Proton Impact Electron Capture Cross Sections from Ba: A BEA Calculation

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Abstract: *Single Electron Capture cross sections for Ba atoms have been calculated using modified Binary Encounter Approximation (BEA). For target electrons, the Hartree-Fock velocity distribution has been taken into account throughout the calculations. The angular divergence as a correction factor has also been considered. The present calculated results show fairly good agreement with the experimental results.*

Keywords: Electron capture, Binary Encounter Approximation, Hartree-Fock velocity distribution, Angular divergence.

1. INTRODUCTION

The study of charge exchange is important not only in order to obtain an understanding of the basic mechanism of rearrangement collisions, but also because charge exchange is a process which plays a vital role in the formation and decay of both astrophysical and laboratory plasmas. In addition, the state selective nature of charge exchange can be employed in diagnostic systems for laboratory plasmas, in pumping atomic levels which exhibit laser action and also in some other applications (Bransden and McDowell[1]). The charge transfer 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 state which 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 McCarrol[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 an important role in accelerator technology, particularly in design of tandom accelerators. These processes are also important in thermonuclear fusion and useful in plasma diagnostics (see McDowell 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 McDowell[1], Dcxon and Elton[7]). In light of a large number of applications, the interest has grown rapidly in studying charge transfer processes in recent past. However, the electron capture process is rather a complicated problem so far its theoretical as well as experimental studies are concerned (See Shevelko[8]). Instead a large no. of workers have investigated experimentally and theoretically eg. Bates and McCarrol[9], Bransden[10], Bates and Kingston[11], Mapleton[12], Biswas et al[13], F.Fremont[14], Bau et al.[15], A Amaya-tapia et al.[16] etc. Still, the investigations are limited especially for heavier targets. Fully quantal and Semi-quantal calculations of cross-sections require a 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 thanking of models for ion-atom collisions based on classical picture which can be expected to provide cross-sections of atleast moderate accuracy. Among the classical models, the classical trajectory Monte Carlo (CTMC) method and the Binary Encounter Model have been found to be the most successful. Here it has been noticed that CTMC model still requires heavy numerical computations more or less similar to quantum formalism. On the other hand Thomas[17] proposed a classical theory for electron capture. Later on it was improved and extended by Bates and Mapleton[18]. Use of original and modified models of Thomas[17] is found to give satisfactory estimates of cross sections for electron capture from heavy atoms by fast light nuclei. In recent past, starting from the theory of Thomas[17], Roy and Rai[19] have given a detailed discussion of the method of calculating charge-transfer cross-sections in Grizinski's[20] model. They have calculated the capture cross-sections for noble gas atoms due to proton impact and found satisfactory agreement with experiment. Their modified binary encounter model was then applied by Kumar and Roy[21], Shrivastava and Roy[22], Chatterjee and Roy[23], S. Kumari et al.[24] etc. Similar modified version of binary encounter model was also given by Tan and Lee[25] independently which may be considered as the generalization of the modified version of Roy and Rai.[19]

Inspired by these facts I think it worthwhile to calculate electron capture cross-sections of Ba atoms due to proton impact for which the experimental results are available.

2. THEORETICAL CONSIDERATIONS

The theoretical descriptions for calculating positive ion impact single electron capture cross sections of atoms have been outlined in detail by Roy and Rai[19], Shrivastava et al[26] and Chatterjee and Roy[23]. The expression for electron capture cross sections in Grizinki's[20] approach for single Binary encounter model can be given by

$$Q = n_e \int_{\Delta E_l}^{\Delta E_u} \sigma_{\Delta E}\,(\Delta E) \qquad (1)$$

Where $\sigma_{\Delta E}$ is the cross section for energy transfer ΔE and n_e is the number of equivalent electrons in the shell under investigation. ΔE_l and ΔE_u are the lower and upper energy limits of energy transfer. Here two dimensionless variables s and t (see also Cattow and McDowell[27]) have been introduced and defined by

$$s^2 = \frac{v_1^2}{v_0^2} \text{ and } s^2 = \frac{v_2^2}{v_0^2}$$

where, $v_0^2 = U_i$ is the binding energy of the target electron 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 capture can be given respectively by

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

and,

$$\Delta E_u = (s^2+1)U_i + g - 2s(U_i g)^{1/2} \qquad (3)$$

where, $g = \frac{2zs}{r(s^2+t^2)^{1/2}}$ (4)

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 shall considered. It is expressed in atomic units.

Here 'g, has been used in place of 'f as mentioned by Roy and Rai[19].

There electron capture cross sections have been found by integrating Vrien's[28] expression for $\sigma_{\Delta E}$ in terms of dimensionless variables s and t which take the form.

$$\int \sigma_{\Delta E} d(\Delta E) = \frac{4z^2}{s^2U}\left(-\frac{1}{\Delta E} - \frac{2t^2U}{3(\Delta E)^2}\right)(\pi a_0)^2;\ \Delta E \le 4sU(s-t) \qquad (5)$$

$$\int \sigma_{\Delta E} d(\Delta E) = \frac{4z^2}{s^2U}\left[\frac{2U}{3t(\Delta E)^2}\left\{\left(\frac{\Delta E}{U} + t^2\right)^{\frac{3}{2}} - \right\} - \frac{1}{\Delta E}\right](\pi a_0^2);\ 4su(s-t) \le \Delta E \le 4su(s+t) \qquad (6)$$

Following Tan and Lee[25] (see also Chatterjee and Roy[23]) there are found six expressions for cross sections, denoted by Q(s,t) corresponding to various values of ΔE_l and ΔEu falling under different energy ranges. In order to take the effect of angular divergence into account, the solid angle correction factor is given by

$$C = \frac{1}{2}\left\{1 - \left(1 - \frac{g}{s^2u}\right)^{1/2}\right\} \qquad \text{see Tan and Lee}^{25} \qquad (7)$$

For s^2 U < g, electron capture is possible even if the energy transferred by the projectile to the target electron is less than $\Delta E_l (or\ \Delta Eu)$. Corresponding to various values of ΔE_l and ΔEu

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[23]). 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[25]).

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

$$Q(S) = ne \int_0^\infty Q(s,t) f(t) U^{1/2}\, dt \qquad (8)$$

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 Mclean & Mclean[29]. The atomic radii and shell radii have been taken from Lotz[30] and Desclaux[31] respectively.

Thus the final expression for electron capture is given by

$$Q = Q(s) \times C \qquad (9)$$

where, C is the solid angle correction factor (Eqn. 7).

3. RESULTS AND DISCUSSION

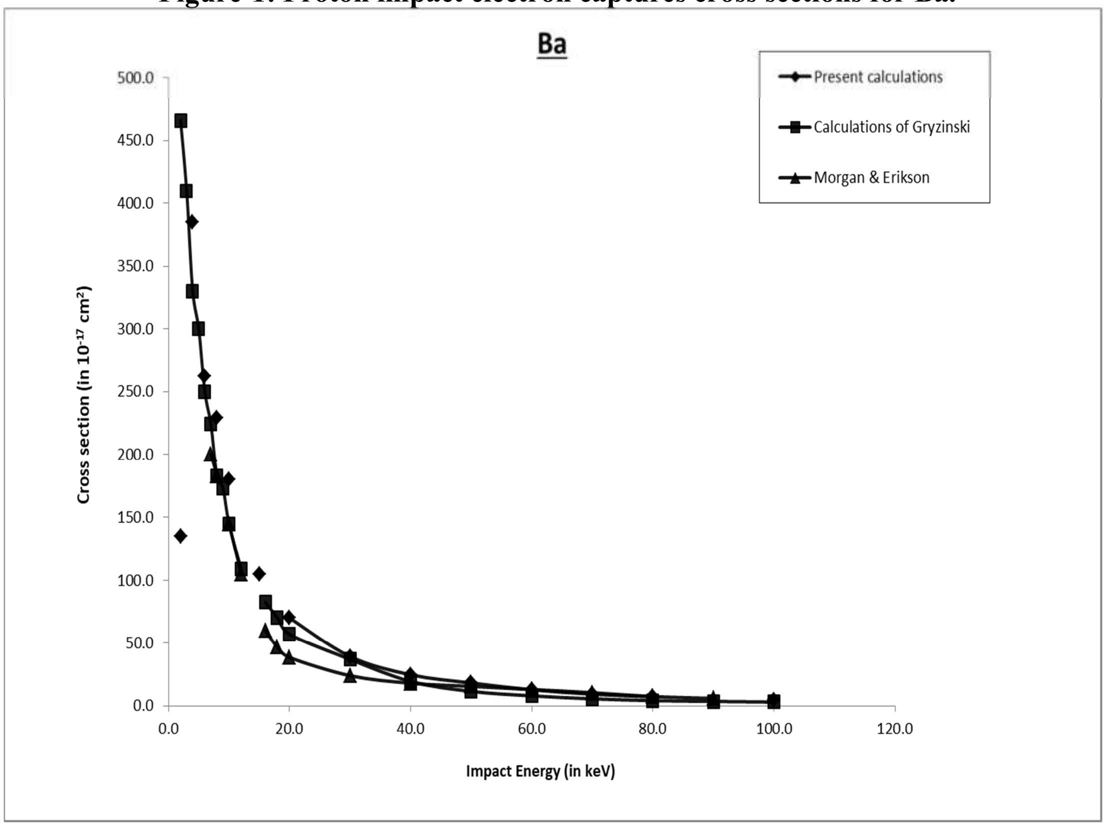
The single electron capture cross sections due to impact of protons for Ba have been calculated along the line discussed in sec .2 (Theoretical consideration). The present calculated as well as experimental cross sections for Ba (See Morgan and Eriksen[32]) along with the available theoretical results of Gryzinski[20] have been shown in Table -1 and Fig. 1 respectively due to proton impact.

Table-1: Proton impact electron captures cross sections for Ba. (in units of 10^{-17} cm^2)

Impact energy (KeV)	Present calculations	Calculations of Gryzinski[20]	Experiment
			Morgan & Eriksen[32]
2.0	135.0	466.0	
3.0		410.0	
4.0	385.0	330.0	
5.0		300.0	
6.0	262.0	250.0	
7.0		224.0	200.0
8.0	229.0	183.0	183.0
9.0		173.0	
10.0	180.0	145.0	145.0
12.0		109.0	105.0
15.0	105.0		
16.0		82.5	60.0
18.0		70.1	46.5
20.0	70.0	57.0	38.5
30.0	39.2	37.0	24.0
40.0	24.7	19.4	18.0
50.0	18.2	11.5	15.5
60.0	12.8	8.0	13.0
70.0	9.3	5.6	10.5
80.0	7.2	4.2	7.4
90.0		3.6	5.9
100.0	4.58	3.0	
150.0	2.23		
200.0	1.38		
300.0	0.58		
400.0	0.23		
500.0	0.12		

The single electron capture cross sections for Ba due to proton impact have been calculated upto impact energy 500 kev. The present calculations for cross sections have been plotted as a function of incident energy shown in fig 1. The fig. 1 includes, in addition to the present cross section, the theoretical results of Gryzinslc[20] and the experimental observations of Morgan and Eriksen[32]. For the sake of convenience in comparison, the graph has been plotted only upto 100.0 KeV because the theoretical results of Gryzinski[20] are only limited upto 100 KeV. Also the experimental observations of Morgan and Eriksen are limited up 90.0 KeV only. The present calculated cross sections are always within a factor of 2 of the experimental observations throughout the energy range available for comparison. Due to non-availability of the experimental results in low energy range (i.e. below > 7 KeV), the present calculated cross sections can't be compared with experimental observations. In the energy range 7 KeV - 40 KeV, the present calculated results overestimate the experiment. The present calculated cross-sections correspond well with the experimental observations. It is to be mentioned that in case of Ba, Hartree-Fock radial functions have been taken from Mclean and Mclean.[29]

Figure-1: Proton impact electron captures cross sections for Ba.



4. CONCLUSIONS

Thus, it can be concluded that the modified Binary Encounter Approximation (BEA) gives a good account of experimental observations in case of charge transfer processes. It has also been noticed that the agreement with experiment improves with increase in impact energy of projectile. Further it is observed that the present model is well suited for heavier atomic targets compared to other quantal or semi-quantal approximations.

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