Indian J Phys. **75B** (2), 85–90 (2001)

I J P B
— an international journal

Charge transfer in the interactions of partially stripped ions with atoms at intermediate and high energies

A Dhara, M Purkait**, S Sounda and C R Mandal*
Department of Physics, Jadavpur University, Calcutta-700 032, India
E-mail : crm@juphys.ernet.in

Received 29 December 2000, accepted 7 February 2001

Abstract The Coulomb-Born (CB) approximation has been employed to study charge transfer cross sections in collisions of C^{q+}, N^{q+} and O^{q+} (q = 1–5) with atomic hydrogen in ground state in the energy range of 30–200 keV/amu The interaction of the active electron with the incoming projectile ion has been approximated by a model potential containing both a long-range part and a short-range part Variations of total capture cross sections with impact energy compare favourable well with the available experimental observations and with other theoretical findings In addition, sub-shell distributions of total capture cross sections are given in graphical form However, we are unable to find any oscillation in the charge-state dependence of total capture cross sections

Keywords . Heavy ion-atom collisions, charge transfer, cross sections.

PACS No. 34 70 +e

1. Introduction

Charge transfer data in heavy ion-atom collisions are in demand for their interdisciplinary applications [1–5] in various branches of physics. For this reason, a lot of investigations [6,7] have so far been made in studies of inelastic processes in heavy ion-atom interactions during last two decades. In this respect, most of the theoretical investigations are confined to the collisions of fully stripped ions with neutral atoms. However, some theoretical studies [8–10] have been performed for the collisions of partially stripped ions with atoms. Under such unbalanced circumstances, experimental investigations [11,12] are well balanced on both counts. Due to the growing need of accurate atomic database, studies on inelastic processes in collisions of partially stripped ions with neutral atoms are still in full swing. Due to non-existence of exhaustive charge transfer data for the collisions of C^{q+}, N^{q+} and O^{q+} (q = 1–5) with atomic hydrogen in ground state, we are motivated to study such processes. A brief review of the investigations carried out so far, for these collisional systems, are narrated below.

Olson and Salop [13] have employed the classical trajectory Monte Carlo (CTMC) stimulation method to study charge transfer cross sections in collisions of B^{q+}, C^{q+}, N^{q+} and O^{q+} ($q > 3$) with ground state atomic hydrogen. They have treated the interaction of the active electron with the projectile ion as Coulombic with an effective charge obtained from spectroscopic data. However, sub-shell distributions of total charge transfer cross sections are not available from their calculations. Eichler *et al* [14] have calculated charge transfer cross sections in collisions of different degree ions of Li, C, N and O with atomic hydrogen within the framework of Oppenheimer-Brinkman-Kramers (OBK) approximation. In their investigations, they have treated the partially stripped projectile ion as bare ion with charge equal to the asymptotic charge of the partially stripped ions. In order to compensate the over-simplified assumptions, they have successively multiplied the calculated cross sections in OBK approximation by a reduction factor obtained from eikonal approximation and the Pauli blocking factor [14]. In this calculation as well, the charge transfer cross sections into each individual sub-shell are not available.

* Corresponding Author
** Present address : Ramakrishna Mission Residential College, Narendrapur, Calcutta-700 103, West Bengal, India

Under the prevailing circumstances, we are motivated to study total charge transfer cross sections and their distributions into shell/sub-shells in collisions of C^{q+}, N^{q+} and O^{q+} (q = 1–5) with ground state atomic hydrogen within the energy range of 30–200 keV/amu. In this specified energy range, different perturbative methods are usually applied. The strength and weakness of such perturbative methods in the application of heavy ion-atom collision have been well discussed by Dewangan and Eichler [15] in their review article. We have formulated our problem in the frame-work of the Coulomb-Born (CB) approximation. The essence of the CB approximation has been well understood after the formulation of the boundary corrected first Born (B1B) [15] approximation. Applications [16–19] of the CB approximation in the three- and four-body processes have received considerable success in depicting experimental observations.

The organization of the paper is as follows. Theoretical formulations are narrated in brief in Section 2. Calculated results are discussed with graphs and tables in Sections 3. Finally, the paper ends with a concluding remark in Section 4. Atomic units are used throughout the work.

2. Theoretical formalism

The coordinate system for the charge transfer reaction

$$X^{q+} + H(1s) \rightarrow X^{(q-1)+}(nl) + H^{+}$$

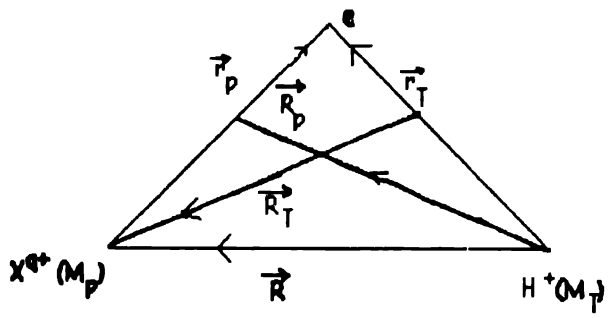

Figure 1. Coordinate representation for the reaction $X^{q+} + H(1s) \rightarrow X^{(q-1)+}(nl) + H^{+}$ (X = C, N, O and q = 1–5).

is shown in Figure 1, where X^{q+} represents C^{q+}, N^{q+} and O^{q+} (q = 1–5) ions respectively. The total hamiltonian of the whole collisional system may be written as

$$H = H_0 + V_{Te}(\boldsymbol{r}_T) + V_{pe}(\boldsymbol{r}_P) + V_{TP}(\boldsymbol{R}) \qquad (1)$$

where

$$H_0 = -\frac{1}{2\mu_i}\nabla^2_{R_T} - \frac{1}{2a}\nabla^2_{r_T} \quad \text{(entrance channel)} \qquad (2a)$$

$$\frac{1}{2\mu_f}\nabla^2_{R_P} - \frac{1}{2b}\nabla^2_{r_P} \quad \text{(exit channel)} \qquad (2b)$$

μ_i, μ_f, a and b are the reduced masses associated with relative coordinates $\boldsymbol{R}_i$, $\boldsymbol{R}_P$, $\boldsymbol{r}_i$ and $\boldsymbol{r}_P$ respectively. V subscripted by two indices represents the pair interaction between two objects which are identified as active electron (e), target ion (T), and projectile ion (P) respectively.

Constructions of these two body potentials are considered as follows. $V_{Te}(r_T)$ is uniquely determined by Coulomb potentials *i.e.* $V_{Te}(r_T) = -\frac{1}{r_T}$. Interaction of the active electron with the partially stripped projectile ion has been approximated by

$$V_{pe}(r_P) = -\frac{q}{r_P} - \frac{e^{-\lambda r_P}}{r_P}\{(Z-q) + br_P\}, \qquad (3)$$

where Z and q are respectively the nuclear charge and asymptotic charge of the projectile ion. λ and b are two arbitrary parameters chosen variationally in such a way that the corresponding hamiltonian of the active electron in the final state is diagonalised to reproduce correct binding energies with respect to a Slater basis set. Potential parameters for different ions are given in Table 1. However, accuracies

Table 1. Model potential parameters λ and b in eq. (3) are given for different

Ion	λ	b
C^{+}	2 0333	3.2930
C^{2+}	3.2280	9 2930
C^{3+}	4 2280	6 6850
C^{4+}	8 0080	8 9850
C^{5+}	10 008	3 5700
N^{+}	1 9533	1 5679
N^{2+}	3 2790	9 9932
N^{3+}	4.0074	9.9432
N^{4+}	5 4670	9 9897
N^{5+}	9.0074	9.8132
O^{+}	2 0110	0 7132
O^{2+}	3 0010	7.4682
O^{3+}	3 9490	9.9222
O^{4+}	5.3670	9.9997
O^{5+}	8.3333	5 5597

of the final state wavefunctions have been tested by the virial theorem and have been found to be accurate within 0.01%. The interaction of the projectile ion with the target nucleus has been treated as Coulombic with asymptotic charge q *i.e.* $V_{TP}(R) = \frac{q}{R}$. This is well justified because, even if some short-range part exits, charge transfer cross sections will not be affected.

With all these considerations, channel hamiltonians and interactions may be written as

Entrance channel :

$$H_i = -\frac{1}{2\mu_i}\nabla^2_{R_T} - \frac{1}{2a}\nabla^2_{r_T} - \frac{1}{r_T}, \qquad (4a)$$

$$V_i = \frac{q}{R} - \frac{q}{r_P} - \frac{e^{-\lambda r_P}}{r_P}\{(Z-q) + br_P\}, \qquad (4b)$$

Exit channel :

$$H_f = -\frac{1}{2\mu_f}\nabla^2_{R_P} - \frac{1}{2b}\nabla^2_{r_P} + \frac{q-1}{R} - \frac{q}{r_P} - \frac{e^{-\lambda r_P}}{r_P}\{(Z-q)+br_P\}, \quad (4c)$$

$$V_f = \frac{1}{R} - \frac{1}{r_T}. \quad (4d)$$

The corresponding transition matrix element may be written as

$$T_{if} = \langle \chi_f^- / V / \psi_i \rangle, \quad (5)$$

where $V = V_i$ (prior) or V_f (post). (6)

Here ψ_i and χ_f^- are defined by

$$(E - H_i)\psi_i = 0, \quad (7a)$$

$$(E - H_f)\chi_f^- = 0. \quad (7b)$$

The solution for ψ_i and χ_f^- may be written as

$$\psi_i = e^{ik_i \cdot R_T}\phi_i(r_T), \quad (8a)$$

$$\chi_f^- = e^{-\pi\alpha/2}\Gamma(1-i\alpha)e^{ik_f \cdot R_P} \times {}_1F_1\left(i\alpha;\ 1;\ -i(k_f R_P + k_f \cdot R_P)\right)\phi_f(r_P). \quad (8b)$$

Using the integral representation of a confluent hypergeometric function and choosing either form of interaction potential, the transition matrix element (T_{if}) may be written in a general form as

$$T_{if} = Ce^{-\pi\alpha/2}\Gamma(1+i\alpha)\lim_{\varepsilon_1 \to 0} D(\varepsilon_1,\beta,\lambda) \frac{1}{2\pi i}\oint dt\, t^{-i\alpha-1}(t-1)^{i\alpha} J, \quad (9)$$

where C is some constant originating from initial and final bound state wave function, $D(\varepsilon_1, \beta, \lambda)$ being the parametric differential operators to generate different higher excited states and the explicit form of J may be written as

$$J = \int dr_P dR_P e^{-ik_f \cdot R_P} \frac{e^{-\lambda r_P}}{r_P} \frac{e^{-\varepsilon R_P}}{R_P} \times e^{ik_f \cdot R_P t, ik_i \cdot R_i} \frac{e^{-\beta r_T}}{} \quad (10)$$

Here $\varepsilon = \varepsilon_1 - ik_f t$.

Taking Fourier transform of terms involving r_T, r_P and R_P and using the properties of delta function, J may be reduced as

$$J = \frac{8}{b^2}\int \frac{dQ}{\left\{|Q-q_1|^2 + \mu_1^2\right\}\left\{|Q-q_2|^2 + \mu_2^2\right\}(Q^2+\beta^2)} \quad (11)$$

where $q_1 = (1/b - a)k_i$, (12a)

$$q_2 = (1-t)k_f - a k_i, \quad (12b)$$

$$\mu_1 = \lambda/b, \quad \mu_2 = \varepsilon_1 - ik_f t. \quad (12c)$$

Using the integral representation of a general three-denominator integral of Lewis [20], J may be reduced to a simplified form as

$$J = \frac{16\pi^2}{b^2}\int_0^\infty \frac{dx}{P+Qt} \quad (13)$$

So the transition matrix element in the reduced form may be written as

$$T_{if} = Ce^{-\pi\alpha/2}\Gamma(1+i\alpha)\lim_{\varepsilon_1 \to 0} D(\varepsilon_1,\beta,\lambda)\frac{16\pi^2}{b^2} \int^\infty dx \frac{1}{2\pi i}\oint dt\, t^{-i\alpha-1}(t-1)^{i\alpha}\frac{1}{P+Qt}. \quad (14)$$

Now, the complex integration may be evaluated by Cauchy's residue to obtain the final form of the transition matrix element (T_{if}) as

$$T_{if} = Ce^{-\pi\alpha/2}\Gamma(1+i\alpha)\lim_{\varepsilon_1 \to 0} D(\varepsilon_1,\beta,\lambda) \int^\infty dx\, P^{-i\alpha-1}(P+Q)^{i\alpha}. \quad (15)$$

This one dimensional integral and the integration over scattering angles are performed numerically using 60- and 30-point Gauss Legendre quadrature method respectively to obtain the final charge transfer cross section with an accuracy of 0.1%. However, it may be pointed out that higher excited states are generated by parametric differentiations which go upto sixth order for all the purposes. All these differentiations have been carried out analytically in the present investigation.

3. Results and discussion

Charge transfer cross sections into each individual sub-shell have been obtained by multiplying the calculated cross sections for the corresponding shell by Pauli blocking factor given by

$$Q_{nl} = \left[1 - \frac{N_{nl}}{2(2l+1)}\right]Q^c_{nl}, \quad (16)$$

where Q^c_{nl} is the calculated cross sections and N_{nl} is the number of electrons occupying the sub-shell (n, l) of the incoming partially stripped projectile ion. We have displayed our calculated results for total charge transfer cross sections in comparison with other existing results (both theoretical and experimental) in Figures 2–4. Here, total cross sections have been obtained by summing up all cross sections upto the maximum principal shell, $n = 5$. Under such circumstances, it may be mentioned that the total cross sections are convergent within 20% even with the projectile ion of charge

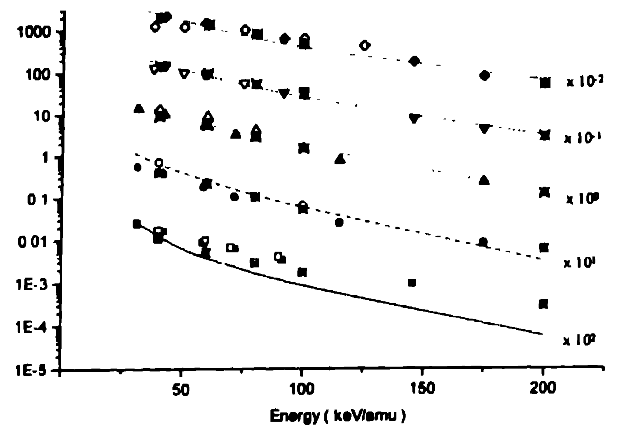

Figure 2. Variation of total capture cross sections with energies for C^{q+} (q = 1–5) + $H(1s)$ interaction.
Theory : (—, q = 1, – – –, q = 2, . . , q = 3, -----, q = 4, . . , q = 5), present CB results, (□, q = 1, O, q = 2, Δ, q = 3,), the theoretical result of Eichler *et al* [14], (∇, q = 4; ◊, q = 5), the CTMC result of Olson and Salop [13]; (⊠, q = 1; ⊗, q = 2; ▲, q = 3, ▼, q = 4, ◆, q = 5), the CTMC results of Purkait *et al* [21]
Experimental results (■, q = 1; ●, q = 2, ▲, q = 3, ▼, q = 4, ◆, q = 5), of Goffe *et al* [11]

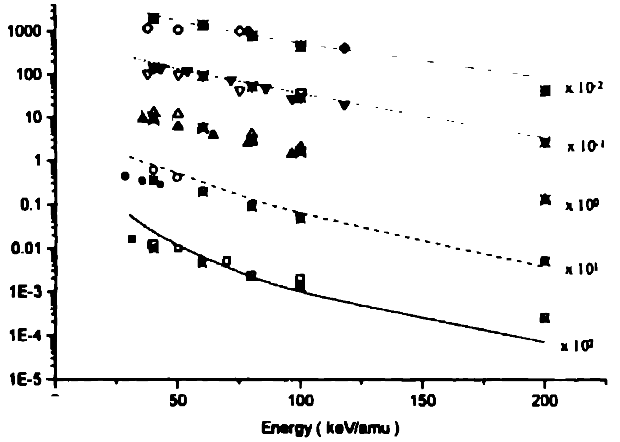

Figure 3. Variation of total capture cross sections with energies for N^{q+} (q = 1–5) + $H(1s)$ interaction.
Notations same as Figure 2 except the experimental results of Phaneuf *et al* [12].

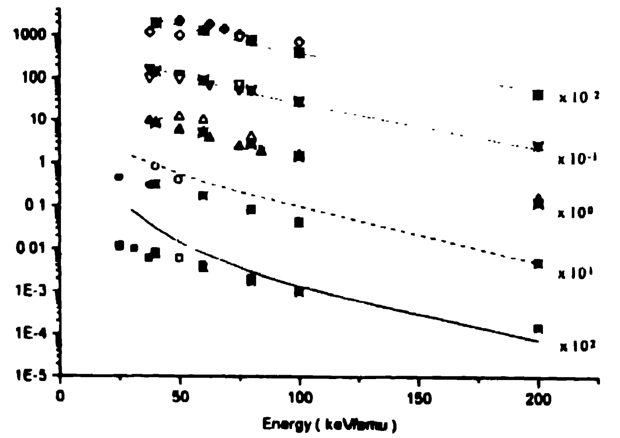

Figure 4. Variation of total capture cross sections with energies for O^{q+} (q = 1–5) + $H(1s)$ interaction
Notations same as in Figure 3

state q = 5 over the entire energy region under study. However, convergence gradually improves with decreasing charge state of the projectile ion and becomes 3% for q = 1. In the present investigation, quantitative data for sub-shell distribution of total charge transfer cross sections have not been given in tabular form and may be obtained on request. However, sub-shell distribution for total charge transfer cross sections have been given in diagrammatic form in comparison with the results of Purkait *et al* [21] in CTMC method in Figures 5–9 for N^{q+} (q = 1–5) as projectile ions

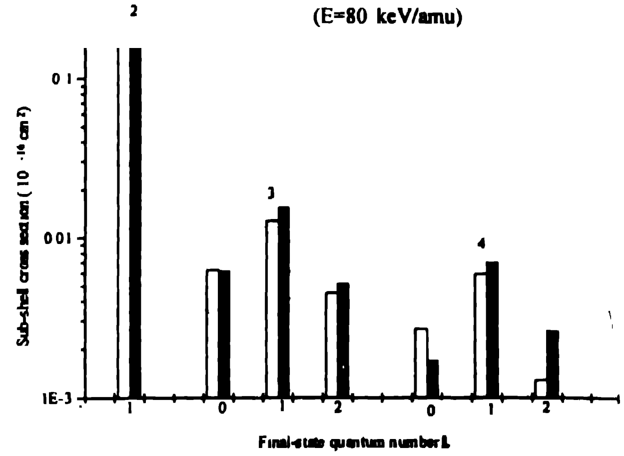

Figure 5. Electron capture into nl levels for 80 keV/amu collisions of nitrogen in charge state q = 1 with atomic hydrogen. X-axis gives the orbital-angular-momentum quantum number l.
□, CB (present work); ■, the CTMC results of Purkait *et al* [21].

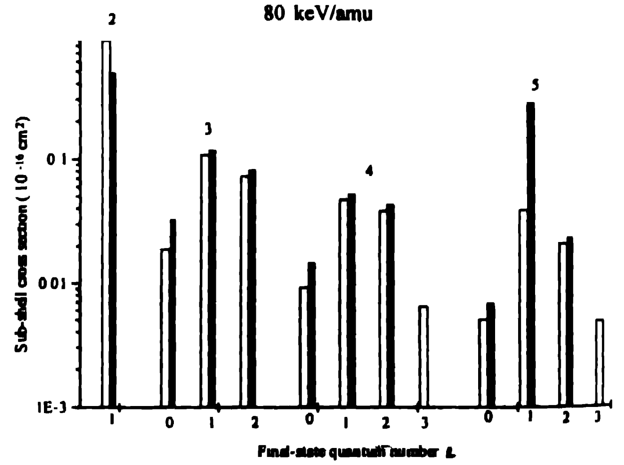

Figure 6. Same as Figure 5 except for incident ion charge state q =

only. There is no specific reason for this choice of such projectile ion because the charge transfer cross sections for other ions as well bear almost the same resemblance.

Variation of total charge transfer cross sections with impact energy for collisions of C^{q+} (q = 1–5) with atomic hydrogen has been displayed in Figure 2. From the figure, we may find that the results for C^+ ion as projectile have fair agreement with CTMC results of Purkait *et al* [21] at lower energies but disagreements are observed with increasing projectile energies. Similar pattern is observed in comparison with the eikonal results of Eichler *et al* [14] and the

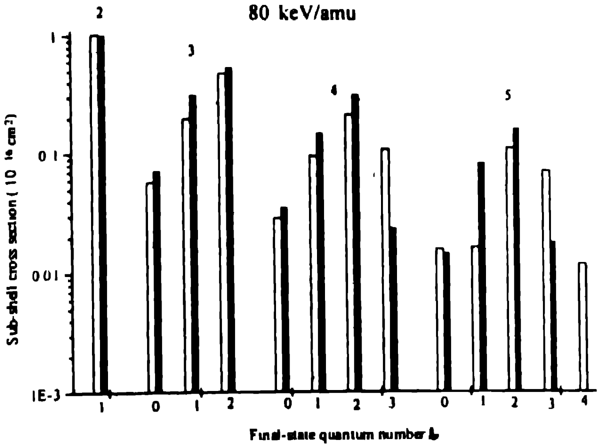

Figure 7. Same as Figure 5 except for incident ion charge state q = 3

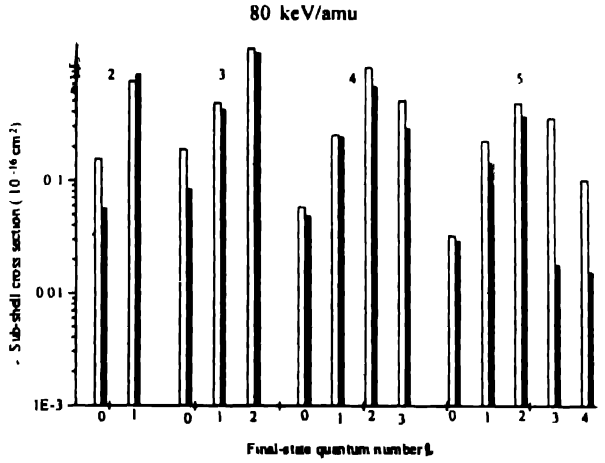

Figure 8. Same as Figure 5 except for incident ion charge state q = 4

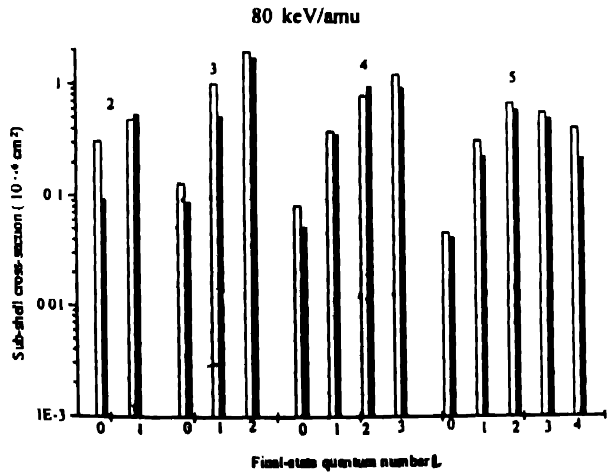

Figure 9. Same as Figure 5 except for incident ion charge state q = 5.

experimental observations of Goffe *et al* [11]. For collisions of C^{2+} ions with atomic hydrogen, our present results compare favourably well with those of Purkait *et al* [21] and the results of Eicher *et al*. Experimental results of Goffe *et al* [11] however overestimate our findings over the entire energy region. For collision of C^{q+} (q = 3–5) ions with atomic hydrogen, we may find that our calculated results in CB-approximation compare very well with all available theoretical and experimental results [11,14,21]. Exception lies only with the CTMC results of Olson and Salop [13] where their results underestimate our findings with increasing energy for the charge state of carbon ions to be 4 and 5 respectively. Energy dependence of total charge transfer cross sections in N^{q+} + H (q = 1–5) interaction is shown graphically in Figure 3. For N^+ and N^{2+} collisions, present calculated results do not have consistent agreement with the theoretical results of Eichler *et al* [14], Purkait *et al* [21] and experimental results of Phaneuf *et al* [12] over the entire energy region under consideration. However, very good agreement is observed in comparison to all available theoretical and experimental results in case of collisions N^{q+} (q = 3–5) ions with atomic hydrogen in ground state. Present computed results for total charge transfer cross sections for collision of O^{q+} (q = 1–5) with atomic hydrogen have been displayed in Figure 4. We find from the figure that the results have almost the same characteristic features as have been found in case of N^{q+} (q = 1–5) collisions. It is for general observation that the magnitude of the cross section at each energy enhances with increasing charge-state of the projectile ion. This is well justified because the capture probability increases as the strength of the potential between the active electron and the projectile ion increases.

Sub-shell distribution of total charge transfer cross sections for N^{q+} (q = 1–5) + $H(1s)$ interactions have been displayed in Figures 5–9 respectively. Due to non-availability of any other results, we have compared our results with those of Purkait *et al* [21] in CTMC method. From the figures, we may find that our quantum mechanical results in CB-approximation at 80 keV/amu compare favourably well with those of Purkait *et al* [21] in a classical method except for a few occasions. It may be observed that the peak of the charge transfer cross sections for N^+ and N^{2+} ions occurs at the principal shell n = 2. We may find that the results for N^{3+} ion, as projectile ion have their maximum value at the principal shell n = 2. However, contributions from n = 3 shell are quite appreciable in comparison to the earlier one. For collision of N^{4+} ion, charge transfer attains their maximum value at the principal shell n = 3 but significant contribution comes from n = 4 shell as well. In case of collisions with N^{5+} ion, cross sections attain their peak values at n = 3 shell. However, charge transfer into n = 4 shell is quite competitive to the previous one in this case under consideration. It is observed that the sub-shell distributions of charge transfer cross sections into a principal shell (n) have largest value at $l_{max} = n - 1$. All these characteristic features may be explained in terms of energy resonance (or near resonance) and velocity matching of the active electron in the initial and final state. However, the situation changes gradually with increasing impact energy. Non-dependence of total charge transfer cross sections on the structure of the projectile ions with charge state $q > 2$ may be due to the fact that the maximum contribution to the total cross sections come from $n \geq 3$ shell and as such, coulomb interaction is predominant in the electron-projectile sub-system in such circumstances.

Kim *et al* [22] have observed oscillations in charge dependance 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 feature in terms of interference between the amplitudes obtained from the short-range part and long-range part of the interaction of the active electron with the lighter projectile ion. However, they have found no such oscillation in case of collisions with projectiles *viz.* Si^{q+}, Fe^{q+} and Mo^{q+}. From Figure 10, we find that no such oscillation exists in our calculation. The theoretical explanation for such

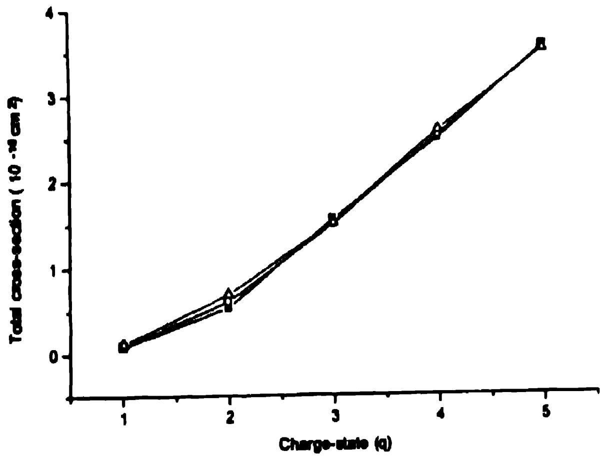

Figure 10. Variation of total cross sections with charge-state for C^{q+}, N^{q+} and O^{q+} (q = 1–5) at 100 keV/amu. ■–carbon; o–nitrogen; Δ–oxygen

oscillations given in the experimental paper by Kim *et al* [22] does not seem to be appealing because, as the charge-state of the projectile increases, charge transfer into excited states dominates. So the effect of short-range part of the potential is negligibly small in comparison to the long-range part. As a consequence, we cannot expect significant contribution from the interference term. In addition, ions under present studies are even lighter than Si^{q+}.

4. Concluding remarks

In comparison to our computed results with the experimental observations and other theoretical findings, it is evident that fair estimate of cross section may be obtained by CB-approximation in the framework of model potential approach in case of collisions of partially stripped ions with neutral atoms. However, much care has to be taken in the construction of the model potential particularly for very low charged ions As the charge state of the projectile increases, the differences among the results for charge transfer cross sections for different projectile ions with same charge diminishes as the impact energy increases. Still we are unable to find a simple q-scaling law. Good agreement of the sub-shell distributions of total charge transfer cross sections obtained from a purely quantum mechanical method and a purely classical method indicate that ensemble interpretation may be well accepted in determining the classical limit of quantum mechanical formulation.

References

[1] R K Janev (ed) *Atomic and Molecular Processes in Fusion Edge Plasmas* (New York Plenum) (1995)

[2] B H Bransden and D P Dewangan *Adv At Mol Opt Phys* **25** 343 (1998)

[3] J S Briggs and J H Macek *Adv At. Mol Phys* **28** 1 (1990)

[4] W Fritsch and C D Lin *Phys Rep* **202** 1 (1991)

[5] D S F Crothers and L J Dube *Adv At Mol Opt Phys* **30** 287 (1992)

[6] D Z Belkic, R Gayet and A Salin *At Data Nucl Data Tables* **51** 59 (1992)

[7] D P Dewangan and J Eichler *Phys Rep* **247** 59 (1994)

[8] J P Hansen and A Dubis *Phys Scr* **T62** 55 (1996)

[9] D R Schultz, P S Krstic and C O Reinhold *Phys Scr* **T62** 69 (1996)

[10] M Das, M Purkait and C R Mandal *Phys Rev* **A57** 3573 (1998)

[11] T V Goffe, M B Shah and H B Gilbody *J. Phys* **B12** 3763 (1979)

[12] R A Phaneuf, F W Meyer and R H Mcknight *Phys Rev* **A17** 534 (1978)

[13] R E Olson and A Salop *Phys Rev* **A16** 531 (1977)

[14] J Eichler, A Tsuji and T Ishihara *Phys Rev* **A23** 2833 (1981)

[15] D P Dewangan and J Eichler *J Phys.* **B18** L65 (1985), D P Dewangan and J Eichler *J Phys* **B19** 2039 (1986)

[16] C R Mandal, S Datta and S C Mukherjee *Phys Rev* **A24** 3044 (1981)

[17] D Z Belkic and I Mancev *Phys Scr* **42** 285 (1990)

[18] I Mancev *Phys Rev* **A54** 223 (1996)

[19] M Das, M Purkait and C R Mandal *J. Phys.* **B31** 4387 (1998)

[20] R R Lewis (Jr) *Phys. Rev.* **102** 537 (1956)

[21] M Purkait, A Dhara, S Sounda and C R Mandal *J. Phys* **B34** (2001)

[22] H J Kim, P Hvelplund, F W Meyer, R A Phaneuf, P H Stelson and C Bottcher *Phys. Rev. Lett.* **40** 1635 (1978)