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ORIGINAL ARTICLE

Study Of Ionization Cross Section Of Argon Molecule By Electron Impact

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ABSTRACT

The total ionization cross-sections of Argon molecule due to electron impact for threshold ionization energy to 6000 eV have been studied. The present cross sections are compared to existing experimental cross sections as well as to theoretical predictions. The correlation between the total electron scattering cross section and the number of target-molecule electrons is discussed.

KEYWORDS:

Electron impact, Cross section, Ionization.

INTRODUCTION

In recent years, there has been increased interest in the study of the total cross section for electron scattering from atoms and molecules at intermediate electron energies 16-6000eV. The cross-section measurements at these energies are required to develop theoretical models in understanding the interaction process and in applications in atmospheric physics, astrophysics, plasma physics and chemical physics [1-2]. One of the purposes of this work is to calculate the electron impact ionization cross-sections of the Argon molecule by employing the useful features of Semi-empirical model at given energy.

The upper atmosphere is constantly bombarded by the energetic particles and electromagnetic radiations. Particularly during solar flare the sun emits greatly enhanced electromagnetic radiation in X-ray and UV regions, cosmic particles, ions and electron produce photoelectrons and secondary electrons. These electrons then lose their energy through various elastic and inelastic processes and ultimately get thermalized. Thus the energy spectrum of the electrons is a very important parameter for all atmospheric calculations. From the energy spectrum induced by collision processes one gets an idea of chemical composition, density and temperature of constituent elements of atmosphere. The ionic layers in the ionosphere of earth are mainly formed due to the ionization of the neutral constituent of atmosphere by solar radiations leading to production of energetic free electrons and ions. These energetic electrons further excite the neutral particles and these excited states of particles on decay to lower states give rise to fluorescence. This is an important component of day glow. These ionized and excited species also produce the atmospheric emission known as aurora. Hence for the proper understanding of the different phenomena occurring in upper atmosphere, we need a wide knowledge of atomic and molecular Collision processes [3-5].

II. THEORY

Cross sections of rare gas species have been extensively investigated by various groups with different types of experimental techniques during the last decades. Electron impact ionization of rare gas ions is an important process in high-energy chemical processes, such as in planetary atmospheres and in plasma physics.

Even though the cross sections for singly and multiply charged ions decline rapidly with increasing stage of ionization, multiple ionization processes are important in fusion plasmas and in other environments with an abundance of energetic electrons. Absolute cross sections have been presented for electron impact single ionization of multiply charged Ar^{k+}. The present results of experimental investigations for single and multiple ionization of Ar^{k}:where k (n=1-8).

$$Ar^{+} + e^{-} \rightarrow Ar^{k+} + 2e^{-}$$

$$Ar^{+} + e^{-} \rightarrow Ar^{3+} + 3e^{-}$$

$$Ar^{+} + e^{-} \rightarrow Ar^{4+} + 4e^{-}$$

$$Ar^{+} + e^{-} \rightarrow Ar^{5+} + 5e^{-}$$

$$Ar^{+} + e^{-} \rightarrow Ar^{6+} + 6e^{-}$$

$$Ar^{+} + e^{-} \rightarrow Ar^{7+} + 7e^{-}$$

$$Ar^{+} + e^{-} \rightarrow Ar^{8+} + 8e^{-}$$

Electron impact ionization of a positive ion may occur directly, when one or more electrons are ejected from an outer or from an inner shell or indirectly, via formation of an intermediate auto ionizing state which cans be formed in two ways.

Firstly, the incident electron may excite the target ion from an inner shell into short-lived auto ionizing states, which subsequently decay via Auger transitions. Secondly, direct inner shell ionization may be followed by single or multiple auto ionization, either by cascading transitions or by simultaneous ejection of two or more electrons [6-16].

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 ith 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, 2e) 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:

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

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,

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

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 & DISCUSSION

Now we present calculate the results of the absolute partial ionization cross section measurements for the Argon molecule from threshold to 6000 eV modified Jain-Khare Semi-empirical model.

Table 1

	Partial Ionization Cross Section of Argon Molecule $10^{-20}m^2$				
Energy (eV)	Ar^+	Ar^{2+}	Ar^{3+}	Ar^{4+}	Ar^{5+}
16	0.00561				
20	0.24249				
28	0.93072	0.08741			
30	1.07025	0.29428			
40	1.55551	0.70586			
50	1.79822	0.92134			
60	1.94904	1.15311	0.03492		
70	1.95139	1.16113	0.04929		
100	1.90392	1.2804	0.39072		

120	1.78816	1.28852	0.49639	0.01394	
130	1.78453	1.28858	0.498809	0.017253	
200	1.51694	1.20378	0.62304	0.25921	
400	1.05217	0.92924	0.69751	0.49825	0.40748
600	0.81128	0.74432	0.63758	0.56182	0.61122
800	0.66468	0.62156	0.56676	0.54848	0.662104
1000	0.56565	0.535107	0.505808	0.51534	0.65501
1500	0.41692	0.40054	0.39637	0.42996	0.57896
2000	0.33325	0.322706	0.32628	0.36401	0.50168

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

Energy (eV)	Ar^{+}	Ar^{2+}	Ar^{3+}	Ar^{4+}	Ar^{5+}
2500	0.279114	0.27156	0.278004	0.31493	0.43911
3000	0.24099	0.23524	0.24271	0.27755	0.38951
3500	0.21259	0.208007	0.21579	0.248291	0.349707
3500	0.21259	0.208007	0.21579	0.248291	0.349707
4000	0.19055	0.18676	0.19453	0.22473	0.31723
4500	0.17291	0.169702	0.17727	0.20543	0.29034
5000	0.15845	0.15568	0.162982	0.18927	0.26769
5500	0.14635	0.14394	0.15096	0.17559	0.24438
6000	0.13609	0.13395	0.14065	0.16382	0.23173

Table 2

	Partial Ionization Cross Section of Argon Molecule $10^{-20}m^2$			
Energy (eV)	Ar^{6+}	Ar^{7+}	Ar^{8+}	TOTAL
16				0.00561
20				0.24249
28				1.01813
30				1.36453
40				2.26137
50				2.71956
69				3.13707
70				3.16181
100				3.57504
129				3.58701
130				3.589172

	Partial Ionization Cross Section of Argon Molecule $10^{-20}m^2$			
Energy (eV)	Ar^{6+}	Ar^{7+}	Ar^{8+}	TOTAL
200				3.60297
400	0.18298			3.76763
600	0.41165	0.41165	0.035102	4.224622
800	0.540006	0.540006	0.168149	4.311745
1000	0.58895	0.58895	0.30356	4.258375

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1500	0.581605	0.581605	0.48085	3.86681
2000	0.52951	0.52951	0.52441	3.431356
2500	0.47651	0.47651	0.51962	3.055358
3000	0.43014	0.43014	0.49804	2.74432
3500	0.39088	0.39088	0.47141	2.487555
4000	0.35771	0.35771	0.44432	2.27354
4500	0.32954	0.32954	0.41854	2.093272
5000	0.30545	0.30545	0.39467	1.939642
5500	0.28452	0.28452	0.37281	1.80307
6000	0.2663	0.2663	0.35298	1.69182

Table 1 & Table 2 shows the measured partial cross sections for the formation of Ar^+, Ar^{+2}, Ar^{+3}, Ar^{+4}, Ar^{+5}, Ar^{+6}, Ar^{+7}, Ar^{+8} and Ar (Total) . In figure 1, 2, 3, 4, 5, 6, 7, 8 and 9 represents the production of Ar^+, Ar^{+2}, Ar^{+3}, Ar^{+4}, Ar^{+5}, Ar^{+6}, Ar^{+7}, Ar^{+8} and total ionization cross section of Ar molecule.

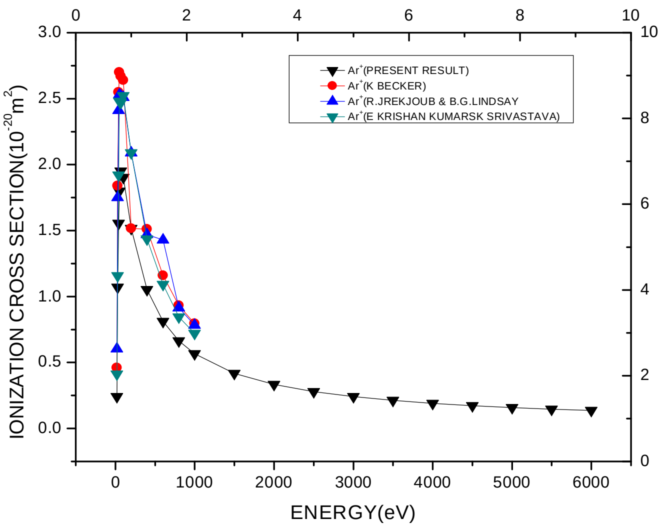

Figure 1: Ionization Cross Section of Ar^+

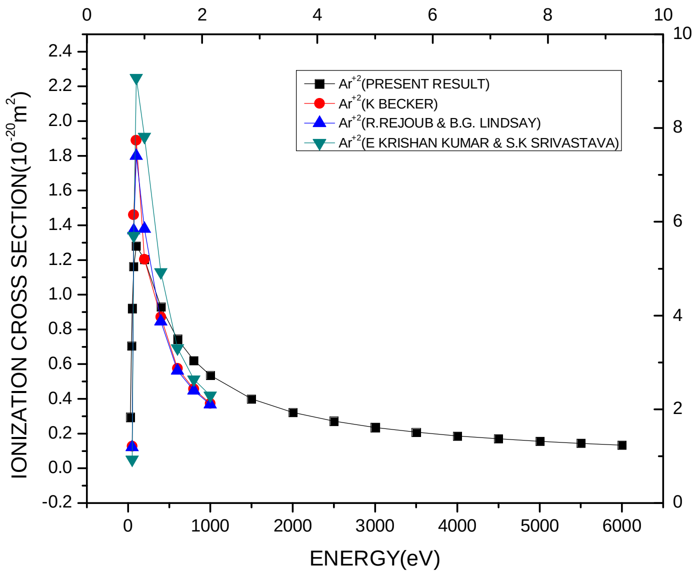

Figure 2: Ionization Cross Section of Ar^{+2}

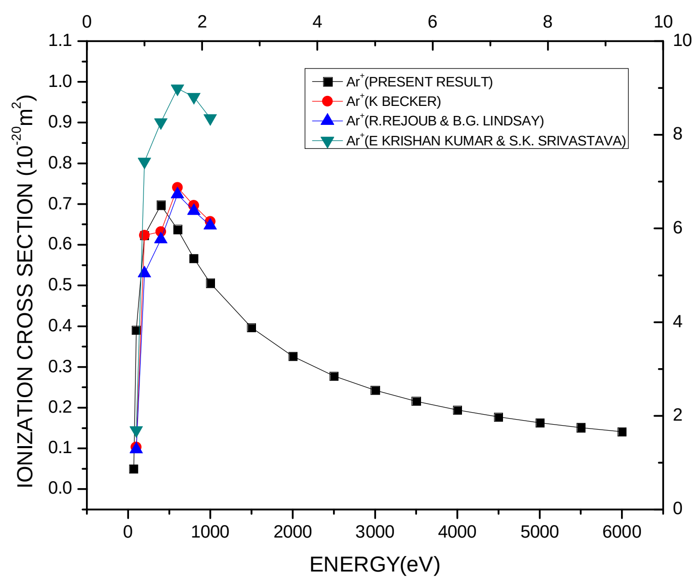

Figure 3: Ionization Cross Section of Ar^{+3}

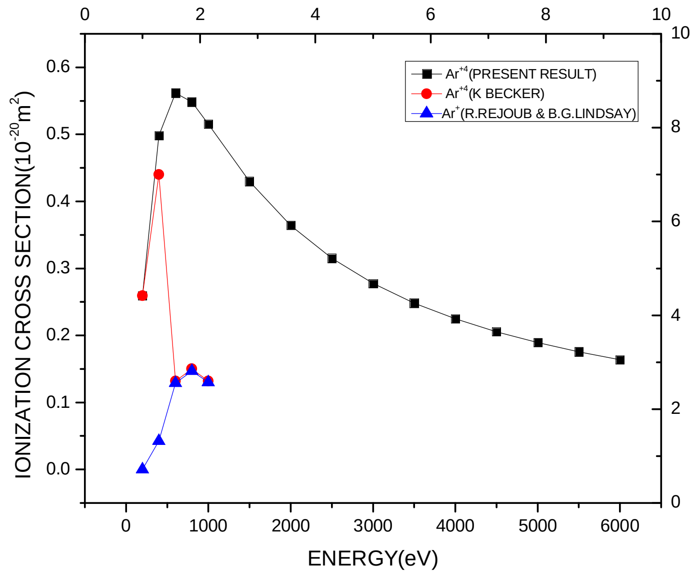

Figure 4: Ionization Cross Section of Ar^{+4}

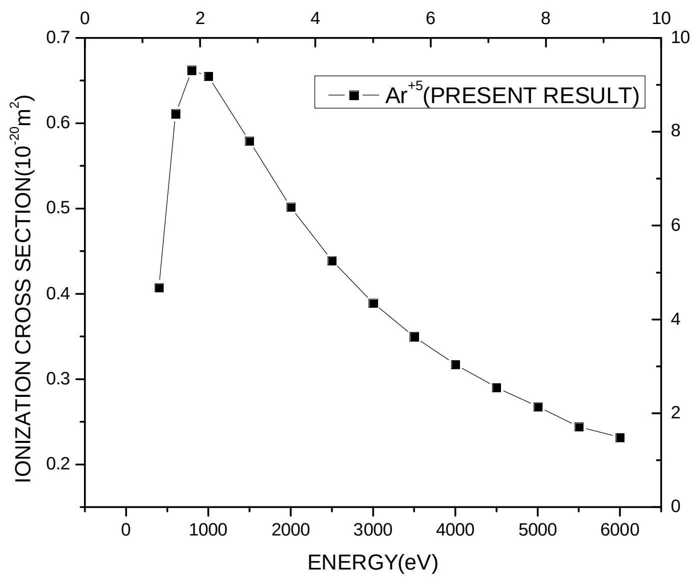

Figure 5: Ionization Cross Section of Ar^{+5}

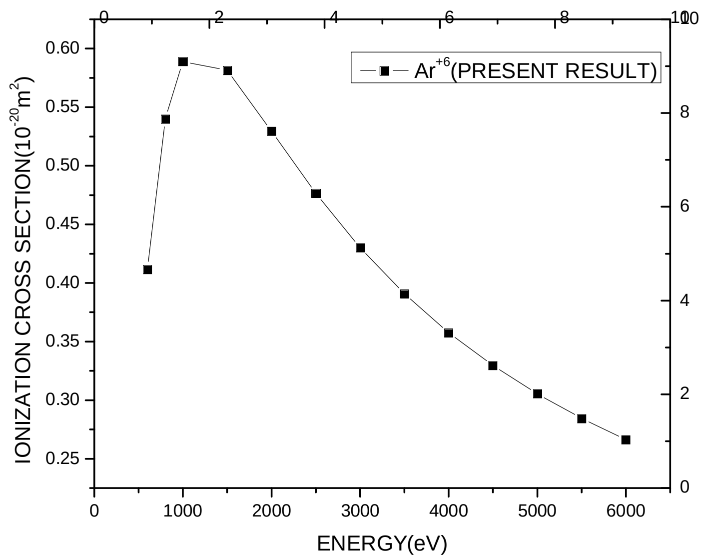

Figure 6: Ionization Cross Section of Ar^{+6}

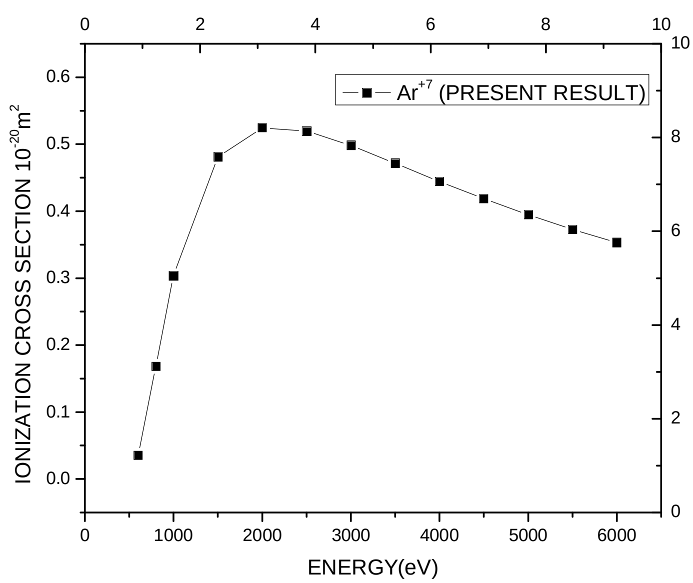

Figure 7: Ionization Cross Section of Ar^{+7}

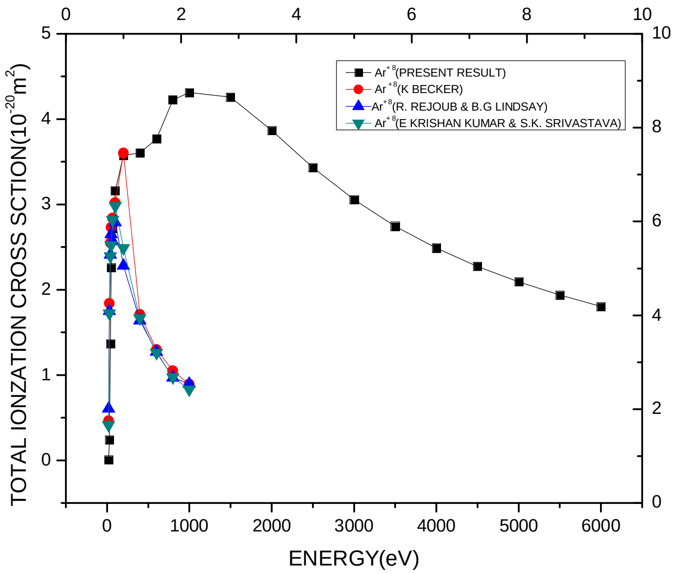

Figure 8: Ionization Cross Section of Ar^{+8}

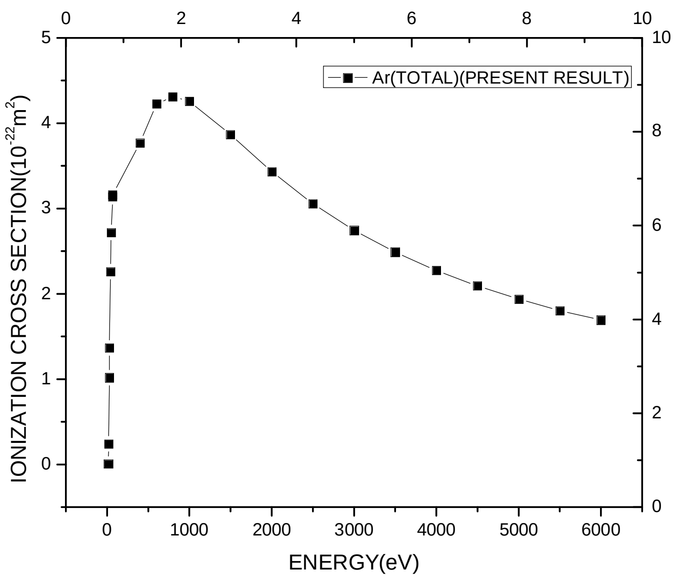

Figure 9: Ionization Cross Section of Ar (total)

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

In the present work Ar^{+} , Ar^{+2} , Ar^{+3} , Ar^{+4} , Ar^{+5} , Ar^{+6} , Ar^{+7} , Ar^{+8} ions from the ion source are calculated at energy 6000eV. The oscillator strengths obtained for the ionic target are observed to be under estimated by the empirical law whereas the latter overestimates the data corresponding to neutral argon. The generalized oscillator strength is deduced from high-energy ionization cross sections. As already observed in earlier experiments for neon ions, at a given incident electron energy multiple ionization cross sections for argon ions are found to decrease exponentially with respect to the final ionization stage of products[17-33].

REFERENCES

[1] G. Garcia and F. Blanco, Phys. Rev. A **62**, 044702 (2000).
[2] A. Zecca, G. P. Karwasz, and R. S. Brusa, J. Phys. B **33**, 843 (2000).
[3] L.G. Christophorou and J.K Olthoff J.Chem. Phys.Vol.30 No.2 (2001) 449-473.
[4] L.G. Christophorou and J.K Olthoff Phys. Chem. Ref. Data Vol.35, No.1 (2006) 31-53.
[5] L.G. Christophorou and J.K Olthoff J. Res Natt. Inst. Stad. Vol.107 (2002) 63-67.
[6] Je Hudson , C Vallance, M Bart And Pw Harlard, J Phys. B. 34, 3025 (2001)
[7] M Bart, Pw Harlard, Je Hudson And C Vallance, Phys. Chem Chem Phys., 3, 800 (2001)
[8] R Rejoub, BG Lindsay And RFStabbings, J Chem. Phys. 115 5053 (2001)
[9] R Rejoub, BG Lindsay And RF Stabbings, J Chem. Phys. 34, 1289 (2001)
[10] R Rejoub, BG Lindsay And RF Stabbings, J Chem. Phys. 114 , 10225 (2001)
[11] K Leiter , P Scherier, G Walder And Td Mark Ijms Ion Processess 87, 209 (1989)
[12] Deutsch H and Mark T D 1987 *Int. J. Mass Spectrum, Ion Process* 79 R1
[13] T.D. Mark, G.H. Dunn (Eds.), Electron Impact Ionziation Springer Verlag, Viena, 1985.
[14] Y-K Kim and M.E. Rudd, Phys, Rev. 50, 3954 (1994).
[15] W. Hwang, Y,-K, Kim and M.E Rudd, J. Chem. Phys. 104, 2956 (1996).
[16] Y.-K. Kim W. Hwang, N.M. Weinberger, M.A. Ali, and M.E. Rudd, J. Chem. Phys. 106, 1026 (1997).
[17] R.S. Schappe, T. Walker, L.W. Anderson and C.C. Lin, Phys. Rev. Lett. 76, 4328 (1996).
[18] C.J. Patton, K.O. Lozhkin, M.B. Shan, J. Geddes and H.B. Gilbody, J. Phys. B: At. Mol. Opt. Phys. 29, 1409(1996).
[18] D.P. Almeida, M.A. Scopel, R.R. Silva and A.C. Fontes, Chem. Phys. Lett. 341, 490 (2001).
[19] R. Rejoub, B.J. Lndsay and R.F. Stebbings Phys. Rev. A65, 042713 (2002).
[20] J.J. Thomson, Phys. Mag. 23, 449 (1912).
[21] M. Gryzinski, Phys. Rev. A138, 305 (1965); *ibid* A138, 322 (196); *ibid* A138 336 (1965).
[22] R.C. Stabler, Phys. Rev. 133, 1268 (1964).

[23] E. Gerjuoy, Phys. Rev. 148, 54 (1966).
[24] A. Buerguess and I.C. Percival, Adv Atom. Mol. Phys. 4, 109 (1968).
[25] A. Burguess, Proc. Symp. Atomic Collision Processes in Plasmas: Culha, 1964, p. 63.
[26] V.I. Ochkur, Proc. Liningrad State Universe. “The Problems of Atomic Collision Theory” N. 1, p. 42 (1975) (in Russian).
[27] L. Vreins, Phys. Rev. 141, 88 (1966).
[28] L. Vriens, Proc. Phys. Soc. 89, 13 (1966).
[29] L. Vriens, in Case Studies in Atomic Physics, edited by E.W McDaniel and M.R.C. McDowel (North-Holland, Amsterdam, 1969), Vol. 1, p. 336.
[30] H. Bethe, Ann. Physik 5, 325 (1930).
[31] J.B. Mann, J. Chem. Phys. 46, 1646 (1967).
[32] H. Deutsch and T.D. Mark, Int. J. Mass Spectrum, Ion Processes 79 R1 (1987).
[33] P. Desclaux, Atomic Data and Nuclear Data Tables 12 311 (1973).