

State selective electron capture in partially stripped ion-atom interaction at intermediate and high energies

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Abstract. Post form of “boundary corrected continuum intermediate state (BCIS)” approximation has been employed to study charge transfer cross-sections in collision of C^{q+} , N^{q+} and O^{q+} ($q = 1-5$) with ground state atomic hydrogen in the energy range of 50–200 keV/amu. In this formalism we have adopted model potential for the interaction of the active electron with the projectile ion. Calculated results for total charge transfer cross-sections have significant improvement over other existing theoretical results in their comparison to the available experimental findings except for singly charge ions. Sub-shell distribution for total charge transfer cross-section has also been reported in graphical form. Predictions suggested by Olson in connection with the sub-shell distribution of total charge transfer cross-section has been reaffirmed. However, an oscillatory structure of charge state dependence of the total charge transfer cross-sections has not been found in the present investigation.

PACS. 34.70.+e Charge transfer

1 Introduction

Due to diverse application of atomic collision data in diverse branches of Physics, efforts are still going in full swing both theoretically as well as experimentally to generate very accurate atomic collision database during last two decades. In addition, more refined experiment, on ion-atom interactions are expected to be carried out in near future due to technological advancement. Partial survey of inelastic collision processes involving multi-charged ions and atoms may be found in the present literature [1–6]. Most of the research work carried out so far in this area is confined to fully stripped ion-atom interactions. However, some theoretical [7–17] and experimental research work [18–20] have been carried out in connection with the collision of partially stripped ions with atoms or collisions of fully stripped ions with multi electron atoms.

After the detection of inherent difficulties in tackling with the coulomb interaction and the prescription for its solution, the first Born approximation (B1) [21,22] had its new appearance to study different inelastic processes in ion-atom interactions [23–25]. To obtain more accurate theoretical results, various attempts have been made to go beyond first order in the framework of distorted wave formalism. These attempts gave birth to different theories viz. Continuum distorted wave-eikonal initial state (CDW-EIS) [16,17,26], eikonal final state-continuum distorted wave (EFS-CDW) [27], boundary corrected contin-

uum intermediate state (BCIS) [28,29] etc. However, the theory of CDW-EIS has been found to be successful in its application to the study of ionization of L-shell electron in $H^+ + Ar$ interaction by Fainstein et al. [30] and in the study of angular distribution of L or M -shell capture in $H^+ + Ar$ collision by Gulays et al. [31]. Mandal et al. [32] has applied the BCIS theory to study positronium formation cross-sections in $e^+ + H$ collision. However, it is to be mentioned that Mandal et al. has re-derived the theory to make it applicable to comparatively lower energy region. Later, Belkic [33] has extended the BCIS theory to four-body problem to calculate double electron capture cross-sections in collision of He^{2+} with He.

Olson and Salop [13] have calculated charge transfer cross-sections in collisions of B^{q+} , C^{q+} , N^{q+} and O^{q+} ($q \geq 3$) with atomic hydrogen in the framework of classical trajectory Monte Carlo (CTMC) simulation method. They have treated the partially stripped ions as hydrogenic ions with effective charge determined from spectroscopic data. However, charge transfer cross-section into each individual sub-shell are not available from their calculations. Eichler et al. [14] have studied the same collision processes in Oppenheimer-Brinkman-Kramers (OBK) approximation. Multiplying the OBK cross-sections by a reduction factor obtained from eikonal approximation yielded final results in reasonable agreement with experimental observation. In the frame-work of three-body formalism, Hanssen et al. [15] have employed molecular state expansion method to study charge transfer cross-sections in collisions of C^{4+} , N^{5+} and O^{6+} with atomic hydrogen

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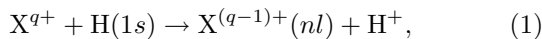
in the energy range of 0.25 to 25 keV/amu using model potential of the active electron with the projectile ion. Calculated results are very encouraging. Martinez et al. [16] have also used Roothan-Hartree Fock potential for the active electron-target nuclear interaction to study inner shell charge transfer with Ne and Ar as target in CDW-EIS theory. Later Abufager et al. [17] have applied the same theory to study inner shell capture in collisions of H^+ , He^{2+} , Li^{3+} with He, Ne, Ar respectively using model potential of same type. However, in this work they have modified the theory in such a way that orthogonality of bound and continuum states of the corresponding potential has been preserved. As a consequence improved results have been obtained. Purkait et al. [11] have employed CTMC method to calculate charge transfer cross-section in collisions of C^{q+} , N^{q+} and O^{q+} ($q = 1-5$) with atomic hydrogen. In their calculation, they have treated the interaction of the active electron with the partially stripped projectile ion by a model potential and as such, significant improvement over the CTMC results of Olson and Salop [13] have been observed in their comparison to experimental observations [19,20]. Dhara et al. [12] have studied the above-mentioned processes in Coulomb–Born (CB) approximation. Their computed results have reasonable agreement with experimental findings. Sub-shell distribution of total charge transfer cross-sections is also available from both of these works [11,12].

Under the prevailing circumstances, we are motivated to study the above-mentioned processes in quantum mechanical framework taking into account of the intermediate continuum states. However, we have in our mind that the theoretical formulation should include the interaction of the active electron with the partially stripped projectile ion to be improved over coulomb interaction. Briggs [34] has shown that the prior (or Post) form of Peaking Impulse Approximation is best suitable when the target charge (or projectile charge) is much greater than the projectile charge (or target charge). With all these considerations, we have employed the post form of Boundary Corrected Continuum Intermediate State (BCIS) approximation to study the charge transfer cross-sections in collisions of C^{q+} , N^{q+} and O^{q+} ($q = 1-5$) with atomic hydrogen within the impact energy range of 50–200 keV/amu.

The organization of the paper is as follows. Theoretical formulation has been described in Section 2. Results and discussion are the contents of Section 3. Finally the paper ends with concluding remarks in Section 4. Atomic units are used unless otherwise mentioned.

2 Theory

All the reactions under the study may generally be represented by



where X^{q+} represents C^{q+} , N^{q+} and O^{q+} ($q = 1-5$) respectively. Let r_T and r_P are the relative position vector

Table 1. Model potential parameters λ and b .

Ion	λ	b
C^+	2.033	3.293
C^{2+}	3.228	9.293
C^{3+}	4.2280	6.6850
C^{4+}	8.008	8.985
C^{5+}	10.008	3.57
N^+	1.9533	1.5679
N^{2+}	3.2793	9.9932
N^{3+}	4.0074	9.9432
N^{4+}	5.467	9.9897
N^{5+}	9.0074	9.8166
O^+	2.011	0.7132
O^{2+}	3.001	7.468
O^{3+}	3.819	9.9222
O^{4+}	4.367	9.9997
O^{5+}	4.7960	11.5978

of the active electron with respect to the target and projectile nuclei respectively. R_T be the position vector of the projectile ion with respect to the center of mass of the target atom, R_P be the relative position vector of the center of mass of the projectile ion after electron capture from the target nucleus and R is the internuclear distance.

Total Hamiltonian of the whole system may be written as

$$H = H_0 + V_{Te}(\vec{r}_T) + V_{Pe}(\vec{r}_P) + V_{TP}(\vec{R}), \quad (2)$$

where V subscripted by any pair of e (active electron), P (projectile) and T (target ion) represents the corresponding two-body interaction. There is no ambiguity in the construction of $V_{Te}(r_T)$ and it is uniquely determined by the Coulomb potential. The interaction of the active electron with the projectile ion has been estimated by a model potential as

$$V_{Pe}(\vec{r}_P) = -\frac{q}{r_P} - \frac{e^{-\lambda r_P}}{r_P} \{(Z - q) + b r_P\}, \quad (3)$$

where Z and q are respectively the nuclear and asymptotic charge of the projectile ion. b and λ are two arbitrary parameters chosen variationally with respect to a slater basis set in such a way that the corresponding Hamiltonian of the active electron in the final state is diagonalised to reproduce correct binding energies. These binding energies of the active electron on different projectile ions are calculated from the tables of Clementi and Roetti [35] and works of Clark and Abdallah [36]. Model Potential parameters λ and b for different projectile ions are given in Table 1.

It has been observed that a unique set of parameters for the potentials reproduce binding energies of the captured electron in a different sub-shell with greater accuracy for a particular shell of the projectile ion, which has initially a closed shell or sub-shell structure. For the capture to the open shell of the projectile ion, potential parameters have to change a little to find out the binding energies of the active electron in each of the different sub-shells to which the capture occurs. However, the

virial theorem has been tested and is found to be accurate within 0.01% in all cases. We have treated the interaction of the projectile ion and the target nucleus as a coulomb interaction between two charges of magnitude q and 1, respectively. This is well-justified even if some short-range part exists that will not affect the charge transfer cross-sections.

The post form of the transition amplitude in the framework of BCIS approximations may be written as

$$T_{if}^+ = \left\langle \chi_f^- \left| \frac{1}{R_P} - \frac{1}{r_T} \right| \psi_i^{BCIS(+)} \right\rangle \quad (4)$$

where,

$$\begin{aligned} \chi_f^- &= e^{-\frac{\pi\alpha_3}{2}} \Gamma(1 - i\alpha_3) e^{i\vec{K}_f \cdot \vec{R}_P} \phi_f(\vec{r}_P) \\ &\quad \times {}_1F_1\left(i\alpha_3; 1; -i\left(K_f R_P + \vec{K}_f \cdot \vec{R}_P\right)\right) \\ \psi_i^{BCIS(+)} &= \phi_i(\vec{r}_T) G_i^+ \\ G_i^+ &= e^{\frac{i\pi}{2}(\alpha_1 - \alpha_2)} \Gamma(1 - i\alpha_1) \Gamma(1 + i\alpha_2) e^{i\vec{k}_i \cdot \vec{R}_T} \\ &\quad \times {}_1F_1\left(i\alpha_1; 1; i b(v_i r_P + \vec{v}_i \cdot \vec{r}_P)\right) \\ &\quad \times {}_1F_1\left(-i\alpha_2; 1; i a\left(k_i R_P - \vec{k}_i \cdot \vec{R}_P\right)\right). \end{aligned}$$

Following Belkic [33], the six dimensional integral in the transition amplitude may be reduced to two-dimensional integral. One of the two is an infinite integral and the other one is from 0 to 1.

Inner integral with infinite upper limit has been evaluated numerically by 40-point Gauss Legendre quadrature method with suitable co-ordinate transformation. The real integral from 0 to 1 has been divided into a number of sub-intervals and each of such sub-intervals has been integrated numerically by 36-point Gauss-Laguerre quadrature method by proper co-ordinate transformation. Finally charge transfer cross-sections are obtained by numerical integration over scattering angles with an overall accuracy of 0.1%. Higher excited states are generated by additional parametric differentiation. In our present investigation, the order of differentiation goes up to six, which have been performed analytically.

3 Results and discussions

Total charge transfer cross-sections have been obtained by summing over all contributions into each shell up to $n = 5$ and the contribution to each shell is determined by adding all sub-shell data obtained by multiplying the calculated results by Pauli blocking factor [14] given by

$$Q_{nl} = \left[1 - \frac{N_{nl}}{2(2l+1)} \right] Q_{nl}^c, \quad (5)$$

where N_{nl} is the number of electrons occupying the sub-shell of the projectile ion and Q_{nl}^c is the calculated cross-sections into the corresponding sub-shell. Variation of total charge transfer cross-sections with the incident energy

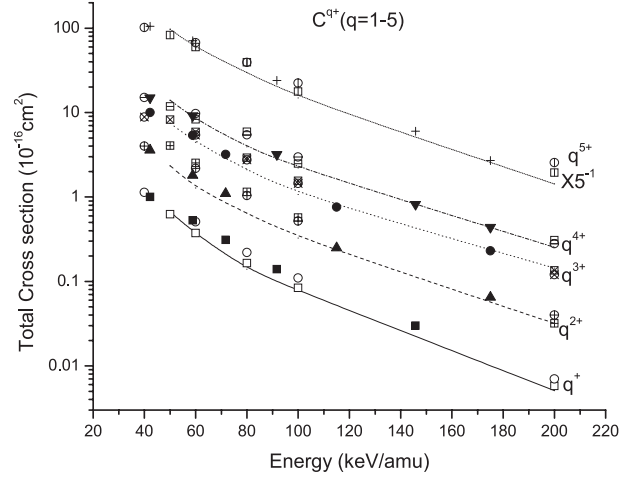


Fig. 1. Variation of total charge transfer cross-sections with energy for C^{q+} ($q = 1-5$) + H ($1s$) interaction. Theory: (—) present results; (□) CB results of Dhara et al. [12]; (○) CTMC results of Purkait et al. [11]; for charge state $q = 1$. (---) Present results; (⊞) CB results of Dhara et al. [12]; (⊕) CTMC results of Purkait et al. [11]; for $q = 2$. (....) Present results; (⊠) CB results of Dhara et al. [12]; (⊗) CTMC results of Purkait et al. [11]; for $q = 3$. (- · - · -) Present results; (⊚) CB results of Dhara et al. [12]; (⊖) CTMC results of Purkait et al. [11]; for $q = 4$. (.....) Present results; (⊛) CB results of Dhara et al. [12]; (⊙) CTMC results of Purkait et al. [11]; for $q = 5$. Experimental results: $q = 1$ (■); $q = 2$ (▲); $q = 3$ (●); $q = 4$ (▼); $q = 5$ (+); of Shah and Gilbody [20].

of the projectile ion are reported in graphical form for all the ions in Figures 1–3. Sub-shell distribution of total charge transfer cross-sections at 80 keV/amu are displayed in Figures 4–8 for carbon ions only. This is because such distribution bears more or less the same characteristic features for all other ions. However, it may be mentioned that explicit numerical data for all the ions may be obtained on request. Finally charge state dependence of total charge transfer cross-section is shown in Figure 9.

Variation of total charge transfer cross-sections with projectile energy in collision of C^{q+} , N^{q+} and O^{q+} ($q = 1-5$) with ground state of atomic hydrogen are displayed in Figures 1–3 respectively. Figure 1 displays the present results of $C^{q+} + H$ ($q = 1-5$) collision. From the figures, we may find that the present results are in excellent agreement with the experimental results of Shah and Gilbody [20] in comparison to the CB results of Dhara et al. [12] and CTMC results of Purkait et al. [11] except for $C^+ + H$ interaction. However it may be found that, for $C^+ + H$ interaction, present results and the previous results in CB approximation are in close agreement. This may be due to the fact that Wilson-Sommerfeld parameters (α_1 and α_2) have small values for $q = 1$ and as such, contributions of two coulomb functions in the initial state (ψ^{BCIS}) has smaller contributions. This may be verified from the observation that these two formalism (CB and BCIS) are identical if we substitute $\alpha_1 = \alpha_2 = 0$. As a consequence agreement of present results and CB results become increasingly poorer, CTMC results of Purkait et al. for all

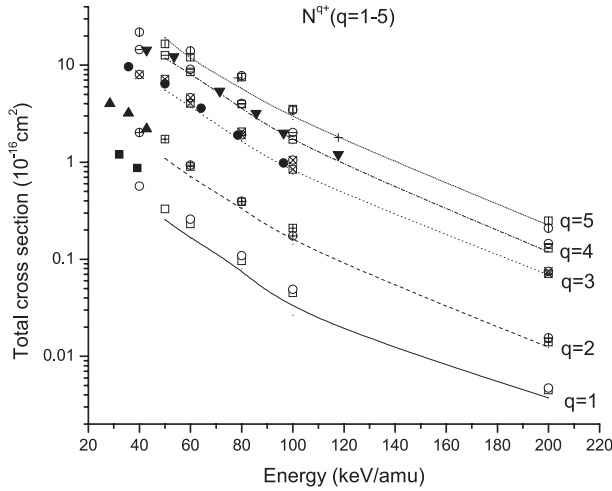


Fig. 2. Variation of total charge transfer cross-sections with energy for N^{q+} ($q = 1-5$) + $H(1s)$ interaction. Same as Figure 1 except the experimental results of Phaneuf et al. [18].

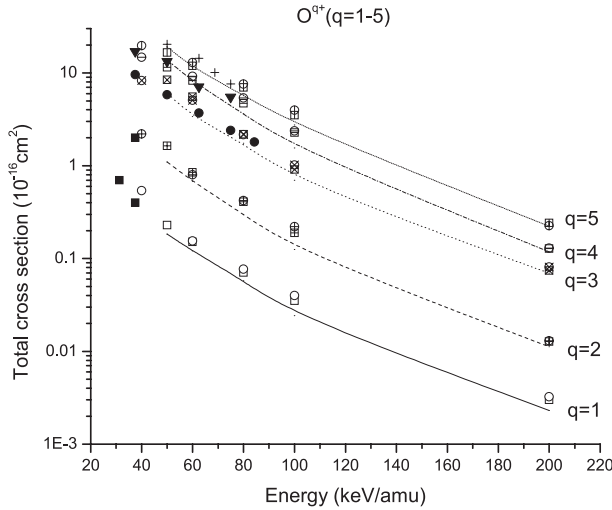


Fig. 3. Variation of total charge transfer cross-sections with energy for O^{q+} ($q = 1-5$) + $H(1s)$ interaction. Same as Figure 1 except the experimental results of Phaneuf et al. [18].

the carbon ions as projectiles overestimate the experimental findings. It may also be noted that, with increasing charge of carbon ions, present results become increasingly improved in their comparison to experimental results [20]. This observation may be explained in terms of strong continuum interaction of the active electron with the projectile ion, which is an essential feature of the present formalism. Figure 2 shows the present results for the collisions of N^{q+} ($q = 1-5$) with hydrogen atom. Here we may also notice that present calculated results agree favorably with the experimental results of Phaneuf et al. [18] except for $N^+ + H$ interaction. All the features observed in $C^{q+} + H$ interaction remain unaltered in this case as well. Figure 3 shows the comparison of our present results with the theoretical results of Dhara et al. [12], Purkait et al. [11] and the experimental observations of Phaneuf et al. [18] for $O^{q+} + H$ ($q = 1-5$) interactions. Here, we also find that

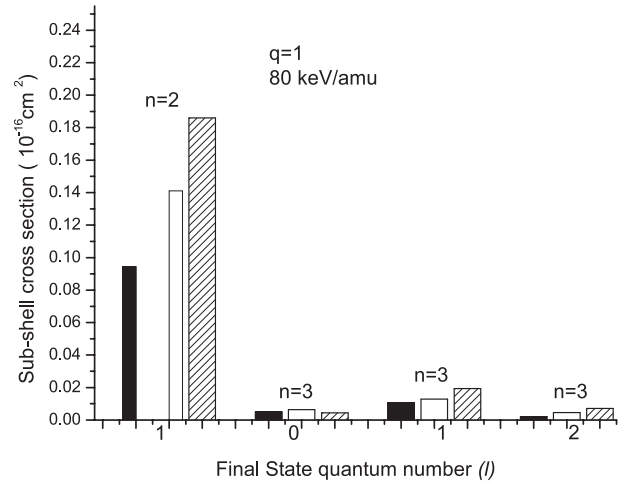


Fig. 4. Electron capture into nl levels for 80 keV/amu collision of carbon in charge state $q = 1$ with atomic hydrogen. X-axis gives the orbital-angular momentum quantum number l : (■) BCIS post (present result); (□) CB results of Dhara et al. [12]; (▨) CTMC results of Purkait et al. [11].

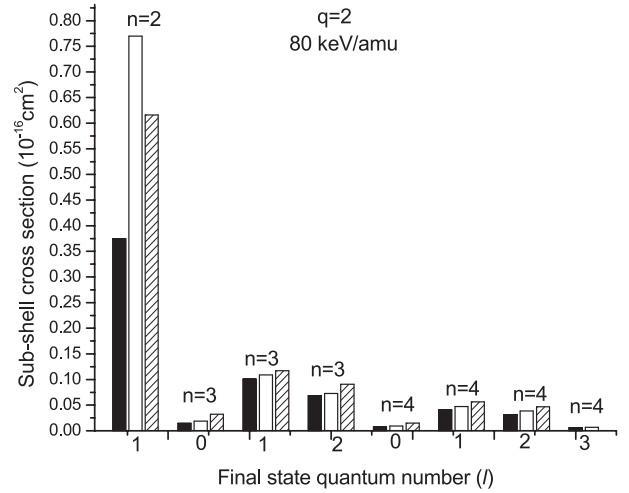


Fig. 5. Same as Figure 4. except for incident ion charge state $q = 2$.

present computed results are in better agreement with the experimental findings of Phaneuf et al. [18] in comparison to the CB results of Dhara et al. and CTMC results of Purkait et al. except for the collision of singly charged oxygen ion and atomic hydrogen. However, it may be mentioned that experimental results are available in much lower energy region for $O^+ + H$ interaction. In this case as well, observed characteristics in carbon and nitrogen ion interactions with atomic hydrogen remain unchanged. However, it may be found that, as the charge state of ions increases, discrepancies among the different sets of results for total charge transfer cross-sections for different classes of ions with same charge state diminishes. This may be due to the fact that, as charge state increases, resonant or near resonant charge transfer takes place into higher excited states and as such, the short-range part of the model potential loses its significance gradually. Again

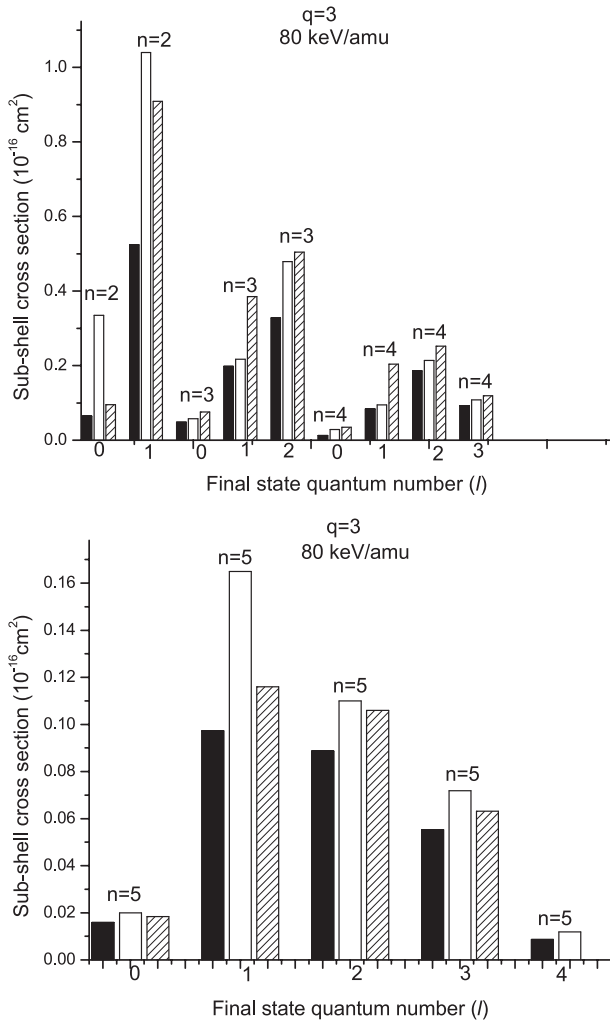


Fig. 6. Same as Figure 4 except for incident ion charge state $q = 3$.

this may be the cause of complexity for failing to find a simple q -scaling law. CTMC method is based on classical theory. Even if we accept ensemble interpretation (EI) of quantum mechanics, we may not expect very accurate data from CTMC calculation. It is well-known that the inclusion of intermediate continuum state is very important to take into account to describe a charge transfer event. Since the inclusion of intermediate continuum states is beyond the scope of CB formalism, we cannot expect very good results from such an approximation.

Sub-shell distribution of total charge transfer cross-sections for C^{q+} ($q = 1-5$) + H ($1s$) interactions have been displayed in Figures 5–8 respectively at 80 keV/amu. Due to non-availability of any other experimental results, we have compared our present computed results with those theoretical results of Purkait et al. [11] in CTMC method and of Dhara et al. [12] in CB approximation. From Figures 4 and 5, we may find that maximum contribution of total charge transfer cross-sections comes from $n = 2$ state and other shells have small contributions for C^+ and C^{2+} ions. Though the magnitude of cross-sections in dif-

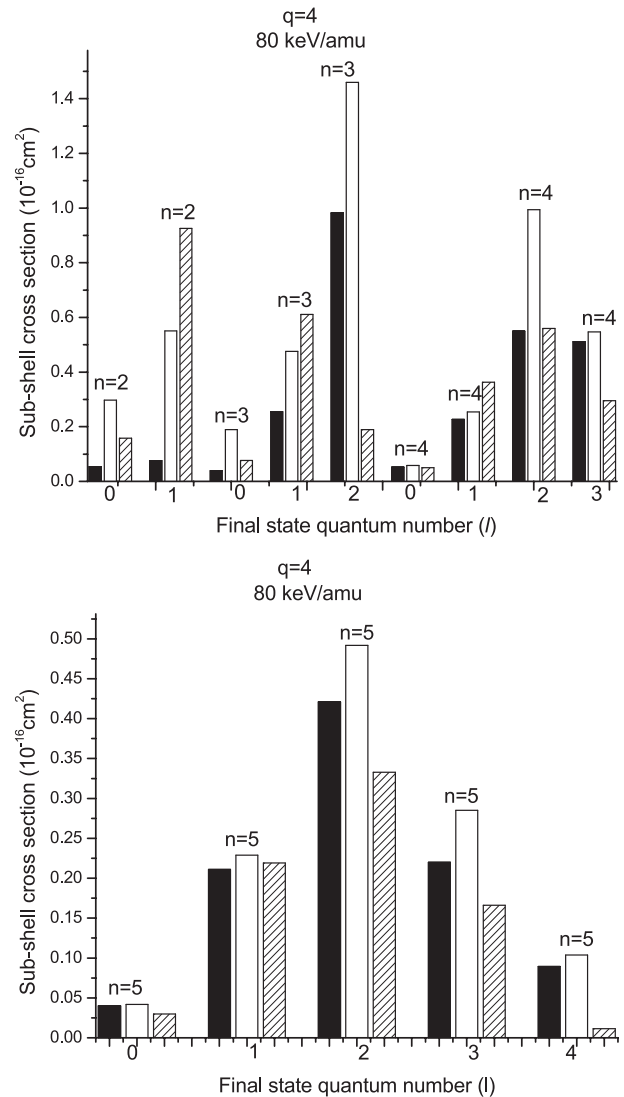


Fig. 7. Same as Figure 4 except for incident ion charge state $q = 4$.

ferent sub-shells obtained from different theoretical methods disagree to an extent, characteristic features of distribution bear more or less the same resemblance. For C^{3+} , C^{4+} and C^{5+} ions, we may find (Figs. 6–8) that the distributions of total charge transfer cross-sections obtained from different theoretical methods have marked discrepancies in magnitude but characteristic features have close resemblance. From Figures 6–8, we may find that the peaks of the cross-sections occur at $n = 3, 4$ and 4 for C^{3+} , C^{4+} and C^{5+} ions respectively. However, contribution from $n = 5$ shell is quite significant for C^{5+} ion and the total charge transfer cross-sections are convergent within 30% at all energies. For all other ions, total charge transfer cross-sections are convergent within 20%. Up to the resonating shell, it has been observed that the sub-shell distributions of total charge transfer cross-sections into a principal shell (n) have largest values at $l_{max} = n - 1$. All these characteristic features may be explained in terms of energy resonance (or near resonance)

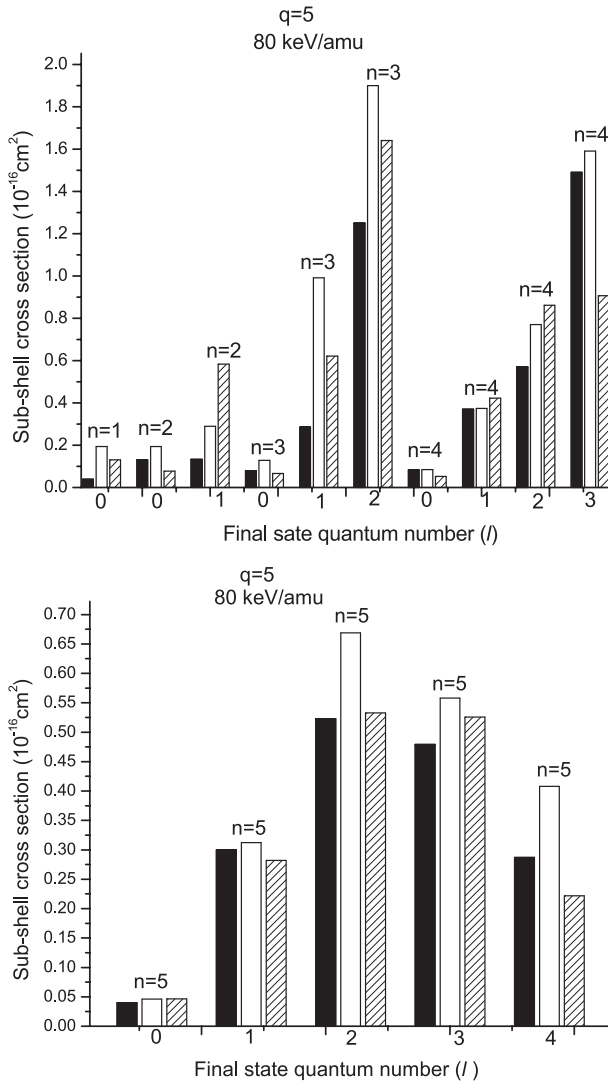


Fig. 8. Same as Figure 4 except for incident ion charge state $q = 5$.

and velocity matching of the active electron in the initial and final state. If the active electron preserves its orbital energy after the electron capture processes, Olson [37] has shown qualitatively that

$$n_f = n_i (q_f/q_i) \quad (6)$$

where n_i , n_f , q_i and q_f are the initial, final principal quantum numbers and nuclear charge seen by the active electron before and after the collision. Similarly if the electron keeps its dimension of the electron's orbit before and after the collision then

$$n_f = n_i (q_f/q_i)^{1/2}. \quad (7)$$

If these two physical properties (energy and orbital radius) are to be honoured on equal emphasis, Olson [37] has suggested that charge transfer will be maximum into a final level n_m where

$$n_m \approx n_i (q_f/q_i)^{3/4}. \quad (8)$$

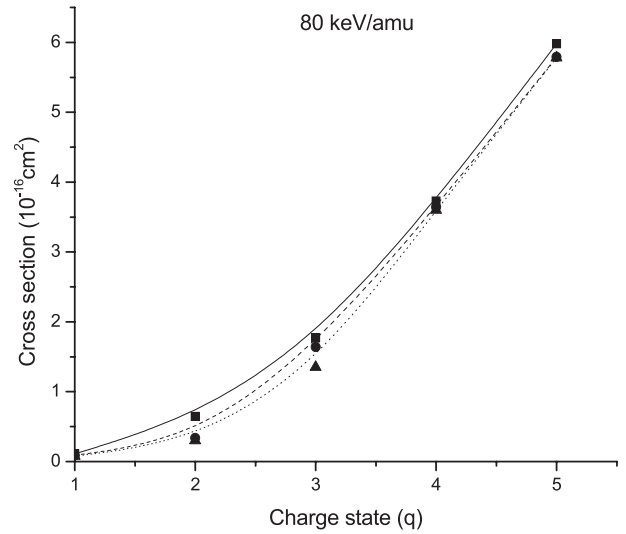


Fig. 9. Variation of total cross-sections with charge state for C^{q+} , N^{q+} and O^{q+} ($q = 1-5$) at 80 keV/amu; (■) carbon; (●) nitrogen; (▲) oxygen.

He also suggested that, for a particular n , maximum permissible l will have the dominant charge transfer cross-sections if $n < n_m$ and $l \approx n_m$ if $n > n_m$. We find by surprise that nl -distribution of our present calculated results bear more or less the same pattern as prescribed by Olson [37], and is in good agreement with Unitarized Distorted Wave (UDWA) calculations of Ryufuku and Watnabe [38].

Kim et al. [39] have observed oscillatory structure in charge state dependence of total electron capture cross-sections in collisions of Ti^{q+} , W^{q+} and Au^{q+} with atomic and molecular hydrogen at impact energies of 25–102 keV/amu. They have explained this observation in terms of interference between the amplitude obtained from short-range part and long-range part of the interaction of the active electron with the projectile ion. However, they have detected no such oscillation in case of collisions with projectiles viz. Si^{q+} , Fe^{q+} and Mo^{q+} . From Figure 9, we find no such oscillation in our calculation. The theoretical explanation for such oscillation given in the experimental paper by Kim et al. does not seem to be appealing because, as the charge state of the projectile ion increases, charge transfer into higher excited states dominate. So the effect of the short-range part of the model potential becomes increasingly small in comparison to that obtained from long-range part. As a consequence, we cannot expect significant contribution from the interference term. In addition, projectile ions under present studies are even lighter than Si^{q+} .

4 Concluding remarks

In comparison to our present theoretical findings on total charge transfer cross-sections in partially stripped ion-atom interaction with the experimental observations, it is evident that the post form of BCIS approximation in

the framework of model potential approach is reliable in case of collision problems where the asymptotic charge of the projectile ion is greater than the charge of the target nucleus. So it may be expected that the application of the prior form of BCIS approximation in the framework of model potential approach may yield good results in case of theoretical studies on ion-atom interactions where projectile charge is less than the nuclear charge. Qualitative estimates, prescribed by Olson, of the nl -distribution of the total charge transfer cross-sections has been verified satisfactorily. However, experimental investigations on sub-shell distribution of total charge transfer cross-sections for partially stripped ion-atom interactions may confirm the truth.

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