Section A-Research paper
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Partial Ionization Cross Section of C_2H_6 (Ethane) Atom by Electron Impact

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ABSTRACT: Total ionization cross-sections of an atom Ethane caused by electron impact for a single ionization. Total ionization cross-sections (TICS) have been calculated from threshold ionization energy to 1100 eV. The modified model, developed by Jain and Khare, has been used to calculate the TICS for ethane.
Keyword: ionization, cross section

I.INTRODUCTION

An accurate hypothetical treatment of the low energy electron impact ionization problem is unfeasible at present due to the complexity of representing the asymptotic form of the wave function when two slow electrons are in the continuum. It is however possible to think about ionization by a very fast incident electron ($k^2_0 > 1$), in which the ejected electron has a low energy. It is now possible, however to use the Born approximation (or Coulomb-Born approximation) with a well correlated multi configuration initial states wave function and *R*-matrix final state wave function. A detailed theoretical description of this has been offered by Robb et al (1975)[1].

Even though the physical processes of interest in astrophysics and plasma chemistry/physics involve mainly low energy incident electrons ($k^2_0 = 1$), exact Born calculations can be helpful in two respects. First, they can be used to normalize experimental data and second, they can offer estimates for many applications where, at the moment, no other reasonable estimates exist.

Protons in the beam may be scattered from the edges of collimator apertures and also from collisions with the target gas. If the scattered protons hit metal surfaces such as the grid or the beam suppressor, secondary electrons are formed [1-5]. It is hard to estimate the scattering from the collimator, but it can be minimized. This is accomplished by making the edges of the aperture as sharp as possible, thus limiting the area from which scattering into the measuring region can take place, and by having a shield past the collimator just large enough to permit the main beam pass but little enough to prevent most scattered particles. The scattering from target gas atoms is appreciable only for extremely low proton energies and for heavy targets, excluding for unusual geometries, must not generate many secondary electrons [6-9].

Electron Impact Ionization

The main atomic processes that give rise to the line spectra of astronomical objects are of two sorts, radiative or collisional. In the first type the atom or ion interacts with a photon while the second type involves collisions between an atom (ion) and an electron. The most important processes are:

Photo-excitation and radiative decay:

$$X_i + h\nu \rightleftharpoons X_f$$

Photo-ionization:

$$X_i + h\nu \rightarrow A_f + e^-$$

Recombination:

$$X_i + e^- \rightarrow X_f + h\nu$$

Electron impact excitation:

$$X_i + e^- \rightleftharpoons X_f(N) + e^-$$

where X corresponds to the target ion, X indicates that the ion has $+1$ electrons.

The subscripts i and f are for initial and final states.

In order to explain such processes and derive atomic data of use for applications, we have to signify a system made of a nucleus of nuclear charge Z and 'many' electrons. The full description can be achieved by solving the time independent Schrodinger equation,

$$H\Psi = E\Psi$$

Where H is the Hamiltonian, Ψ is the Eigen function linked to the Eigen energy E.

Here the atomic unit system in which e = m = ħ = 1.

In order to be complete the Hamiltonian should account for all the interactions among the different particles present in the system. This includes kinetic energy of electrons, their potential energy generated by the nucleus, the repulsive interaction between electrons, the spin-orbit for each electron, the spin-spin, spin-other orbit and orbit-orbit interactions between electrons. A light element of low charge, we can use the non-relativistic Hamiltonian.

II. Theoretical Methodology:-

Even on the theoretical side several more methods are available to compute the cross sections over a wide range of atoms and molecules.

The formula is useful for finding the rate coefficient of any atoms and molecules. Semi-empirical formalism developed by Jain and Khare [10-13].This formula is also applicable to calculate partial, photo, integral ionization cross sections of atoms and molecules. The formula is useful for finding the rate coefficient of any atoms and molecules. This is a theoretical approach. The single differential cross sections in the complete solid angle ($\Omega = 4\Pi = \int 2\pi \sin\theta d\theta$) as a function of secondary electron energy ε corresponding to the production of i^{th} type ion in the ionization of a molecule by incident electron of energy E is given by equation 1:

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

where, $W = (\varepsilon + I_i)$ is energy loss 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.

The oscillator strength is directly proportional to the photo ionization cross section [10-17]. 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 $df_i(W,K,\theta)$, the differential generalized oscillator strength (DGOS) in the optical limit $(K \to 0)$ has been used. From Lassettre's Theorem [8-9] 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.

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

where β is the asymmetric parameter and $P_2(\cos\theta) = \frac{1}{2}(3\cos^2\theta - 1)$ 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. The oscillator strengths are directly proportional to the photo ionization cross sections.

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. RESULTS AND DISCUSSION

In this paper the results of the absolute partial ionization cross section measurements for the Ethane atom are calculated from threshold to 1100 eV by the use of modified Jain-Khare approach.

The Partial ionization cross sections are also summarized in Table 1 (a) and 1(b)

Table1 (a)

Energy (eV)	**$C_2H_6^+$**	**$C_2H_5^+$**	**$C_2H_4^+$**	**$C_2H_3^+$**	**$C_2H_2^+$**	**C_2H^+**	**C_2^+**	**CH_3^+**
13	**0.1375**		**0.1375**					
15	**0.399693**	**0.226548**	**0.399693**	**0.040241**				
20	**1.067572**	**0.846343**	**1.067572**	**0.557076**	**0.48166**			**0.48166**
25	**1.55397**	**1.343026**	**1.55397**	**1.054288**	**0.969418**			**0.969418**
30	**1.872495**	**1.683905**	**1.872495**	**1.419903**	**1.338959**	**0.054096**		**1.338959**
35	**2.074725**	**1.908407**	**2.074725**	**1.672984**	**1.599299**	**0.257633**		**1.599299**
40	**2.199104**	**2.053209**	**2.199104**	**1.844456**	**1.77835**	**0.483284**		**1.77835**
45	**2.272273**	**2.143189**	**2.272273**	**1.957907**	**1.898794**	**0.686179**	**0.063027**	**1.898794**
50	**2.310353**	**2.196338**	**2.310353**	**2.031234**	**1.978307**	**0.85645**	**0.186095**	**1.978307**
55	**2.325433**	**2.223251**	**2.325433**	**2.075451**	**2.027906**	**0.99564**	**0.320544**	**2.027906**
60	**2.323886**	**2.232806**	**2.323886**	**2.099826**	**2.056955**	**1.107444**	**0.448451**	**2.056955**
65	**2.311925**	**2.229208**	**2.311925**	**2.108997**	**2.07017**	**1.197097**	**0.563408**	**2.07017**
70	**2.291761**	**2.217471**	**2.291761**	**2.108293**	**2.073006**	**1.267893**	**0.664298**	**2.073006**
75	**2.267164**	**2.198869**	**2.267164**	**2.099303**	**2.067093**	**1.324285**	**0.751235**	**2.067093**

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80	**2.238413**	**2.176739**	**2.238413**	**2.085592**	**2.0561**	**1.367965**	**0.826086**	**2.0561**
90	**2.175935**	**2.123979**	**2.175935**	**2.046795**	**2.021818**	**1.428329**	**0.944125**	**2.021818**
100	**2.11049**	**2.066193**	**2.11049**	**2.00006**	**1.978686**	**1.462433**	**1.029378**	**1.978686**
120	**1.98194**	**1.948825**	**1.98194**	**1.898941**	**1.882867**	**1.483708**	**1.134079**	**1.882867**
140	**1.863584**	**1.838156**	**1.863584**	**1.799524**	**1.787116**	**1.471599**	**1.185456**	**1.787116**
160	**1.757363**	**1.737472**	**1.757363**	**1.707013**	**1.69727**	**1.444017**	**1.207231**	**1.69727**
200	**1.57786**	**1.565268**	**1.57786**	**1.545726**	**1.539523**	**1.371867**	**1.206387**	**1.539523**
240	**1.433226**	**1.425066**	**1.433226**	**1.412279**	**1.408252**	**1.295408**	**1.178372**	**1.408252**
260	**1.371036**	**1.364458**	**1.371036**	**1.354093**	**1.350839**	**1.258146**	**1.159646**	**1.350839**
300	**1.262568**	**1.258321**	**1.262568**	**1.251568**	**1.249467**	**1.1873**	**1.117779**	**1.249467**
350	**1.150435**	**1.148087**	**1.150435**	**1.14431**	**1.143152**	**1.106675**	**1.06255**	**1.143152**
400	**1.057893**	**1.056792**	**1.057893**	**1.054927**	**1.05438**	**1.034928**	**1.008216**	**1.05438**
Energy (eV)	**$C_2H_6^+$**	**$C_2H_5^+$**	**$C_2H_4^+$**	**$C_2H_3^+$**	**$C_2H_2^+$**	**C_2H^+**	**C_2^+**	**CH_3^+**
450	**0.980179**	**0.979891**	**0.980179**	**0.979323**	**0.979188**	**0.971308**	**0.956798**	**0.979188**
500	**0.913941**	**0.914218**	**0.913941**	**0.914533**	**0.914684**	**0.914852**	**0.909061**	**0.914684**
550	**0.856789**	**0.857452**	**0.856789**	**0.858378**	**0.858724**	**0.864604**	**0.865141**	**0.858724**
600	**0.806922**	**0.807863**	**0.806922**	**0.80923**	**0.809709**	**0.819674**	**0.824859**	**0.809709**
650	**0.763016**	**0.764152**	**0.763016**	**0.765826**	**0.766416**	**0.779338**	**0.787968**	**0.766416**
700	**0.724026**	**0.725308**	**0.724026**	**0.727205**	**0.727853**	**0.742939**	**0.754154**	**0.727853**
750	**0.689172**	**0.690543**	**0.689172**	**0.692605**	**0.693302**	**0.709949**	**0.723103**	**0.693302**
800	**0.657792**	**0.659235**	**0.657792**	**0.6614**	**0.662143**	**0.679912**	**0.694522**	**0.662143**
850	**0.629389**	**0.630883**	**0.629389**	**0.633127**	**0.633887**	**0.652458**	**0.668151**	**0.633887**
900	**0.603556**	**0.605072**	**0.603556**	**0.607365**	**0.608141**	**0.627268**	**0.643776**	**0.608141**
950	**0.579926**	**0.581471**	**0.579926**	**0.583791**	**0.58458**	**0.604066**	**0.621184**	**0.58458**
1000	**0.558246**	**0.559799**	**0.558246**	**0.562131**	**0.562917**	**0.582637**	**0.600174**	**0.562917**
1050	**0.538264**	**0.53981**	**0.538264**	**0.542148**	**0.542943**	**0.562774**	**0.580596**	**0.542943**
1100	**0.519783**	**0.521328**	**0.519783**	**0.523661**	**0.524454**	**0.544303**	**0.562309**	**0.524454**

Table 1(b) - Ionization cross section of C_2H_6

Energy (eV)	**CH_2^+**	**CH^+**	**C^+**	**H_3^+**	**H_2^+**	**H^+**	**Total**
13							**0.275**
15							**1.066175**
20							**4.501883**
25						**0.167405**	**7.611495**
30	**0.144917**				**0.003172**	**0.49119**	**10.22009**
35	**0.392464**	**0.068777**		**0.017979**	**0.123941**	**0.788692**	**12.57893**
40	**0.630839**	**0.243321**		**0.151738**	**0.323095**	**1.029026**	**14.71388**
45	**0.833664**	**0.431701**	**0.010804**	**0.324773**	**0.519808**	**1.215291**	**16.52848**
50	**0.998415**	**0.603671**	**0.095842**	**0.492673**	**0.693059**	**1.356658**	**18.08776**
55	**1.129971**	**0.751737**	**0.213452**	**0.641914**	**0.838779**	**1.463276**	**19.36069**

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60	**1.233449**	**0.875581**	**0.334701**	**0.769469**	**0.959195**	**1.542299**	**20.3649**
65	**1.314877**	**0.978221**	**0.448531**	**0.876896**	**1.057204**	**1.600851**	**21.13948**
70	**1.377788**	**1.062114**	**0.550834**	**0.96603**	**1.13706**	**1.642621**	**21.72394**
75	**1.426856**	**1.131034**	**0.641158**	**1.040187**	**1.201106**	**1.672474**	**22.15502**
80	**1.463727**	**1.186619**	**0.719582**	**1.100895**	**1.253084**	**1.691835**	**22.46115**
90	**1.51214**	**1.268321**	**0.846179**	**1.192032**	**1.327241**	**1.710014**	**22.79466**
100	**1.5362**	**1.320681**	**0.939904**	**1.252649**	**1.373081**	**1.709116**	**22.86805**
120	**1.541835**	**1.370881**	**1.05951**	**1.316177**	**1.41286**	**1.676488**	**22.57292**
140	**1.518264**	**1.380276**	**1.122858**	**1.335636**	**1.414453**	**1.625304**	**21.99293**
160	**1.481985**	**1.369168**	**1.154265**	**1.332314**	**1.397332**	**1.56832**	**21.30838**
200	**1.397617**	**1.320447**	**1.167876**	**1.294802**	**1.339979**	**1.45525**	**19.89999**
240	**1.313121**	**1.259606**	**1.150181**	**1.241544**	**1.273308**	**1.352198**	**18.58404**
Energy (eV)	**CH_2^+**	**CH^+**	**C^+**	**H_3^+**	**H_2^+**	**H^+**	**Total**
260	**1.272849**	**1.22825**	**1.135535**	**1.213086**	**1.239744**	**1.305079**	**17.97464**
300	**1.19739**	**1.166533**	**1.100227**	**1.155887**	**1.174578**	**1.219168**	**16.85282**
350	**1.112819**	**1.09381**	**1.050905**	**1.087097**	**1.098844**	**1.125765**	**15.61804**
400	**1.038407**	**1.027413**	**1.000717**	**1.023382**	**1.030397**	**1.045455**	**14.54518**
450	**0.972959**	**0.967508**	**0.952266**	**0.965354**	**0.96907**	**0.97598**	**13.60919**
500	**0.915217**	**0.913673**	**0.906683**	**0.912869**	**0.914243**	**0.915418**	**12.78802**
550	**0.86404**	**0.865322**	**0.864344**	**0.865485**	**0.865156**	**0.862241**	**12.06319**
600	**0.818458**	**0.821783**	**0.825248**	**0.822642**	**0.821079**	**0.815216**	**11.41931**
650	**0.777619**	**0.782459**	**0.789245**	**0.78385**	**0.781354**	**0.77334**	**10.84402**
700	**0.74086**	**0.746809**	**0.756098**	**0.748593**	**0.745427**	**0.73581**	**10.32696**
750	**0.707589**	**0.714374**	**0.725561**	**0.716458**	**0.712766**	**0.701983**	**9.859879**
800	**0.677367**	**0.684755**	**0.697371**	**0.68706**	**0.682987**	**0.67136**	**9.435839**
850	**0.649768**	**0.657606**	**0.671299**	**0.660068**	**0.655712**	**0.643474**	**9.049098**
900	**0.624479**	**0.632643**	**0.647158**	**0.635215**	**0.630658**	**0.617963**	**8.694991**
950	**0.601205**	**0.609595**	**0.624724**	**0.612275**	**0.607567**	**0.594569**	**8.369459**
1000	**0.579737**	**0.588282**	**0.60385**	**0.591018**	**0.586195**	**0.572998**	**8.069147**
1050	**0.559836**	**0.568489**	**0.584368**	**0.57126**	**0.56637**	**0.553055**	**7.79112**
1100	**0.541366**	**0.550065**	**0.566168**	**0.552871**	**0.547932**	**0.534561**	**7.533038**

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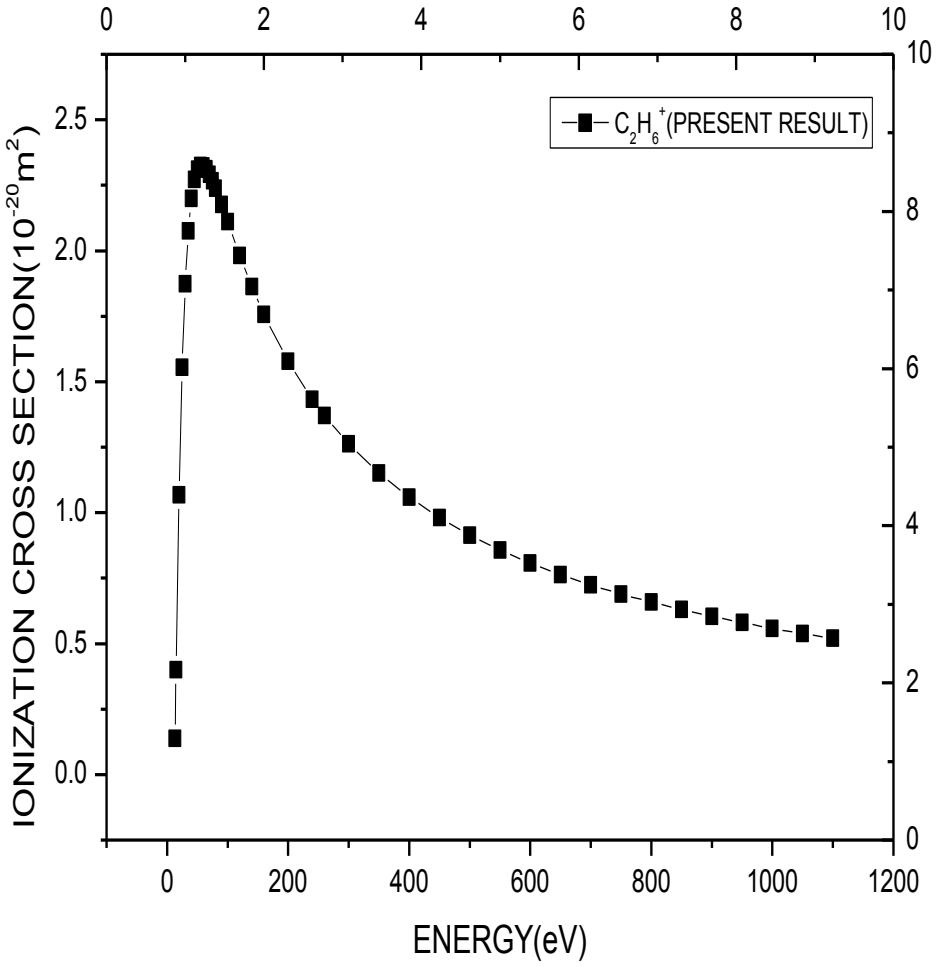

1)Graph representing cross section of $C_2H_6^+$ due to ionization of C_2H_6

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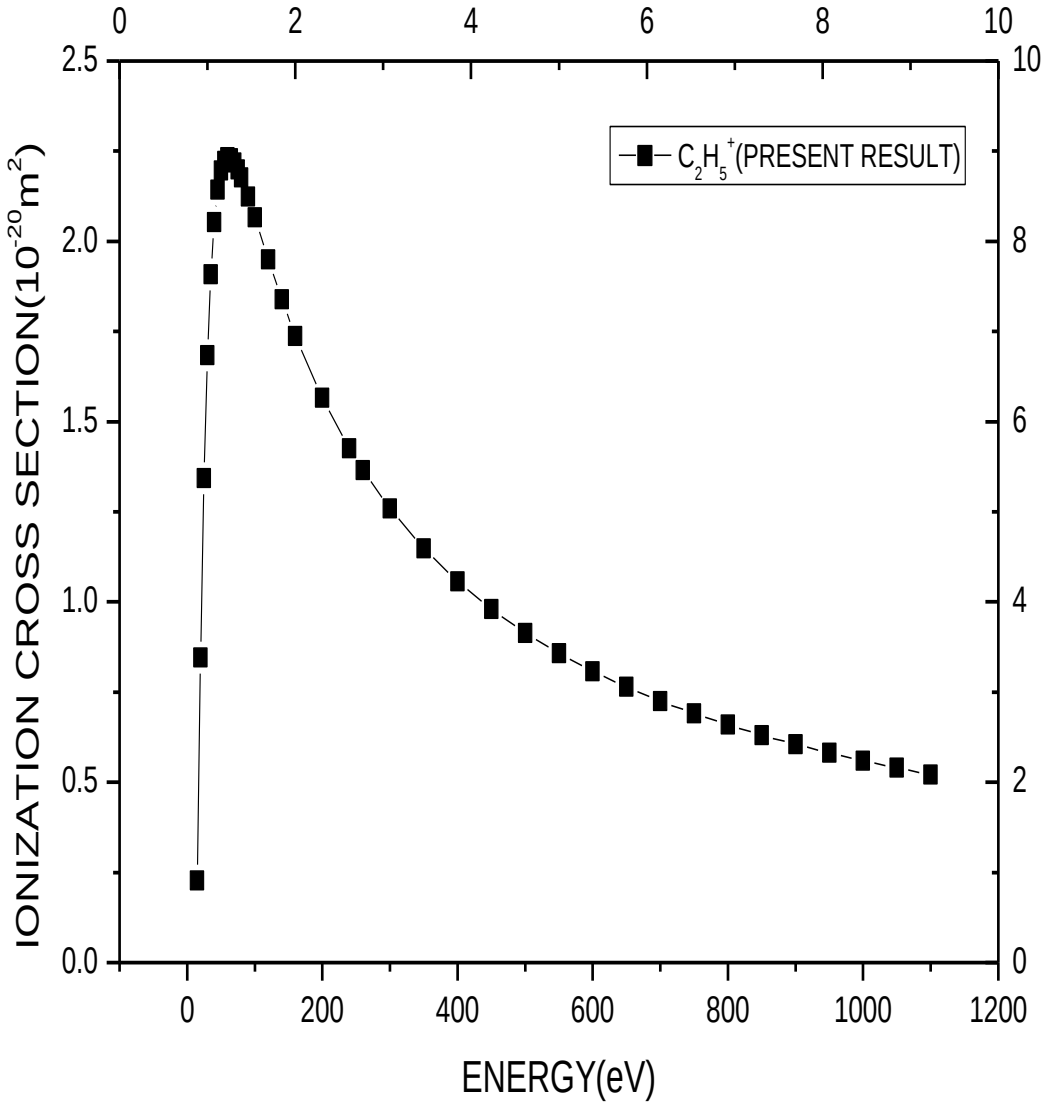
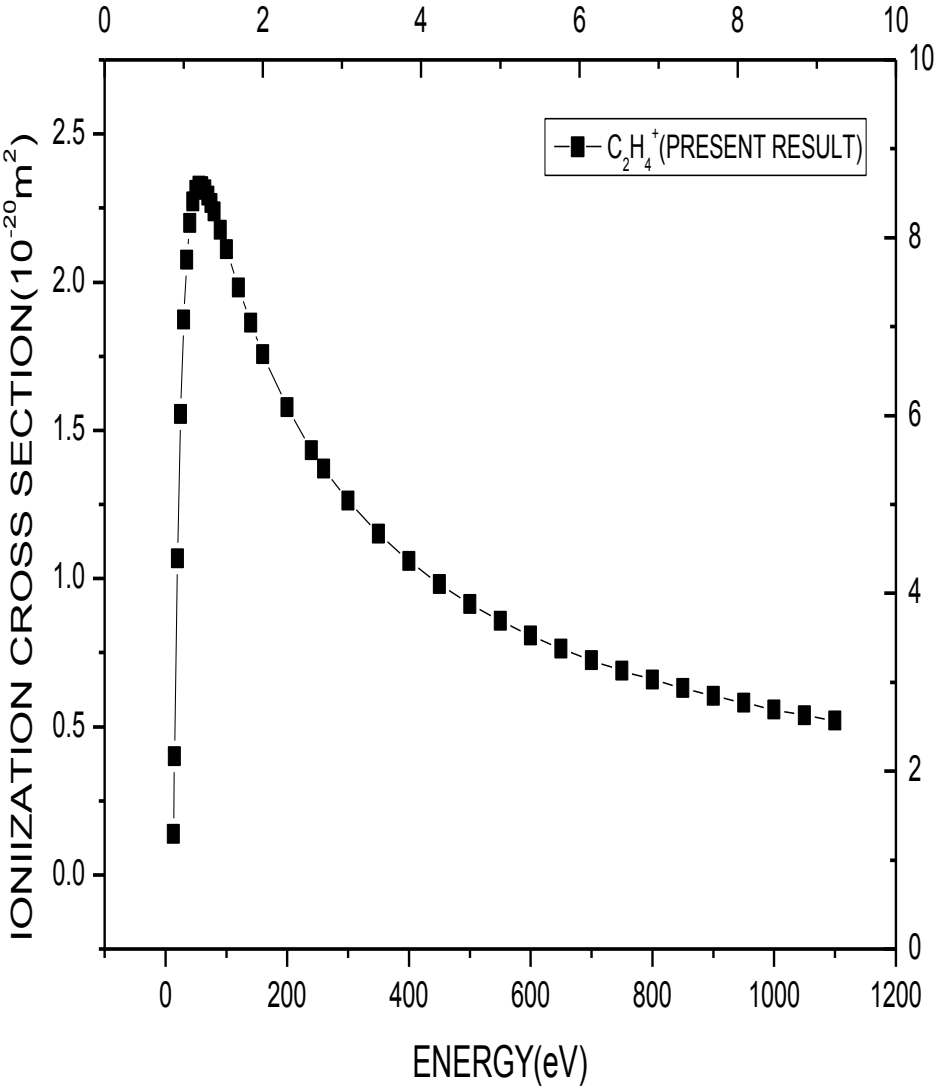


2)Graph representing cross section of $C_2H_5^+$ due to ionization of C_2H_6



3)Graph representing cross section of $C_2H_4^+$ due to ionization of C_2H_6

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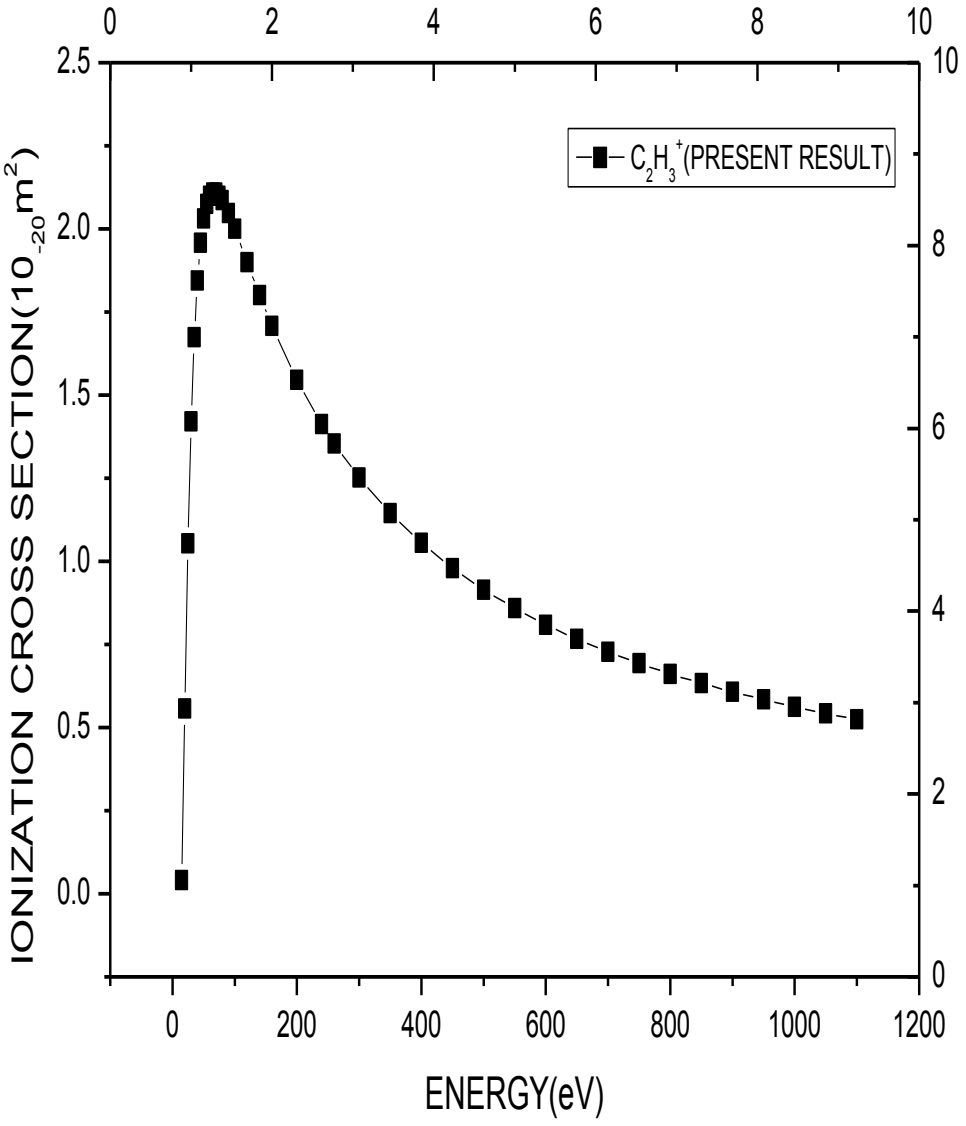
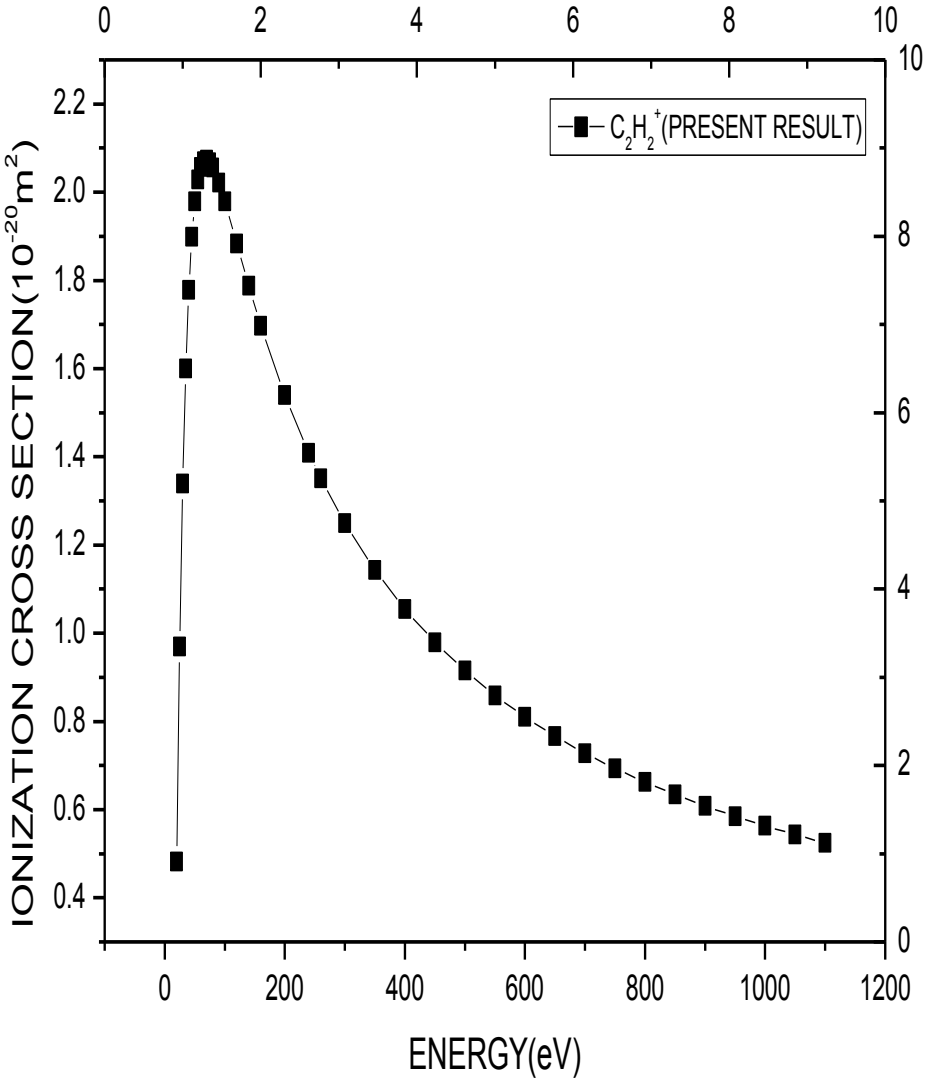


4) Graph representing cross section of $C_2H_3^+$ due to ionization of C_2H_6



5)Graph representing cross section of $C_2H_2^+$ due to ionization of C_2H_6

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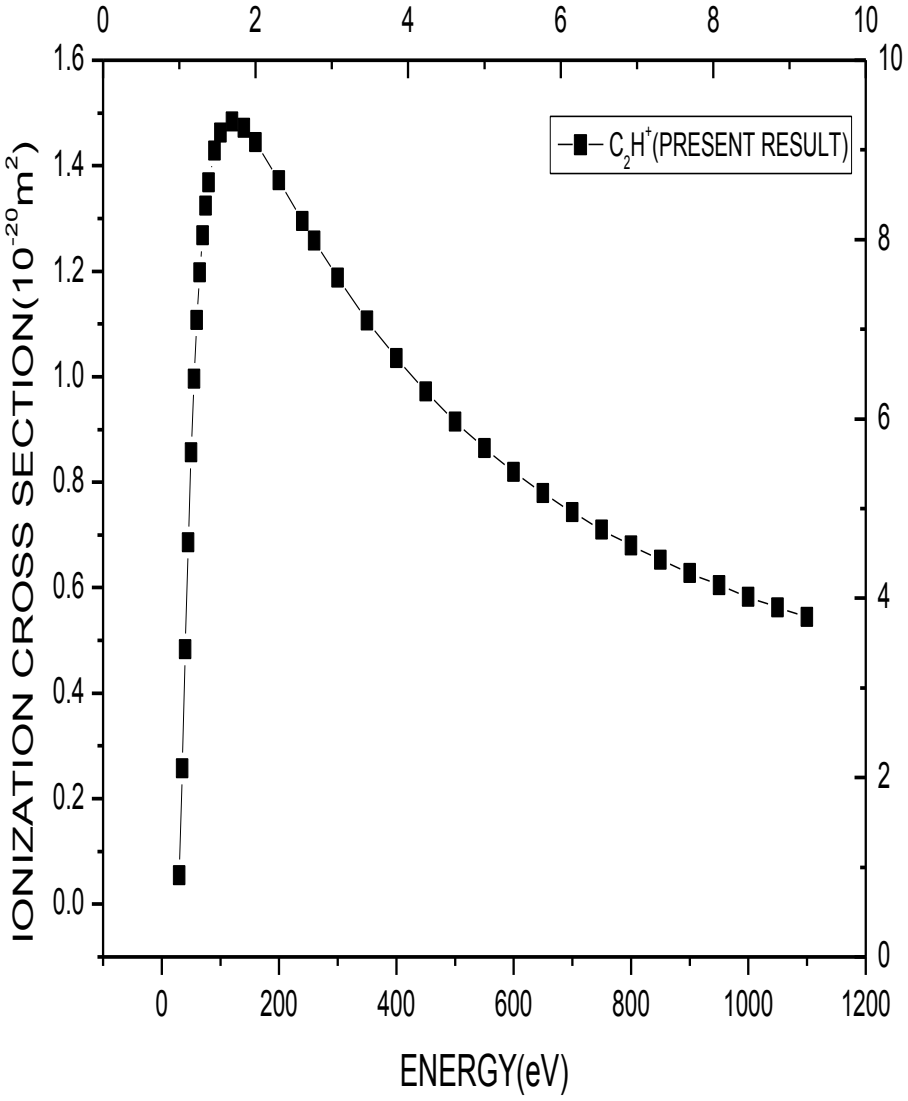
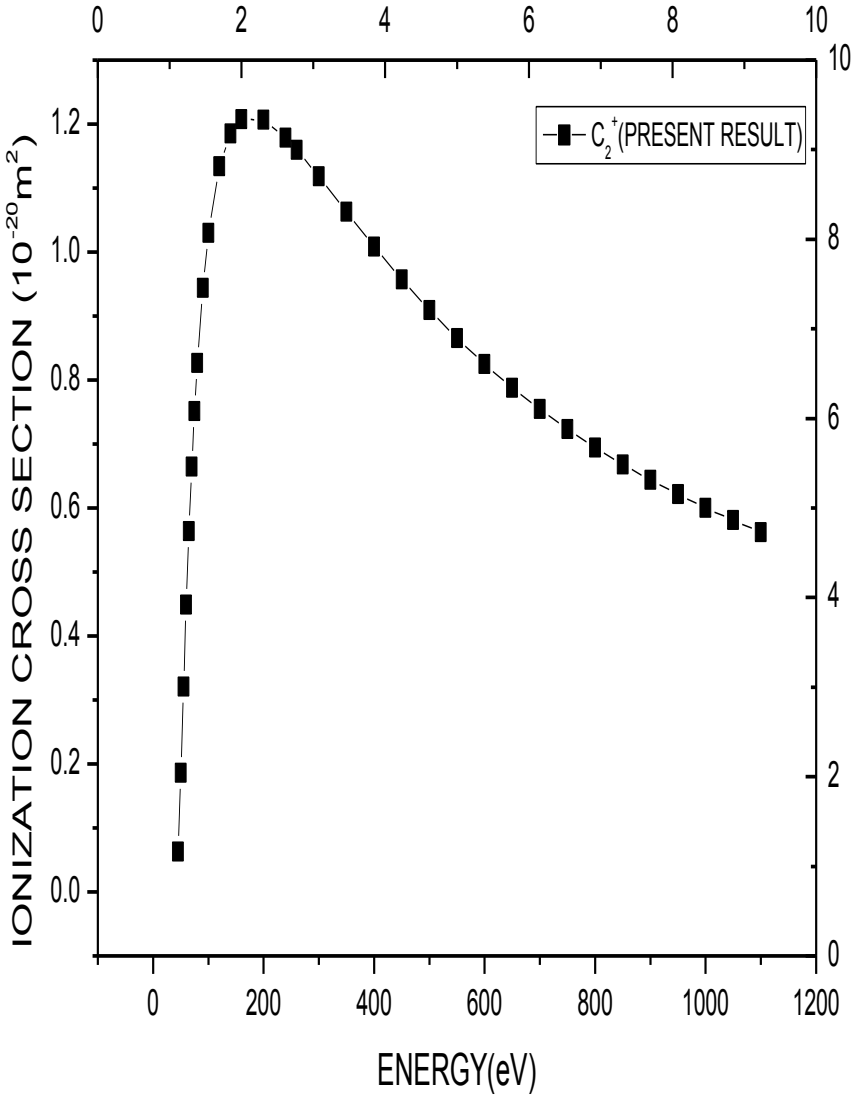


6) Graph representing cross section of C_2H^+ due to ionization of C_2H_6



7)Graph representing cross section of C_2^+ due to ionization of C_2H_6

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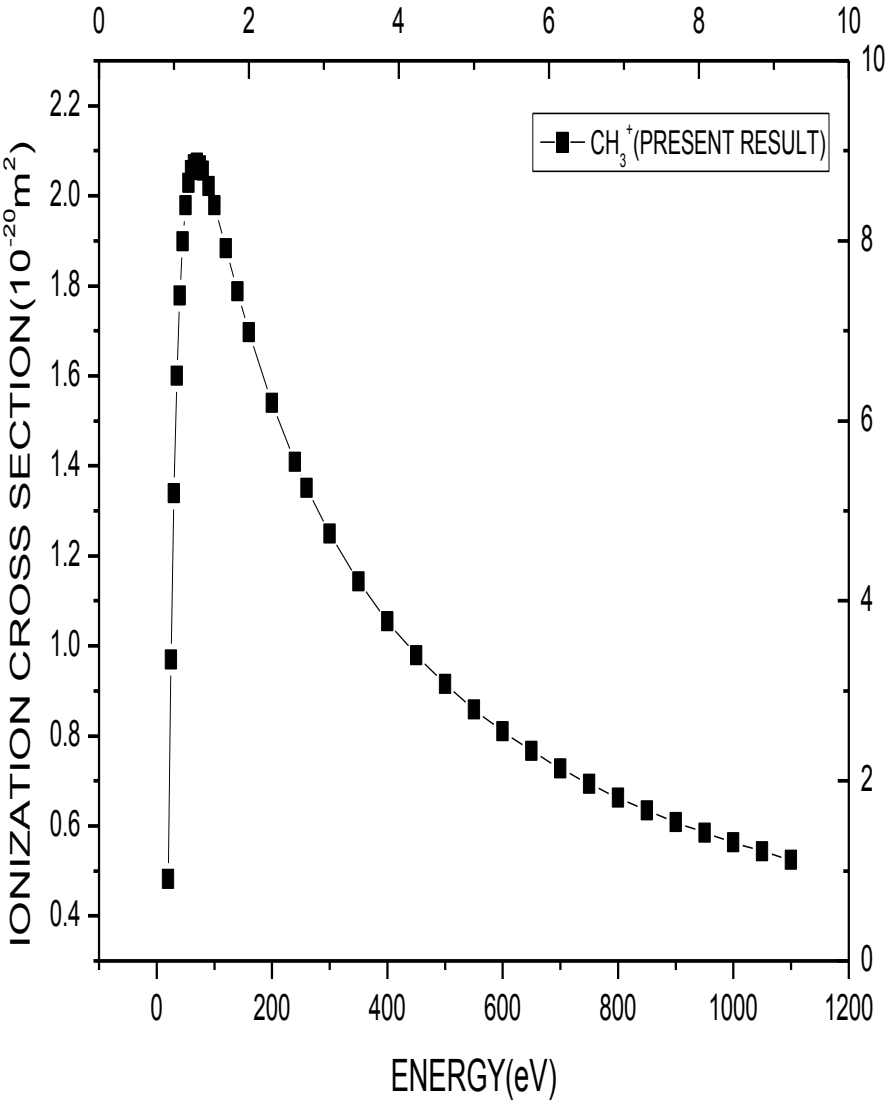

8)Graph representing cross section of CH_3^+ due to ionization of C_2H_6

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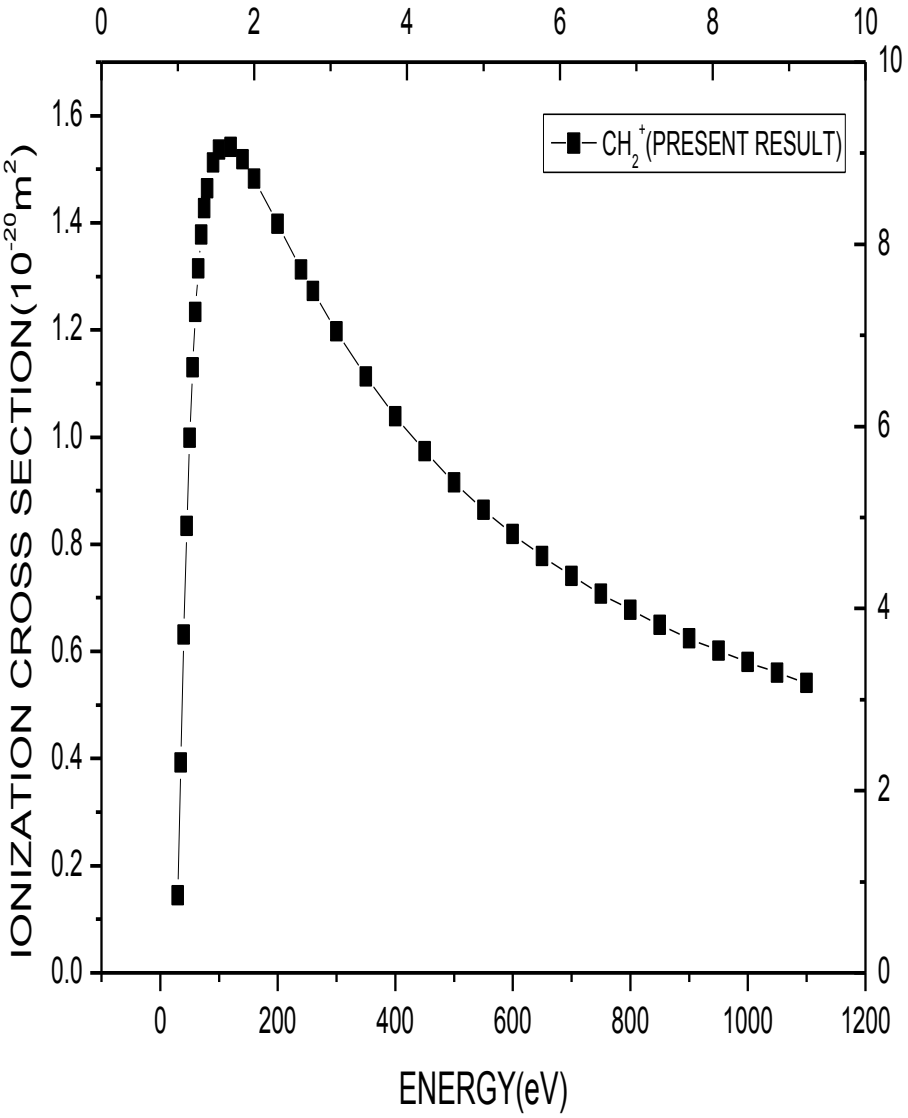
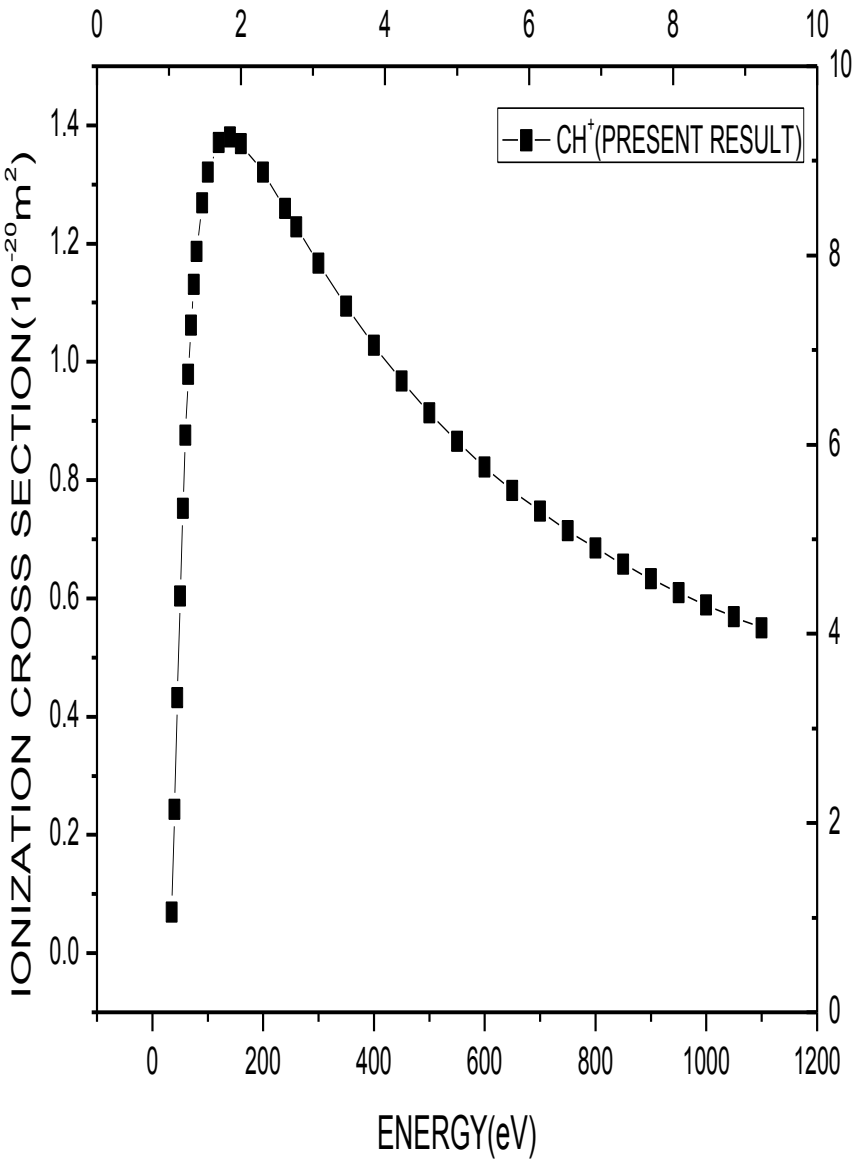
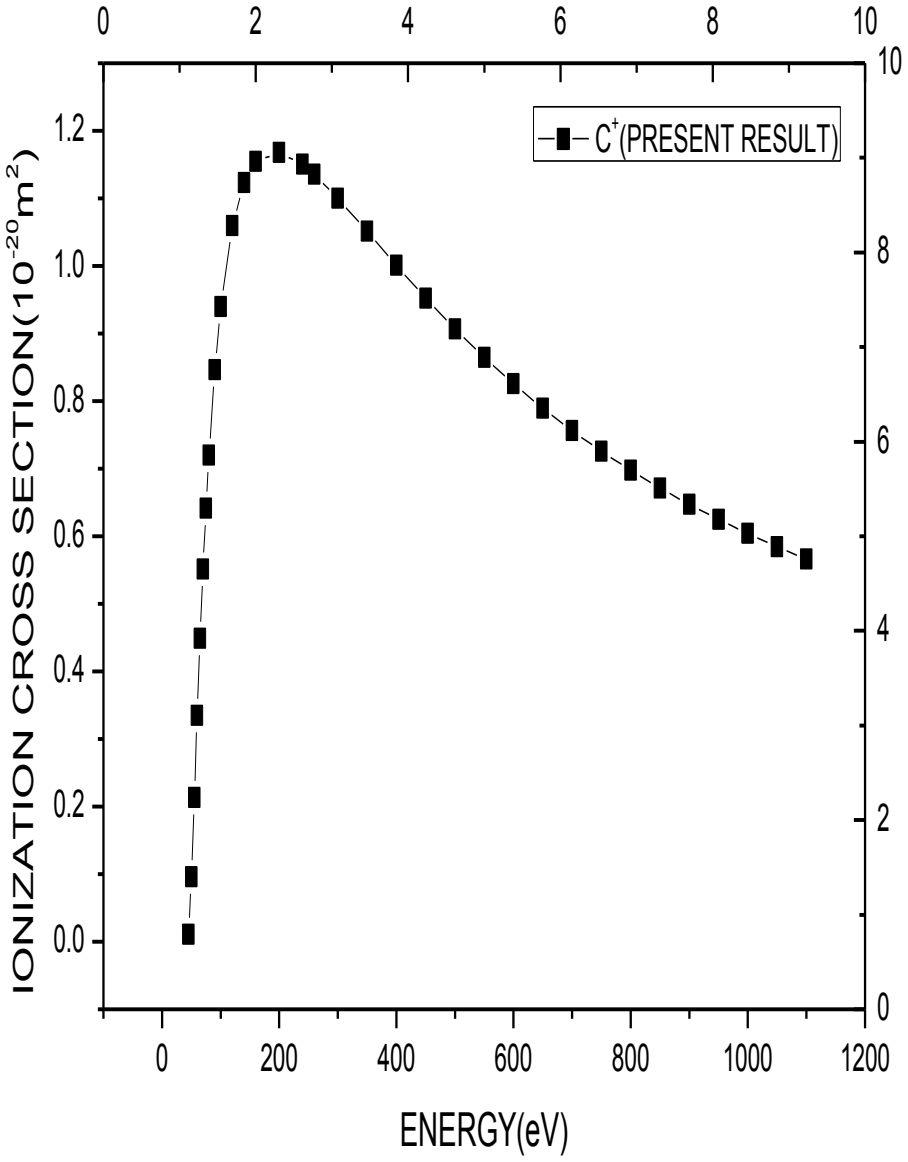


9)Graph representing cross section of CH_2^+ due to ionization of C_2H_6



10) Graph representing cross section of CH^+ due to ionization of C_2H_6



11) Graph representing cross section of C^+ due to ionization of C_2H_6

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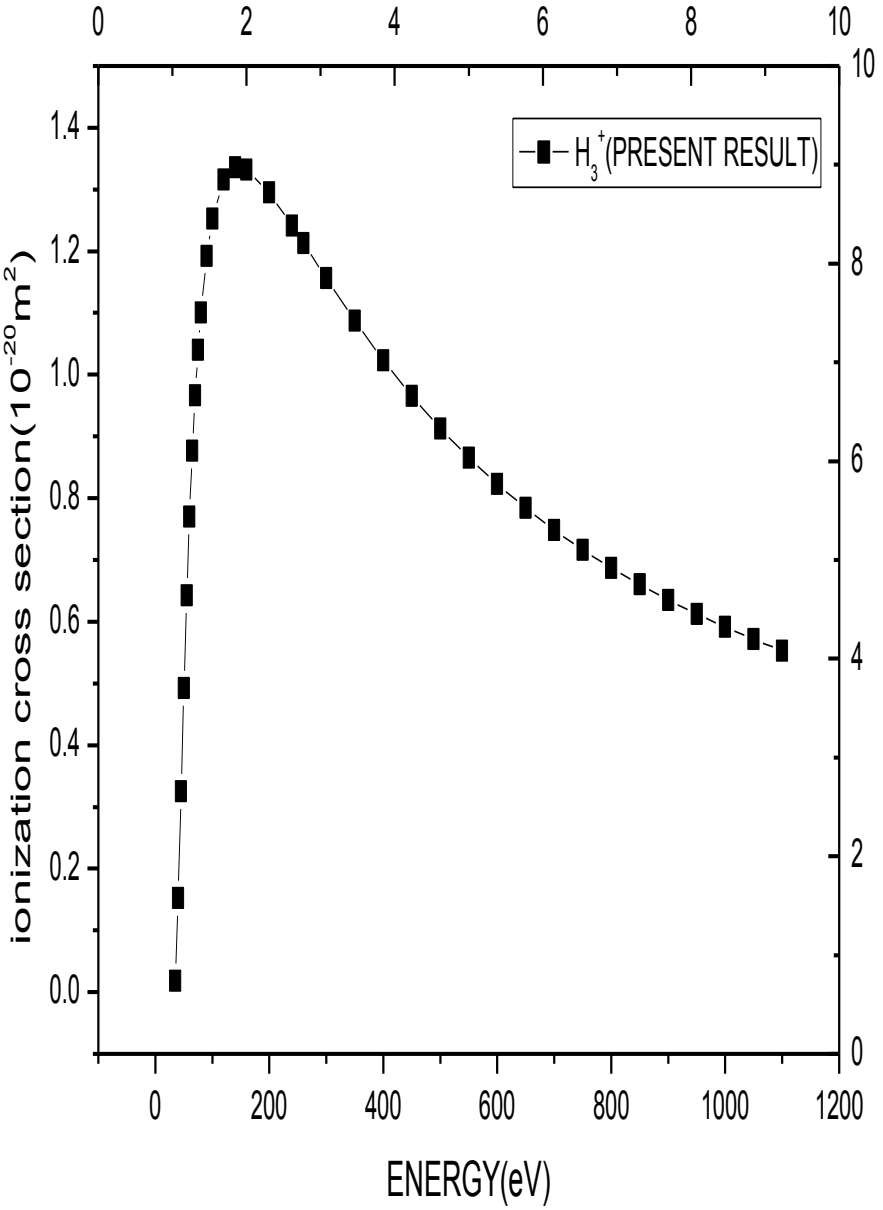
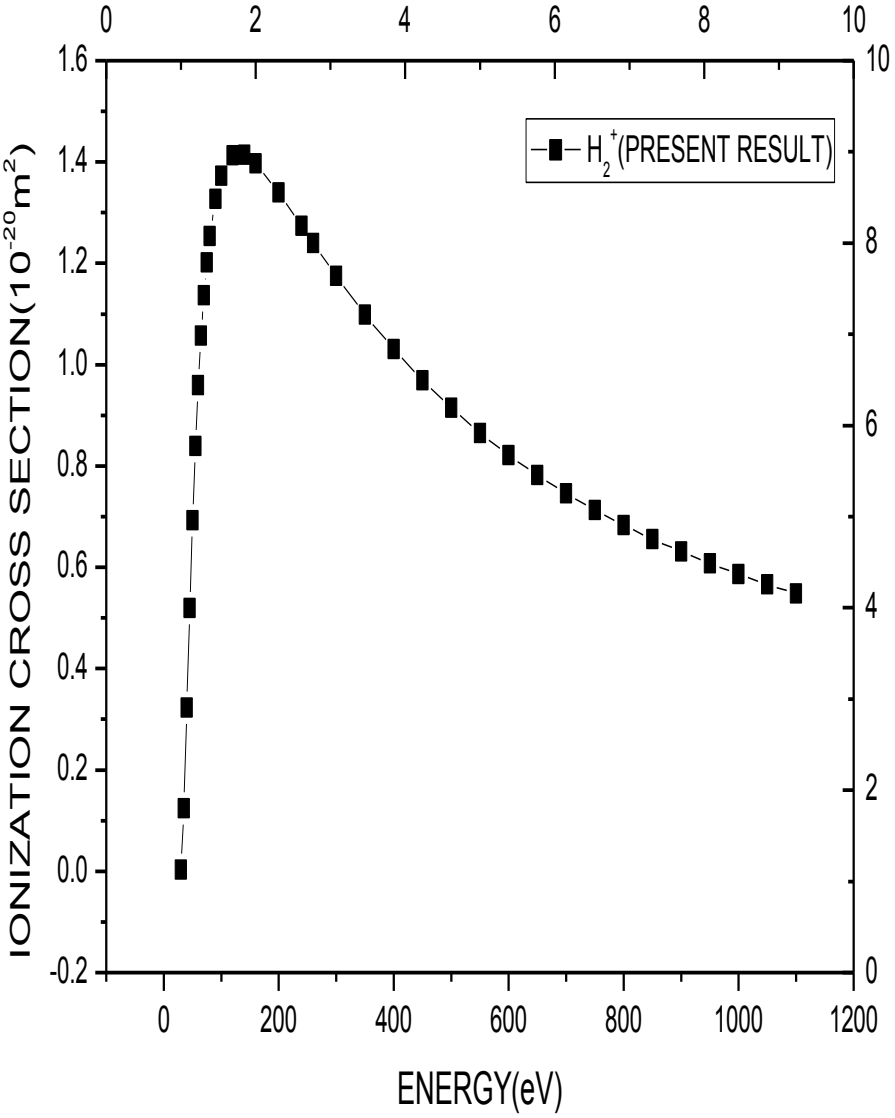
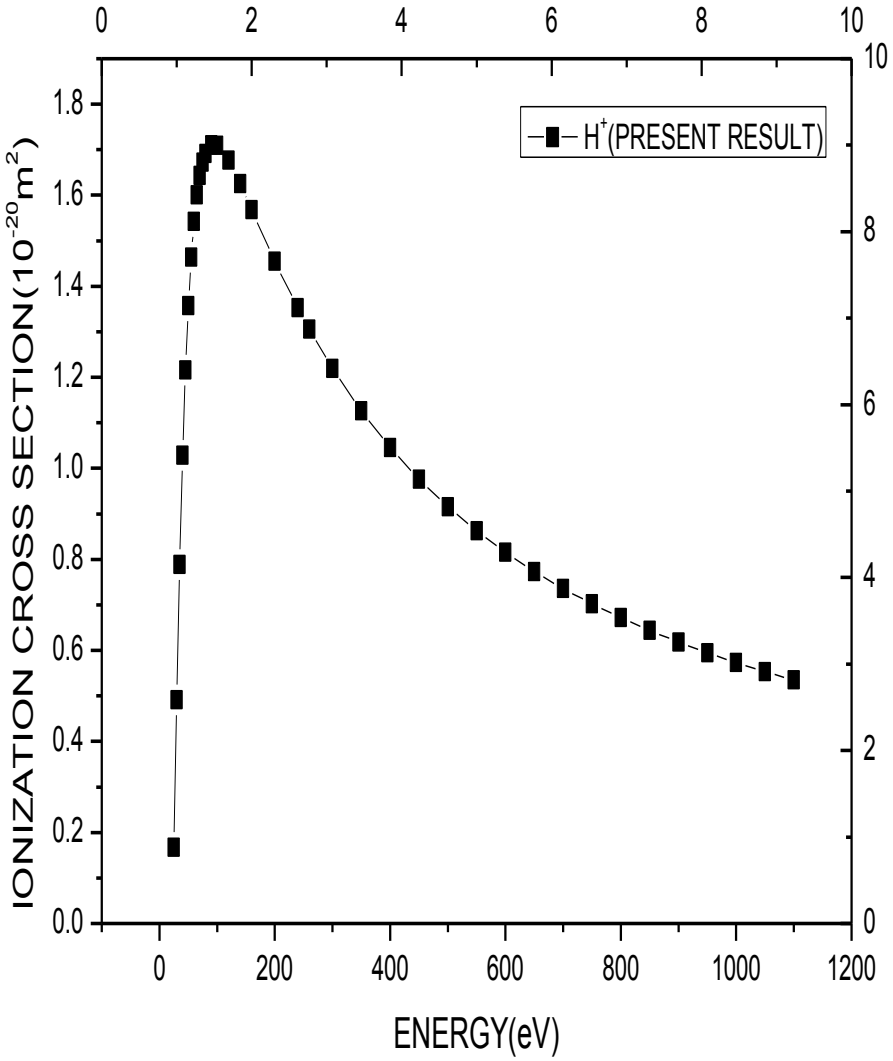


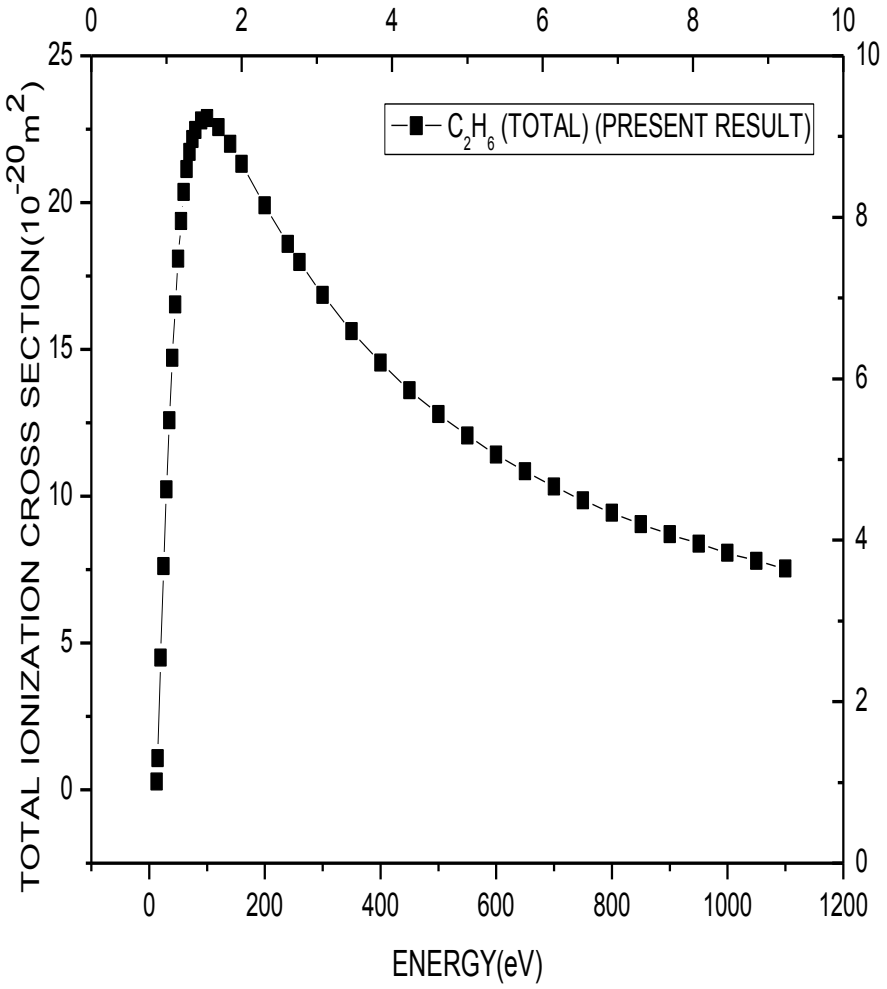
12) Graph representing cross section of H_3^+ due to ionization of C_2H_6



13) Graph representing cross section of H_2^+ due to ionization of C_2H_6



14) Graph representing cross section of H^+ due to ionization of C_2H_6



15) Graph representing total ionization cross section of C_2H_6

Conclusion:

Electron-impact ionization of many atoms has been investigated in the present study for which data are fragmentary in the literature. Many theoretical and experimental approaches have been developed over the years to give reliable cross section data to the atomic and molecular community. However, there still remains an avenue of research to produce cross section data for many systems as the cross section data for most of the systems vary remarkably. Hence there is a need for a simple method that can quantify reliable results

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