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Calculations of Electron Capture Cross-Sections of Mg Atoms due to Proton, $^3He^+$ and $^3He^{2+}$ Ions Impact

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ABSTRACT Proton, $^3He^+$ and $^3He^{2+}$ ions impact Electron Capture Cross sections for Mg atoms have been calculated in the Modified Binary Encounter Approximation. The Hartree Fock Velocity distribution for the target electrons has been used throughout the calculations. The effect of angular divergence as correction factor has also been taken into account. The present calculations show fairly good agreement with the experimental observations.

KEYWORDS Electron Capture Cross Section, Modified Binary Encounter Approximation, Hartree- Fock Velocity distribution, Angular divergence Correction factor.

INTRODUCTION

There are various physical Phenomena in Atomic Collision Physics. One of the most needed amongst them is charge transfer process in which electron capture cross-sections have been investigated.

Charge exchange is a process which plays a vital role in the formation and decay of both astrophysical and Laboratory Plasma. In addition, state selective nature of charge exchange can be employed in diagnostic systems for laboratory plasmas, in pumping atomic levels which exhibits laser action and in some other applications (Bransden and Mc Dowell)[1]. Furthermore, the charge exchange processes are specially relevant to upper atmosphere researches. Bare nuclei present in low energy cosmic rays interact with the interstellar gas atoms and the electrons captured by the cosmic rays nuclei lead to the formation of atoms and ions in excited states. These formation yield x-rays through radiative decay and the x-rays so produced give a direct measure of the interstellar Cosmic ray intensity (see Belkic and Mc Carrol[2], Belkic and Gayat[3]). Charge changing processes provide valuable information about the radiation damage and design of radiation detectors. These processes are helpful in the production of negatively charged ions which play important role in accelerator technology, particularly in design of tandom accelerators. Moreover, the study of these processes is also important in thermonuclear fusion. Charge exchange is also useful in plasma diagnostics (See Mc Dowell and Ferendeci[4], Jochain and Post[5]). It also finds applications in the production of Vacuum ultra violet and x-radiation (Vinogradov and Soblemen[6], Bransden and Mc Dowell[1], Dixon and Elton[7]).

Due to a large number of applications, the interest has grown rapidly in studying charge transfer phenomena in recent years. Charge transfer process, the basic mechanism of rearrangement collision, is rather a complicated problem so far its theoretical as well as experimental studies are concerned (see Shevelko[8]). Despite the complexities existing therein, the charge transfer process due to impact of different positively charged particles has been investigated experimentally and theoretically by a number of workers but still are less and limited especially for heavier targets. In recent past Bates and Mc Carrol[9], Bransden[10], Bates and Kigston[11], Mapleton[12], Biswas et al.[13], F. Fremont[14A], Basu et al.[14B], A Amaya-Tapiya et al.[14C] etc. have reviewed the theoretical investigations of charge exchange processes in different quantal and semiquantal approximations.

Fully quantal and semi-classical calculations of cross sections require large scale numerical computations. Due to inherent numerical complexities these calculations are restricted to the lighter targets only. For this reason there has always been an interest in thinking of models for ion-atoms collisions based on classical picture which can be expected to provide cross sections of at least moderate accuracy. Among the classical models, the classical trajectory Monte Carlo (CTMC) method and the Binary Encounter model have been found to the most successful. In case of CTMC, still the numerical complexities are more or less similar to the quantum formalism.

On the other hand, a theoretical model was constructed by Thomas[15] based on classical considerations as early as 1927. Later on it was improved and extended by Bates and Mapleton[16] and Mapleton[12]. The original as well as modified theories are based on the theories of two binary encounters-one between the incident ion and the target electron and the other between the ejected electron and the target nucleus to account for electron capture. Use of the original and the modified models of Thomas[15] is found to give satisfactory estimates of cross sections for electron capture from heavy atoms by fast light nuclei. Later on a classical model for electron capture involving single binary encounter between the incident ion and the target electron was proposed by Bates and Snyder[17] in which the idea of finite characteristic collision time was introduced. However, they themselves have expressed doubt about the suitability of the model in case of capture from heavier targets. Later on a classical model for charge transfer with single binary encounter was proposed by Gryzinski[18]. In recent past Roy and Rai[19] have derived new limits for energy transfer depending on the Thomas[15] condition and gave a detailed discussion of the Model for calculating charge transfer cross sections in GryZinski's[18] model. They have calculated single electron capture cross sections for noble gas due to proton impact & found satisfactory agreement with experiments. Their modified binary encounter model was then also applied by Kumar and Roy[20], Shrivastava and Roy[21], Chatterjee & Roy[22] etc. Similar modified version of binary encounter was also given by Tan and Lee[24] independently which may be considered as the generalisation of the modified version of Roy and Rai[19].

Inspired by the above facts, I have considered it worthwhile to calculate single electron capture cross section of Mg atoms due to impact of Protons, He^+ and He^{2+} ions along the line suggested by Tan and Lee[24] and Shrivastava et al.[25] in the modified binary encounter model.

THEORETICAL CONSIDERATIONS

The theoretical descriptions for calculating ion impact single electron capture cross sections of atoms have been outlined in detail by Roy and Rai[19] and Shrivastava et al.[25]. We now introduce two dimensionless variables s and t (see also Catlow and McDowell[26]) defined by $s^2 = \frac{v_1^2}{v_0^2}$ and $t^2 = \frac{v_2^2}{v_0^2}$ where $v_0^2 = U_i$ is the binding energy of the target atom in rydbergs and v_1 and v_2 are respectively the velocities of the projectile and the target electron in atomic units. In terms of these dimensionless variables, the lower and upper limits of energy transfer for electron cap lure can be given respectively by

$$\Delta E_l = (s^2 + 1)U_i + g - 2s(U_i g)^{\frac{1}{2}} \quad (1)$$

and $$\Delta E_u = (s^2 + 1)U_i + g + 2s(U_i g)^{\frac{1}{2}} \quad (2)$$

where $$g = {2zs}\Big/{r(s^2 + t^2)^{\frac{1}{2}}} \quad (3)$$

Here z is the charge and r is the modules of the position vector of the bound electron with respect to the target nucleus which may be taken to be the radius of the Shell considered. It is exprened in atomic units.
Here, ʻg has been used in place of f as mentioned by Roy and Rai[19].

The electron capture cross sections have been found by integrating Vrien's expression for $6_{\Delta E}$ and found six expressions for cross sections, denoted by Q (s, t), corresponding to various values of ΔE_l and ΔE_u falling under different energy ranges (see Shrivastava et. Ql[25], Chatterjee and Roy[22], see also Tan and Lee[24]). In order to take the effect of angular divergence into account, the solid angle correction factor is given by

$$c = \frac{1}{2}\left\{1 - \left(1 - \frac{g}{s^2 u}\right)^{\frac{1}{2}}\right\} \quad (4)$$

(See Tan and Lee[24])

For $s^2U<g$, electron capture is possible even if the energy transferred by the projectile to the target electron is less than ΔE_l (or ΔE_u). Corresponding to various values of ΔE_l and ΔE_u relative to the values of quantities *s*, *4su (s–t)* and *4su (s+t)* there are ten expressions for electron capture (see Chatterjee and Roy[22]). In all those ten expressions, it has been assumed that the Projectile captures all the electrons ejected due to energy transfer ΔE satisfying the condition $U \leq \Delta E \leq \Delta E_u$. Where only half of the ejected electrons, corresponding to $\Delta E_l \leq \Delta E \leq \Delta E_u$ are captured by the projectile (See Tan and Lee[24]).

The expressions so obtained are integrated over the Hartree-Fock Velocity distribution for the target electron in the Shell under consideration so that the electron capture cross-section reduces to

$$Q(s) = n_e \int_0^{\infty} Q(s,t)\, f(t) U^{\frac{1}{2}} dt \quad (5)$$

Where n_e is the no. of equivalent electrons in the shell; $f(t)$ is the momentum distribution function constructed by making use of the Hartree-Fock radial functions given by Clementi and Roetti[28]. The atomic radii and shell radii have been taken from Lotz[29] and Desclaux[30] respectively.
Thus the final expression for electron capture

is given by $Q = Q(s) \times c$ (6)

Where C is the solid angle correction factor (Eqn. 4).

RESULTS AND DISCUSSIONS

The single electron capture cross sections due to impact of Protons, He^{+} and He^{2+} for Mg atoms have been calculated along the line discussed in section 2 (Theoretical considerations). The present calculated as well as experimental cross sections for Mg[31] have been shown in the figs.1, 2, 3 and Table 1, 2, 3 respectively, due to proton, $^{3}He^{+}$ ion and $^{3}He^{2+}$ ion impact.

Proton impact single electron capture cross-sections calculated for Mg have been plotted as a function of energy in fig. 1. The fig. includes in addition to the present cross-sections, the experimental observations of Dubois and Toburen[31] and Morgan and Eriksen[35]. The present calculations have been done upto energy 1000.0 KeV but the experimental observations are available upto 100 KeV so for convenience to comparison of the graph in fig. is limited to 100 KeV energy. The present calculated cross sections underestimate the experimental results in low energy range below 2.0 KeV energy. At 2.0 KeV impact energy the underestimation is more but beyond this energy it improves gradually with increase of impact energy. After impact energy 15.0 KeV, the present calculated cross sections are in better agreement with the experimental results. The agreement still improves as energy increases. The discrepancy may partly be attributed to the non-suitability of Binary Encounter

Approximation (BEA) in the lower energy range and the better agreement in the higher energy range is the general feature of the success of BEA. The present calculated results have not been compared with other theoretical calculations due to non-availability of others in the energy range of interest.

Table 1: Proton impact electron captures cross sections for Mg.

(in units of 10^{-17} cm^2)

Impact Energy (in keV)	Present calculations	Doubis & Toburen[31]	Morgan & Erikson[35]
1.0			89.0
2.0	36.0	81.4	10.9
3.0	69.0	142.0	
4.0	85.0	145.0	167.0
5.0	132.0		215.0
6.0	151.0	227.0	
7.0			258.0
8.0	155.0	217.0	250.0
10.0	150.0	195.0	210.0
15.0	103.0	145.0	125.0
20.0	62.4	81.0	72.0
30.0	19.8	20.0	
40.0	9.6	10.5	9.4
60.0	3.5	2.48	4.41
80.0	2.0	1.37	2.23
90.0			2.05
100.0	1.4	1.35	

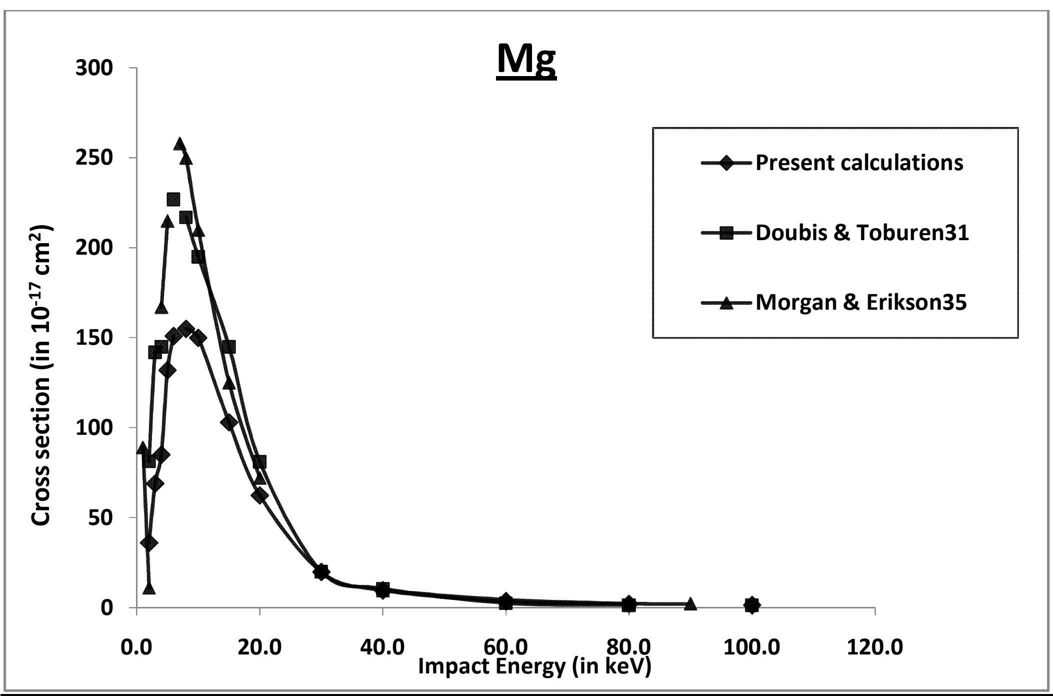

Figure 1: Proton impact electron capture cross sections for Mg.

In case of $^3He^+$ ion impact single electron capture cross sections for Mg, the calculations have been done with Z_{eff}=1.22 and Z_{eff}=1.0. As pointed out by Martin et al[33], the He^+ ion can be considered equivalent to an effective change Z_{eff} lying somewhere between the actual net charge and the total nuclear charge. A He^+ ion at high energy (corresponding to 800 KeV) can be considered equivalent to a point charge with Z_{eff}=1.22. Though, Pivovar et al[23] have pointed out that Z_{eff} for He^+ ion is slightly energy dependent and increases from 1.17 to 1.30 (corresponding to energy from 800 KeV to 1800.0 KeV) but I have taken Z_{eff}=1.22 throughout the calculations as suggested by Martin et al[33] & supported by de Heer et al[34].

Here it has been observed that the present calculations with Z_{eff}=1.22 in case of $^3He^+$ ion impact, agrees well with the experimental observations in low energy range whereas the tendency of agreement seems to be that with Z_{eff}=1.0 in higher energy range. It has also been noticed that the cross sections corresponding to Z_{eff}=1.22 and Z_{eff} =1.0 for He^+ ions are correct almost within a factor of 2 throughout the energy range. The concept of Z_{eff} is appropriate for ionisation processes (Martin et al) but for charge transfer process, no experimental evidences regarding effective charge of He^+ ion are available in literature.

$^3He^{2+}$ ion impact single electron capture cross sections for Mg calculated presently have been presented in fig. 3 along with the experimental observations of Dubois and Toburen[31]. The present calculations have been done upto energy range 1000.00 KeV whereas the experimental results are available only upto 200.0 KeV. In case of $^3He^{2+}$ ion impact electron capture cross sections for Mg, the present calculations are in better agreement with the experiment. However in the lower energy range the present results are in slightly less agreement with experiment than that in higher energy range. Overall, the agreement is fairly good.

Table 2: $^3He^+$ impact electron capture cross sections for Mg

(in units of 10^{-17} cm^2)

Impact energy (in keV)	Present calculations (Z=1.0)	Present calculations (Z=1.22)	Dubois & Toubren[31]	II'in et al.[36]
2.0	10.8	12.6	19.5	168.0
3.0	20.0	25.0	35.0	255.0
4.0	29.4	38.0	42.9	170.0
5.0				145.0
6.0	54.0	64.0	81.2	75.0
8.0	75.3	97.0	92.3	42.0
10.0	94.4	129.0	119.0	19.7
15.0	132.0	192.0	181.0	10.3
20.0	173.0	240.0	229.0	
25.0		254.0		
30.0	136.0	217.0	160.0	
40.0	96.0	158.0	76.4	
50.0	75.0	136.0		
60.0	54.0	120.0	63.5	
80.0	26.2	55.0	29.8	
90.0	20.0	41.0		
100.0	15.6	29.5	16.1	

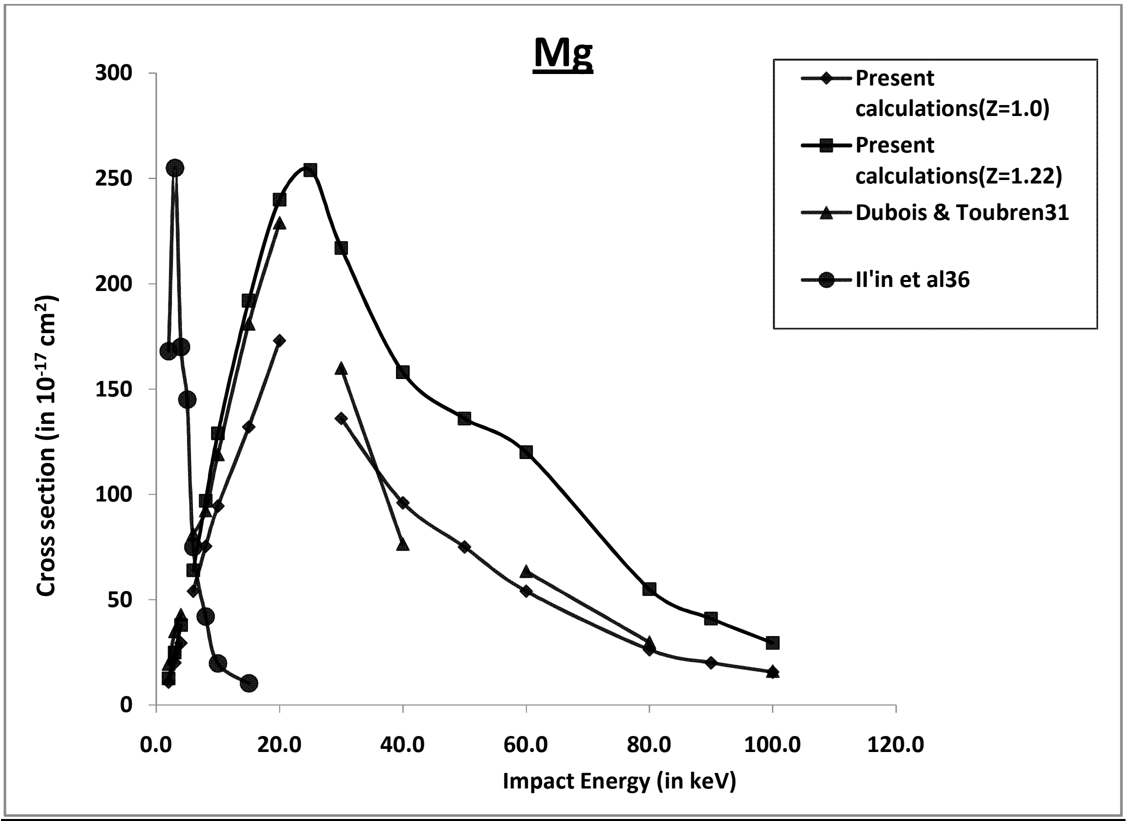

Figure 2: $^3He^+$ impact electron capture cross sections for Mg.

From the fig. 3 and Table-3 presented here one can see that the present calculated cross sections are always within a factor of 2 of the experimental observations throughout the energy range investigated. Furthermore it has also been noticed the degree of suitability of this approximation improves for more and more massive projectile which possess more and more classical behaviour.

Table 3: $^3He^{2+}$ impact electron captures cross sections for Mg.

(in units of 10^{-17} cm^2)

Impact Energy (in keV)	Present calculations	Duboris & Toburen[31]
4.0	221.0	395.0
6.0	356.0	540.0
8.0	412.0	437.0
10.0	490.0	
12.0		483.0
15.0	560.0	
16.0	650.0	610.0
20.0	650.0	539.0
30.0	630.0	576.0
40.0	540.0	525.0
50.0	443.0	
60.0	315.0	276.0

80.0	240.0	231.0
100.0	160.0	
120.0	97.0	75.0
150.0	34.0	
160.0		27.0
200.0	20.0	18.7
250.0	18.6	
300.0	14.0	
400.0	11.0	
500.0	9.8	

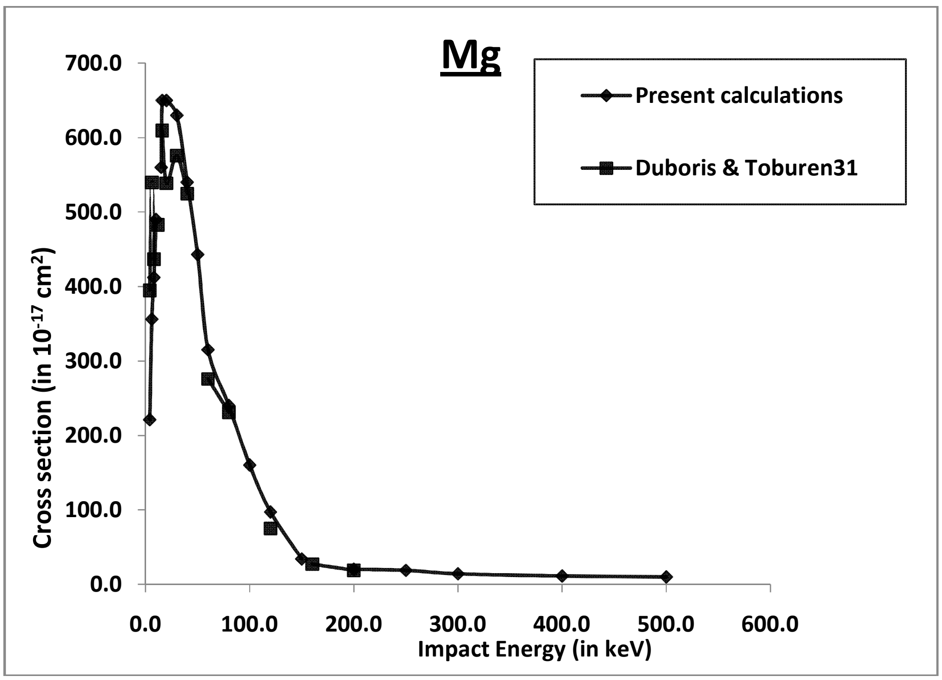

Figure 3: $^3He^{2+}$ impact electron capture cross sections for Mg.

CONCLUSION

Thus, it can be concluded that the Modified BEA gives a good account of the experimental observations in case of charge transfer process. It has also been noticed that the agreement with experiment improve with increase in charge state of the projectile. Further it is observed that the present model is well suited for heavier atomic targets compared to other quantal or semi quantal approximations. Also it has been found that the present Model is more favourable for more massive projectiles. Also it is found that the present model is more favourable for more massive projectile.

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