REVIEW OF RESEARCH
ISSN: 2249-894X
IMPACT FACTOR : 5.7631(UIF)
VOLUME - 10 | ISSUE - 12 | SEPTEMBER - 2021

ELECTRON IMPACT IONIZATION CROSS SECTIONS OF 1-HYDROXYPROPANE

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ABSTRACT:

In the present study the total ionization cross sections of 1-Hydroxypropane (C_3H_7OH) molecule due to electron impact for single ionization have been employed. Electron impact ionization cross sections (EIICS) have been calculated from threshold ionization energy to 14 MeV. The theoretical model, developed by Jain-Khare has been used to calculate the electron impact ionization cross section for 1-Hydroxypropane. The Present work is in good agreement with the available theoretical and experimental data.

KEYWORDS: *Cross sections, Electron impact ionization, 1-Hydroxypropane.*

I. INTRODUCTION

The study of ionization cross section by electron impact of molecules are required in mass spectrometry, ionization in gas discharge, plasma diagnostic, astronomy, modeling of radiation effect for both materials and medical research[1-2]. Electron impact ionization cross sections (EIICS) at high energy have great importance in various accelerator applications. Electron impact ionization of 1-Hydroxypropane is widely used in the plasma modelling.

1-Hydroxypropane is very complex target because it contains three atoms of carbon, eight atoms of hydrogen and one atom of oxygen, Therefore, it is a very difficult task to evaluate the electron impact ionization cross sections theoretically. Many investigations were carried out for experimental and theoretical evaluations of the ionization cross sections of 1-Hydroxypropane. Recently, Vinod Kumar et al. [3] calculated the total ionization cross section for these molecules. They used the complex scattering potential ionization contribution method. Hudson et al [4] calculated ionization cross section for 1-Hydroxypropane from the ionization threshold to 300 eV using the Deutch–Mark (DM) and Kim binary-encounter-Bethe (BEB) models. Deutch et al [5] calculated the ionization cross section of 1-Hydroxypropane. They used additive rule and weight factors, which depend on the atomic radii. Recently, Y.Kumar et al [6] calculated the ionization cross section of 1-Hydroxypropane. They used the plane-wave Born approximation for finding total ionization cross section of 1-Hydroxypropane from threshold to 10 MeV.

Hudson et al [4] measured the total ionization cross sections in the energy range 16 to 207 eV and Djuric et al [7] also reported the total ionization cross sections of 1-Hydroxypropane. Djuric et al [7] employed the parallel plate method.

II.THEORETICAL METHODOLOGY

The present calculations are carried out using the modified semi empirical formalism developed by Jain-Khare [10-13].In brief, the single differential cross sections in the complete solid angle (Ω

$=\int 2\pi sin\theta d\theta$)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

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

Where, $W\ (=\varepsilon + I_i)$ 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,
ε_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. The oscillator strength is directly proportional to the photo ionization cross section [10-13]. 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 [14] 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.

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

where β is the asymmetric parameter and $P_2(\cos\theta)=\frac{1}{2}\left(3\cos^2\theta-1\right)$ 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. 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.

III. RESULT AND DISCUSSION

Total ionization-cross section (TICS) values for electron impact ionization of 1-Hydroxypropane in 10^{-20} m^2 are given in below table.

Energy (eV)	TIC of 1-Hydroxypropane	Energy (eV)	TIC of 1-Hydroxypropane
1.50E+01	1.17E+00	2.00E+03	1.96E+00
2.00E+01	3.87E+00	4.00E+03	1.11E+00
3.00E+01	8.01E+00	6.00E+03	7.90E-01
4.00E+01	1.02E+01	8.00E+03	6.19E-01
5.00E+01	1.14E+01	1.00E+04	5.13E-01
6.00E+01	1.19E+01	2.00E+04	2.86E-01
7.00E+01	1.21E+01	4.00E+04	1.63E-01
8.00E+01	1.21E+01	6.00E+04	1.19E-01
9.00E+01	1.20E+01	8.00E+04	9.57E-02
1.00E+02	1.18E+01	1.00E+05	8.25E-02
2.00E+02	9.43E+00	2.00E+05	5.39E-02
3.00E+02	7.64E+00	4.00E+05	4.07E-02
4.00E+02	6.43E+00	6.00E+05	3.63E-02
5.00E+02	5.56E+00	8.00E+05	3.52E-02
6.00E+02	4.90E+00	1.00E+06	3.41E-02
7.00E+02	4.40E+00	5.00E+06	3.63E-02
8.00E+02	3.99E+00	1.00E+07	3.96E-02
9.00E+02	3.66E+00	1.20E+07	4.18E-02
1.00E+03	3.38E+00	1.40E+07	4.05E-02

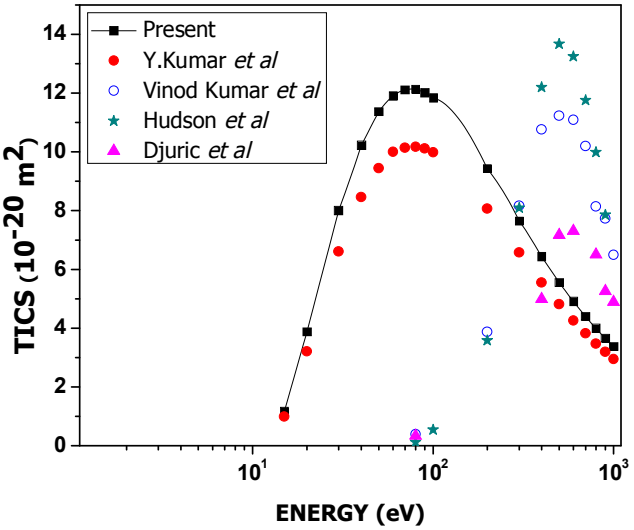

Figure: Total ionization cross sections of 1-Hydroxypropane (C_3H_7OH)

Total ionization cross sections (TICSs) for C_3H_7OH in 10^{-20} m^2, the solid square line represents the present results, the filled hexagonal represents the theoretical results calculated by Y. Kumar et al [6], the hollow circles represents the theoretical results calculated by Vinod Kumar et al [3], the filled stars represents the theoretical results caculated by Hudson et al [4], the filled triangles represents the experimental results of Djuric et al [7].

Figure shows total ionization cross sections for 1-Hydroxypropane in the energy region from threshold to 1000 eV together with the earlier results of Vinod Kumar et al [3], Hudson et al [4], Deutsch et al [5], Y.Kumar et al [6] and Djuric et al [7] in the same energy region. The required ionization energies are taken from Irikura [8] and Rejoub et al [9]. In the present investigation total ionization cross section reaches its maximum at 80 eV. There is good agreement between our cross sections and the data of Y.Kumar et al [6] both in terms of cross section values and cross section shapes. The corresponding cross section of Hudson et al [4] is comparatively higher at 500 eV energy, declining faster towards higher impact energies in comparison with the results of Hudson et al [4], Deutsch et al [5], Y.kumar et al [6] and Djuric et al [7]. The present calculated cross section data appears to consistently higher than the experimental results reported by Djuric et al [7] and theoretical result of Vinod Kumar et al [3].

IV. CONCLUSION

In this present work we have calculated total ionization cross sections for electron impact ionization of 1-Hydroxypropane molecule using semi-empirical model developed by Jain and Khare. The present study investigates total electron impact ionization cross sections for 1-Hydroxypropane from threshold to 14 MeV. The present calculations are compared with the theoretical results and experimental data of Vinod Kumar et al [3], Hudson et al [4], Y.Kumar et al [6] and Djuric et al [7].

The present cross sections consistently show a good agreement with the results of Y.Kumar et al [6] from lower to upper range of energies. However, they are greater than the experimental data measured by Djuric et al [7]. At relativistic energies, the calculated data are also found in good agreement with the theoretical data of Y.kumar et al [6]. The present method can be used for calculation of ionization cross sections for organic molecules even with high incident energy range.

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