J. At. Mol. Sci.
doi: 10.4208/jams.061810.071610a

Vol. **1**, No. 4, pp. 301-307
November 2010

Electron impact ionization cross sections of C_2H_2 and CH molecules at low and high energy range

Neelam Tiwari[a,*], Yogesh Kumar[b], and Surekha Tomar[a]

[a] *Department of Physics, R.B.S College, Agra-282002, U.P, India*
[b] *D.A.V College, Muzzaffarnagar-251001, U.P., India*

Received 18 June 2010; Accepted (in revised version) 16 July 2010
Published online 2 August 2010

Abstract. In this communication, studies of the total ionization cross sections of hydrocarbon molecules (CH, C_2H_2) due to electron impact are presented. Electron impact ionization cross sections (EIICS) have been calculated from threshold ionization energy to high energy (10 MeV). Apart from EIICS calculation the values of collisional parameters are also calculated. The theoretical model, developed by Khare, has been modified to calculate the total ionization cross section for molecules. Obtained theoretical cross sections are compared extensively with a number of experimental and theoretical data. The obtained values of collisional parameter compared with the available experimental values.

PACS: 34.80.Gs
Key words: ionization cross section, C_2H_2 and CH molecules, electron impact

1 Introduction

The study total ionization cross-sections by electron impact of molecules 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. Electron impact ionization cross sections (EIICS) at high energy have great importance in many accelerator applications. Cross sections due to ionization are needed for modeling of radiation effects in materials and in biomedical research and modeling of fusion plasmas in tokomaks. The computed data on cross sections are necessary in studying the problems of radiative association [1, 2]. The hydrocarbon molecules are one of the Earth's most important energy resources, and also an important part of the plasma processing. Hydrocarbons are currently the main source of the world's electric energy and heat sources.

*Corresponding author. *Email address:* neelutiwari5@gmail.com (N. Tiwari)

Acetylene (C_2H_2) is used to volatilize carbon in radiocarbon dating which is widely used as a fuel and a chemical building block.

The EIICS for acetylene molecule electron impact ionization cross sections have been calculated by many researchers [3,4]. Kim *et al.* [3] theoretically calculated the total cross section for C_2H_2 from threshold to 1 keV by using Binary Encounter Bethe theory and Vinodkumar *et al.* [4] calculated from threshold to 2 keV. Vinodkumar *et al.* [4] calculated total cross section for elastic and inelastic collisions and total ionization cross sections are calculated by 'complex scattering potential-ionization contribution' method. Experimentally total ionization cross section for C_2H_2 is measured by Zheng and Srivastava [5] for energy range threshold to 800 eV. For high energy the total cross section measured by Reike and Prepejchal [6] from 0.1 MeV to 2.7 MeV. For Methylidene (CH) molecule total ionization cross section measured by Tarnovsky *et al.* [7] for energy range threshold to 200 eV and calculated by Kim *et al.* [3] for energy range from threshold to 1 keV while Vinodkumar calculated up to 2 keV. For CH there is no experimental and theoretical data available for high energy range according to best of our knowledge. Experimentally total cross section for high energy range is available for acetylene only by Reike and Prepejchal [6].

One of the purposes of this work to calculate the electron impact ionization cross sections of the molecules by employing the useful features of Kim model with Saksena model to remove the deficiency of the later model at low temperature. For CH_4 molecule Khare *et al.* [8] replaced $(1-\omega/E)$ by $(E'/E'+U+I)$, where ω is the energy lose suffered by incident electron in the ionizing collision, E is the kinetic energy of incident electron, E' is the relativistic energy, I is the ionization energy, U is the average kinetic energy of bound electron. Here $U+I$ represent the increase in kinetic energy of the incident electron due to its acceleration by the field of the target nucleus. In the present work we have extended Khare *et al.* [8] model to study the EIICS of CH and C_2H_2 molecule in such a way that it yield better agreement between theory and experiments. To the best of our knowledge, this is the only theory which is applicable for such a wide energy range varies from threshold to several MeV.

2 Theory

Saksena *et al.* [9] have proposed a model for the molecular ionization cross sections. They started with the plane wave born approximation (PWBA) but later on included exchange and relativistic corrections. The transverse interaction through emission and the re-absorption of the virtual photons along with the longitudinal interaction through the static unretarded coulomb field are also included. However, PWBA requires continuum generalized oscillator strengths (CGOS), which are very difficult to evaluate. Hence, they employ a semi-phenomenological relation of Mayol and Salvet [10] 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 or-

bital into two terms one representing the Bethe term (Soft collision) and other one the Mott term (hard collision). But it is found that their model has been found to underestimate the cross section at low impact energies. Hence to remove the deficiency of the former model at low E, another model was developed by Khare *et al.* [8] by combining the useful features of Saksena *et al.* [9] model and the Binary Encounter Bethe models of Hwang *et al.* [11] dropping the contribution of the exchange to the Bethe term and the adhoc cut off factor from it. Furthermore the effect of the acceleration of the incident electron by the molecular field is included through the classical binary encounter theory for COOS, the present total ionization cross section for the j^{th} molecular orbital for incident energy E is given by

$$\sigma_{jt}=\sigma_{jpBB}+\sigma_{jpMB}+\sigma_{jjt}, \tag{1}$$

where

$$\sigma_{jpBB}=\frac{AN_jI_j}{(E'+U_j+I_j)}\int_{I_j}^{E'}\frac{1}{\omega^3}\ln\left[\frac{\omega}{Q_-}\right]d\omega. \tag{2}$$

The recoil energy Q_- is given by [8]

$$Q_-=0.5mc^2[\{E(E-\omega)\}^{1/2}-\{(E-\omega)(E-\omega+2mc^2)\}^{1/2}]^2. \tag{3}$$

It is due to the assumption that a large contribution to the integral comes from the small values of ω. Hence for $\omega \ll E$ we obtain from Eq. (3)

$$Q_-=\frac{\omega^2}{4}\left[0.5mc^2+\frac{1}{E}\right]. \tag{4}$$

Now putting this in Eq. (2) and evaluating the integral we obtain

$$\begin{aligned}\sigma_{jpBB}=&\frac{AN_jI_j}{(E'+U_j+I_j)I_j}\left[0.4431\left(1-\frac{1}{t^2}\right)\right.\\&\left.-0.5\ln\left(\frac{1}{t}+\frac{I_j}{2mc^2}\right)+\frac{1}{2t^2}\ln\left(1+\frac{E'}{2mc^2}\right)\right],\end{aligned} \tag{5}$$

$$\begin{aligned}\sigma_{jpMB}=&\left[\frac{AN_j}{(E'+U_j+I_j)I_j}\right]\left[\left(1-\frac{2}{t+1}+\frac{t-1}{2t^2}\right)\right.\\&\left.+\left(\frac{5-t^2}{2(t+1)^2}-\frac{1}{t(t+1)}\right)-\left(\frac{(t+1)}{t^2}\ln\left(\frac{t+1}{2}\right)\right)\right],\end{aligned} \tag{6}$$

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

where σ_{jpBB}, σ_{jpMB} and σ_{jjt} are the Bethe's, Mott's cross section and the cross section due to transverse interaction respectively with the following values of t and β

$$t=\frac{E'}{I_j},\quad \beta=\frac{v}{c}$$

with

$$E' = \frac{1}{2}mv^2 = \frac{1}{2}mc^2\left[1 - \frac{1}{(1+E/mc^2)^2}\right],$$

where U_j is the average kinetic energy of the bound electron of the j^{th} orbital, $A{=}4\pi {a_0}^2 R^2$, R is Rydberg energy, a_0 is first Bohr radius, N_j is the number of electrons, I_j is the ionization thresholds, m is the rest mass of electron, E' is the relativistic energy, v is the incident velocity, c is the velocity of light, Q_- is the recoil energy, ω is the energy loss, ${M_j}^2$ is the total dipole matrix squared for the ionization. Reike and Prepejchal [6] have expressed their molecular cross-section measured in the energy of 0.1 to 2.7 MeV in terms of two collision parameters ${M_j}^2$ and C is given by

$$\sigma_{jjt} = -\frac{A}{RE}[M_j^2\{\ln(1-\beta^2)+\beta^2\}+C]. \tag{8}$$

3 Results and discussion

In the present investigation EIICS have been calculated for the two hydrocarbon molecules CH and C_2H_2 by the modified formula. From Eq. (1) the ionization cross sections σ_{jt} have been calculated for each orbital of the molecules for incident energy E' varying from threshold ionization energy to high energy (10 MeV). Using present method the EIICS is the sum of Eqs. (5), (6) and (7).

The calculated cross section for each orbital, contributes to the total ionization cross section of whole molecule. The term σ_{jjt} is ignored since it is of significance only at high energies. With best of our knowledge there is no experimental data available for energy range 12 keV to 0.1 MeV for the present molecules. Table 1 contained the calculated collision parameters C and ${M_j}^2$ of considered molecules which are obtained by employing the COOS given by Khare *et al.* [8] at large E.

Table 1: C, ${M_j}^2$: Collision parameters [6]

Molecules	Calculated		Experimental [6]	
	C	${M_j}^2$	C	${M_j}^2$
C_2H_2	53.71	4.34	53.76	5.12
CH	28.64	2.30		

The ionization cross sections for both molecules are compared with the available experimental and theoretical data as following.

In Fig. 1 which shows the comparison of present cross sections for C_2H_2 along with the experimental data given by Zheng and Srivastava [5], and theoretical data set of Kim *et al.* [3], Vinodkumar *et al.* [4]. Overall data (theoretical and present) maintain same shape and slightly overestimate in comparison with the other data till 100 eV. Present data find very good comparison with the measurements of Zheng and Srivastava [5] till around 100 eV and then falls slightly below the experimental data.

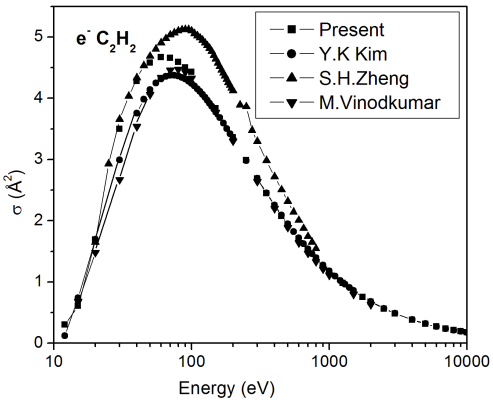

Figure 1: The figure compares the present theoretical total cross section and experimental total cross section for C_2H_2. Square, present work; triangles, experimental data by Zheng [5]; circle, theoretical data by Kim [3]; inverted triangles, theoretical data by Vinodkumar [4].

Fig. 2 shows the modified theoretical calculation for C_2H_2 at $E > 10$ keV. Although theories behind EIICS have a tendency to underestimate the cross sections, the total cross sections are in good agreement with experimental data measured by Reike and Prepejchal [6]. The calculated values of collisional parameter C and ${M_j}^2$ obtained at 1 MeV are 53.71 and 4.34, respectively. These values are about 13% and 0.09% lower than the corresponding experimental values of Reike and Prepejchal [6]. All these values of the collision parameter do not change with the increase of E.

In Fig. 3 the graph depicted the total ionization cross section for CH molecule and

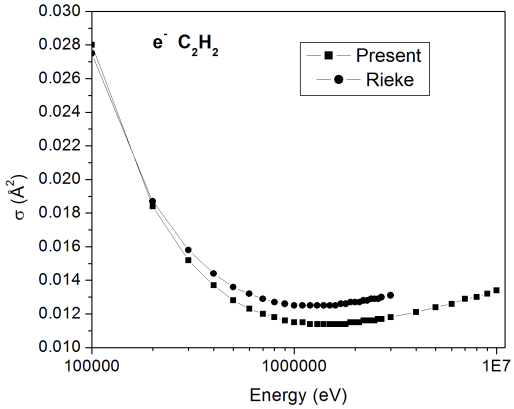

Figure 2: This figure showing the comparison of the present theoretical total cross section to experimental data for C_2H_2. Square, the present work; circle, the experimental data by Reike and Prepejchal [6].

compared with theoretical values of Kim *et al.* [3], Vinodkumar *et al.* [4] and the only measurement of Tarnovsky *et al.* [7]. However, present data compares very well with the theoretical results after 100 eV. Present result gives a better comparison with the other theoretical data. Experimental results from Tarnovsky *et al.* [7] gives surprisingly small cross section and under estimate all the theoretical values by near about 1.4 times at the peak. Since there is no any other experimental data available, so it is quite difficult to make any conclusions.

Fig. 4 shows the total cross sections for CH from 0.1 MeV to 10 MeV. The present value of M_j^2 and C obtained at 1 MeV are 2.30 and 28.64 respectively. However there is no experimental and theoretical data available to compare with present calculation to the

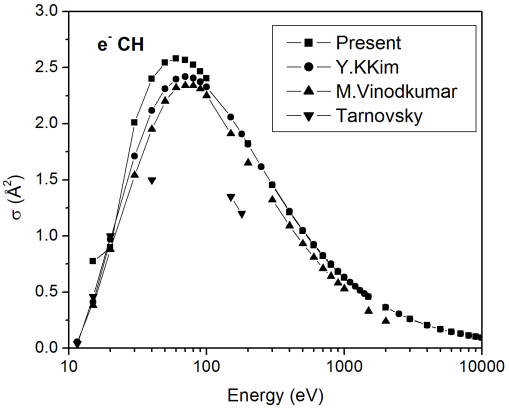

Figure 3: This figure compares of the present theoretical total cross section to experimental total cross section for CH. Square, present work; circle, Kim *et al.* [3]; triangles, theoretical data by Vinodkumar *et al.* [4]; inverted triangles, experimental data by Tarnovsky *et al.* [7].

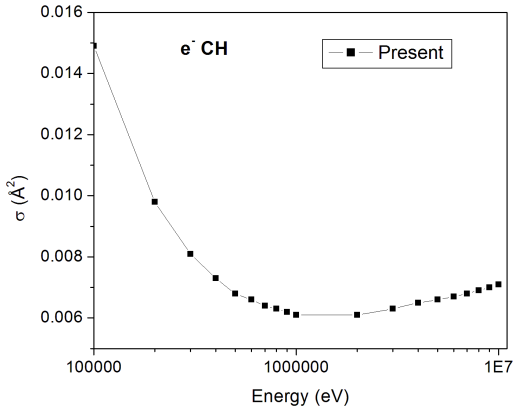

Figure 4: This figure shows the present theoretical total cross section for CH.

best of our knowledge.

4 Conclusion

From the present study it is concluded that the theoretical predicted and measured value of the total ionization cross sections for C_2H_2 and CH hydrocarbon molecules are in good concurrence. Furthermore we have extended Khare model [8] which has considerably improved the agreement between the experimental and theoretical data at low and high energy range. Although it is clear from the results of the various measurements reported in the literature sometimes disagree with theoretical data.

At higher values of energy, there is hardly any difference between the present and data measured by Reike and Prepejchal [6]. Thus the experimental data is in good agreement with the present data over a high energy range. The present value of collisional parameters seems to be in reasonable agreement with the experimental data by Reike and Prepejchal [6]. The present modification gives satisfactory results for low and high energy range. To the best of our knowledge this is the first calculation for C_2H_2 and CH hydrocarbon molecules over a wide energy range from threshold to 10 MeV.

The application of the present model to the ionization of other molecules and atoms, including inner-shell and dissociative ionizations is of interest.

Acknowledgments. The authors are grateful to the University Grants Commission, New Delhi for financial support. Neelam Tiwari acknowledges the IUAC New Delhi for providing the hospitality.

References

[1] W. Lindinger and F. Howorka, in: Electron Impact Ionization, eds. T. D. Mark and G. H. Dunn (Springer, Berlin, 1985).
[2] D. R. Bates and I. Mendas, Proc. R. Soc. A 402 (1985) 245.
[3] Y. K. Kim, M. A. Ali, and M. E. Rudd, J. Res. Natl. Inst. Stand. Technol 102 (1997) 693.
[4] M. Vinodkumar, K. N. Joshipura, C. G. Limbachiya, and B. K. Antony, Eur. Phys. J. D 37 (2006) 67.
[5] S. H. Zheng and S. K. Srivastava, J. Phys. B: At. Mol. Opt. Phys. 29 (1996) 3235.
[6] F. F. Rieke and W. Prepejchal, Phys. Rev. A 6 (1972) 1507.
[7] V. Tarnovsky, A. Levin, H. Deutsch, and K. Becker, J. Phys. B: At. Mol. Opt. Phys. 29 (1996) 139.
[8] S. P. Khare, M. K. Sharma, and S. Tomar, J. Phys. B: At. Mol. Opt. Phys. 32 (1999) 3147.
[9] V. Saksena, M. S. Kushwha, and S. P. Khare, Physica B 233 (1997) 201.
[10] R. Mayol and F. Salvat, J. Phys. B: At. Mol. Opt. Phys. 23 (1990) 2117.
[11] W. Hwang, Y. K. Kim, and M. E. Rudd, J. Chem. Phys 104 (1996) 2956.