

Proton Impact K-Shell Ionisation of Atoms in Modified Binary Encounter Model

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Abstract: *The Binary Encounter Approximation has been used for calculations of Proton impact K-Shell ionization cross-sections of atoms. The effects of coulomb deflection of the incident projectiles and increase in binding of the target electrons have been investigated. Hartree-Fock velocity distributions for the target electrons have been used in the present calculations. The calculated cross-sections have been compared with experimental result and other theoretical calculations wherever available. The present calculations give a good account of experimental observations.*

Keywords: **K-Shell ionization cross-sections, Binary Encounter Approximation, Coulomb deflection, Hartree-Fock velocity distribution.**

1. Introduction:

Investigation of inner shell ionization of atoms by heavy charged particles impact has long been an interesting subject in the field of atomic collisions. The study of inner-shell ionization remained almost slow between 1940 to seventies. This field received considerable attention in seventies, mainly due to improvement in the experimental technique e.g. improved availability of accelerated heavy ions and much improved experimental counters based on coincidence technique (See Hansteen¹, Burhop²). A good number of experimental and theoretical studies of inner-shell ionization of atoms by the impact of heavy charged particles is available in the literature.

The inner-shell ionization and x-ray production by charged particles has been extensively studied in the last few decades, mainly because of its importance for the particle induced x-ray emission (PIXE) in analytical studies. Theoretical studies of these processes are of much practical importance as they provide cross-sections for the emission of x-rays from various inner shells which can be used for the interpretation of experimental data (Sarter et al.³). These cross sections find applications in characterization of ionizing atomic collisions, trace-element analysis of biological and environmental samples and accurate determination of beam intensities in various particle accelerators experiments (Hardt and Watson⁴).

Ionization from inner-shell of an atomic target takes place due to impact of heavy energetic structureless charged particles when these penetrate deep into the atomic inner shell.

The contribution to the ionization cross-sections come from the direct coulomb excitation of the target electron by the projectiles. Theoretical investigations of inner-shell ionization of atoms by incident heavy charged particles involving direct coulomb excitation have been done initially in the plane wave Born approximation (PWBA) (See Merzbacher and Lewis⁵) and in the semi Classical approximation (SCA) (See Bang and Hansteen⁶). In recent past the same processes has been investigated by Garcia^{7a,b} in the Binary Encounter Approximation (BEA). This being an impulse approximation gives results similar to those obtained in PWBA at high impact energies (Hansteen¹). Specially, in case of inner shell ionization, apart from its simplicity the BE cross sections are competing with those obtained using SCA and PWBA and are in agreement with experimental observations (See Bearse et al⁸).

The Theoretical values of inner-shell ionization cross-sections due to heavy charged particle impact in any one of the above mentioned approximations do not show agreement with the experimental observations. The discrepancy between theory and experiment can be reduced to a large extent by incorporating two important physical processes. These two processes are coulomb deflection of the projectile in the field of target nucleus and increase in binding of the target electron in the presence of the projectile (See Brandt et al⁹).

Garcia⁷ has incorporated the effect of coulomb deflection of the incident proton in the binary encounter approximation. The effects of increase in binding of the target electron as well as coulomb deflection of the projectile in BEA calculations of heavy positively charged particle impact inner-shell ionisation cross-section of atoms have been incorporated by *Singhal and Singh*¹⁰ kumar and Roy¹¹, Chatterjee et al¹², Shrivastava and Roy.¹³ Kumar and Roy¹¹ have used the correct expression for $\sigma_{\Delta E}$ (Cross-sections for energy transfer ΔE by the projectile to the target) as given by vriens^{14a,b} in their calculations but the factor used by them for the increase in binding of the target electron is independent of impact velocity, which is not physical justified. Later on Shrivastava and Roy¹³ used a velocity dependent correction factor incorporating the effects of increase in the binding of the target electron (See Basbas et al¹⁵, Brandt and Lapicki^{16a,b}) in their calculations of heavy charged particle impact K-Shell ionization cross-section of atoms.

Keeping in view the above mentioned fact, I consider it worthwhile to calculate K-Shell ionization cross-sections of atoms due to impact of protons taking into account the physical processes properly along with accurate quantum mechanical velocity distribution for the target electron (See Shrivastava and Roy¹³).

2. Theoretical Considerations

Vriens¹⁴ expressions for ionization Cross-sections of atoms by proton impact have been used by incorporating the coulomb repulsion of the proton in the field of target nucleus suggested by Thomas and Garcia¹⁷ (See also Kumar and Roy¹¹). The effect of coulomb repulsion is introduced analytically through the relation (See Shrivastava et al.^{13a,b} Chatterjee et al¹²)

$$\sigma(E_1) = \sigma(E'_1) \left[\frac{1}{2} + \frac{1}{2} \left(1 - \frac{Z_1 Z_{2k} e^2}{E_1 a_{2k}} \right)^{1/2} \right] \quad (1)$$

where $\sigma(E'_1)$ is the ionisation cross-section at the reduced energy.

$$E'_1 = E_1 - \frac{Z_1 Z_{2k} e^2}{a_{2k}}$$

and $Z_{2k} = Z_2 - S_{2k}$

Z_1 and Z_2 are the nuclear charges of the projectile and of the target under consideration respectively a_{2k} and S_{2k} are the radius and the screening constant for the K-Shell respectively.

The effect of the increase in binding of the target electron in the presence of the positively charged particle (protons) can be incorporated in the ionization expression for cross-sections by replacing the unperturbed binding energy U_{2k} of atomic K-shell by $U_C = \epsilon U_{2k}$, where U_C is the corrected binding energy and ϵ is a correction factor given by (See Brandt and Lapicki^{16a,b})

$$\epsilon = 1 + \left(\frac{2Z_1}{Z_{2k} \theta_{2k}} \right) g \quad (2)$$

Where θ_{2k} is the reduced binding energy and for K-shell electron it is given by

$$\theta_{2k} = \frac{U_{2k}}{Z_{2k}^2 (13.6)} \quad (3)$$

The factor g is a velocity dependent term and for K-shell it is given by (See Basbas et al.^{15a,b,c})

$$g = \frac{(1+5x+7.14x^2+4.27x^3+0.94x^4)}{(1+x)^5} \quad (4)$$

where $x = \frac{V_1}{\left(\frac{1}{2} \theta_{2k} V_{2k} \right)}$

Finally Vriens¹⁴ expressions for ionization cross-sections incorporating the contributions of above mentioned effects in terms of two dimensionless variables s and t (see Catlow and McDowell)¹⁸, can be expressed as

$$Q(s,t) = \begin{cases} \frac{(s+s')^2 Z_1^2}{s^2 s'^2 U_c^2} \left(1 + \frac{2t^2}{3} - \frac{1}{4(s'^2 - t^2)}\right) \pi a_0^2; & 1 \leq 4s'(s' - t) \\ \frac{(s + s')^2 Z_1^2}{2s^2 s'^2 U_c^2 t} \left[\frac{1}{4(s' + t)} + t + \frac{2}{3} \left\{ 2s'^3 + t^3 - (1 + t^2)^{\frac{3}{2}} \right\} \right] \pi a_0^2; & 4s'(s' - t) \leq 1 \leq 4s'(s' + t) \\ 0 & | > 4s'(s' + t) \end{cases} \quad (5)$$

The two dimensionless variable have been defined

$$\text{as } t^2 = \frac{\vartheta_{2k}^2}{\vartheta_0^2}, s^2 = \frac{\vartheta_1^2}{\vartheta_0^2} \text{ and } s'^2 = s^2 - (1.058Z_1 Z_{2k}) / (1836 M a_{2k} U_c)$$

ϑ_0^2 is the corrected ionization energy in Rydberg units of the shell under consideration $\vartheta_1, \vartheta_{2k}, \vartheta_0$, and M (Mass of Projectile) are expressed in atomic units.

The resulting expression for ionization cross-sections have been integrated over Hartree-Fock Velocity distribution for the bound electron, reduces to

$$Q(s) = n_e \int_0^\infty Q(s,t) f(t) U_c^{1/2} dt$$

Where n_e is the number of equivalent electron in the shell under consideration and $f(t)$ is momentum distribution functions for the target electrons constructed by Hartree-Fock radial function which is given by clement & Roetti¹⁹ (See Kumar and Roy¹¹). The binding energies of the target electrons have been taken from the table of clement and Roetti.¹⁹ The quantum-mechanical values of the points of maximum radial probability reported by Desclaux²⁰ have been used as the shell radii. For K-Shell, the screening constant has been taken equal to 0.30 (See slater²¹, Basbas et al¹⁵, Langerberg²²).

3. Results and Discussion

Proton impact K-Shell ionization Cross Sections for Ne, Mg, Cl and Ar have been calculated along the line discussed in Sec. 2 (Theoretical consideration). Three sets of calculation have been done for every target atoms and the result of which are presented in figures 1 to 4 and tables

1 to 4. The experimental results of K-Shell ionization cross-sections (σ_1) for atoms have been determined from x-ray production cross-section (σ_x).

$$\sigma_1 = \frac{\sigma_x}{W_k} \text{ where } W_k \text{ is the fluorescence yield of the K-shell of the atomic target.}$$

In the present work, the values of W_k for different targets has been taken from the review article by Lapicki.²³ The present calculations of K-Shell ionization cross-sections have been compared with the experimental Observations of different workers and different calculations in ECPSSR as reported in the review article of Lapicki.²³

In case of proton impact K-Shell ionization cross-sections of Neon (Ne), three sets of present calculations along with two sets of experimental observations and one other theoretical results have been presented in fig. 1 and table 1. The two sets of experimental observations have been reported by Lapicki²³, one set due to Harrison et al.²⁴ which is limited to low energy region (48.0 KeV to 135.0 KeV) whereas the other set due to Langenberg and VanEck²⁵ is in the energy range 125.0 KeV to 1000 KeV. Present results including all modifications overestimate the experimental results at low impact energies but the agreement improves with increase in impact energy. It is a general feature of cross-sections calculated in the BEA. The present results including all modifications are always within a factor of two as compared to the experimental observations. The present calculated cross-section are also in reasonably good agreement with the calculation of ECPSSR throughout energy range. Further, it is observed that inclusion of effects of coulomb deflection of the projectile in the field of target nucleus and the effect of increase in binding of the target electron in the presence of the project lowers the cross-sections at low impact energies. With increase in impact energy the effects of these two physical processes on the ionization cross-sections decrease and at high impact energies, the three sets of calculations give cross-sections which are very close to each other. These observations are as expected from the physical considerations. At high impact energies, the projectile will get little time to be deflected appreciably from its path. Moreover, the probability of formation of quasi molecule leading to increase in binding of the target electron is also very small at high impact energies.

Present results of atomic magnesium have been presented in table-2 and fig. 2 along with the experimental observations of Khan et al²⁶, Shima²⁷ and Khan and Potter.²⁸ The calculated results using ECPSSR theory are also shown in Fig. Experimental results due to Shima²⁷ have been reported only for two impact energies whereas those of Khan and Potter²⁸ are over a limited energy ranges (60.0 KeV to 500.0 KeV). Observations of Khan et. al²⁶ are available over an extended energy range (50.0 KeV to 1700.0 KeV). The present calculations show reasonably good agreement with all the three sets of experiments, always being within a factor of two to the observed values. The present calculated cross-sections are also in reasonable agreement with the results of ECPSSR calculations. As far as the effects of the physical processes included in the present calculations are concerned, the observations are similar as in the case of neon.

Experimental values of K-Shell ionization cross-section for atomic chlorine are available over the energy range 800 KeV to 5000 KeV (As reported by Lapicki)²³. Experiments have been performed by the three group of workers- Avaldi et. al²⁹, Olabanji and Martinsson³⁰ and Szokefalvi-Nagi and Demeter³¹ which are spread over the impact energy range 600.0 KeV to 5000.0 KeV. The present calculations of cross-sections, over the energy range used by Experimentalist mentioned here, have been performed and presented the results along with the experimental observations and calculationis in ECPSSR in Table 3 and fig. 3. The overall agreement of the present calculations with the experimental observations is reasonably good. Present results are higher than the experimental cross sections but always within a factor of 2. The present calculations also show satisfactory agreement with the values of cross-sections calculated in ECPSSR.

In case of argon, the proton impact K-Shell ionization cross-sections have been reported from 125.0 KeV to 1000.0 KeV by Langerberg and VanEck²⁵ whereas from 1500.0 KeV to 5000.0 KeV by winters et al.³² Winters et.al³³ have performed experiments for 1500.0 KeV to 5000.0 KeV impact energies. Present calculations have seen carried out from 125.0 KeV to 5000.0 KeV impact energies. The results have been presented along with the experimental observations and ECPSSR values in table 4 and fig. 4 At low impact energies the present calculated results of cross-sections are higher than that of the experimental values but with increase in impact energy the agreement improves. This is the general trend of BEA cross sections. Over all the agreement of my calculated results with the experiment is satisfactory. They are always within a factor of 2. The present results are also in satisfactory agreement with the values of cross-sections calculated using ECPSSR.

4. Conclusion:

A critical study of the results presented in See 3 it is concluded that Binary Encounter Approximation (BEA) incorporating the corrections for two physical effects namely the coulomb deflection of the projectile in the field of the target nucleus and increase in binding of the target electron in the presence of the projectile gives a reasonable estimate of K-Shell ionization cross-sections of atomic targets due to impact of heavy bare nuclei. The present results in general overestimates the experimental cross-sections, which is more prominent at low impact energies. As the impact energy increases, the calculated cross-sections come closer to the experimental observations.

The present method is simple and gives results in reasonable agreement with experiments and complex calculations like ECPSSR. Hence the method is useful whenever fast calculations of such cross sections are required.

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Table-1

H^+ impact K-Shell ionization cross sections of Ne

(in units of 10^{-23} Cm^2)

Impact Energy (KeV)	Exp. Of Harrison et.al ²⁴	Exp. Of Langenberg and VanEck ²⁵	Cal (Cm ²) ECPSSR (D)	Present Cal (cm ²)		
				A	B	C
48.0	7.83		6.93	35.8	19.3	9.71
58.0	14.8		15.2	62.3	33.2	21.0
68.0	26.0		28.5	158.0	72.1	43.0
77.0	43.5		45.8	118.0	102.0	81.2
97.0	99.4		105.0	283.0	210.0	184.0
116.0	183.0		192.0	376.0	289.0	242.0
125.0		178.0	245.0			
135.0	300.0		315.0	571.0	421.0	385.0

150.0		317.0	424.0	1420.0	620.0	522.0
200.0		694.0	925.0	1580.0	1380.0	1210.0
300.0		1770.0	2250.0	3760.0	2950.0	2820.0
400.0		3130.0	3660.0	4880.0	4580.0	4350.0
500.0		3910.0	4920.0	6830.0	5430.0	5400.0
600.0		4650.0	6010.0	7430.0	6710.0	6600.0
700.0		5330.0	6010.0	7880.0	7290.0	7240.0
800.0		5830.0	7630.0	8590.0	8180.0	8130.0
900.0		6770.0	8840.0	9730.0	9280.0	9230.0
1000.0		7220.0	8690.0	10002.0	9630.0	9580.0

Figure-1

H⁺ impact K-Shell ionisation Cross-Sections of Ne

(in units of 10⁻²³ Cm²)

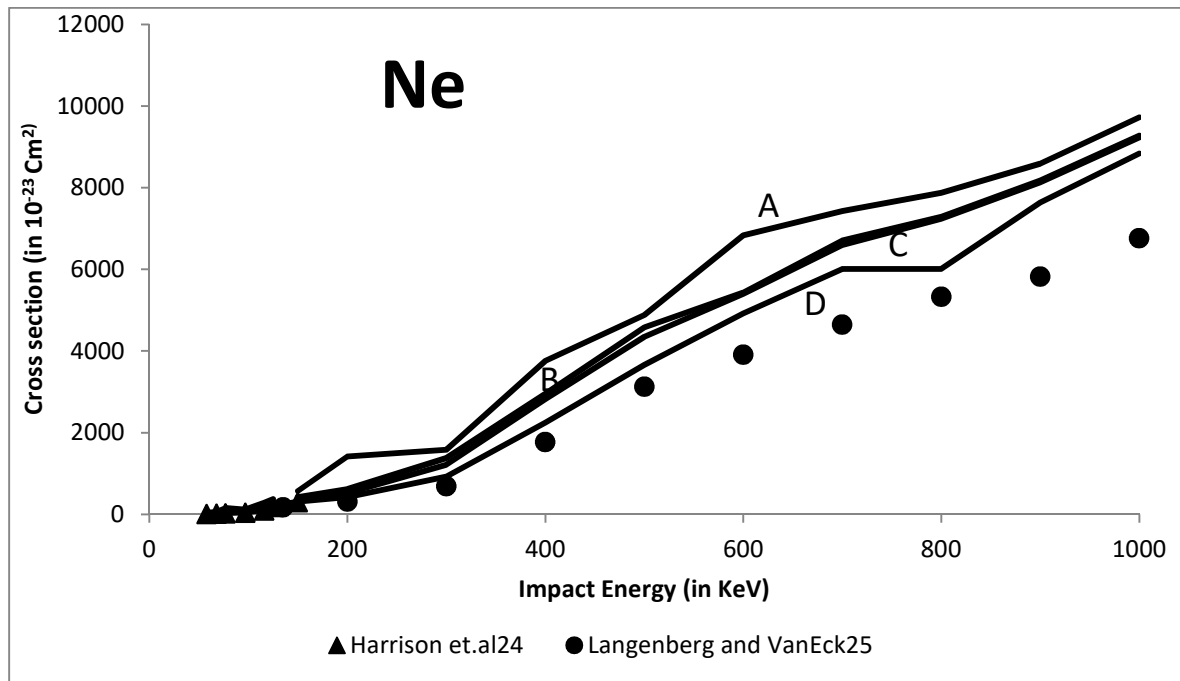


Table-2

H⁺ impact K-Shell ionization cross sections of Mg(in units of 10^{-24} Cm^2)

Impact Energy (KeV)	Exp of Khan et.al ²⁶	Exp. Of Shima ²⁷	Exp. Of Khan and Potter ²⁸	Cal (Cm ²) ECPSSR (D)	Present Cal (cm ²)		
					A	B	C
50.0	7.57	6.67		7.80	48.6	26.3	18.2
60.0	14.8	16.0	11.7	17.5	92.4	50.2	27.8
70.0	28.4			33.8	152.0	91.8	49.2
80.0	61.7			58.1	242.0	155.0	81.4
90.0	80.3			92.2	326.0	226.0	132.0
100.0	115.0		93.3	137.0	461.0	322.0	175.0
150.0			400.0	575.0	1820.0	1120.0	700.0
200.0			933.0	1420.0	2750.0	2120.0	1720.0
300.0			3130.0	4210.0	5420.0	4950.0	4680.0
400.0			6000.0	7930.0	14200.0	9530.0	9210.0
500.0			6670.0	12000.0	18300.0	15300.0	13800.0
600.0	14200.0			16200.0	25600.0	20200.0	18300.0
686.0	15000.0			19300.0	28300.0	23200.0	22100.0
800.0	16900.0			23200.0	33100.0	27300.0	26500.0
900.0	19200.0			26200.0	36100.0	31200.0	29300.0
1000.0	21400.0			28800.0	37500.0	35200.0	33800.0
1100.0	24200.0			31400.0	43200.0	38700.0	35200.0
1200.0	25800.0			33300.0	44400.0	39500.0	37200.0
1300.0	29300.0			35200.0	46200.0	40200.0	39200.0
1400.0	31500.0			36400.0	45100.0	41200.0	40100.0
1500.0	34300.0			37500.0	44200.0	38800.0	38300.0
1600.0	35700.0			39000.0	42000.0	35800.0	35600.0
1700.0	38000.0			40000.0	40100.0	34500.0	34200.0

Figure-2

H⁺ impact K-Shell ionization cross sections of Mg

(in units of 10⁻²⁴ Cm²)

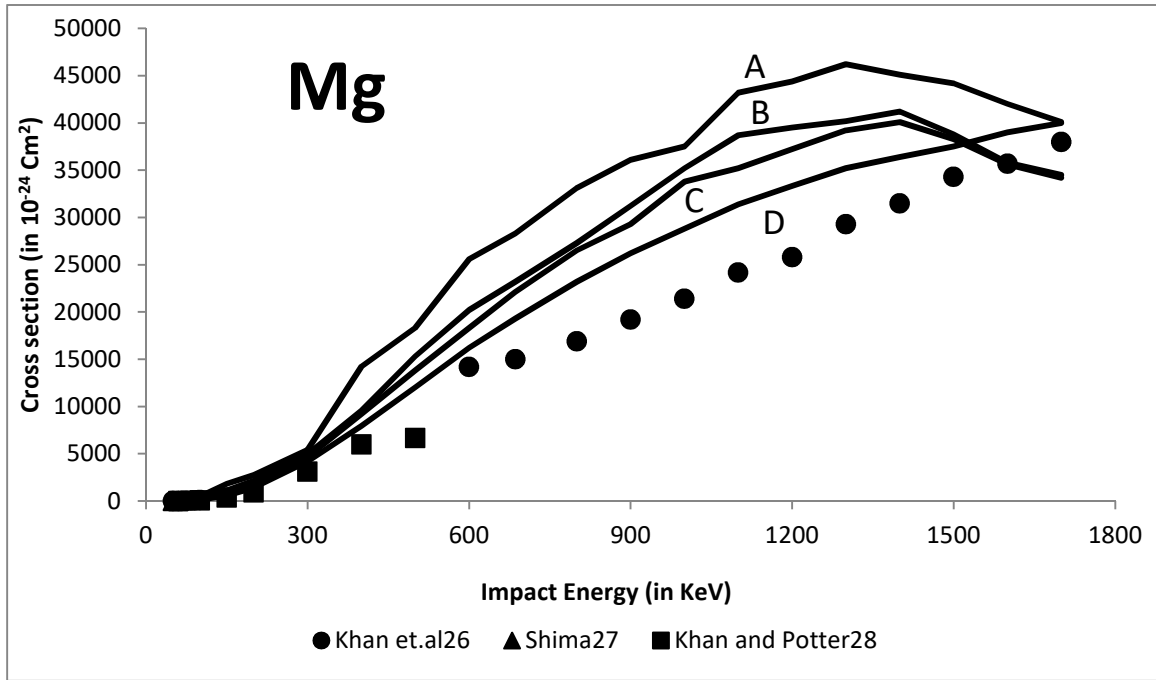


Table-3

H⁺ impact K-Shell ionization cross sections of Cl

(in units of 10⁻²¹ Cm²)

Impact Energy (KeV)	Exp. Of Avaldi et.al ²⁹	Exp. Of Szokefalvi-Nagi and Demeter ³¹	Exp. Of Olabanji and Martinsson ³⁰	Cal (Cm ²) ECPSSR (D)	Present Cal (cm ²)		
					A	B	C
800.0	1.68			1.51	4.91	3.64	2.6
1000.0	2.72		2.77	2.31	7.20	5.42	3.93
1200.0	2.89			3.10	8.78	6.70	5.21
1300.0			4.12	3.43	9.36	6.26	5.42
1400.0	3.41	3.74		3.86	9.96	7.84	5.42

1500.0		3.86		4.22	10.1	8.23	5.94
1600.0	4.31	4.14		4.56	10.6	8.52	6.66
1700.0		4.57		4.90	11.1	8.84	6.96
1800.0	4.95	5.41		5.20	10.9	8.89	7.17
1900.0		5.31	6.28	5.50	10.6	9.21	7.37
2000.0	5.48	5.30		5.76	10.5	9.30	7.42
2200.0	5.63			6.28	10.4	9.43	7.67
2250.0			6.84	6.39	10.3	9.43	7.73
2400.0	5.49			6.72	10.4	9.75	8.06
2550.0			7.44	7.02	10.3	9.85	8.35
2600.0	5.89			7.14	9.67	9.60	8.35
2800.0	5.70		7.86	7.48	9.62	9.63	8.60
3000.0			8.33	7.78	9.68	9.66	8.87
3500.0			8.68	8.35	9.42	9.73	8.18
4000.0			9.64	8.76	9.15	10.0	9.46
4500.0			10.2	9.11	9.02	9.10	8.43
5000.0			10.5	9.21	9.91	9.92	8.83

Figure-3

H⁺ impact K-Shell ionization cross sections of Cl

(in units of 10⁻²¹ Cm²)

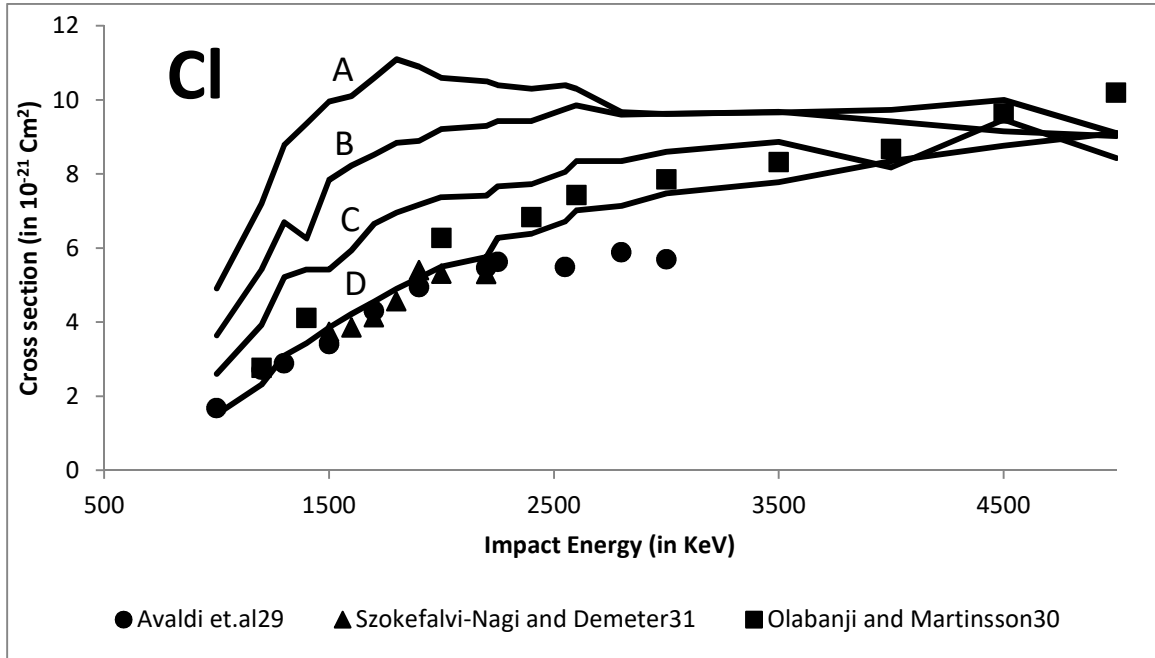


Table-4

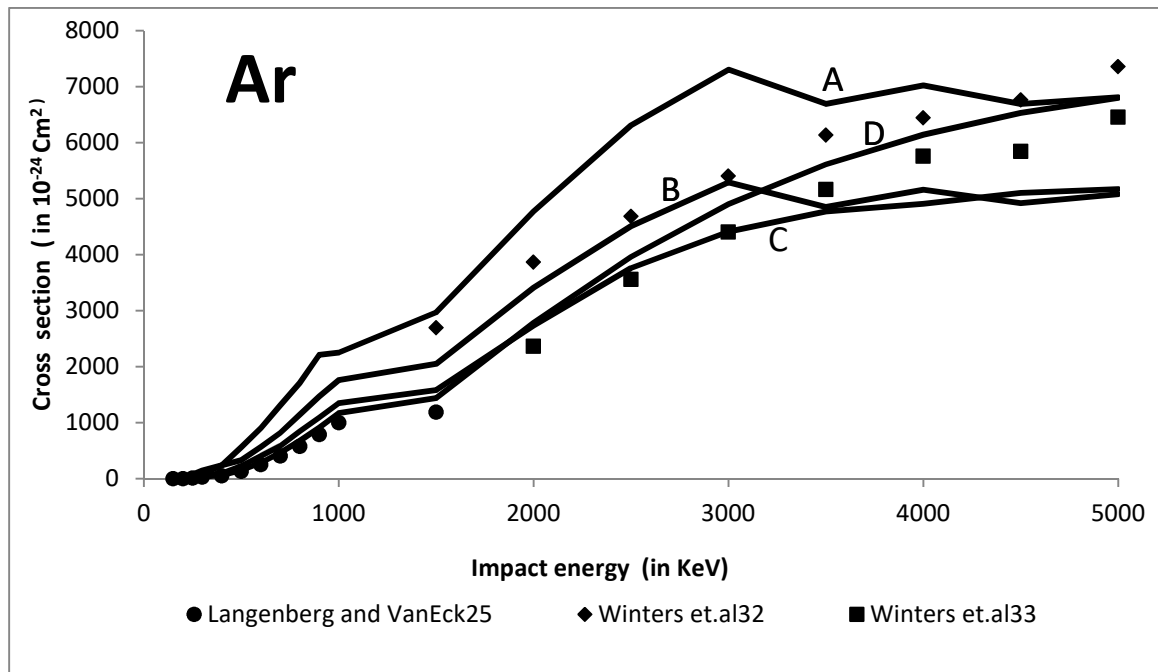
H⁺ impact K-Shell ionization cross sections of Ar

(in units of 10⁻²⁴ Cm²)

Impact Energy (KeV)	Exp. Of Langenberg and VanEck ²⁵	Exp. Of Winters et.al ³²	Exp. Of Winters et.al ³³	Cal (Cm ²) ECPSSR (D)	Present Cal (cm ²)		
					A	B	C
125.0	2.64			2.22	13.5	7.10	4.44
150.0	5.02			4.78	26.6	14.1	9.10
200.0	13.5			14.7	71.5	39.7	26.5
250.0	30.2			32.8	151.0	83.7	55.8
300.0	55.2			61.2	241.0	242.0	97.9
400.0	134.0			152.0	563.0	331.0	228.0

500.0	254.0			288.0	902.0	564.0	403.0
600.0	406.0			465.0	1310.0	819.0	585.0
700.0	581.0			677.0	1710.0	1140.0	846.0
800.0	792.0			911.0	2210.0	1470.0	1090.0
900.0	1000.0			1170.0	2250.0	1760.0	1350.0
1000.0	1190.0			1440.0	2970.0	2050.0	1580.0
1500.0		2700.0	2370.0	2780.0	4770.0	3410.0	2730.0
2000.0		3870.0	3560.0	3960.0	6310.0	4510.0	3760.0
2500.0		4690.0	4410.0	4900.0	7300.0	5290.0	4410.0
3000.0		5410.0	5170.0	5610.0	6690.0	4850.0	4770.0
3500.0		6140.0	5760.0	6140.0	7020.0	5160.0	4910.0
4000.0		6450.0	5850.0	6530.0	6690.0	4920.0	5100.0
4500.0		6770.0	6460.0	6800.0	6810.0	5080.0	5170.0
5000.0		7360.0		7010.0	6910.0	5160.0	5190.0

Figure-4

H⁺ impact K-Shell ionization cross sections of Ar(in units of 10^{-24} Cm^2)**References:**

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