Calculation of Electron Capture Cross-Section for Potassium (K) Due to Proton-Impact

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Abstract - A number of classical and quantum formulations have been developed to study the charge transfer process from a very low energy range to a very high energy range. However, there are some restrictions for lighter targets due to inherent mathematical complexities.

Keywords - cross-section for Potassium, Proton-impact

I. INTRODUCTION

Gryzinski[1] proposed a simplified Binary Encounter Model to account for the electron capture process. In this model a single Binary Encounter between the incident ion and the target electron may give rise to the phenomenon of electron capture by the projectile provided the energy transferred by the projectile to the target electrons between specified limits. Some attempts were made by *Garcia et al*[2]. and *Variens*[3] *t*o modify the energy limits for electron capture, as prescribed by *Gryzinski*, but failed to show any improvement in the results.

Roy and Rai[4]specify the limits for energy transfer after the implication of Thomas's theory. *Thomas*[5]model, a classical model for electron capture, was improved and extended by *Bates and Mapleton*[6] Method.

Presently, Roy and *Rai,* before *Tan and Lee*[7]*,* based on Thomas's second condition for electron capture, have established new energy limits in Gryzinski's model.

The equation has given the expression for electron capture cross-section

$$Q = n_e^u \sigma_{\Delta E} d(\Delta E) \quad (1)$$

Where Q is the cross-section for energy transfer E and n_e is the number of equivalent electrons in the shell under investigation.

And,

$$E_i = \frac{1}{2} mv^{2} + U_i + g - v(2mg)^{½} \quad \ldots\ldots\ldots\ldots (2)$$

$$E_u = \frac{1}{2} mv^{2} + U_i + g + v(2mg)^{½} \quad \ldots\ldots\ldots\ldots\ldots (3)$$

We now introduce dimensionless variables

$$S^2 = \frac{v_1^2}{v_0^2} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (4)$$

and

$$t^2 = \frac{v_2^2}{v_0^2} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (5)$$

where U_i is the binding energy of the target atom in Rydbergs; v_1 and v_2 are the velocities of incident particle and target orbiting electron in atomic units respectively and v_0 is the root mean square velocity of orbital electrons. (See *Catlow and* Mc *Dowell*). In terms of these dimensionless variables E_i, and E_u, can be given below

$$E_i = (s^2+1)\, U_i + g - 2s(U_i g)^{1/2} \ldots\ldots\ldots\ldots..(6)$$

And

$$E_u = (s^2+1)\, U_i + g + 2s(U_i g)^{½} \ldots\ldots\ldots\ldots (7)$$

Where,

$$g = \frac{2zs}{(r^2+t^2)^{\frac{3}{2}}} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (8)$$

Here s is the charge and r is the modules of the position vector of the bound electron with respect to target nucleus and may be taken as the radius of the shell (in atomic units).

The electron capture cross-sections have been found by integrating *Vriens* expression for two different ranges of energy transfer

$$f_{\Delta E}\, d(\Delta E) = \frac{2e^4 z^2}{mv_1^2} \left[\frac{1}{E} - \frac{mv_2^2}{2(\Delta E)^2}\right];\ E <= 2\, mv_1 (v_1 - v_2) \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (9)$$

And

$$f_{\Delta g}\, d(\Delta E) = \frac{ne^4 z^2}{mv_1^2} \cdot \left[\frac{m}{(\Delta E)^2}\left\{ \left(\frac{2\Delta E}{m} + v_2^2\right)^{3/2} - (2v_1^3 + v_2^3) - \frac{1}{\Delta E} \right\}\right];$$

$$2\, mv_1 (v_1 - v_2) <= E <= 2\, mv_1 (v_1 + v_2) \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (10)$$

Integrating the above expressions (in terms of s and t) over the Hartree-Fock velocity distribution for the target electron in the shell under consideration the electron capture cross section reduces to

$$Q^i(s) = n_e \int_0^\infty Q^i(s,t) f(t) U^{1/2} \mathrm{d}t. \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots.. (11)$$

Where f (t) is the momentum distribution function constructed by making use of the Hartree-Fock radial function given by *Clementi and Roetti*[9].

The atomic radii and shell radii have been taken from *Lotz*[10] and *Desclaux*[11] respectively.

Table 1: Proton impact electron capture cross-section for K (in Units of cm^2)

Impact Energy (KeV)	Present Calculation	Experiment Du Bois and Tobure
4.0	2.88,-15	………
6.0	7.88,-15	………
8.0	10.27,-15	1.25.-14
10.0	2.38,-14	………
12.0	1.73,-14	………
14.0	1.98,-14	………
16.0	1.67,-14	1.42,-14
40.0	5.24,-15	7.96,-15
200.0	3.7,-16	3.39,-16
1000.0	2.48,-17	………

2.88,-15 stands for 2.88×10^{-15}

II. RESULTS AND DISCUSSION

The cross-section for K due to protons have been shown in the above table. The present calculated capture cross-section is always within a factor 2 of the experimental values except in the energy range below 6 kev in case of proton impact.

The discrepancy in low energy may be partly attributed to the non-suitability of the Binary Encounter approximation. The range of agreement of our calculated cross-sections with experimental observations shifts in a higher energy range as the mass of the projectile increases.

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