

# Investigations and Analysis of Single Electron Capture Cross Sections from Mg Atoms by Proton Impact

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## Abstract

Critical investigations for the process of single charge transfer by the impact of  $H^+$  ions with magnesium atoms have been done for the comparative study of theoretical and experimental observations. The data for the capture cross section is compiled for the different impact energy range from 1 KeV/amu to 500 KeV/amu. The mechanism for the electron capture process in the different energy range is pointed out and the experimental and the theoretical capture cross section peak obtained by the different workers is analyzed for the different impact energy.

**Keywords:** Capture Cross Sections, Proton Impact, Mg Atoms and  $H^+$  Ions

## Introduction

Study of Electron capture and charge transfer in collisions between incident energetic ions and atomic target is an important classical discipline in atomic collision physics. Charge transfer reaction in several ion-atom collisions plays a significant role in various field of interest. A positively charged particle incident to the target atom captures the electron from the atom. During the process of electron capture or charge exchange phenomena the charge state of the incident ion as good as and the ionization energy of the target electron plays the role of decisive parameters. Due to great interest and importance of charge exchange reaction, several studies have been done for the process of multiply charged ions-atom collisions. Owing to the large number of applications such as study of solar corona [1], Production of Vacuum ultra violet radiations and X-rays [2], controlled thermo nuclear fission development, ion penetration and radiation physics [3], astrophysics and upper atmospheric studies. In accelerator technology the contribution to the negatively charged ions through charge transfer processes explicitly in the modeling of Tandem accelerators [4] is equally important. In the study of upper atmospheric physics electron capture process having vital role.

The cross section for electron capture is estimated in various cases of ionic and atomic collisions [5-7]. Single and double electron capture processes by the impact of  $He^{+2}$  particles have been explained by McCullough et al. [8] and Post et al. [9]. Various quantal calculations are reported for single electron capture cross section of lighter atoms. The quantal calculations are limited for small atoms. Mathematical complexities are involved in case of heavy atoms. Using an independent particle model (IPM) by McGuire and Weaver [10] and Crothers and Mc Caroll [11] proposed the theory for the study of two electron capture process. Also an independent electron model (IEM) of a quantum mechanical four body formulation for

double electron transfer by the impact of bare ions to He atoms is proposed by Belkic and Mancev [12-13]. A theory proposed by Oppenheimer-Brikman-Kramers (OBK) for the calculation of electron capture cross-sections following omission of nucleus-nucleus (n-n) interaction. The several approaches like continuum distorted wave (CDW), Belkie and Gayet Crothers and Todd and Crothers (1981), fixed scattered approximations by Roy and Ghosh (1979), the multi-state perturbation stationary state approximation of Crothers and Hugges and impact parameter method of Morrison and Opik, were implemented for the study of electron capture processes.

Charge transfer processes gives the important information about design of radiation detector, radiation damage and plasma diagnostics (see McDowell and Ferendeci [14]), Jochain and Post [15]. In recent pasts, the attraction of the workers in the field of collisional and charge changing studies has rapidly grown. A large number of theoretical and experimental observations for the charge changing processes have been done in recent decades. Different quantal and semi-quantal approximations are applied by Amaya-Tapaiya et al. [16], Basu et al. [17], F Feremon [18], Bates and McCaroll [19], Bates and Kigston [20] and Mapleton [21-24]. Due to challenging and interesting problems of charge capture process, it is always a matter of great interest for developing different models for the study of ion-atom collisions. These models are assumed to provide information about capture cross-sections with accuracy. The classical models such as Classical Trajectory Monte Carlo (CTMC) and Binary Encounter Approximations (BEA) have been found more accurate for the theoretical investigations of ionic and atomic collisions.

Thomas [25] introduced classical impulse approximation for the estimation of cross-sections for single capture by fast light particle from heavy atoms for the first time. Thomas classical model in 1927 improved and extended by Bates and Mapleton [26] and Mapleton [21-24]. Later on a classical model for charge transfer with single binary encounter was proposed by Gryzinski [27] also by Roy and Rai [28] giving a new limit for energy transfer  $\Delta E$  using Thomas [25] condition.

Considerable experimental investigations on  $H^+$  and  $He^{2+}$  impact single and double electron captures are performed by the Belfast group during last two decades. A close beam techniques incorporating TOF spectroscopy has been used in those works and measured cross-sections for several atomic targets including magnesium atoms. The magnesium atom is important due its presence in the study of upper atmosphere and hence its emission spectra have been investigated by several ground based and spacecraft based [29] instruments. Some other calculations for the charge transfer of Mg by  $H^+$  impact is reported by Mapleton and Grossbard [30]. The charge changing process is particularly important to take up the problem of theoretical calculation and critical investigations of capture cross-sections of Mg atoms by the incidence of  $H^+$  particles using the BEA suggested by Tan and Lee [31], Chatterjee and Roy [32] respectively. Charge transfer in collisions with Mg are important due to its various applications in the field of astrophysics, plasma physics and emission of spectral lines, Shah and Gilbody [33] and Shah et al. [34] have described about the measurements of transfer ionization cross-sections of He and Li atoms by the impact of  $H^+$  and alpha particles. Theoretical calculations of electron capture and transfer ionization processes are limited (see McDowell and Janev [35], Bhattacharya et al. [36], Janev and Kristic [37]). The mechanism involved in the process of electron capture is complicated especially in case of heavy atoms and very few literatures are available.

The experimental observation for the electron capture process with Mg atoms is reports by Berkner et al. [38]. The experiment for the calculations of capture cross sections have been performed for the different impact energy from 5 KeV- 70 KeV. The experimental capture cross sections by proton and He ions impact from Li, Na, and Mg atoms are reported by DuBuois and Toburen [39]. Shah et al. [40] also calculated the experimental cross sections for the electron capture on the different impact energy range by  $H^+$  and alpha particle impact with Mg atoms. The experimental results for the total electron capture cross section of Mg atoms by the impact of proton is reported by Morgan et al. [41]. The theoretical calculations for the total single and double electron capture cross sections by the impact of  $H^+$  and  $He^{2+}$  for the impact energy range 90 KeV/amu - 500 KeV/amu have been reported by Kumari et al. [42].

The objective of this study and investigation is to compile, evaluate and represent the available experimental and theoretical results of electron capture cross sections at different impact energy of incident proton to Mg target atoms. The data and reported results of the single electron capture cross section is represented in the tabular form for the comparative study of the capture cross sections. The experimental and the theoretical findings for the total electron capture cross sections are compiled together to analysis of the different approaches adopted for the calculation of single electron capture cross section of Mg atoms by the impact of proton. The theoretical and experimental data for the capture cross section of Mg atoms by  $H^+$  impact is taken from impact energy range 1 KeV/amu - 500 KeV/amu.

### Methodology

There are several theoretical methodology and experimental techniques and methodology have been formulated for the calculation of cross sections like perturbed-stationary sates (PSS) Projected valence bond (PVB) method, Landau-Zener (LZ) methods, continuum distorted wave (CDW), classical models such as Classical Trajectory Monte Carlo (CTMC), close beam techniques, quantum mechanical (QM), Atomic orbital (AO) methods and binary encounter approximations (BEA). The experimental techniques are quite enough for the measurements of electron capture cross section in by the impact of positively charged projectile to the heavy atoms. The theoretical description for the ionization and charge changing process for the heavy atoms is rarely available. Involving mathematical complexities and complicated computational work the theoretical results are less reported in the literature. The quantal calculations are limited for the two-electron systems and for the heavy atoms classical models are adopted for the calculations for electron capture and charge changing processes. Apart from different theoretical models binary encounter approximation (BEA) gives suitable and viable explanation of the charge changing mechanism also in the case of heavy atomic targets.

In case of Binary encounter approximation the incident charged particle is allowed to collides with target electron/ atomic electron it gets ejected providing the energy transfer  $\Delta E$  greater than the electronic binding energy. Taan and Lee (1981) based on Thomas (1927) second condition, proposed a theoretical framework for the calculation electron capture cross section by the impact of positively charged particle following condition.

$$F(\Delta E, \theta) = (\Delta E - U) + \frac{1}{2} m V^2 - V \quad (1)$$

Where  $g = Ze^2 / \left( \frac{rU}{V} \right)$  and  $\theta$  is the angle between impact velocity ( $V$ ) and the velocity of the ejected electron.  $r$  is the shell radius,  $Ze$  represents charge on the projectile,  $m$  is electronic charge,  $U$  is given for the binding energy of the electron and  $u = \sqrt{V^2 + v^2}$  where  $v$  is the velocity of the bound electron.

In this case the electron capture cross-section and impact ionization is given by

$$\sigma_{cap} = n_e C \int_{\Delta E_1}^{\Delta E_u} \sigma_{\Delta E} d(\Delta E) \quad (2)$$

where,  $\sigma_{\Delta E}$  represents cross-section for energy transfer  $\Delta E$  to the bound electron and  $n_e$  number of equivalent electron in the shell.

Following the the Gryzinsky model [27] and Thomas condition [25] Kumari et al. [42] calculated the theoretical single electron capture cross sections of Mg atoms by the impact of proton in the using BEA methods.

### Result and Analysis

Berkner et al. [38] reported experimental electron capture cross-sections for the impact of proton in energy range 5 KeV - 70 KeV from Mg vapor and pointed out about the difficulties in estimation of capture cross-section from heavy atoms and considerable interest in classical approximations and semi-empirical methods due to reasonable good agreement with the experimental findings of capture cross-sections with Mg atom using Brikman Kramers (BK) approximation [43-44]. The experimental cross-sections of single electron capture indicated  $\pm 20\%$  error due to uncertainty in the Mg vapor pressure. The classical and BK approximation for the single electron capture is most suitable at higher energies but the experiment at aforesaid energy range in not reasonably good for Mg than Ne and Ar.

Dubois and Toburen [39] also performed experiment for the calculation of single electron capture cross section by the proton impact in the energy range 2 KeV - 100 KeV for Mg atoms. Due to availability of two loosely bound outer shell electrons in Mg, the capture cross-section estimation is more complex and little experimental and theoretical study is reported for ionic impact with Mg target. In case of charge transfer by the collision of proton with Mg atoms tabulated errors are reported as  $\pm 15\%$ . The experimental observations for single capture cross-sections  $\sigma_{10}$  increases and reach a maximum value and then decreases. The cross-section reported by Dubois and Toburen [39] below 10 KeV/amu is not constant like Li and Na targets.

In the experimental calculation for electron capture for obtaining electron capture cross-sections by the proton impact is reported by Shah et al. [40] using closed beam technique and time of flight spectroscopy. The experimental data is obtained for the impact energy range 90 KeV - 500 KeV/amu. In this experimental

observation, results extended the available data to energies involving inner 2s and 2p electrons in addition to 3s electron. The uncertainty arising due to normalization procedure is estimated to be  $\pm 15\%$ . The experimental results for the single capture are listed by Morgan et al. [41]. Experimental results for the impact energy range 1 KeV/amu - 200 KeV/amu. The ion beam technique for the experimental observation is given by Morgan et al. [41]. The experimental capture cross-section increases from 1 KeV to 7 KeV and then decreases. The peak of the capture cross-section is achieved at the impact energy 7 KeV/amu.

Kumari et al. [42] theoretical results reported for single electron capture cross-section of Mg by proton impact is reported for the impact energy 90 KeV/amu - 500 KeV/amu. Using the classical model, BEA method is implemented for the theoretical estimation of capture cross-sections in case of heavy atoms. The result shows the high degree of success for the theoretical calculations of capture cross-sections in case of heavy atoms. The result overestimates the single electron capture cross-section throughout the investigated energy range. At the higher energy region 150-240 KeV/amu, the experimental data is 2-3 times smaller than the theoretical observations. The contribution of 3s, 2p and 2s shells are taken into the account for single electron capture cross-section of Mg by H<sup>+</sup> impact. The theoretical data are in good agreement with the experimental observations.

Table 1: Proton Impact Single Capture Cross-sections of Mg in Units of  $10^{-16} \text{ cm}^2$

| Energy (keV /amu) | Expt. [38] | Expt. [39] | Expt. [40] | Expt. [41] | Theo. [42] |
|-------------------|------------|------------|------------|------------|------------|
| 1                 | -          | -          | -          | 8.0        | -          |
| 2                 | -          | 8.14       | -          | 9.3        | -          |
| 3                 | -          | 14.4       | -          | 13.0       | -          |
| 4                 | -          | 14.5       | -          | -          | -          |
| 5                 | 15.2       | -          | -          | 18.0       | -          |
| 6                 | -          | 22.7       | -          | -          | -          |
| 7                 | -          | -          | -          | 21.0       | -          |
| 7.5               | 22.5       | -          | -          | -          | -          |
| 8                 | -          | 21.70      | -          | -          | -          |
| 10                | 15.6       | 19.5       | -          | 20         | -          |
| 15                | 10.7       | 14.5       | -          | -          | -          |
| 20                | 6.16       | 8.10       | -          | 8.0        | -          |
| 25                | 3.94       | -          | -          | -          | -          |
| 30                | 2.22       | 2.00       | -          | -          | -          |
| 35                | 1.42       | -          | -          | -          | -          |
| 40                | 0.83       | 1.05       | -          | -          | -          |
| 45                | -          | -          | -          | -          | -          |
| 50                | 0.408      | -          | -          | 0.49       | -          |

|     |       |       |      |      |      |
|-----|-------|-------|------|------|------|
| 60  | 0.278 | 0.248 | -    | -    | -    |
| 70  | 0.213 | -     | -    | 0.19 | -    |
| 80  | -     | 0.137 | -    | -    | -    |
| 90  | -     | -     | 5.8  | -    | 8.44 |
| 100 | -     | 0.135 | -    | 0.11 | -    |
| 110 | -     | -     | 4.1  | -    | 5.98 |
| 130 | -     | -     | 2.5  | -    | 4.61 |
| 150 | -     | -     | 1.61 | -    | 3.69 |
| 170 | -     | -     | 1.18 | -    | 3.00 |
| 190 | -     | -     | 0.90 | -    | 2.48 |
| 200 | -     | -     | -    | 0.09 | -    |
| 210 | -     | -     | 0.71 | -    | 2.05 |
| 240 | -     | -     | 0.51 | -    | 1.56 |
| 280 | -     | -     | 0.28 | -    | 1.11 |
| 330 | -     | -     | 0.21 | -    | 0.75 |
| 370 | -     | -     | 0.11 | -    | 0.56 |
| 430 | -     | -     | 0.09 | -    | 0.36 |
| 500 | -     | -     | 0.05 | -    | 0.23 |

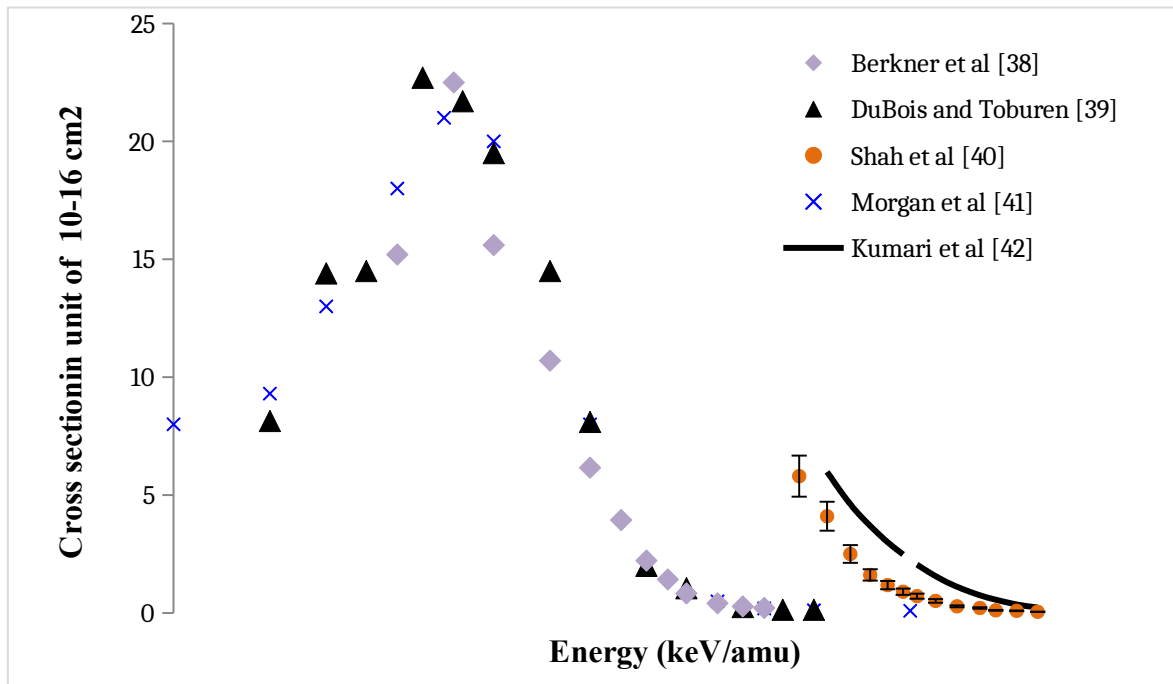


Figure 1: Single Electron Capture Cross-section by Impact of Proton for Mg Atoms

## Conclusion

Experimental and theoretical calculations of electron capture cross sections by the proton impact with magnesium atoms the available data is very less. Most of the experiments are done for the study of ionic/atomic collisions. Investigations and the study of electron capture process from the heavy atomic target, situation is less satisfactory. On the basis analysis and evaluation of the available data it infer that the magnesium atom behave different than the other atoms. The capture cross section trend is quite different than other atoms. At lower impact energy the different experimental observations shows single electron capture cross sections with slight deviations. At the lower impact energy significant experimental data is available but for the higher energy impact less observation is found. Although the theoretical observation using BEA methods is in agreement with experimental data but still less theoretical work is reported and need more theoretical frame work and calculations for the measurement of capture cross section of heavy atoms with ionic impact.

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