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Electron impact total ionization cross sections of BH_2 , SH, F_2O , HCN , C_2 and C_3 molecules.

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Abstract: *Total ionization cross sections for BH_2, F_2O,SH , HCN ,C_2 and C_3 molecules are studied theoretically in the energy range from ionization threshold to 2 Kev . The total ionization cross sections are calculated by Binary Encounter Bethe (BEB) and modified BEB model. There are no measurements available in the literature to the best of my knowledge with which the present results can be compared . From theoretical side a few comparisons for C_2 and C_3 molecules are available. The present results are compared with the available theoretical data.*

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Key words : total ionization cross section, electron molecule collision .

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I. Introduction

BH_2 is an important impurity in Tokamak edge and divertor plasmas . Experimental work of the absorption spectrum in the flash photolysis of H_3BCO to the free BH_2 radical and accurate determination of the geometrical structure of the ground and first excited states of BH_2 was studied by Herzberg and Johns [1] in 1967. No other experiments have been reported for this molecule since then. The properties of first two states of BH_2 were studied theoretically by several people in 1970s and 1990s [2–7]. Recently differential, integral, and momentum-transfer cross sections for the rotationally elastic and inelastic scattering of electron by the BH_2 molecule at low collision energies (0–8 eV) are reported using the *R*-matrix method by Zhang et al. [8].SH is produced in the upper atmosphere due to the photolysis of H_2S. It is found as an intermediate in many naturally occurring reactions yielding sulfur containing pollutants . In fossil fuel combustion processes , SH is also important. Λ -type doublet structure of SH in its ground state possesses electric dipole radio spectra of high intensity [9] hence it has very importance in astrophysical studies. The only theoretical study of electron impact on the open-shell radical SH is reported by Baluja and Msezane [10]. For understanding the ozone depletion [11-13] , electron Cl_xO_y collision studies is very important. F_2O has an isovalence electronic structure with Cl_2O and belongs to the same point group C_{2v}. However, the study of F_2O is neglected both theoretically and experimentally. Its experimental absorption spectrum is still unknown and the only theoretical studies for elastic differential, integral, momentum transfer and excitation cross sections for incident electron energies up to 15 eV using the *R*-matrix method is reported by Gupta and Baluja [14] . HCN is a linear and very polar molecule well-known astrophysically. HCN is one of the most abundant molecules in the

interstellar medium (ISM) after H_2 and CO . Electron-molecule scattering have many important applications in astrophysics, including the computation of electron densities in shocked regions of the ISM [15] and population analysis in comets, where electron collisions can provide a significant excitation mechanism for rotational transitions in the HCN molecule [16]. Theoretical Results are presented for the electron impact electronic excitation of HCN molecules by Varambhia and Tennyson [17] at low energies using R-matrix method but it is not studied at high energy.

Astronomical studies of C_2 and C_3 are very important , C_2 is main constituent of carbon stars[18]and it is also detected substantially in comets , interstellar clouds and stellar atmosphere [19].C_3 is detected in cometry tails , stellar and interstellar clouds and cool carbon rich stars [20,21].Carbon materials are extensively used in plasma for magnetic confinement of high temperature plasma . Electron impact ionization cross sections data by carbon clusters are helpful for modeling fusion edge plasma [22,23]. For C_2 molecule , Michelin et al[24] have calculated total ionization cross section using Schwinger variational iterative method and distorted wave approximation , Deutch et al[25] have computed the total ionization cross sections using semi empirical method called DM formalism. Deutch et al [26] have also calculated the total ionization cross sections for C_2 and C_3 molecules applying defect concept. Recently Pindzola [27] have also estimated total ionization cross section for C_2 by configuration averaged distorted wave method. Very recently Rahla and Antony [28] have published total ionization cross sections of C_2 and C_3 molecules using their CSP-ic approach but the reliable data for these molecules are still lacking.

The binary-encounter-Bethe (BEB) model of Kim and Rudd [29] has produced total ionization cross -sections for many molecules and the results have excellent agreement with experimental data. This model is a useful tool for supplying cross-section data and also for identifying reliable sets of experimental data . As Hwang et al [30] have found that the BEB model was underestimating the cross-section by a significant margin for heavy atoms with the highest principal quantum number $n \geq 3$, or molecules containing heavy atoms , they modified the BEB model.

Thus in the present work , the total ionization cross sections for BH_2 , SH , F_2O , HCN, C_2 and C_3 molecules are calculated by these models.

2 Theory

In electron impact ionization of atoms and molecules , to get an expression of singly differential ionization cross section , Kim and Rudd [29] presented a theoretical model for ionizing an electron out of an orbital i at an incident energy T

$$\boldsymbol{\sigma_i} = \frac{S_i}{t+u_i+1}\left[\frac{\ln t}{2}\left(1-\frac{1}{t^2}\right)+1-\frac{1}{t}-\frac{\ln t}{t+1}\right] \qquad [1]$$

Where ,

$$\boldsymbol{t = \frac{T}{B_i}}\ ,\mathbf{U_i} = \frac{U_i}{B_i}, \boldsymbol{S = 4\pi a_o^2\left(\frac{R^2}{B_i^2}\right)} \qquad [2]$$

Here a_o and R are Bohr radius and Rydberg energy constant, respectively. The total ionization cross section in the BEB model is given by ,

$$\boldsymbol{\sigma_{BEB} = \sum_i N_i\sigma_i} \qquad [3]$$

With N_i the electron occupation number of orbital i.

This model is applied successfully to many molecules [31-35] and the results agreed well with experimental data over a wide energy range of incident electron-impact energy from the ionization threshold to a few keV.

Hwang et al.[30] have modified the BEB model for heavy atoms or molecules containing heavy atoms. This modified BEB model given by Hwang et al.[30] is as follows.

$$\Sigma_I = \frac{S_I}{T+(U_I+1)/N_I}\left[\frac{Lnt}{2}\left(1-\frac{1}{T^2}\right)+1-\frac{1}{T}-\frac{Lnt}{T+1}\right] \qquad [4]$$

In the present work all physical quantities occurring in equations [1] and [4] are calculated for the ground state of the molecules by the same method as in the paper by Pandya [36]. The target properties used here are tabulated in table 1.

Table 1. Target Properties[37]

Target	Ip(Ev)	Bond Length(Angstrom)	Bond Angle (Degree)
BH_2	9.8	1.18	131.04
SH	10.42	1.34	------
F_2O	13.11	1.41	103.16
HCN	13.6	1.56(N-C) 1.06(H-C)	180.00
C_2	11.4	1.24	------
C_3	13	1.27	180.00

II. Results And Discussion

BH_2 , SH , F_2O and HCN molecules :

The total ionization cross sections for BH_2 , SH , F_2O and HCN molecules are depicted in figures 1 to 4 respectively. SH is made of the atom that consisted of M shell electrons which have radial nodes in their atomic orbitals and hence the U values are very high. These large U values decrease the contributions to the ionization cross sections from the valence electrons which are dominant ones. To overcome this, the U values of the molecular orbitals identified with 3s and 3p electrons of S were divided by their principal quantum number. The BEB cross sections with this modified U values are also plotted in the figure 2 . The curves marked "BEB/3" represent BEB cross sections with the modified U values, while the curves marked " BEB " used the unmodified values. The ionization cross sections calculated by modified U values are higher than that of unmodified U values as per expectation.

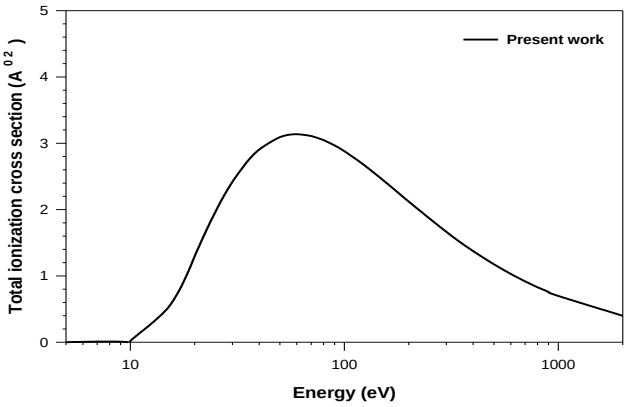

Fig. 1. Total Ionization Cross Sections Of Bh_2 By Electron Impact. Solid Line –Present Beb Model Qion .

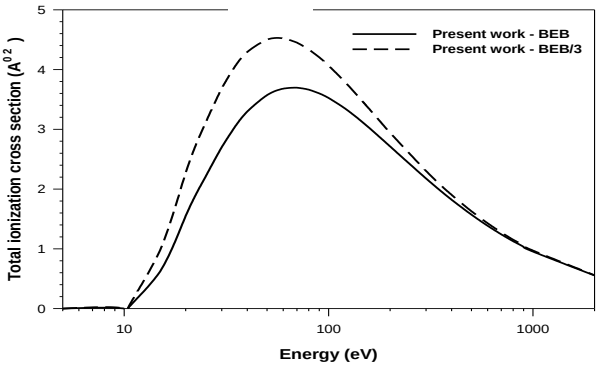

Fig. 2. Total Ionization Cross Sections Of Sh By Electron Impact. Solid Line – Present Beb Model Qion ; Small Dash – Modified Values Of U In The Beb Model.

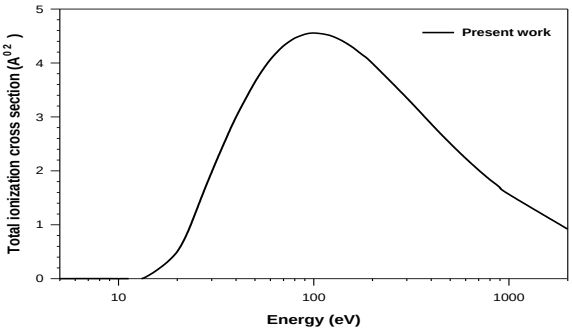

Fig. 3. Total Ionization Cross Sections Of F_2o By Electron Impact. Solid Line – Present Beb Model .

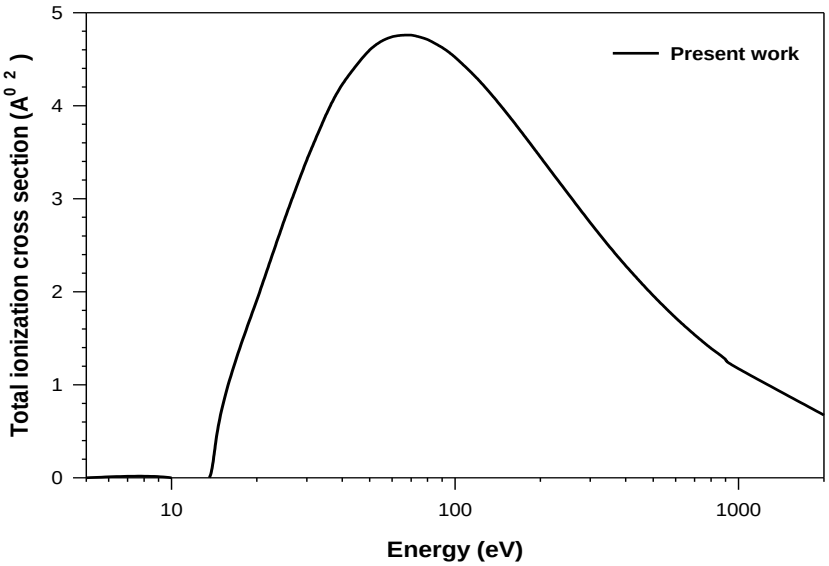

Fig. 4. Total Ionization Cross Sections Of Hcn By Electron Impact. Solid Line –Present Beb Model.

In absence of any other high energy electron collision theoretical or experimental data it is difficult to draw any sort of conclusion. It is true to say that the BEB has consistently yielded the cross sections that are in very good agreement with experiment (see http://physics.nist.gov/PhysRefData/Ionization/molTable.html for example). Thus, the results obtained over here can be considered very reliable and can be compared with other theoretical or experimental work in future.

C2 and C3 molecules :

Total ionization cross sections calculated for C_2 and C_3 molecules are shown in figures 5 and 6. The calculations are compared with the theoretical results of Mechelin et al[24],Deutch et al[25,26]and very recent calculations of Rahla and Antony [28] .

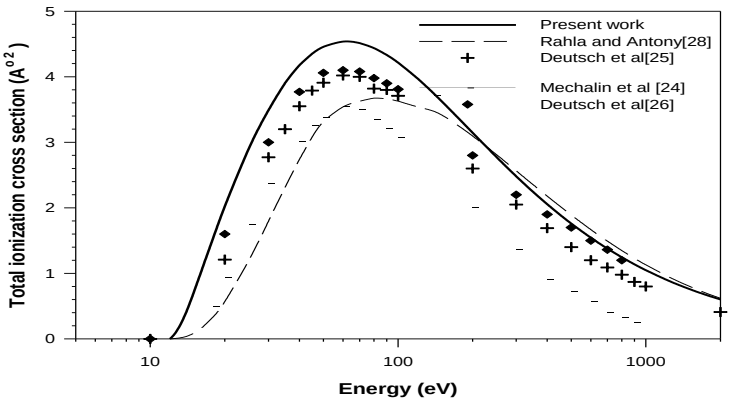

Fig. 5 . Total Ionization Cross Sections Of C_2 By Electron Impact. Solid Line Present Results, Rahla And Antony [28] , Duetsch Et Al.[25,26], - Mechalin Et Al.[24].

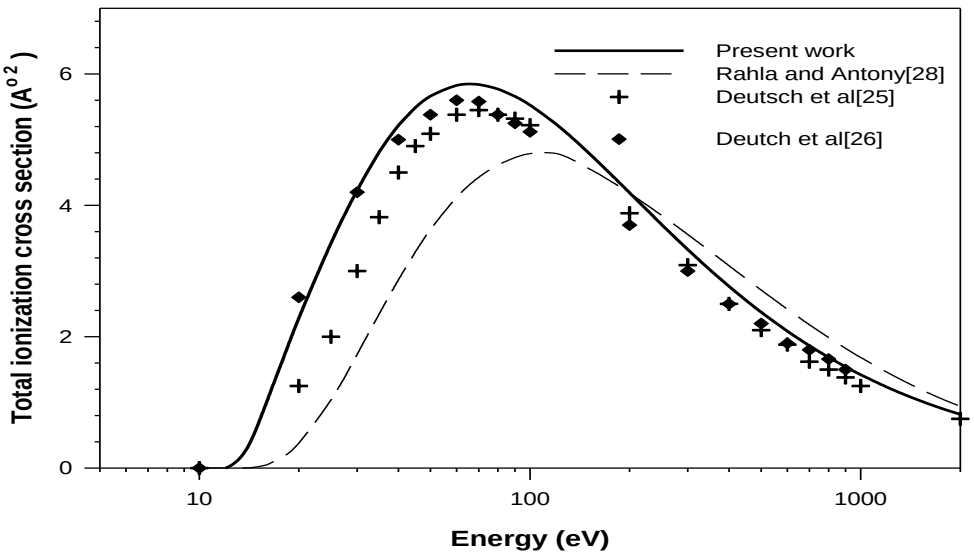

Fig.6. Total Ionization Cross Sections Of C_3 By Electron Impact. Solid Line Present Results, Rahla And Antony[28] , Duetsch Et Al.[25,26] .

For both the molecules , the results of Rahla and Antony [28] much differ from the present BEB calculations and that of Duetsch et al [25 ,26] . Here it is observed that below 100 eV the total flux loss in the ionization channel is not strong .It is very much less than expectation because the total potential calculated by Rahla and Antony[28] in their CSP-ic method is weak. It is also observed that at high T , the results of Rahla and Antony [28]are above the BEB and Duetsch results [25,26] . This indicates that the dipole contribution in their CPS-ic model is not correct which dominates at high T.

The total ionization cross sections calculated for Br_2 and I_2 molecules by Joshipura and Limbachiya [38] are also much higher than the BEB calculations of Ali and Kim [39] at higher T indicating wrong asymptotic behavior of their wave function.

In case of C_2 , the results of Mechelin et al [24] also considerably underestimates the BEB and Duetsch [25,26] results.

III. Conclusion

In the present studies of electron impact total ionization cross section calculations for BH_2, SH, F_2O , HCN ,C_2 and C_3 molecules , no experimental or theoretical data are available for comparison for BH_2, SH, F_2O and HCN molecules. I am quite sure that the present work will inspire experimentalist to perform studies on these spices. For C_2 and C_3 molecules , present results are compared with the theoretical data of Rahla and Antony[28] , Duetsch et al. [25,26] and Mechelin et al[24]. The results of Rahla and Antony [28] are much differ from the present calculations and Duetsch et al .[25,26] values.

The results of Rahla and Antony[28] have not satisfactory agreement with other theoretical results . In their CSP-ic model they require a proper value of R_p which requires a lot of experimental data [40] .They have carried out the calculations though no experimental data for C_2 and C_3 are available .Second important thing is

that the CSP-ic model [40] basically comes from the modified additivity rule proposed by Joshipura and Patel [41] for electron-molecule scattering. In this approach they have separated electron – molecule interactions into short range and long range parts. For short range part , basic atomic properties were used and the molecular average spherical dipole polarizability was used for the long-range part. This model was modified by Joshipura et al.[40] to calculate total ionization cross sections for molecules. The atomic charge density derived from Cox and Bonham [42] by Rahla and Antony [28] is a basic input in the CSP-ic model to calculate all various potentials of electron molecule collision cross sections. In this treatment , the true nature of the molecular charge distribution and potentials are missing. It should be noted that accurate evaluation of the charge density and potentials are very important in such types of calculations and Jain and Baluja [43] have reported electron scattering cross sections for many diatomic and polyatomic molecular targets for which they have employed various single centre expansion programs to determine the charge density and various potentials for linear and non-linear molecules and for linear molecules the molecular wave functions were obtained from McLean and Yoshmine [44] while for nonlinear cases they have employed the MOLMON computer code [45].

The BEB cross-sections are determined entirely by the properties of the target and bound state properties and it doesn't depend on any adjusting parameters , fitting parameters or experimental data. The BEB cross sections require only a minimum set of molecular constants for the initial state of a target molecule and such constants can be calculated from the molecular structure codes and hence it provides an efficient means of determining total ionization cross sections . This model has reliably predicted the Q_{ion} for many molecules [31-35] and hence this study will be useful for experimental work in future.

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