Protons Impact Transfer Ionization Cross sections for Gallium

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Abstract:*In the present work we have performed calculations of transfer ionization cross sections for gallium due to impact of protons in Binary EncounterApproximation method. Method of Tan and Lee has been used for calculations for single ionization and transfer ionization. In these calculations binding energies are taken as the Hartree-Fock shell energies and for shell radii we have used the values of radial distributions of maximum probability as reported by Desclaux. Calculated results have been compared with available experimental observation.*

Keywords: **Transfer Ionization, Binary Encounter Approximation Method, Proton Impact**

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1. Introduction

Study of charge exchange reactions in various types of ion-atom collisions is of much interest due to their applications in different fields of research. Detail understanding of these processes is important for investigation of properties of upper atmosphere and some auroral phenomena (Basu et.al.[1]). In the interstellar gaseous medium a large number of elements are present in natural and ionized form. The bare nuclei present in the low energy cosmic rays in course of their interaction with these atoms and ions capture one or more electrons from them leading to formation of atoms and ions in excited states. These excited products may de-excited themselves via radiative transition yielding x-rays. The intensity of x-rays so emitted gives a measure of interstellar cosmic ray intensity (see Belkic and McCarroll,[2]Belkic and Gayet[3]). Electron capture processes are also of much significance because of their applications in the study of high temperature systems such as sun, solar wind, fusion reactors, particle and energy losses in plasmas (Bayfield and Khayrallah[4]) and in the production of ultraviolet and x-radiation (Vinogradov and Sobelmann[5]). Charge exchange collisions also provide a method for production of negatively charged ions which play significant role in design of tandem accelerator and cyclotron. Further, study of these processes provides valuable information about the radiation damage and design of radiation detector (Roy and Rai[6]). Moreover, at low energies electron capture is an important mechanism of ionization of atoms and molecules due to impact of charged particles.Further study of ionization of atoms and molecules due to bare ion impact are important in the study of processes related to physics and chemistry (Tachino et.al.[7]).

In the transfer ionization process two electrons are ejected by the projectile from the target out of which is captured by the projectile and other is left free. This process has significant contribution to double ionization of atoms at low energies. However, it may partly explain the structures observed in single electron capture cross section curves of atoms due to impact of charged particles.

Theoretical studies of transfer ionization process are very few in Literature (McDowell and Janev[8], Bhattacharya et.al.[9], Janev and Kristic[10]). While the mechanisms responsible for these processes in the case when more than two electrons participate is still not well understood, the following mechanisms have been proposed in the case when only two electrons are active (Kishinevaskii and Parilis[11]).

(i) Direct ionization and capture (DIC) (Transfer Ionization) :

$$A\,(e_1, e_2) + B^{Z+} \longrightarrow A^{2+} + B_{e_1}^{(z-1)+} + e_2 \qquad (0.1)$$

(ii) Single electron capture followed by molecular Auger or Penning ionization (SCAPI):

$$A\,(e_1, e_2) + B^{Z+} \longrightarrow A^{+}\,(e_2) + B_{e_1}^{(z-1)+}$$

$$\longrightarrow A^{2+} + B^{(z-1)+} + (e_1) + e_2 \quad (AI)$$

$$\longrightarrow A^{2+} + B^{(z-1)+} + (e_2) + e_1 \quad (PI) \qquad (0.2)$$

(iii) Double electron capture followed by autoionization (DCAI) :

$$A\,(e_1, e_2) + B^{Z+} \longrightarrow A^{2+} + B^{(z-2)+**} + (e_1, e_2)$$

$$\longrightarrow A^{2+} + B^{(z-1)+} + (e_1) + e_2$$

$$\longrightarrow A^{2+} + B^{(z-1)+*} A^{2+} + B^{(z-2)+**} + (e_1, e_2)$$

$$A^{2+} + B^{(z-2)+} + (e_1) + e_2 \quad (0.3)$$

Chatterjee et.al.[12]proposed a method in the framework of the binary encounter approximation (BEA) for calculation of transfer ionization cross sections for the mechanics (0.1). The calculations are based on Gryzinski's[13] model for double ionization by incident of atoms or ions and the method proposed by Tan and Lee[14] for calculations of pure ionization and electron capture cross section by impact of ions with atoms successfully applied for H^+ and He^{2+} incident on He and Li. In the present work we apply the method of Chatterjeeet.al.[12]in more complex processes i.e. H^+ and He^{2+} incident on gallium.

2. Theoretical Method

The present theory is based on the method proposed by Tan and Lee[14] for calculation of electron capture and ionization cross section of atoms due to impact of fast light nuclei and the work of Chatterjee and Roy[15] on the BEA calculations of double electron capture cross sections from atoms due to impact of light multicharged nuclei. The transfer ionization process is supposed to take place via two successive binary encounters between the incident ions and the target atom. In the first binary encounter the projectile with energy E_q transfer energy ΔE to one of the bound electrons; as a result of which the electron is emitted into free space leading to impact ionization. The projectile with the remaining energy $(E_q - \Delta E)$ makes a second binary encounter with the residue target capturing one of its electrons. Hence the cross section for the transfer ionization processes may be written as

$$Q = \frac{n_e(n_e-1)}{4\pi\bar{r}^2}\left[\int_{U_i}^{\Delta E_l} \sigma_{\Delta E}\left(E_q\right) C' \left\{\int_{\Delta E'_L}^{\Delta E'_U} \sigma_{\Delta E'}\left(E_q - \Delta E\right) d(\Delta E')\right\}\right] d(\Delta E)$$

$$+ (1-C) \int_{\Delta E_l}^{\Delta E_u} \sigma_{\Delta E}\left(E_q\right) C' \left\{\int_{\Delta E'_L}^{\Delta E'_U} \sigma_{\Delta E'}\left(E_q - \Delta E\right) d(\Delta E')\right\}\, d(\Delta E)$$

$$+ \int_{\Delta E_u}^{E} \sigma_{\Delta E}\left(E_q\right) C' \{\int_{\Delta E'_L}^{\Delta E'_U} \sigma_{\Delta E'}\left(E_q - \Delta E\right) d(\Delta E')\}\ d(\Delta E)] \quad (1.1)$$

Here all the primed quantities correspond to the second process and $\bar{r} = \frac{r}{n_e^{1/3}}$ is the average distance between the two electrons in the shell. All other quantities have been defined earlier.

It is apparent from the above expression for transfer ionization cross section that the energy ΔE transfer in course of ionization should be taken into account while considering the electron capturing processes. In this situation continually varying fractions of the projectile energy to be given to the target electron in the successive encounters. However, this consideration would involve complicated numerical integrations because $\sigma_{\Delta E'}$, as well as $\Delta E'_l$, $\Delta E'_u$ and C' will depend on ΔE . Since only a small fraction of the energy of the incident ion is transferred to the atomic electron during the first process, the energy of the projectile can be assumed to be remains practically unchanged for the second process. Hence we put $E_q - \Delta E \simeq E_q$, so that $\sigma_{\Delta E'}$, $\Delta E'_l$, $\Delta E'_u$ and C' become function of E_q only. Consequently the transfer ionization cross section becomes

$$Q = \frac{n_e(n_e-1)}{4\pi\bar{r}^2}\left[\int_{U_i}^{\Delta E_l} \sigma_{\Delta E}\left(E_q\right) d(\Delta E) + (1-C)\int_{\Delta E_l}^{\Delta E_u} \sigma_{\Delta E}\left(E_q\right) d(\Delta E) + \int_{\Delta E_l}^{\Delta E_u} \sigma_{\Delta E}\left(E_q\right) d(\Delta E)\right] \text{x} \left[C' \int_{\Delta E'_L}^{\Delta E'_U} \sigma_{\Delta E'}\left(E_q\right) d(\Delta E')\}\right]$$

$$= \frac{n_e(n_e-1)}{4\pi\bar{r}^2} Q_1\ x\ Q_2$$

Where $Q_1\ and\ Q_2$ refer to the quantities within the square brackets.

Let us put $s^2 = \frac{{V_1}^2}{{V_0}^2}$ and $t^2 = \frac{{V_{2k}}^2}{{V_0}^2}$ Where ${V_0}^2 = U_i$ is the first ionization potential of the target in rydbergs and V_1 and V_2 are respectively the velocities of the projectiles and the bound electron in atomic units. In terms of these dimensionless quantities $\Delta E_l\ and\ \Delta E_u$ are respectively given by

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

and $\Delta E_u = (s^2+1)U_i + g + 2s(U_i\ g)^{1/2}$ (1.2)

where $g = 2Zs/r(s^2+t^2)^{1/2}$.

The expression for $\Delta E_l'\ and\ \Delta E_u'$ are similar to those of $\Delta E_l\ and\ \Delta E_u$ with s, t, and g replaced by the corresponding quantities s, t, and g respectively. In terms of s and t, using Vriens expression for $\sigma_{\Delta E}$, the integral in (4.20) may be written as

$$\int (\sigma_{\Delta E})_a d(\Delta E) = \frac{4}{s^2 U_i}\left[-\frac{1}{\Delta E} - \frac{2t^2 U}{3(\Delta E)^2}\right](\pi a_0^2);\ \Delta E \leq E_1 \quad (1.3)$$

$$\int (\sigma_{\Delta E})_b\, d(\Delta E) = \frac{2}{s^2 U_i}\left[\frac{2U_i}{3t(\Delta E)^2}\left\{\left(\frac{\Delta E}{U} + t^2\right)^{3/2} - (2s^3 + t^3)\right\} - \frac{1}{\Delta E}\right](\pi a_0^2);$$

$E_1 \leq \Delta E \leq E_2$ (1.4)

and $\int (\sigma_{\Delta E})_c\, d(\Delta E) = 0$, $\Delta E > E_2$

whereas $E_1 = 4sU_i(s-t)$ and $E_2 = 4sU_i(s+t)$.

Depending on the relative values of Depending on the relative values of S^2U_i and g the following two cases arise (see Tan and Lee[14])

Case 1: If $S^2U_i > g$ $(S'^2U_{ii} > g')$, corresponding to the values of ΔE_l and ΔE_u ($\Delta E_l'$ *and* $\Delta E_u'$) relative to E_1 *and* E_2 (E_1' *and* E_2') Q_1 and Q_2 have one of the following values:

$$Q_1(s,t) = \begin{cases} \int_{U_i}^{E_1}(\sigma_{\Delta E})_a\, d(\Delta E) - c\left[\int_{\Delta E_l}^{\Delta E_u}(\sigma_{\Delta E})_a d(\Delta E) + \int_{E_1}^{E_2}(\sigma_{\Delta E})_b d(\Delta E)\right]; U_i \le \Delta E_l \le \Delta E_u \le E_1 \le E_2 \\ \int_{U_i}^{E_1}(\sigma_{\Delta E})_a\, d(\Delta E) - c\left[\int_{\Delta E_l}^{E_1}(\sigma_{\Delta E})_a d(\Delta E) + \int_{E_1}^{\Delta E_u}(\sigma_{\Delta E})_b d(\Delta E)\right]\int_{E_1}^{E_2}(\sigma_{\Delta E})_b d(\Delta E); \\ \quad U_i \le \Delta E_l \le E_1 \le \Delta E_u \le E_2 \\ \int_{U_i}^{\Delta E_l}(\sigma_{\Delta E})_a\, d(\Delta E) + (1-c)\left[\int_{\Delta E_l}^{E_1}(\sigma_{\Delta E})_a d(\Delta E) + \int_{E_1}^{E_2}(\sigma_{\Delta E})_b d(\Delta E)\right]; \\ \quad U_i \le \Delta E_l \le E_1 \le E_2 \le \Delta E_u \\ \int_{U_i}^{E_1}(\sigma_{\Delta E})_a\, d(\Delta E) + \int_{E_1}^{E_2}(\sigma_{\Delta E})_b d(\Delta E) - c\left[\int_{\Delta E_l}^{\Delta E_u}(\sigma_{\Delta E})_b d(\Delta E)\right]; \\ \quad U_i \le E_1 \le \Delta E_l \le E_2 \le \Delta E_u \\ \int_{U_i}^{E_1}(\sigma_{\Delta E})_a\, d(\Delta E) + \int_{E_1}^{\Delta E_l}(\sigma_{\Delta E})_b d(\Delta E) + (1-c)\left[\int_{\Delta E_l}^{E_2}(\sigma_{\Delta E})_b d(\Delta E)\right]; \\ \quad U_i \le E_1 \le \Delta E_l \le E_2 \le \Delta E_u \\ \int_{U_i}^{E_1}(\sigma_{\Delta E})_a\, d(\Delta E) + \int_{E_1}^{E_2}(\sigma_{\Delta E})_b d(\Delta E); U_i \le E_1 \le E_2 \le \Delta E_l \le \Delta E_u \end{cases}$$

and

$$Q_2'(s',t') = \begin{cases} c'\int_{\Delta E_l'}^{\Delta E_u'}(\sigma_{\Delta E})_a d(\Delta E); \Delta E_l' \le \Delta E_u' \le E_1' \le E_2' \\ c'\left[\int_{\Delta E_l'}^{E_1'}(\sigma_{\Delta E})_a d(\Delta E) + \int_{E_1'}^{\Delta E_u'}(\sigma_{\Delta E})_b d(\Delta E)\right]; \Delta E_l' \le E_1' \le \Delta E_u' \le E_2' \\ c'\left[\int_{\Delta E_l'}^{E_1'}(\sigma_{\Delta E})_a d(\Delta E) + \int_{E_1'}^{E_2'}(\sigma_{\Delta E})_b d(\Delta E)\right]; \Delta E_l' \le E_1' \le E_2' \le \\ \Delta E_u' c'\int_{\Delta E_l'}^{\Delta E_u'}(\sigma_{\Delta E})_b d(\Delta E); E_1' \le \Delta E_l' \le \Delta E_u' \le E_2' \\ c'\int_{\Delta E_l'}^{E_2'}(\sigma_{\Delta E})_b d(\Delta E); E_1' \le \Delta E_l' \le E_2' \le \Delta E_u' \\ 0; E_1' \le E_2' \le \Delta E_l' \le \Delta E_u \end{cases} \quad (1.5)$$

Case 2: similarly for S^2U_i (S'^2U_{ii}) , less than g (g') the values of $Q_1(s,t)$ and $Q_1'(s',t')$ are given by :

$$Q_1(s,t) = \begin{cases} 0.5\int_{\Delta E_l}^{\Delta E_u}(\sigma_{\Delta E})_a\,d(\Delta E) + \int_{\Delta E_u}^{E_1}(\sigma_{\Delta E})_a d(\Delta E) + \int_{E_1}^{E_2}(\sigma_{\Delta E})_b d(\Delta E); \\ \qquad U_i \le \Delta E_l \le \Delta E_u \le E_1 \le E_2 \\ 0.5\left[\int_{\Delta E_l}^{E_1}(\sigma_{\Delta E})_a d(\Delta E) + \int_{E_1}^{\Delta E_u}(\sigma_{\Delta E})_b d(\Delta E)\right] + \int_{\Delta E_u}^{E_2}(\sigma_{\Delta E})_b d(\Delta E); \\ \qquad U_i \le \Delta E_l \le E_1 \le \Delta E_u \le E_2 \\ 0.5\left[\int_{\Delta E_l}^{E_1}(\sigma_{\Delta E})_a d(\Delta E) + \int_{E_1}^{E_2}(\sigma_{\Delta E})_b d(\Delta E)\right] + \int_{\Delta E_u}^{E_2}(\sigma_{\Delta E})_b d(\Delta E); \\ \qquad U_i \le \Delta E_l \le E_1 \le E_2 \le \Delta E_u \\ 0.5\int_{\Delta E_l}^{\Delta E_u}(\sigma_{\Delta E})_b\,d(\Delta E) + \int_{\Delta E_u}^{E_2}(\sigma_{\Delta E})_b d(\Delta E); \\ \qquad U_i \le E_1 \le \Delta E_l \le \Delta E_u \le E_2 \\ 0.5\int_{\Delta E_l}^{\Delta E_u}(\sigma_{\Delta E})_b\,d(\Delta E) + \int_{\Delta E_u}^{E_2}(\sigma_{\Delta E})_b d(\Delta E); \\ \qquad E_1 \le U_i \le \Delta E_l \le \Delta E_u \le E_2 \\ 0.5\int_{\Delta E_l}^{E_2}(\sigma_{\Delta E})_b\,d(\Delta E); \qquad U_i \le E_1 \le \Delta E_l \le E_2 \le \Delta E_u \\ 0.5\int_{\Delta E_l}^{E_2}(\sigma_{\Delta E})_b\,d(\Delta E); E_1 \le U_i \le \Delta E_l \le E_2 \le \Delta E_u \\ 0 \quad ; U_i \le E_1 \le E_2 \le \Delta E_l \le \Delta E_u \\ 0 \quad ; E_1 \le U_i \le E_2 \le \Delta E_l \le \Delta E_u \\ 0 \quad ; E_1 \le E_2 \le U_i \le \Delta E_l \le \Delta E_u \end{cases}$$

(1.6)

$$Q_2'(s',t') = \begin{cases} \int_{U_{ii}}^{\Delta E_l'}(\sigma_{\Delta E})_a d(\Delta E) + 0.5\int_{\Delta E_l'}^{\Delta E_u'}(\sigma_{\Delta E})_a d(\Delta E); \\ \qquad U_{ii} \le \Delta E_l' \le \Delta E_u' \le E_1' \le E_2' \\ \int_{U_{ii}}^{\Delta E_l'}(\sigma_{\Delta E})_a d(\Delta E) + 0.5\left[\int_{\Delta E_l'}^{E_1'}(\sigma_{\Delta E})_a d(\Delta E) + \int_{E_1'}^{\Delta E_u'}(\sigma_{\Delta E})_b d(\Delta E)\right]; \\ \qquad U_{ii} \le \Delta E_l' \le E_1' \le \Delta E_u' \le E_2' \\ \int_{U_{ii}}^{\Delta E_l'}(\sigma_{\Delta E})_a d(\Delta E) + 0.5\left[\int_{\Delta E_l'}^{E_1'}(\sigma_{\Delta E})_a d(\Delta E) + \int_{E_1'}^{E_2'}(\sigma_{\Delta E})_b d(\Delta E)\right]; \\ \qquad U_{ii} \le \Delta E_l' \le E_1' \le E_2' \le \Delta E_u' \\ \int_{U_{ii}}^{E_1'}(\sigma_{\Delta E})_a d(\Delta E) + \int_{E_1'}^{\Delta E_l'}(\sigma_{\Delta E})_b d(\Delta E) + 0.5\int_{\Delta E_l'}^{\Delta E_u'}(\sigma_{\Delta E})_b d(\Delta E); \\ \qquad U_{ii} \le E_1' \le \Delta E_l' \le \Delta E_u' \le E_2' \\ \int_{U_{ii}}^{\Delta E_l'}(\sigma_{\Delta E})_b d(\Delta E) + 0.5\int_{\Delta E_l'}^{\Delta E_u'}(\sigma_{\Delta E})_b d(\Delta E); \\ \qquad E_1' \le U_{ii} \le \Delta E_l' \le \Delta E_u' \le E_2' \\ \int_{U_{ii}}^{E_1'}(\sigma_{\Delta E})_a d(\Delta E) + \int_{E_1'}^{\Delta E_l'}(\sigma_{\Delta E})_b d(\Delta E) + 0.5\int_{\Delta E_l'}^{E_2'}(\sigma_{\Delta E})_b d(\Delta E); \\ \qquad U_{ii} \le E_1' \le \Delta E_l' \le E_2' \le \Delta E_u' \end{cases}$$

$\int_{U_{ii}}^{\Delta E_l'} (\sigma_{\Delta E})_b d(\Delta E) + 0.5 \int_{\Delta E_l'}^{\Delta E_u'} (\sigma_{\Delta E})_b d(\Delta E) \;\; ; E_1' \le U_{ii} \le \Delta E_l' \le \Delta E_u' \le E_2'$

$\int_{U_{ii}}^{\Delta E_l'} (\sigma_{\Delta E})_b d(\Delta E) + 0.5 \int_{\Delta E_l'}^{E_2'} (\sigma_{\Delta E})_b d(\Delta E) \;\; ; \;\; E_1' \le U_{ii} \le \Delta E_l' \le E_2' \le \Delta E_u'$

$\int_{U_{ii}}^{E_1'} (\sigma_{\Delta E})_a d(\Delta E) + \int_{E_1'}^{E_2'} (\sigma_{\Delta E})_b d(\Delta E); \;\; U_{ii} \le E_1' \le E_2' \le \Delta E_l' \le \Delta E_u'$

$\int_{U_{ii}}^{E_2'} (\sigma_{\Delta E})_b d(\Delta E) \;\; ; \quad E_1' \le U_{ii} \le E_2' \le \Delta E_l' \le \Delta E_u' \qquad 0 \qquad ; E_1' \le E_2' \le U_{ii} \le$

$\Delta E_l' \le \Delta E_u'$ (1.7)

The values of Q_1 and Q_2 have been averaged over the Hartree-Fock velocity distribution for the target electron under consideration.

3. Results and discussion

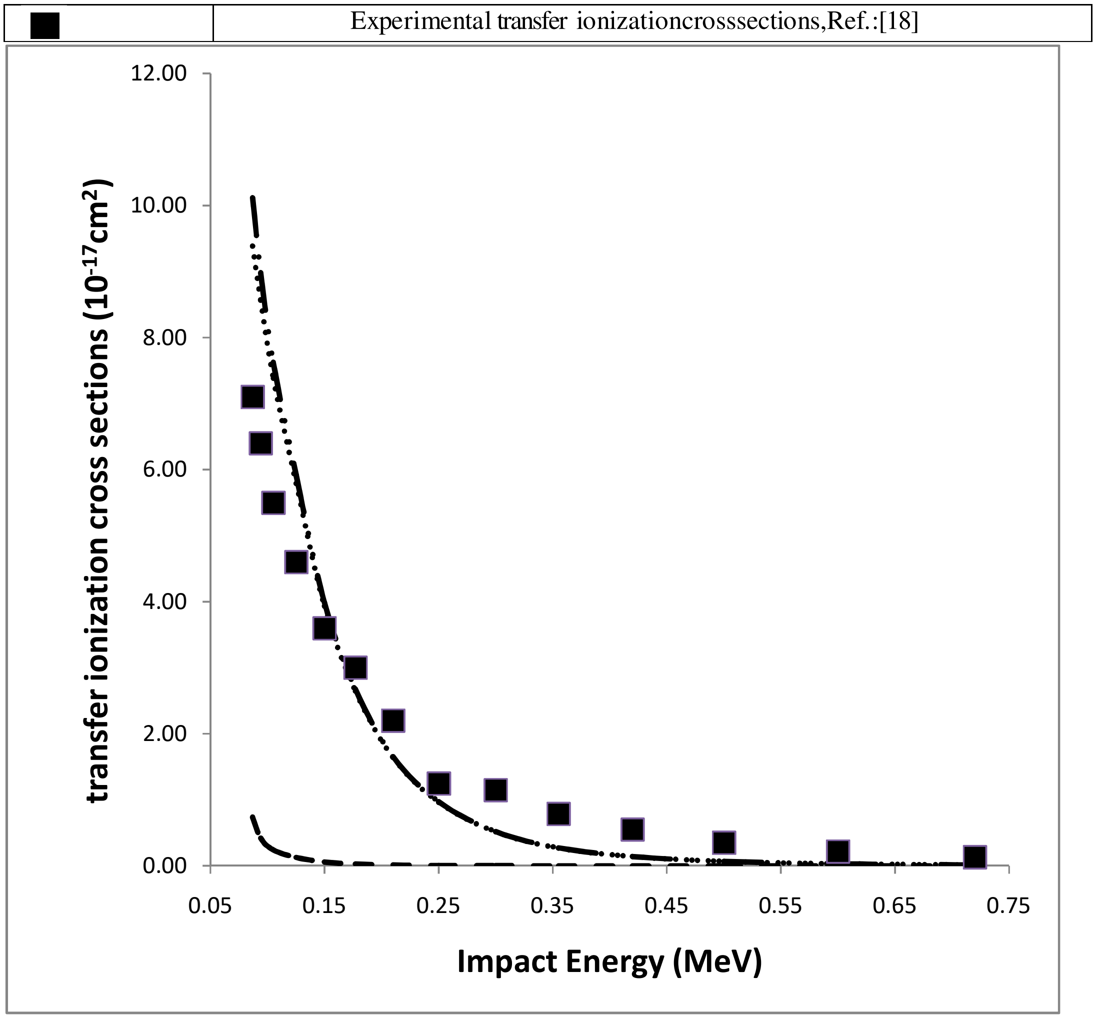
We have performed calculations of H^+ impact transfer ionization cross sections of gallium using the method described in the previous section. In these calculations the binding energies for target electron have been taken as the Hartree-Fock shell energies reported by Clementi and Roetti [16]. For shell radii we have used the radial distance of maximum probability as reported by Desclaux [17]. Our calculated results of H^+ impact transfer ionization cross sections have been presented in Table 1.1 and Figure 1.1 along with the experimental observations of Lozhkin et.al.[18].

Table :- 1.1:Transfer Ionization Cross sections of Gallium By Proton Impact

Impact Energy (kev)	Present calculated transfer ionization cross sections ($10^{-17}cm^2$)		Total calculated transfer ionization cross sections ($10^{-17}cm^2$)	Experimental Transfer ionization cross sections (10^{-17} cm^2) Ref.:[18]
	4p-4s contribution	4p-3d contribution		
87.0	0.74	9.38	10.12	7.1
94.0	0.42	8.57	8.98	6.4
105.0	0.24	7.38	7.62	5.5
125.0	0.13	5.79	5.91	4.6
150.0	0.06	3.93	3.99	3.6
177.0	0.03	2.65	2.68	3.0
210.0	0.01	1.64	1.65	2.2
250.0	0.01	0.96	0.97	1.25
300.0	0.00	0.52	0.52	1.15
355.0	0.00	0.27	0.27	0.79
420.0	0.00	0.14	0.14	0.55
500.0	0.00	0.07	0.07	0.35
600.0	0.00	0.03	0.03	0.22
720.0	0.00	0.01	0.01	0.13

Fig. 1.1: Transfer Ionization Cross sections of Gallium by Proton Impact

— — — — —	Presentcalculated transfer ionization crosssectionsof Ga(4p-4s contribution)
....	Presentcalculated transfer ionization crosssectionsof Ga(4p-3d contribution)
—— •• ——	Totaltransfer ionization crosssectionsof Gallium



In calculations of transfer ionization cross sections we have assumed that the incident particles first produces pure ionization in 4p shell of gallium and then it follows an electron capture by the projectile form the ion produced. We have presented the results of two sets of calculations, in the first set after ionization of 4p shell as the electron capture take place from 4s shell of resulting Ga^+ ion where as in the second set capture is supposed to take place from 3d shell of Ga^+. Below 300.0 keV impact energy our calculated cross sections for electron capture by H^+ from 4s shell of Ga^+ are found to be about 10^3 times smaller than the ionization cross sections of H^+ for 4p shell of Ga and hence the contribution to transfer ionization cross sections for 4p-4s is very small below 300.0 keV impact energy. Our total transfer ionization cross sections are in reasonable agreement with the experimental observations.

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