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ORIGINAL ARTICLE

Partial Ionization Cross Section Of Ccl_2f_2 Molecule By Electron Impact

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ABSTRACT

Electron impact ionization cross sections have been evaluated for atoms at incident energies ranging from ionization threshold to 1100 eV. The proposed model by incorporating it in exchange, coulomb and relativistic effects along with the contributions of transverse interaction to ionization cross sections. Adequate comparisons have been made with other theoretical methods, empirical formulae. Obtained results are in good agreements with available experimental data.

KEYWORDS:

cross section, electron impact and ionization.

INTRODUCTION

In the recent years there has been used in the evaluation of the cross section of atoms and molecules due to photon, electron and heavy particle impact because of their useful in various fields such as the example cross section for the indexed for modeling ionization in the material in the biological and biomedical research and modeling of fusion plasma in the tokomaks. There is a strong impact on much other scientific area, such as astrophysics, astrochemistry, atmospheric physics, radiobiological area, biological chemistry, x-ray laser and fusion research. Electron impact ionization cross section at high energy has very importance.

Electron impact ionization of molecules are considered the most interesting collision processes. Data are required for electron impact ionization of molecular targets to understand the

physics of a wide range of environments, and great development of quantitative indicators, as well as the theoretical description of this fundamental process. The different cross sections absolute partial and total electron impact ionization of CCl_2F_2 are reported for electron energies from threshold to 1100 eV. The product ions were analyzed therefore the mass using a time of flight mass spectrometer and were detected with a position sensitive detector whose output shows that all ion species collected product with nearly the same efficiency irrespective of their initial kinetic energies. The total cross section for each target is obtained as the sum of partial cross sections. The present partial cross sections for fragments ions are found to be considerably higher than had been previously reported. Total ionization cross sections are calculated as the sum of measured partial cross sections.

Very few multiply charged ions are produced however and the two cross sections are thus essentially identical. For CCl_4 the data of Hudson et al agree well with the present measurements; the cross section of Leiter et al is considerably smaller than the other measurements as expected given their collection efficiency problems. For CCl_2F_2 it is gratifying to see that very good agreement exists between all three experiments. Calculations by Hudson et al and Bart et al obtained by semi classical Deustch Mark_formalism(DM) and the Binary Encounter Bethe (BEB)model. Evidently neither theory is consistently able to reproduce the experimental cross section .When all of the partial cross section plots are viewed the most obvious trend observed cross section become progressively smaller relative to present measurements as the mass of fragment ion decreases [1-3].

II. THEORY

For CCl_4 the ion peaks are well resolved by mass spectrometer. However for CCl_2F_2 some of the product ions are formed with very nearly the same mass to charge ratios and cannot be separated by time of flight mass spectrometer. Fortunately when multiply charged species with very small cross sections are formed in the vicinity of a much larger singly charged ion peak their presence may be neglected without compromising the quoted uncertainties.

The tiny cross sections for production of doubly charged species provide quantitative support for this approach. In one instance two singly charged ions, $CClF_2^+$ and CCl_2^+ are formed in very close proximity to each other, but because the CCl_2^+ cross section has been found to be more than two orders of magnitude smaller than that for $CClF_2^+$ this peak is attributed to the dominant $CClF_2^+$ ion only. Furthermore the Cl^+ and CF^+ time of flight peaks to allow the individual cross section to be determined by fitting the sum of two modified Gaussian distributions to the spectra. For CCl^+ and CF_2^+ none of these approaches is applicable and the aggregate cross section is reported. Cross section for production of ($CCl_2^+ + Cl^+$) and ($CCl^+ + Cl^+$) ion pairs were obtained by utilizing an electronic gating technique which has been described previously. Observations of ion pair production from CCl_2F_2 have been discussed that the uncertainty in the total cross section is ± 5 %. near the threshold for formation of each

species the uncertainties in the cross section are typically greater than those quoted in tables. The mean energy of electron beam was established to within ± 5eV.

This is consistent with incomplete collection of lighter more energetic fragment ions in the earlier study. Such effects are extremely common and are almost invariably present when secondary ions are analyzed with mass spectrometers embodying long path lengths. Even the large discrepancies for Cl^+ and C^+ are not surprising when it is remembered that these are the lightest and most energetic ions formed. Recently noted that CCl_4 data are too low because of incomplete ion collection and they attempted to correct the data to account for this.

The BEB approach predicts the energy at which the cross section peak more accurately than the DM theory which predicts lower maxima than are observed. However an improved version of DM theory which has been applied to atomic targets, predicts slightly higher energy maxima than the version used for calculations [4-15].

III.FORMULATION

The present calculations are carried out using the modified semi empirical formalism developed by Jain-Khare. In brief, the single differential cross sections in the complete solid angle ($= \Omega = 4\pi = \int 2\pi sin\theta d\theta$) is known 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

$$Q_i(E, W, \square) = \frac{a_0^2 R^2}{E}\left[\int_0^{E-I_i}\left\{\frac{E-W}{E-I_i}\frac{1}{W}df_i(W, K, \square)\ x\ ln[1 + C_i(E-I_i)] + \frac{E-I_i}{E(\epsilon_0^3+\epsilon^3)}x\ s_i\left(\epsilon - \frac{\epsilon^2}{E-\epsilon} + \frac{\epsilon^2}{(E-\epsilon)^2}\right)\right\}\right] 2\pi sin\theta d\theta$$

Where

W (=ε + I_i) is defined as energy loss suffered by the incident electron.

I_i = the ionization threshold for the production of ith 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 or appearance potential is in direct ratio or directly proportional to the photo ionization cross section. We have used partial photo ionization cross section data set in the energy range provided by Brion using (e, e) spectroscopy. The accuracy of the determined oscillator strength scales was estimated to be better.

In the photon energy range, we have used their measured total valence photo absorption oscillator strength data and for higher photon energy range the same were extrapolated by Thomas-Reiche-Kuhn (TRK) sum rule. The total photo absorption cross sections have been distributed into ionic fragments considering the constant ionization efficiency to be above the dipole breakdown limit of ~25eV. However, its evaluation is possible quantum mechanically using the suitable wave functions and transition probabilities corresponding to the production of cations. In case of dissociative ionization of polyatomic molecule, we have no reliable probabilities corresponding to different dissociative ionization processes. The collision parameter and energy parameter ε_0 are evaluated as for other polyatomic molecules. The vertical onsets or the ionization potentials corresponding to the various cations are also given along with the photo ionization measurements. In the present evaluations of cross sections, the estimated uncertainty is more or less the same as for the measurement of photo-ionization cross sections. The double differential cross sections as a function of energy and angle were evaluated by the differentiation of equation of semi empirical formula with respect to the solid angle Ω as follows:

$$Q_i^2(E, W, \theta) = \sum_i Q_i(E, W. \theta)$$

The double differential cross sections are angular dependant in all the scattering geometries and hence the oscillator strength must be angle dependent. In this context, we have used the angular oscillator strengths that were derived in the optical limit (Bethe regime) where angular-momentum-transfer k→ 0,

$$\frac{df_i(W,0,\theta)}{dW d\,\Omega} = \frac{1}{4\pi}\frac{df_i(W,0)}{dW}[1 + \beta/2(3\cos^2\theta - 1)]$$

where β is an energy dependent asymmetric parameter. Its evaluation is difficult due to the lack of wave functions of molecular ions in ground and excited states. In valence shell ionization of atomic molecules, we have computed β as the ratio of the Bethe spectral transitions $S_i(W)$ to the dipole matrix squared M_i^2 (W). The oscillator strength appeared in equation is simply a derived form in the forward scattering corresponding to k→ 0 and θ→0.

The partial ionization cross section is obtained by the integration of the energy dependent single differential cross sections over the entire energy loss as follows:

$$Q_i(E) = \int Q_i(E,W)dW$$

and the counting or total electron impact ionization cross section is obtained by

$$Q_i^T(E,W) = \sum_i Q_i(E,W)$$

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

$$R_i = \int_{-\infty}^{\infty} 4\pi \left(\frac{1}{2\pi mkt}\right)^{3/2} me^{(-e/kT)} Qi(E)$$

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

IV. RESULTS AND DISCUSSION

Now we calculate the results of the absolute partial ionization cross section measurements for the CCl_2F_2 molecule from threshold to 1100 eV modified Jain-Khare Semi-empirical model. Table 1 & Table 2 shows the measured partial cross sections for the formation of CF_2Cl^+, $CF_2Cl_2^+$, $CFCl_2^+$, CF_2^+, Cl_2^+, $CFCl^+$, Cl^+, CF^+, F^+, ClF^+, CCl and CCl_2F_2 (Total) . In figure 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11 and 12 represents the production of CF_2Cl^+, $CF_2Cl_2^+$, $CFCl_2^+$, CF_2^+, Cl_2^+, $CFCl^+$, Cl^+, CF^+, F^+, ClF^+, CCl and total ionization cross section of CCl_2F_2 molecule. There is a good agreement between theoretical and experimental results.

TABLE 1

	Partial Ionization Cross Section of CCl_2F_2 Molecule $10^{-20}m^2$						
ENERGY (eV)	CF_2Cl^+	$CF_2Cl_2^+$	$CFCl_2^+$	CF_2^+	Cl_2^+	$CFCl^+$	Cl^+
15							
16	0.247031				0.376181		
17	0.351364	0.37668			0.738976		
20	0.672947	0.740021	0.358564	0.157682	1.239293	0.077445	0.268386

25	1.136527	1.241389	0.731929	0.629644	1.589364	0.562102	0.684931
30	1.472485	1.592381	1.000524	0.882497	1.824003	0.814723	0.943815
35	1.703313	1.827718	1.201951	1.082584	1.977515	1.013318	1.145439
40	1.858636	1.981729	1.35071	1.237768	2.090126	1.169321	1.298448
45	1.960413	2.080322	1.458735	1.35521	2.143922	1.289471	1.412618
50	2.025271	2.140009	1.53655	1.44305	2.172368	1.380171	1.496082
55	2.06331	2.173397	1.591027	1.507237	2.18391	1.44818	1.556611
60	2.083147	2.187451	1.628724	1.553874	2.182513	1.497738	1.59887
65	2.088997	2.188839	1.652854	1.586094	2.173032	1.533784	1.628056
70	2.08585	2.180177	1.667739	1.608162	2.156663	1.558342	1.646202

Partial Ionization Cross Section of CCl_2F_2 Molecule $10^{-20}m^2$

ENERGY (eV)	CF_2Cl^+	$CF_2Cl_2^+$	$CFCl_2^+$	CF_2^+	Cl_2^+	$CFCl^+$	Cl^+
75	2.075086	2.165562	1.674428	1.621254	2.136686	1.57501	1.657013
80	2.060097	2.145521	1.676118	1.628632	2.112918	1.584328	1.660913
85	2.040769	2.123001	1.672636	1.630196	2.087939	1.589169	1.660845
90	2.019783	2.09745	1.666649	1.628703	2.060787	1.589092	1.656264
95	1.996237	2.07129	1.657216	1.623286	2.033712	1.586692	1.649748
100	1.972447	2.043372	1.646794	1.61642	1.894455	1.580855	1.640088
125	1.845924	1.904487	1.57621	1.559017	1.770697	1.532348	1.576678
150	1.726534	1.774434	1.499068	1.490109	1.555126	1.467907	1.501947
200	1.523267	1.558219	1.354105	1.354382	1.387201	1.339598	1.360467
250	1.362946	1.389844	1.231255	1.236191	1.253521	1.225973	1.239091
300	1.234272	1.255805	1.127996	1.135354	1.144637	1.128205	1.136404

350	1.128847	1.146644	1.040647	1.049284	1.05423	1.04414	1.049181
400	1.040997	1.056033	0.96606	0.975329	0.977965	0.971584	0.974474
450	0.966642	0.979601	0.901832	0.911324	0.911603	0.908535	0.91003
500	0.902888	0.914249	0.846005	0.855513	0.806131	0.853441	0.853898
600	0.799247	0.808264	0.753824	0.763047	0.724091	0.761928	0.761128
700	0.718475	0.725909	0.680909	0.689654	0.658958	0.689094	0.687635
800	0.653632	0.659943	0.621751	0.630024	0.604955	0.629811	0.627945
900	0.600388	0.60582	0.572763	0.580543	0.581398	0.580572	0.578517
950	0.577146	0.582226	0.551292	0.558791	0.559771	0.558902	0.556817
1000	0.55578	0.560554	0.531487	0.538783	0.539838	0.538987	0.536827
1050	0.536077	0.540582	0.51318	0.520272	0.536025	0.520495	0.518329
1060	0.532331	0.536774			0.536025		
1100					0.521382		

TABLE 2

	Partial Ionization Cross Section of CCl_2F_2 Molecule $10^{-20}m^2$					
ENERGY (eV)	CF^+	C^+	F^+	ClF	CCl	TOTAL
15						
16						0.623212
17						1.46702
20						3.514338
25	0.107656			0.028642		6.712184

30	0.522833	0.31228	0.065876	0.459821	0.325799	10.21704
35	0.733419	0.558261	0.405163	0.674261	0.580948	12.90389
40	0.887271	0.698879	0.567452	0.833854	0.723164	14.69736
45	1.005387	0.806521	0.686006	0.958633	0.827163	15.9844
50	1.09661	0.894032	0.781461	1.05658	0.908322	16.93051
55	1.167391	0.96564	0.859949	1.133648	0.972651	17.62295
60	1.221601	1.024534	0.925066	1.193515	1.024313	18.12135
65	1.263415	1.072187	0.978527	1.240322	1.065251	18.47136
70	1.294589	1.111141	1.022845	1.275842	1.098199	18.70575
75	1.318264	1.141968	1.058688	1.303286	1.123772	18.85102
80	1.334849	1.167034	1.088372	1.323131	1.144309	18.92622
85	1.346997	1.186143	1.111812	1.338094	1.159544	18.94715
90	1.354211	1.201588	1.13123	1.347755	1.171708	18.92522
95	1.35892	1.212568	1.145925	1.354564	1.179916	18.87007
100	1.360036	1.221346	1.158137	1.357511	1.186368	18.67783
125	1.34306	1.232614	1.1829	1.346709	1.190967	18.06161
150	1.304547	1.21589	1.17648	1.31139	1.17199	17.19542
200	1.215077	1.155101	1.129502	1.224542	1.112223	15.71368

Partial Ionization Cross Section of CCl_2F_2 Molecule $10^{-20}m^2$

ENERGY (eV)	CF^+	C^+	F^+	ClF	CCl	TOTAL
250	1.128165	1.085794	1.06899	1.138257	1.046069	14.4061
300	1.049181	1.018274	1.007268	1.059182	0.98192	13.2785

350	0.978748	0.95557	0.948484	0.988409	0.92231	12.30649
400	0.917634	0.899816	0.89539	0.926873	0.869246	11.4714
450	0.861021	0.847172	0.844599	0.869761	0.818999	10.73112
500	0.811953	0.80024	0.79909	0.820221	0.774161	10.03779
600	0.729185	0.721441	0.722029	0.736648	0.698766	8.979598
700	0.662329	0.657052	0.658543	0.669094	0.636993	8.134645
800	0.607292	0.603645	0.605731	0.613449	0.585704	7.443882
900	0.561247	0.558758	0.5611	0.566923	0.542487	6.890516
950	0.540923	0.538831	0.541272	0.546336	0.523311	6.635618
1000	0.522133	0.520365	0.522886	0.527344	0.505549	6.400533
1050	0.504705	0.503269	0.505873	0.509734	0.489065	6.197606
1060		0.499991	0.502574		0.485896	3.093591
1100		0.487325	0.489955		0.473673	1.972335

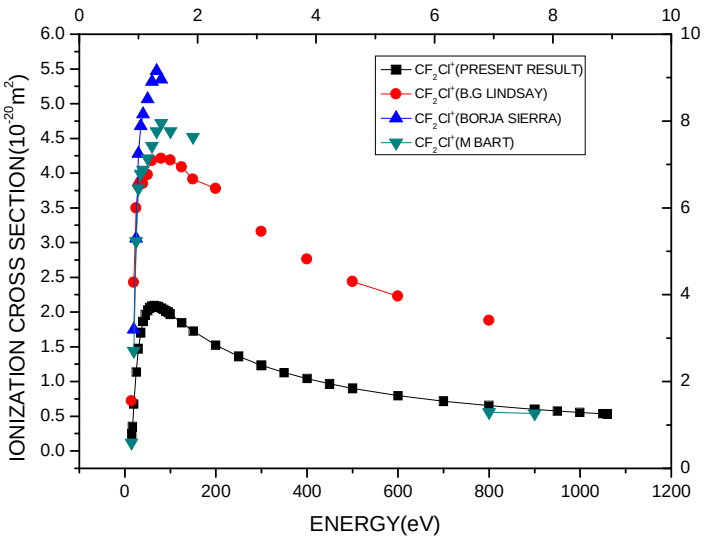

Figure 1: Ionization Cross Section of $CF_2Cl_2^+$

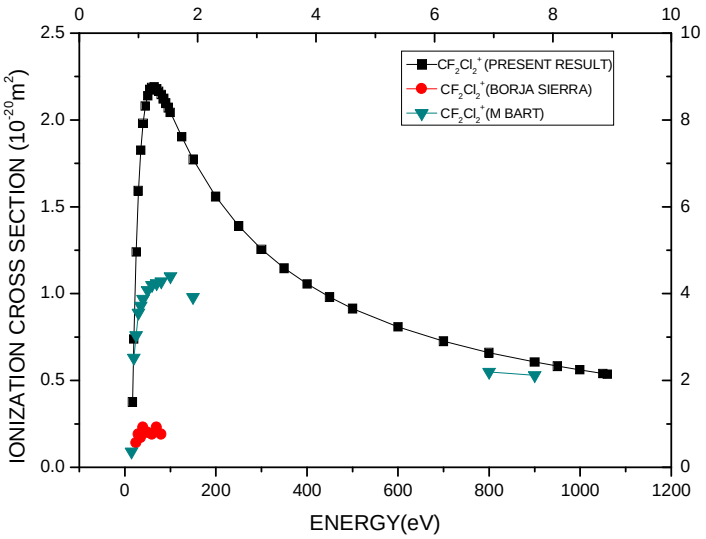

Figure 2: Ionization Cross Section of $CF_2Cl_2^+$

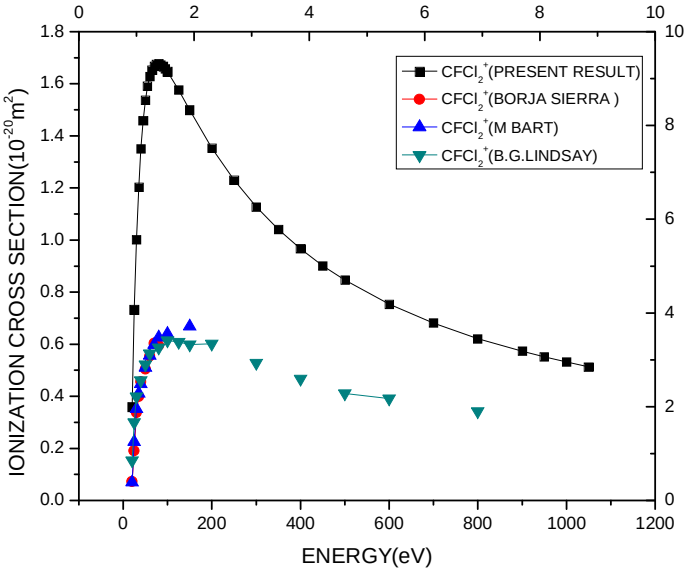

Figure 3: Ionization Cross Section of $CFCl_2^+$

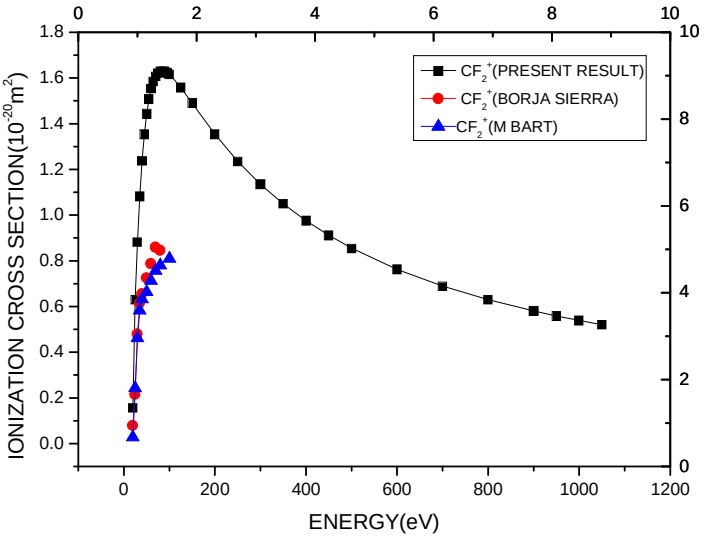

Figure 4: Ionization Cross Section of CF_2^+

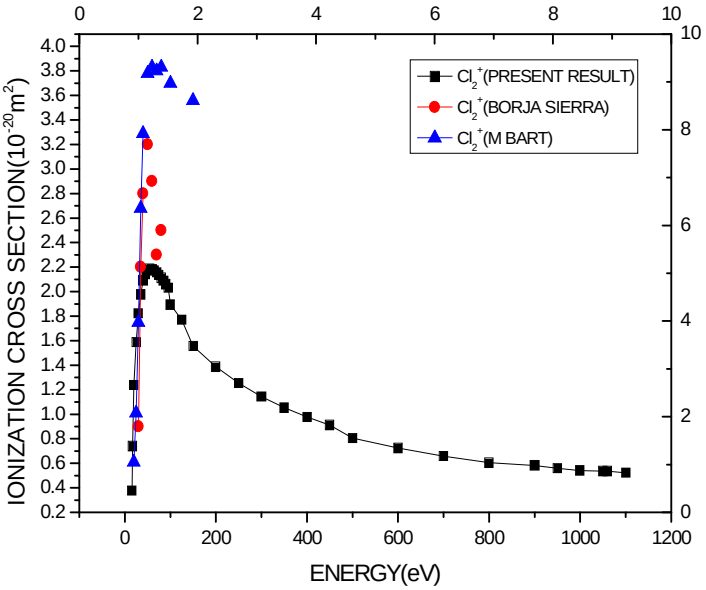

Figure 5: Ionization Cross Section of Cl_2^+

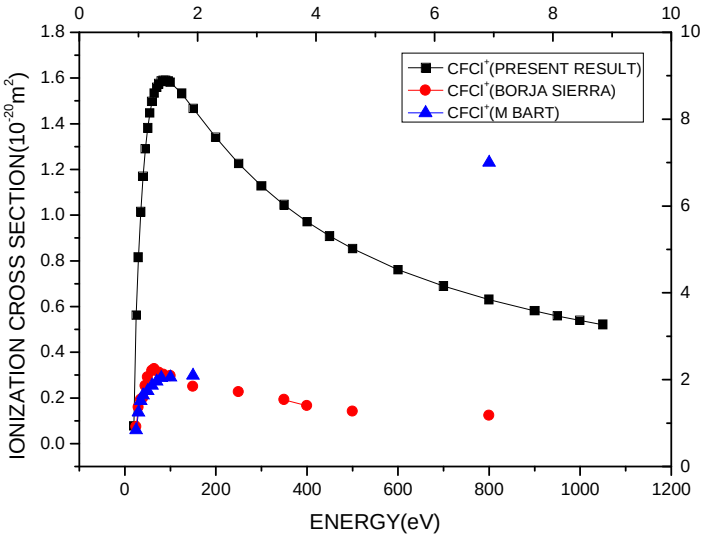

Figure 6: Ionization Cross Section of $CFCl^+$

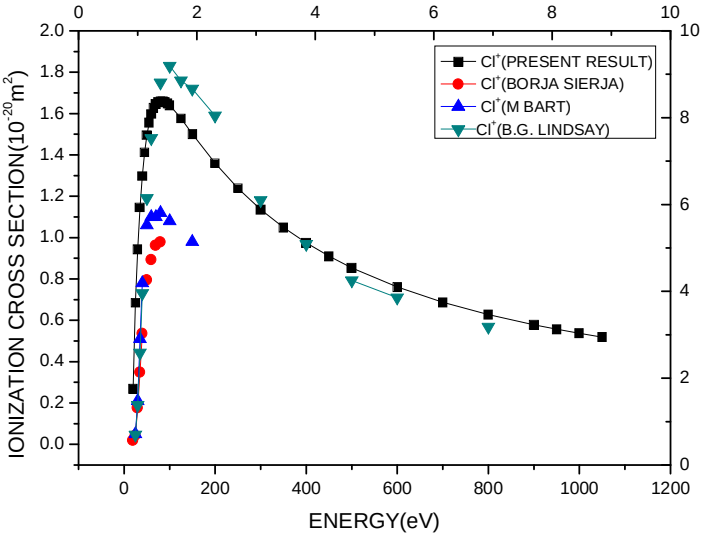

Figure 7: Ionization Cross Section of Cl^+

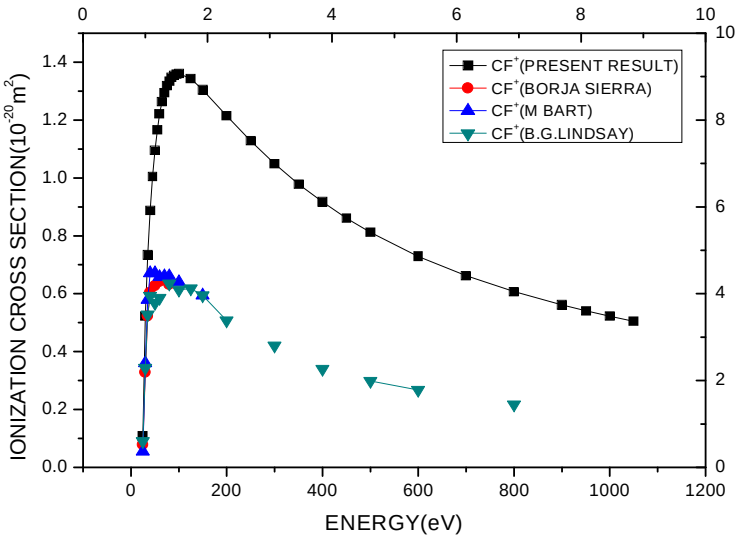

Figure 8: Ionization Cross Section of CF^+

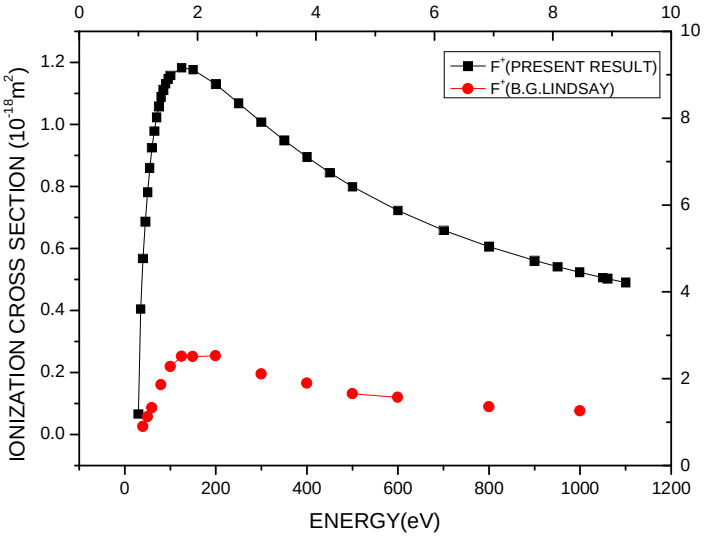

Figure 9: Ionization Cross Section of F^+

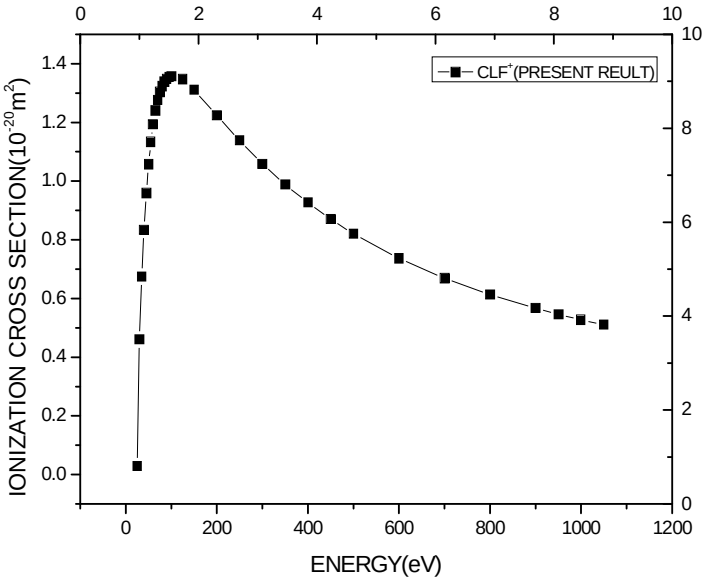

Figure 10: Ionization Cross Section of ClF^+

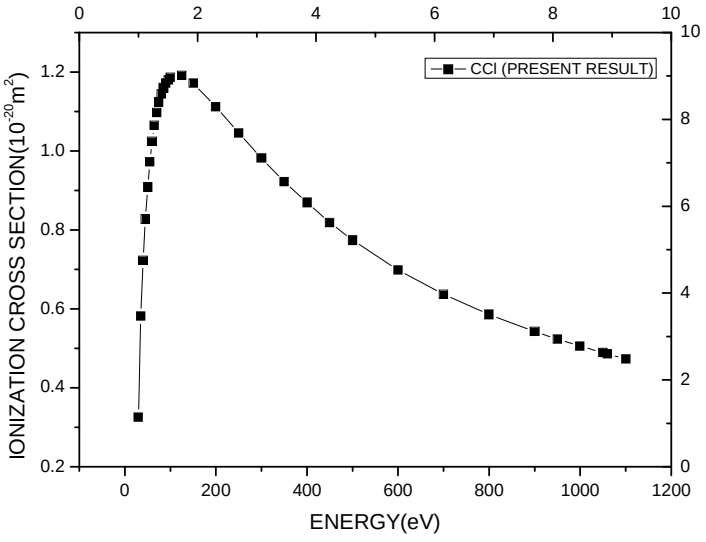

Figure 11: Ionization Cross Section of CCl

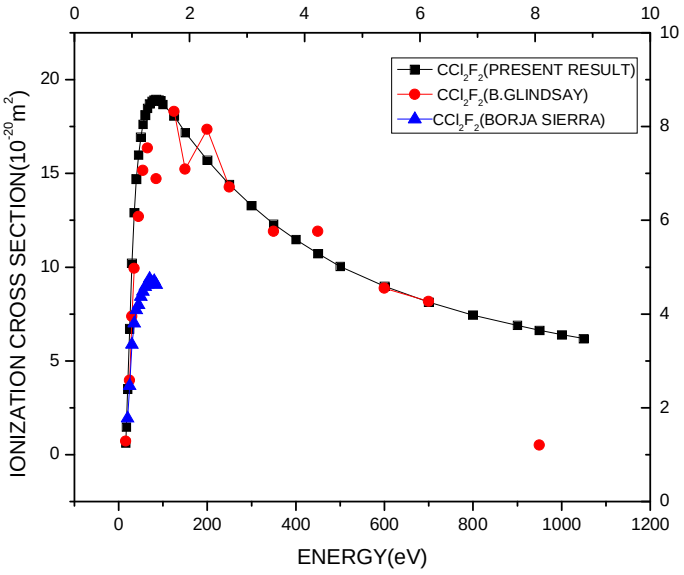

Figure 12: Ionization Cross Section of CCl_2F_2 (Total)

The experimental determination of the partial and total ICSs, considerable effort has been focused on the development of theoretical approaches for computing the total ICS based on semi-empirical methods.

V. CONCLUSION

Absolute partial and total cross section are reported for electron impact ionization of CCl_2F_2 for electron energies from threshold to 1100eV for the ions CF_2Cl+ , $CF_2Cl_2^+$,. $CFCl_2^+$, CF_2^+, Cl_2^+,$CFCl^+$, Cl+, CF^+, C^+ ,F^+, ClF, CCl is calculated.

The apparatus geometry is of simple design embodying a short path length TOFMS and position sensitive detection of the product ions which equivalent demonstrates that all fragment ions species are collected with equal efficiency irrespective of their initial kinetic energy. the present partial cross section for lighter fragments ions are found to be considerably higher than had been previously which is attributed to contributed to incomplete ion collection in the earlier studies. The most recent total cross section measurements agree well with those cross section measurements agree well with those reported here but neither the neither the BEB theory nor the DM Theory was able to reproduce the experimental cross sections for both targets[16-21].

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