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Electron impact ionization cross sections of allene and propane molecules at low and high energy range

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Abstract. We have made a study of the total ionization cross sections of hydrocarbon molecules (allene, propane) due to electron impact for single ionization. Electron impact ionization cross sections (EIICS) have been calculated from threshold ionization energy to high energy (10 MeV). Along with EIICS calculation the values of collisional parameters are also calculated. The theoretical model, developed by Khare, has been modified to calculate the electron impact ionization cross section for molecules and atoms. The predicted EIICS of allene and propane molecules are compared with other theoretical and experimental data. Present model prevail a high degree of goodness of cross sections to the experimental data. Adequate comparisons of collisional parameter have been made with other available experimental values.

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Key words: ionization cross section, molecules, electron impact, collisional parameter

1 Introduction

The study of 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

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cross sections are necessary in studying the problems of radiative association [1, 2]. Allene (C_3H_4) and propane (C_3H_8) are hydrocarbon molecules. Allene is the one of the isomers having the chemical formula C_3H_4 and others are propyne and cyclopropene. These isomers have different ionization potential. In our calculation we have used the isomer, which having the smallest ionization potential. The hydrocarbon molecules are one of the Earth's most important energy resources, and also an important part of the plasma processing. Currently hydrocarbons are the main source of the world's electric energy and heat sources.

Allene is chiefly used in organic synthesis. The EIICS for allene molecule have been calculated by Kim *et al.* [3] but no experimental data is available there. Kim *et al.* [3] theoretically calculated the total cross section for allene from threshold to 1 keV by using Binary Encounter Bethe theory. With best of our knowledge there is no experimental and theoretical data available for allene molecule at high energy range. For propane molecule the ionization cross sections have been calculated by Vinodkumar *et al.* [4] and Hwang *et al.* [5]. Hwang *et al.* [5] calculated the total cross section for propane from threshold to 1 keV by using Binary Encounter Bethe theory while 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.

Propane is a nonrenewable energy source. It is used in semiconductor manufacture to deposit silicon carbide. Experimentally EIICS for propane is measured by various groups [6–10]. Measurement for propane is reported by Nishimura and Tawara [6], Schram *et al.* [7], Defrance and Gomet [8] and Duric *et al.* [9]. For high energy the electron impact ionization cross sections for propane have been measured by Reike and Prepejchal [10] from 0.1 MeV to 2.7 MeV.

One of the purpose of this work to calculate the electron impact ionization cross sections of the molecules by employing the useful features of Kim model [3] with Saksena model [11] to remove the deficiency of the later model at low energy. For CH_4 molecule Khare *et al.* [12] replaced $(1-\omega/E)$ by $(E'/E+U+I)$, where ω is the energy lost by the 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 the 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.* [12] model to study the EIICS of allene and propane 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.* [11] 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 [13] 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 orbital 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.* [12] by combining the useful features of Saksena *et al.* [11] model and the Binary Encounter Bethe models of Hwang *et al.* [5]. Hwang *et al.* [5] dropped the contribution of exchange to Bethe term. Furthermore they included the effect of acceleration of the incident electron by the molecular field through the classical-binary encounter theory and used a simple representation of the COOS.

In present model to calculate the EIICS, we require three constants for each molecule, ionization energy 'I', the occupation number 'N' and the average kinetic energy of bound electron 'U'. The values of these molecular orbital constants (I, N and U) for the considered molecules have given by Kim and co-workers [5, 14]. The present EIICS for the j^{th} molecular orbit for incident energy E is given by

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

where

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

The recoil energy Q_- is given by [12]

$$Q_- = \frac{1}{2mc^2}\left[\Big(E(E-\omega)\Big)^{\frac{1}{2}} - \Big((E-\omega)(E-\omega+2mc^2)\Big)^{\frac{1}{2}}\right]^2. \tag{3}$$

Khare have taken an approximate expression for Q_- [15]

$$Q_- = \frac{\omega^2}{4E}, \tag{4}$$

Now putting the value of Q_- from Eq. (3) in Eq. (2) and evaluating the integral, we obtain

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

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

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

Here 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

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

with

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

Reike and Prepejchal [10] 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

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

The symbols used here are listed as follows:

σ_{jpBB}	=present Bethe's cross section
σ_{jpMB}	=present Mott's cross section
σ_{jjt}	=the cross section due to the transverse interaction
σ_{jt}	=total ionization cross-section for the jth molecular orbital
U_j	=average kinetic energy of the bound electron of the jth orbital
I_j	=ionization thresholds
E	=incident energy
E'	=Kinetic energy
v	=incident velocity
c	=velocity of light
A	$=4\pi a_0^2R^2$
N_j	=number of electrons
ω	=energy lost by the incident electron in the collision
R	=Rydberg energy
M_j^2	=total dipole matrix squared for the ionization
C	=collision parameter
$df/d\omega$	=continuum optical oscillator strengths
m	=rest mass of electron
Q_-	=recoil energy
a_0	=first Bohr radius

3 Result and discussion

Electron impact ionization cross sections (σ_{jt}) have been calculated for the two hydrocarbon molecules allene and propane by the modified formula given by Eq. (1) which is sum

of Eqs. (5), (6) and (7). The calculated cross sections for each orbital of the molecules for incident energy E' varying from threshold ionization energy to high energy (10 MeV), contributes to the total ionization cross section of whole molecule. In the calculation the term σ_{jjt} has been ignored since it is of significance only at high energies ($E \geq 0.1$ MeV). At low impact energies, the relativistic effect is negligible but exchange becomes important. Due to the negligible relativistic effect σ_{jjt} is very small. The total ionization cross section at low impact energies ($E < 1$ keV) is

$$\begin{aligned}\sigma_{jt} &= \sigma_{jpBB} + \sigma_{jpMB} + \sigma_{jjt} \\ &= \sigma_{jpBB} + \sigma_{jpMB}, \qquad \text{(From threshold to 1 keV)}\end{aligned}$$

However, at higher values of E, σ increases with E, whereas $\sigma_{jpBB} + \sigma_{jpMB}$ tend to be constant because the exchange and Coulomb corrections are negligible but relativistic effect becomes more important. Hence σ_{jjt} (due to transverse interaction) highly contributes to the total ionization cross section than $\sigma_{jpBB} + \sigma_{jpMB}$ at energy ≥ 0.1 MeV [16].

With best of our knowledge there are no experimental data available for energy range 12 keV to 0.1 MeV for the same proposed molecules. Table 1 presents the calculated and experimental [6, 7, 10, 17] values of collision parameters C and M_j^2 for the two molecules presently investigated. Collision parameters C and M_j^2 have been calculated by employing COOS given by Khare *et al.* [12] at 1 MeV. To access the level of performance of the present model, its predictions are compared with the result available from the other experimental and theoretical data.

- In Fig. 1 electron impact ionization cross sections for allene molecule are compared to the theoretical values of Kim *et al.* [3]. We can see that calculated EIICS are in good agreement with the theoretical data of Kim by maintaining the same shape of the curve but beyond the peak obtained results seems to be shifted slightly towards left. Since no other data is available, it is quite difficult to make more conclusions.

- The EIICS for allene for high energy from 0.1 MeV to 10 MeV have plotted in Fig. 2. The calculated value of M_j^2 and C obtained at 1 MeV are 7.23 and 89.74 respectively. However, for the present molecule no electron scattering data are yet reported in literature at this energy range, to our knowledge. EIICS at high energy have great importance in many accelerator fields [18].

- In Fig. 3 we have depicted electron impact ionization cross sections for propane molecule and compared with the other available experimental and theoretical result. The present results are in good agreement with the available theoretical result of Hwang *et al.* [5] and M. Vinodkumar *et al.* [4]. However, calculated result compares very well with the theoretical results [4, 5] after 100 eV. The experimental data from Defrance and Gomet [8] gives surprisingly large cross section and over estimate all the theoretical values at the peak. Present result gives a better comparison with the other experimental data given by Nishimura and Tawara [6] but somewhat lower than those by Nishimura

and Tawara [6]. While it over estimate other measurement of Duric and Schram [7,9]. Our calculated result shows better agreement with experimental data than other previous theoretical data.

- Fig. 4 shows the present theoretical calculation for propane at $E > 10$ keV. The EIICS are agree well with experimental data measured by Reike and Prepejchal [10]. The agreement between the experimental and theory is good, although theory has a tendency to underestimate the cross sections. The calculated values of M_j^2 and C obtained at 1 MeV are 8.45 and 104.71, respectively. These values are about 8% and 8.2% lower than the corresponding experimental values of Reike and Prepejchal [10]. Due to the difference between the calculated collisional parameter and measured by Reike and Prepejchal [10], discrepancies comes in calculated EIICS and measured by them [10]. The term σ_{jjt} (cross section due to transverse interaction) at MeV energy range highly contributes to total ionization cross section. The obtained value of M_j^2 is also compared with the available value given by Nishimura and Tawara [6], Schram *et al.* [7] and optical by Schoen [17] in Table 1. The calculated values of collisional parameters are in excellent agreement with the other measured value. All these values of the collision parameter do not change with the increase of E.

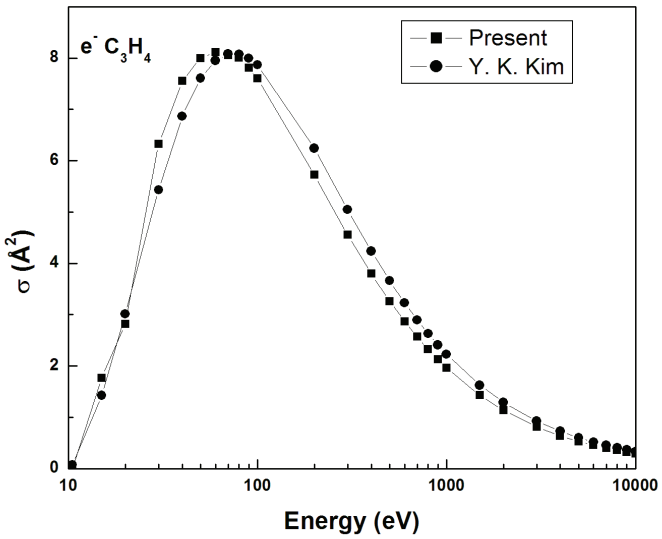

Figure 1: The comparison of the present calculated EIICS and other theoretical EIICS for allene. Square ■, the present work; circle •, theoretical data by Y-K Kim *et al.* [3].

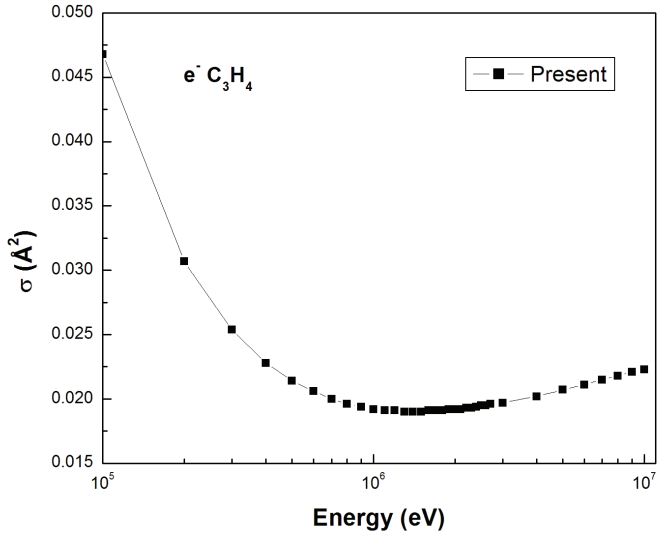

Figure 2: The present theoretical EIICS for allene.

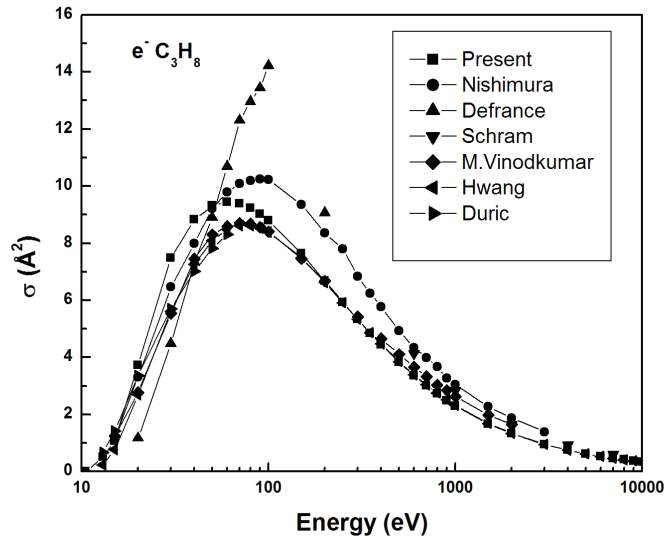

Figure 3: The comparison of the present theoretical EIICS to experimental electron impact ionization cross sections for propane. Squares ■, the present work; Circle •, experimental data by Nishimura and Tawara [6]; triangles ▲, experimental data by Defrance and Gomet [8]; inverted triangles ▼, experimental data by Schram *et al.* [7]; diamond ♦, theoretical data by M. Vinodkumar *et al.* [5]; ◄, theoretical data by Hwang *et al.* [5]; ►, experimental data by Duric *et al.* [9].

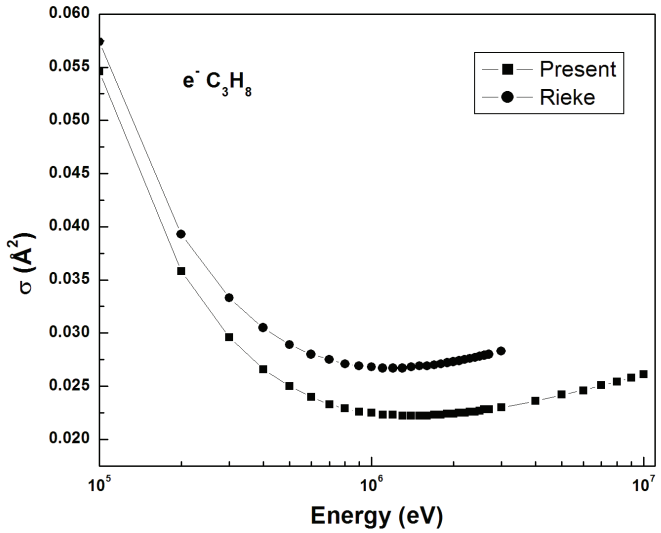

Figure 4: The comparison of the present calculated EIICS to experimental data for propane. Square ■, the present work; circle •, experimental data by Reike and Prepejchal [10].

Table 1: C, M_j^2: Collision parameters [6, 7, 10, 16].

Molecules	Calculated		Reike		Nishimura	Schram	Schoen
	C	M_j^2	C	M_j^2	M_j^2	M_j^2	M_j^2
Allene (C_3H_4)	89.74	7.23	——	——	——	——	——
Propane (C_3H_8)	104.71	8.45	114.10	9.19	20	13.8	7.60

4 Conclusion

In this paper we has been reported comprehensive calculations of EIICS for allene and propane and also compared with the available experimental and theoretical data. Present method has been successfully tested for a number of molecular targets [19–21]. The present study investigates an almost complete picture of EIICS for allene and propane molecule at low and high energy range. Furthermore we have extended Khare model [12] 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 [10]. 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 various groups [6, 7, 10, 17]. As far as we know there is no other single model to apply for such a wide range of

energies and seems to be very use full for applications. To the best of our knowledge this is the first calculation for allene and propane hydrocarbon molecules over a wide energy range from threshold to 10 MeV. The modified formulae have great versatility of obtaining electron impact cross sections for a great variety of molecules and atoms.

The application of the present model is to extend this analysis to the ionization of other complicated molecules and clusters by knowing their molecular orbital constants.

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