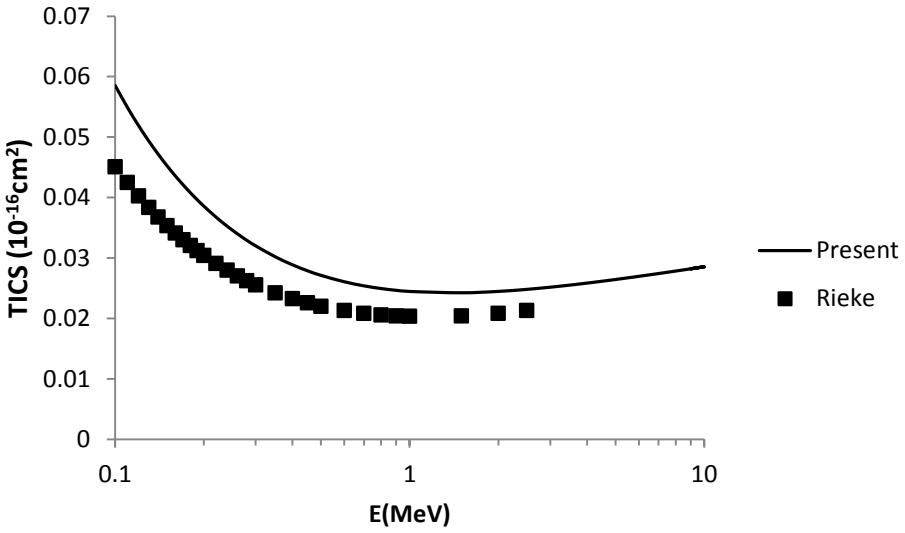

Figure 2: In this figure we compare the present total ionization cross sections in 10^{-16} cm^2 to experimental results of Rieke and Prepejchal [10] (filled rectangles) for carbon tetrafluoride at high energy range .1 MeV to 10 MeV

Figure 2 depicts the present cross sections along with the experimental results of Reike and Prepejchal [10]. In energy range .1MeV to 10 MeV, the present calculations overestimate the experimental results but difference between two results are not large and tends to come closer to each other as impact energy increases. Thus the agreement between the present values and experimental data is satisfactory. The calculated values of collisional parameters C_{RP} and M^2 are 103.62 and 9.356 respectively. The calculated value of C_{RP} is higher than the experimental value (=84.05) by 23.28%, however, the value of M^2 less than experimental result (=10.26) by 8.81%.

IV. CONCLUSION

The Khare-BEB method, previously employed widely for many molecules, has been presently used to evaluate the total ionization cross sections for carbon tetra fluoride from ionization threshold to 10 MeV. We found a good agreement between our calculations and available experimental results. These are the first calculations for the total ionization cross sections of tetrafluoromethane for energy range 10 keV to 10 MeV. The present method will be continued to calculate the cross sections for other molecules.

ACKNOWLEDGMENT

We are grateful to Dr Sachin Kumar, Meerut college, Meerut (India) for fruitful discussion and also thankful to principal, D.A.V. College, Muzaffarnagar, (India) for providing the facilities for research work.

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