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Electron Impact Ionization Cross Sections and Rate Coefficients for the Pyrimidine Molecule

Yogesh Kumar [1], Anushka Tyagi [2], Radhika Saini [3], Tanu, Neeraj Kumar [4*]

[1-4] Department of Physics, D.A.V. College, Muzaffarnagar, Uttar Pradesh, India

Corresponding Author: * Neeraj Kumar

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Abstract

In the present work, the total ionisation cross sections (TICS) of pyrimidine have been calculated using the simplified Khare BEB method. The calculations were performed for incident electron energies spanning from ionization threshold to 10 MeV. Comparisons with available experimental data and other theoretical models demonstrate that the Khare BEB method yields accurate predictions while maintaining computational efficiency. The present findings not only validate the applicability of the simplified Khare BEB formalism to complex heteroaromatic systems but also contribute to the growing database of ionization cross sections essential for radiation biology, astrophysics, and plasma modeling. Using the evaluated ionization cross sections and Maxwell–Boltzmann electron energy distribution we have also calculated the ionization rate coefficients as a function of electron temperature/energy.

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1. INTRODUCTION

Electron impact ionization cross sections are fundamental parameters for understanding the interactions of charged particles with atoms and molecules. It plays a significant role in a wide range of physical, chemical, and biological environments. These cross sections are essential for modeling of plasma processing, astrophysical media, and environmental chemistry, where accurate knowledge of ionization probabilities is required for reliable simulations and experimental interpretation. In particular, the interaction of electrons with molecular targets governs various microscopic processes such as excitation, ionization, and fragmentation, which collectively determine the energy deposition and transport mechanisms in matter exposed to radiation fields [1-3].

In the last few years, the electron impact ionization of DNA and RNA constituent molecules has been an interest of investigation to understand the physical mechanism of damage to biological system on microscopic level. In cancer radiotherapy, the interaction of radiation with bio-molecules creates the low energy secondary electrons, ions and radicals in large quantities. These low energy electrons induced DNA damage with single and double strand breaks by dissociative electron attachment process. Ionizing radiation interacting with biologically important molecules can induce ionization and subsequent fragmentation processes, ultimately leading to molecular damage and structural modifications in cellular environments [4-6]. Among such molecules, heterocyclic aromatic compounds play a crucial role as fundamental building blocks of nucleic acids. Pyrimidine, a six-membered heterocyclic ring containing two nitrogen atoms, forms the structural basis of nucleobases such as cytosine, thymine, and uracil, which are essential constituents of DNA and RNA. Consequently, the study of electron impact ionization of pyrimidine provides valuable insight into radiation-induced damage mechanisms at the molecular level and contributes to the broader understanding of biological radiation effects [7].

Experimental and theoretical investigations of ionization cross sections for molecules have been carried out using a variety of techniques and methods over several decades. Bug et al. [8] have measured the single differential cross sections of pyrimidine molecule along with other constituent molecules of DNA in energy range from 10 eV to 10 keV. They obtained the total ionization cross sections by integrating the experimental data of single differential cross sections. They declared the uncertainty in their experiment in order of 25%. Linert et al. [9] reported the experimental data of pyrimidine molecule from incident energies from 12 eV to 145 eV. They have used the quadrupole mass spectrometer and claimed 20% experimental error in their experiment. Dinger et al. [10] have also produced the total ionization cross sections of the same molecule from doubly differential electron impact ionization cross sections with uncertainty of 30%. Gupta et al. [11] have calculated the electron-impact ionization cross-section of pyrimidine molecules by using the spherical complex optical potential formalism with complex scattering potential ionization contribution method. Recently, Zywicka and Mozejko [7] have employed Kim BEB method to calculate total ionization cross-section. They have obtained the input data for the BEB calculations concerning electronic structure with quantum chemical methods including the Hartree–Fock (H-F) and the outer valence green function (OVGF) methods.

In 1999, Khare et al. [12] proposed the method to calculate the total ionization cross sections due to electron impact that was the sum of three terms, Bethe cross section, Mott cross section and transverse cross section. Kumar et al. [13] simplified the Bethe cross section of Khare BEB model by taking non relativistic recoil energy expression. In present investigation, we have employed the simplified Khare BEB method to calculate the electron impact ionization cross sections of pyrimidine molecule. Beyond the calculation of ionization cross sections, we have also computed the ionization rate coefficients using the calculated cross sections and the Maxwell-Boltzmann electron energy distribution. These rate coefficients are particularly significant for applications in plasma physics, gas discharge systems, and flowing afterglow studies [15 - 17], where they often hold more practical relevance than the cross sections themselves.

2.Theory:

In simplified Khare BEB-model [13], the ionization cross section due to electron impact for j_{th} molecular orbital is given by

$$\sigma_{jT} = \sigma_{jM} + \sigma_{jB} + \sigma_{tj} \qquad (1)$$

where, Mott cross section, σ_{jM} is

$$\sigma_{jM} = \frac{AN}{[E+I+U]I}\left[1 - \frac{2}{t+1} + \frac{t-1}{2t^2} + \frac{5-t^2}{2(t+1)^2} - \frac{1}{t(t+1)} - \frac{t+1}{t^2}\ln\left(\frac{t+1}{2}\right)\right] \qquad (2)$$

where $t = E/I$, $E = \frac{1}{2}mc^2\left[1 - \frac{1}{1+\frac{T}{mc^2}}\right]$, $A = 4\pi a_0^2 R^2$. The notations U, a_0, I, N, T, m, c and R stand for the average kinetic energy of bound electron, the first Bohr radius, the ionization energy, the occupation number of molecular orbital, the kinetic energy of the incident electron, rest mass of electron, velocity of light and Rydberg energy, respectively. The Bethe cross-section σ_{jB} is given by

$$\sigma_{jB} = \frac{AN}{2[E+I+U]I}\left[\frac{1}{2}\left(1 - \frac{1}{t^2}\right) - X\right] \qquad (3)$$

where the term X is given by

$$X = 2ln\left(\sqrt{t} - \sqrt{(t-1)}\right) + \frac{1}{2t^2}\left\{\begin{array}{c} 1 - \frac{1}{2}\left(\frac{t}{t-\sqrt{t(t-1)}}\right)^2 \\ + \frac{1}{2}\left(\frac{t}{t+\sqrt{t(t-1)}}\right) - \left(\frac{t}{t-\sqrt{t(t-1)}}\right) \\ - \frac{3}{4}ln\left(\frac{t+\sqrt{t(t-1)}}{t-\sqrt{t(t-1)}}\right) \end{array}\right\}$$

and the cross section due to the transverse interaction is

$$\sigma_{tj} = -\frac{4\pi a_0^2 R}{E} M_j^2 [\ln(1-\beta^2) + \beta^2] \quad (4)$$

where β is the ratio of the incident velocity v and the velocity of light c, M_j^2 represents the total dipole matrix squared measured in units of a_0^2 and given by

$$M_j^2 = \int_{I_j}^{E} \frac{R}{w} \frac{df_j(w,0)}{dw} dw \quad (5)$$

where $\frac{df_j(w,0)}{dw}$ is the continuum optical oscillator strength (COOS) per unit energy range and given by

$$\frac{df_j(w,0)}{dw} = \frac{NI_j}{w^2} \quad (6)$$

The expression of collision parameter for jth molecular orbit C_{jRP} is given by

$$C_{jRP} = \frac{RE}{A} \sum_j (\sigma_{jB} + \sigma_{jM}) - M_j{}^2 ln\beta^2 \quad (7)$$

To evaluate total ionization cross section and collision parameters of molecule, the contributions that come from all molecular orbital are added.

Table 1: Variation of parameter C_{RP} with the incident energy E (in MeV).

E(MeV)	C_{RP}	E(MeV)	C_{RP}
1	148.64	6	147.77
2	148.00	8	147.75
4	147.82	10	147.00

In plasma processes, the ionization rate coefficients are important quantities which are determined by using our calculated total ionization cross sections and Maxwell-Boltzmann distribution as a function of temperature/energy [17, 18] as follows:

$$R_i = \int_{-\infty}^{+\infty} 4\pi \left(\frac{1}{2\pi mkT}\right)^{\frac{3}{2}} me^{\left(\frac{-E}{kT}\right)} Q_i(E) E \, dE \quad (8)$$

where k, T, and m are the Boltzmann constant, absolute temperature, and mass of the electron, respectively.

3. RESULT AND DISCUSSION

The equation (1) has been used to calculate the total ionisation cross-section from the ionisation threshold to 10 MeV for pyrimidine molecule. The required input parameters binding energies, I, and average kinetic energies, U, of bound electron are taken from Żywicka and Mozejko [7]. Figures (1 & 2) show the present calculations with other available theoretical and experimental results. Our calculations are in good agreement with experimental data measured by Bug et al. [8] within 5% except near the ionization threshold (E<25 eV). For E<25 eV present results are slightly higher than experimental values. The predictions of the present calculation do not agree with experimental results those of measured by Linert et al. [9] except in incident energies range E<20 eV. At above incident energies E >20eV, the present cross sections overestimate the experimental values up to 40%. It may be due to incomplete collection of all formed ions in

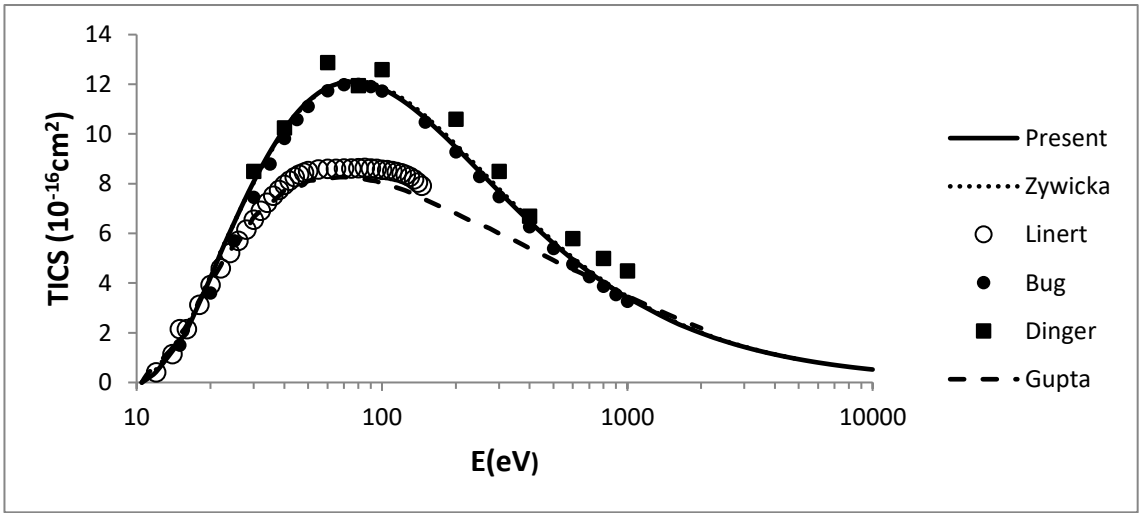

Fig.1 Total ionization cross sections (TICS) due to electron impact on Pyrimidine molecule in 10^{-16} cm^2. Solid line, dashed line, and dotted line represent present results, theoretical results of Gupta et al. [11], and Zywicka and Mozejko calculations [7], respectively. Filled circles, filled squares, and open circles are the experimental results of Bug et al. [8]. Dinger et al. [10], and Linert et al. [9] respectively

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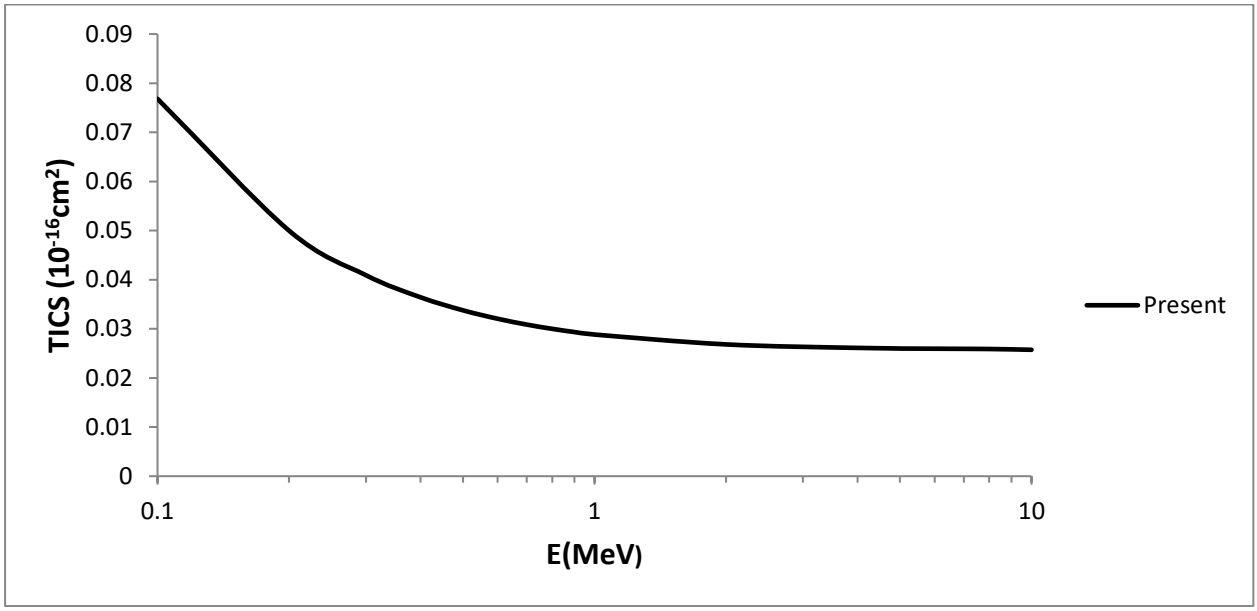

Fig. 2 This figure depicts the present total ionization cross sections in 10^{-16} cm^2 to Pyrimidine at high energy range 0.1 MeV to 10 MeV.

experiment with the time-of-flight mass spectrometer. The present calculations and the experimental data of Dinger et al. [10] are in good agreement within experimental uncertainty for whole range of incident energy. Our predictions and theoretical calculations of Zywicka and Mozejko [7] are very close to each other. For E>20 eV, the difference between both theoretical cross sections is not more than 1.5%. The cross sections calculated by Gupta et al. [11] are lower than present cross sections for incident energy range, 30 eV<E<600 eV.

At relativistic energies, from 0.1 MeV to 10 MeV, the present calculated cross sections of pyrimidine are represented in figure 2. There is no experimental data available at these incident energies to compare our calculations. However, the tendency of curve is found same as previous results. Rieke and Prepejchal [14] have measured the ionization cross sections in terms of two parameters, collisional parameter C_{RP} and dipole matrix squared M^2 (measured in units of a_0^2) for the large number of atoms and molecules. Therefore, both of these parameters are evaluated. We have no experimental data to compare these values for pyrimidine molecule. The calculated values of collisional parameter C_{RP} and dipole matrix squared M^2 are 148.64 at 1 MeV and 12.85 (units of a_0^2) respectively. The change in parameter C_{RP} with the impact energy is not considerable. This is according to expectation. At higher incident energies, these calculations will be useful for normalization of the experimental data in future.

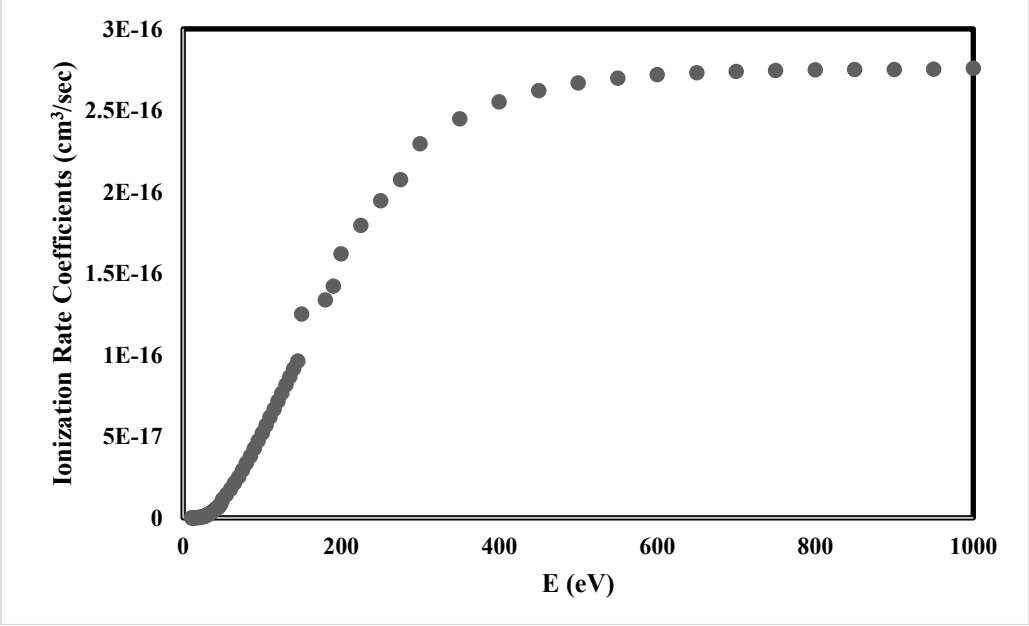

Fig. 3 Ionization rate coefficients (cm^3/s) of pyrimidine molecule in the energy range ionization threshold to 1 keV.

In relation to the applications, particularly in plasma processes, ionization rate coefficients are rather more important than ionization cross sections. We have evaluated the ionization rate coefficients as a function of electron temperature/energy for the electron collision with the pyrimidine molecule. The calculations are made using the calculated ionization cross sections and Maxwell-Boltzmann energy distribution, and the results are presented in Figure 3.

CONCLUSION

The simplified Khare-BEB method, has been previously employed widely for many molecules. This model has been presently used to evaluate the total ionization cross sections for pyrimidine molecule from ionization threshold to 10 MeV. A good agreement between our calculations and available experimental results are found. For energy range 10 keV to 10 MeV, the total ionization cross sections of pyrimidine are evaluated for first time. The present method will be continued to calculate the cross sections for other molecules. The study confirms a strong correlation between calculated data and experimental results. It reports the first evaluation of pyrimidine's total ionization cross sections within 10 keV to 10 MeV. The ongoing research aims to extend this method to analyze other molecules' cross sections, enhancing understanding in molecular ionization processes. Other than calculating the ionization cross-sections, we also calculated the ionization rate coefficients using Maxwell–Boltzmann electron distribution. These coefficients are crucial for accurately modelling plasma chemistry in case of the pyrimidine molecule. By filling gaps in the literature where quantitative data have been ambiguous or absent, our work provides a solid foundation for detailed plasma process simulations.

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