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Absolute Ionization Cross-Section of tetrafluoromethane by electron impact

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ABSTRACT: The fragmentation pattern of halomethane (CF_4) has been studied by electron impact with reference to Jain-Khare semi-empirical formula in the energy range from threshold to around 350 eV. Absolute cross-sections for electron impact single ionization of CF_4 ions leading to the formation of CF_3^+, CF_2^+ and C^+ are measured, having the corresponding threshold energies are 14.63 eV, 18.97 eV and 31.65 eV respectively.The present results are compared with the previously measured results of Ce Ma *et al* [11] and K.Stephan *et al* [12].

KEYWORDS: Ionization Cross Section, Scattering Cross Section.

I.INTRODUCTION

Tetrafluoromethane, It can also be classified as a haloalkane or halomethane. Because of the multiple carbon–fluorine bonds, and the highest electronegativity of fluorine, the carbon in tetrafluoromethane has a significant positive partial charge which strengthens and shortens the four carbon–fluorine bonds by providing additional ionic character. Tetrafluoromethane, like other fluorocarbons, is very stable due to the strength of its carbon-fluorine bonds. The bonds in tetrafluoromethane have a bonding energy of 515 $kJ.mol^{-1}$. As a result, it is inert to acids and hydroxides. However, it reacts explosively with alkali metals. Thermal decomposition or combustion of CF_4 produces toxic gases (carbonyl fluoride and carbon monoxide) and in the presence of water will also yield hydrogen fluoride. It is very slightly soluble in water, but miscible with organic solvents. Tetrafluoromethane is a potent greenhouse gas that contributes to the greenhouse effect. It is very stable, has an atmospheric lifespan of 50,000 years, and a high greenhouse warming potential of 6500 (CO_2 has a factor of 1); however, the low amount in the atmosphere restricts the overall radiative forcing effect.

Although structurally similar to (CFCs), tetrafluoromethane does not deplete the ozone layer. This is because the depletion is caused by the chlorine atoms in CFCs, which dissociate when

struck by UV radiation. Carbon-fluorine bonds are stronger and less likely to dissociate.

Tetrafluoromethane is sometimes used as a low temperature refrigerant. It is used in electronics microfabrication alone or in combination with oxygen as a plasma etchant for silicon, silicon dioxide, and silicon nitride. Depending on the concentration, inhalation of tetrafluoromethane can cause headaches, nausea, dizziness and damage to the cardiovascular system (mainly the heart). Long-term exposure can cause severe heart damage. Due to its density; tetrafluoromethane can displace air, creating an asphyxiation hazard in inadequately ventilated areas.

The role of collision phenomenon is important in theoretical and experimental investigations on the structure of matter on a microscopic scale. Hence, a knowledge of reliable atomic in the molecular collision cross sections are in demand for mass spectroscopy [2] , gas laser, plasma Chemistry, controlled thermonuclear fusion, transport phenomenon, chemical reaction, biophysics gases electronics , airglow etc.

In a scattering experiment a target is bombarded to a well defined collimated homogenous beam of monoenergetic particles from a large distance. After collision the particles of incident beam are scattered in all directions and their distribution is detected over large distances. The number of particles scattered into the detector per unit solid angle per unit incident flux is called the differential cross section for that particular direction. An integration of differential cross sections over all solid angles yields the total cross sections. Thus we note that the total cross section is the cross sectional area which the target presents to the direction of the beam and differential cross section is the effective area which the target presents to the beam for the deflection of the incident particle into a particular solid angle.

All these collision processes are analyzed theoretically by quantum collision theory. The probability that a given type of collision will occur under given conditions is usually expressed in terms of collision cross sections.

II.THEORETICAL METHODOLOGY

Even on the theoretical side several more methods are available to compute the cross sections over a wide range of atoms and molecules. The present calculations are carried out using the modified semi empirical formalism developed by Jain-Khare [1-8].In brief, the single differential cross sections in the complete solid angle ($\Omega = \int 2\pi \sin\theta d\theta$) as a function of secondary electron energy ε corresponding to the production of i^{th} type of ion in the ionization of a molecule by incident electron of energy E is given by equation 1.

$$Q_i(E,W,\theta) = \frac{a_0^2 R^2}{E}\left[\int_{k\to 0}^{E-I_i}\left\{\begin{array}{l}\dfrac{E-W}{E-I_i}\dfrac{1}{W}df_i(W,K,\theta)\times\ln\left[1+C_i(E-I_i)\right]+\\ \dfrac{E-I_i}{E\left(\varepsilon_0^3+\varepsilon^3\right)}\times S_i\left(\varepsilon-\dfrac{\varepsilon^2}{E-\varepsilon}+\dfrac{\varepsilon^2}{(E-\varepsilon)^2}\right)\end{array}\right\}\right]2\pi\sin\theta d\theta \quad \ldots(1)$$

where, W $(=\varepsilon + I_i)$ is defined as energy loss suffered by the incident electron. I_i is the ionization threshold for the production of i^{th} type of ion, a_0 is the Bohr radius, ε_0 is energy parameter, C_i is collision parameter, S_i is number of ionizable electrons, R is Rydberg constant and θ is the scattering angle respectively.

In the present formulation, the dipole oscillator strengths df_i/dw are the key parameters. The oscillator strength is directly proportional to the photo ionization cross section [2-3,5-9]. Summation of PDDCS (Partial double differential cross section) over the system gives the total (DDCS) (Double differential cross section)

$$Q_i^t(E,W,\theta) = \sum_i Q_i(E,W,\theta).$$

Here it is interesting to note that $Q_i(E,W,\theta)$ is isotropic and hence the material property of molecule, i.e., the oscillator strength must be isotropic in nature. Here $df_i(W,K,\theta)$, the differential generalized oscillator strength (DGOS) in the optical limit $(K \to 0)$ has been used. From Lassettre's Theorem [10] the DGOS in the Bethe regime is reduced to the cosine distribution form of the linear optical oscillator strengths $df_i(W,0))/dW$, i.e.

$$df_i(W,K,\theta) \to (1/4\pi)[1+\beta P_2(\cos\theta)] \times df_i(W,0)/dW,$$

where β is the asymmetric parameter and $P_2(\cos\theta) = \frac{1}{2}(3\cos^2\theta - 1)$ is the second order Legendre polynomial. In the present treatment, β is chosen as the probability of ionizing electrons in the ionization processes however, it depends on the ejected electron energy. The oscillator strengths are directly proportional to the photo ionization cross sections.

Further integration of Equation (1) with respect to the scattering angle θ (from 0 to 2π) gives the PSDCS (Partial single differential cross section)

$$Q_i(E,W) = \int Q_i(E,W,\theta)d\Omega,$$

where differential solid angle dΩ is $2\pi \sin\theta d\theta$

Similarly, SDCS (Single differential cross section) are given as

$$Q_i^T(E,W) = \sum_i Q_i(E,W).$$

Further integration of PSDCS with respect to W from I to W_{max} (= .E) results in PICS (Partial integral cross section), i.e.

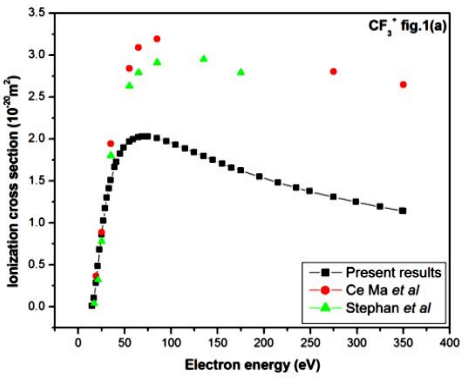
$$Q_i(E) = \int Q_i(E,W)dW.$$

The present formulation requires the major input data of the photo ionization cross-sections in terms of the optical oscillator strengths.

Even on the theoretical side several more methods are available to compute the cross sections over a wide range of atoms, molecules, radicals and even cluster but all of them are partially successful. In this research work, we calculate the ionization cross section of CF_4 ions leading to the formation of CF_3^+, CF_2^+ and C^+. The formula is useful for finding the rate coefficient of any atoms and molecules. But in this paper we are concern with ionization cross section only.

III.RESULTS AND DISCUSSION

In this paper the results of the absolute partial ionization cross section measurements for the CF_4 are calculated from threshold to 350 eV by the use of modified Jain-Khare approach. Table 1 shows the measured partial cross sections for the formation



of the CF_3^+ parent ion and all singly charged fragment ions CF_2^+ , C^+ and CF_4(Total).

Fig.1(a) shows ionization cross section of CF_3^+ ion.

Energy	CF_3^+	CF_2^+	C^+	Total
15	0.009510	-	-	0.009510
17	0.101332	-	-	0.101332
19	0.283199	0.0067	-	0.289899
21	0.484072	0.2667	-	0.750772
23	0.680550	0.4125	-	1.093050
25	0.862600	0.5429	-	1.405500
27	1.026591	0.6648	-	1.691391
29	1.171961	0.7782	-	1.950161
31	1.299575	0.8826	0.07426	2.256435
33	1.410903	0.9778	0.15340	2.542103
35	1.507608	1.0638	0.31760	2.889008
39	1.663649	1.2107	0.49360	3.367949
41	1.725928	1.2720	0.55640	3.554328
45	1.825241	1.3769	0.65690	3.859041
49	1.897539	1.4588	0.73610	4.092439
55	1.968666	1.5489	0.82940	4.346966
59	1.997724	1.5920	0.87930	4.469024
65	2.021726	1.6374	0.94040	4.599526
69	2.027976	1.6576	0.97350	4.659076
75	2.026843	1.6768	1.01430	4.717943
85	2.006151	1.6871	1.06330	4.756551
95	1.971629	1.6800	1.09790	4.749529
105	1.930000	1.6625	1.11480	4.707300
115	1.885096	1.6388	1.12590	4.649796
125	1.839163	1.6116	1.13100	4.581763
135	1.793488	1.5826	1.13170	4.507788
145	1.748814	1.5527	1.12920	4.430714
155	1.705538	1.5227	1.12450	4.352738
165	1.655738	1.4929	1.11800	4.266638
175	1.623895	1.4637	1.11020	4.197795
195	1.548976	1.4074	1.09200	4.048376
215	1.480431	1.3544	1.07170	3.906531
235	1.417668	1.3046	1.05010	3.772368
249	1.376848	1.2717	1.03470	3.683248
275	1.307084	1.2144	1.00550	3.526984
299	1.248871	1.1658	0.97870	3.393371
325	1.191611	1.1172	0.95010	3.258911
349	1.143430	1.0758	0.92430	3.143530
350	1.141300	1.0739	0.92360	3.138800

The results for fragmentations of CF_4 are shown in TABLE 1.

Tale 1.

The present results are compared with the results of Ce Ma *et al* [11] and K.Stephan *et al* [12]. In the figure 1(a), 1(b) and 1(c) represents ionization cross-section for the CF_3^+, CF_2^+, C^+ ions respectively and figure 2 epresents the total differential ionization cross-section of CF_4 by electron impact.

The shape of figure 1(a), 1(b) and 1(c) for ionization cross section of Ce Ma *et al* [11] and K.Stephan *et al* [12] and that of present result is in good agreement irrespective of cross section magnitude.

Present results for cross section value of CF_3^+ ion [fig.1(a)] are lower than that of Ce Ma *et al* [11] and K.Stephan *et al* [12] but are higher for CF_2^+ and C^+ ions.

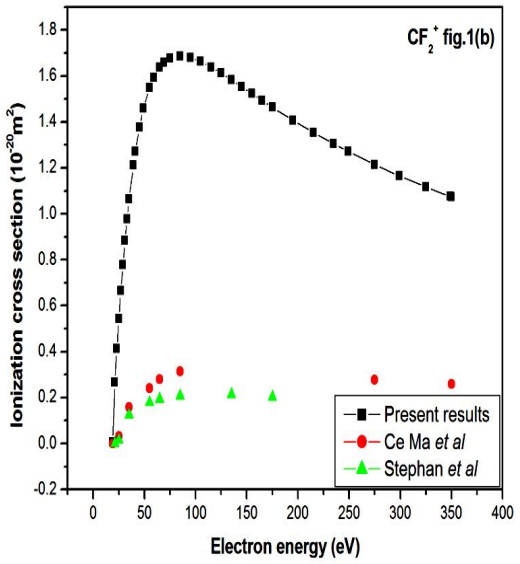


Fig.1(b) shows ionization cross section of CF_2^+ ion.

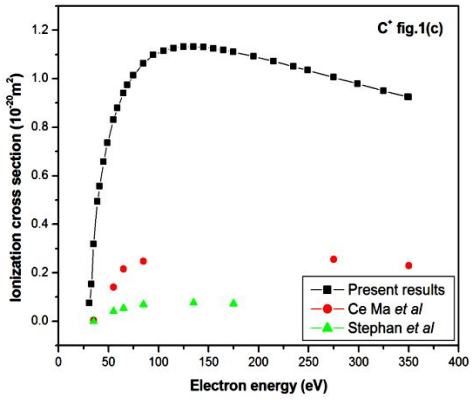


Fig.1(c) shows ionization cross section of C^+ ion.

Fig.1(a),1(b),1(c) represents the production of the CF_3^+,CF_2^+ and C^+ ion.

Maximum cross section of 2.027×10^{-20} m^2 is found for CF_3^+ ion at 69 eV.[shown in fig.1(a)]. Maximum cross section of 1.687×10^{-20} m^2 is found for CF_2^+ ion at 89 eV.[shown in fig.1(b)]. Maximum cross section of 1.1317×10^{-20} m^2 is found for C^+ ion at 135 eV.[shown in fig.1(c)]. Figure 2 shows total ionization cross section of CF_4, the maximum cross section is 4.75×10^{-20} m^2 at 85 eV.Which is in excellent agreement with Ce Ma *et al* [11] and is in good agreement with that of K.Stephan *et al* [12].

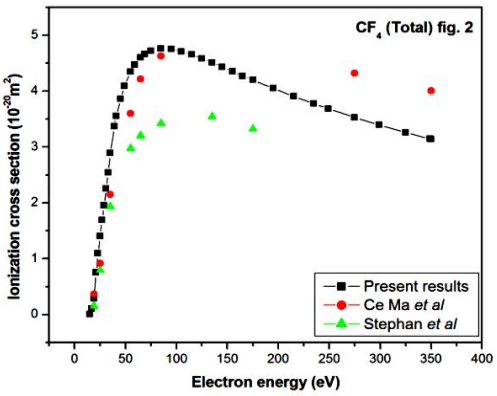


Fig.2 shows the Total ionization cross-section of CF_4 molecule.

IV.CONCLUSION

In this work we measured partial and total ionization cross sections for electron impact ionization of halomethane (CF_4) molecule using semi-empirical model developed by Jain and Khare.The present study investigates partial and total EIICS(Electron Impact Ionization Cross section) for CF_4 from threshold to 350 eV. We compared the present results with Ce Ma *et al* [11] and K.Stephan *et al* [12]. A good agreement is found between our measurements and the earlier results of Ce Ma *et al* [11] and K.Stephan *et al* [12] for total ionization cross section of CF_4.

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