



International Journal of Chemistry and Pharmaceutical Sciences

Journal Home Page: www.pharmaresearchlibrary.com/ijcps



RESEARCH ARTICLE

Total Ionization Cross Section of FCO by Electron Impact

Prof. S.P. Sharma¹, Nidhi Dhull²

¹Dean (Faculty of Sciences), Baba Mastnath University, Rohtak

²Research Scholar, Dept. of Chemistry, Baba Mast Nath University, Rohtak

ABSTRACT

Electron-impact ionization is one of the basic collision processes for atoms and molecules and is studied not only for its intrinsic importance but also for a wide range of applications. Such as in fusion plasma diagnostics, radiation effects on materials. And astrophysics, FCO is one of the more important diagnostic elements for controlled fusion, and recently there has been much interest in its use as a liquid metal wall in tokomaks molecule.

ARTICLE INFO

CORRESPONDING AUTHOR

Prof. S.P. Sharma

Dean (Faculty of Sciences),

Baba Mastnath University, Rohtak

MS-ID: IJCPS3674



PAPER-QR CODE

ARTICLE HISTORY: Received 25 April 2018, Accepted 28 May 2018, Available Online 27 June 2018

Copyright©2018 S.P. Sharma. Production and hosting by Pharma Research Library. All rights reserved.

This is an open-access article distributed under the terms of the Creative Commons Attribution License, which permits unrestricted use, distribution and reproduction in any medium, provided the original work is properly cited.

Citation: S.P. Sharma. Total Ionization Cross Section of FCO by Electron Impact. *Int. J. Chem, Pharm, Sci.*, 2018, 6(6): 164-166.

CONTENTS

1. Introduction.	164
2. Methodology.	165
3. Results and Discussion.	166
4. Conclusion.	166
5. References.	166

1. Introduction

Quantum mechanical studies of the ionization process are still largely limited to the first born approximation of the molecules mentioned only the ionization cross section of CH₄ molecules by inokuti (1962) in first Born approximation however, the result are only in qualitative arrangement with the experimental data the theory overestimates the cross section in the absence of quantum mechanical investigation, wich are quite involved. Ever semi-empirical approach have been developed recently Geen and Sawada (1972 have given an empirical relation similar to a dispersion relation to calculate the energy loss International Journal of Chemistry and Pharmaceutical Sciences

cross section. S(E,W).where E is the energy of the incident electron and W is the energy loss suffered by the incident electron in there ionizing collision. The empirical relation a number of the free parameter which are adjusted so that the result are in agreement with the experimental data of Opal (1972) .S(E,W) has also been integrated to obtain the total ionization cross section Q_i. However, they noticed that to achieve agreement between theory and experiment for Q_i different values of the free parameter have be used. Khare (1969) has also proposed two semi-empirical relation to calculate Q(E,) the ionization cross section per unit energy

range for the production of a secondary electron of the energy ϵ . These relations are used on the well known Born and Moller part formula. Since then the relation have been employed in slightly modified form. To calculate many physical entities related to energy degradation studies, the result obtained in all the investigation were found to be in satisfactory agreement with the available experimental data. However so far these relation have not been applied to the above mentioned molecules. As the calculation are extremely simple and encouraging result are obtained it will be of interest to calculate the energy spectra of secondary electron and the total ionization cross section of $\text{CO}_2, \text{CO}, \text{H}_2\text{O}, \text{CH}_4$ and NH_3 due to electron impact reemploying semi empirical relation similar to those employed by Khare and Co-Workers.

The first attempt to calculate total ionization cross-section for molecule using a combination of theories describing two different types of collision i.e. soft and hard collision was made by Jain and Khare. This work was based on earlier work (i) to calculate energy loss cross-section $d(E, W)/dW$, where E is the energy of incident and W is the energy loss suffered by the incident electron in the ionizing collision (ii) to calculate the single differential ionizing cross section $d(E, W)/d\theta$ for the production of a secondary electron of energy ϵ .

2. Materials and Method

Cross sections of many different types of molecules and atoms can be determined by various experimental techniques during the last decades. Electron impact ionization of rare gas ions is an important process in high-energy chemical processes, such as in planetary atmospheres and in plasma physics. Even though the cross sections for singly and multiply charged ions decline rapidly with increasing stage of ionization, multiple ionization processes are important in fusion plasmas and in other environments with an abundance of energetic electrons. The total ionizing cross-section $\sigma_i(E)$ was obtained by the integration over all possible values of ϵ from 0 to $(E-I)/2$. Moreover, Khare and Meath^{8/} extended their formation for the calculation of partial ionization cross-section for molecules (i.e. the cross section for the production of specific parent or fragment ion. As summarized by these authors, according to Inokuti^(9,10) the single differential ionization cross-section $d(E, W)/d\theta$ was given in the first Born approximation by

$$\frac{d\sigma(E, \nu)}{d\nu} = \frac{4f a_0^2}{EW} \int \frac{\partial f(WK^2 a_0^2)}{\partial W} d[\ln(Ka_0)^2]$$

Where,

a_0 denotes the Bohr's radius,

R is the Rydberg constant

Ionization energy of the hydrogen atom,

$$\frac{\partial f(WK^2 a_0^2)}{\partial W}$$

Is the density of the generalized oscillator strength per unit energy range, and Ka_0 is the change in the momentum International Journal of Chemistry and Pharmaceutical Sciences

vector of the incident electron due to scattering. The generalized oscillator strength may be given in a complete fashion by plotting df/dW versus $\ln[(Ka_0)^2]$ and W/R . Depending on the nature of the energy transfer hard collision are associated with a large energy transfer and soft collision (glancing) with a small energy transfer. Thus the ionizing collision can be divided into two regimes on the Bethe surface. Hence equation (4.1) is reduced to Bethe term for soft collisions where the collisions takes place primarily through the dipoles interaction between the incident electron and the hard collision between the target electron.

Formulation: The present calculations are carried out using the modified semi empirical formalism developed by Jain-Khare. In brief, the single differential cross sections in the complete solid angle ($\Omega = 4\pi = \int 2\pi \sin\theta d\theta$) is known 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 Where,

$W (= E - I_i)$ is defined as energy loss suffered by the incident electron.

I_i = the ionization threshold for the production of i^{th} type of ion.

a_0 = the Bohr radius,

θ_0 = energy parameter,

C_i = collision parameter,

S_i = number of ionizable electrons,

R = Rydberg constant and

θ = the scattering angle respectively.

In the present formulation, the dipole oscillator strengths df_i/dW are the key parameters. In the present formulation, the dipole oscillator strengths df_i/dW are the key parameters. The oscillator strength or appearance potential is in direct ratio or directly proportional to the photo ionization cross section. However, its evaluation is possible quantum mechanically using the suitable wave functions and transition probabilities corresponding to the production of cations.

$$Q_i(E, W, \nu) = \frac{a_0^2 R^2}{E} \left[\int_{k=0}^{E-I_i} \left\{ \frac{E-W}{E-I_i} \frac{1}{W} df_i(W, K, \nu) \times \ln[1 + C_i(E-I_i)] + \frac{E-I_i}{E(\nu_0^3 + \nu^3)} \times S_i \left(\nu - \frac{\nu^2}{E-\nu} + \frac{\nu^2}{(E-\nu)^2} \right) \right\} 2f \sin \theta d\theta \dots \dots \dots \right]$$

Oscillator strengths df_i/dW are the key parameters. The oscillator strength is directly proportional to the photo ionization cross section. Summation of PDDCS (Partial double differential cross section) over the system gives the total (DDCS) (Double differential cross section).

$$Q_i'(E, W, \nu) = \sum_i Q_i(E, W, \nu)$$

Here it is interesting to note that $Q_i(E, W, \nu)$ is isotropic and hence the material property of molecule, i.e., the oscillator strength must be isotropic in nature. Here $df_i(W, K, \nu)$, the differential generalized oscillator strength (DGOS) in the optical limit ($K \rightarrow 0$) has been used from Lassette's Theorem 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.

$$df_i(W, K, \mu) \rightarrow (1/4f) [1 + SP_2(\cos \mu)] \times df_i(W, 0) / dW,$$

Where,

is the asymmetric parameter

$P_2(\cos \mu) = \frac{1}{2}(3\cos^2 \mu - 1)$ is the second order Legendre polynomial.

In the present treatment, f_i 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).

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

Where differential solid angle $d\Omega$ 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.

3. Results and Discussions

The present result for TICS 2500 eV with respect to the energy loss function or the secondary electron energy. As mentioned earlier, no previous data exist with which comparison of TICS at either energy can be made. To check the accuracy of present result, we have carried out a comparison of TICS with the available experimental data. In the figures, represent the TICS for the FCO molecules by electron impact FCO. Table for the ionization rate coefficients (in the units of $10^{-20} \text{cm}^3/\text{s}$) corresponding to the formation of cations in electron.

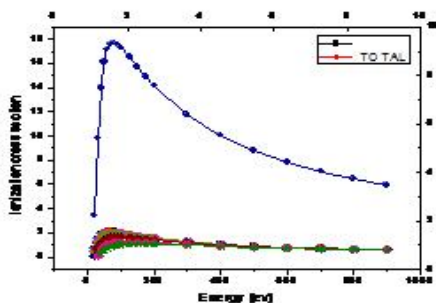


Figure 1: Graphs represent Electron impact ionization

4. Conclusion

The Rate coefficient is obtained for the ionic target is observed to be under estimated by the empirical law whereas the latter overestimates the data corresponding to neutral Difluoromethane.

5. References

- [1] S. Pal, “Determination of single differential and partial cross sections for the production of cations

in electron-methanol collision,” *Chemical Physics*, 2004, 302 (1–3): 119–12.

- [2] S. Pal, J. Kumar, and T. D. Mark, “Differential, partial and total electron impact ionization cross sections for SF₆,” *The Journal of Chemical Physics*, 2004, 120(10):4658–4663.
- [3] P. Bhatt and S. Pal, “Determination of cross sections and rate coefficients for the electron impact dissociation of NO₂,” *Chemical Physics*, 2006, 327(2–3):452–456.
- [4] S. Pal, “Differential and partial ionization cross sections for electron impact ionization of plasma processing molecules: CF₄ and PF₅,” *Physica Scripta*, 2008, 77(5): 7.
- [5] M. Capitelli, R. Celiberto, and M. Cocciatore, “Needs for cross sections in plasma chemistry,” *Advances in Atomic, Molecular, and Optical Physics*, 1994, 33: 321–372.
- [6] T. Fujimoto, “Semi-empirical cross sections and rate coefficients for excitation and ionization by electron collision and photo ionization of Helium,” *Institute of Plasma Physics Report, IIPJ-AM-8*, Nagoya University, Nagoya, Japan, 1978.
- [7] S. Pal and S. Prakash, “Partial differential cross sections for the ionization of the SO₂ molecule by electron impact,” *Rapid Communications in Mass Spectrometry*, 1998, 12(6):297–301.
- [8] M. Inokuti, “Inelastic collisions of fast charged particles with atoms and molecules—the bethe theory revisited,” *Reviews of Modern Physics*, 1971, 43 (3): 297–347.