

SINGLE ELECTRON CAPTURE INTO ARBITRARY STATES OF BARE PROJECTILES FROM MULTI-ELECTRON TARGETS

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Abstract. *The prior form of four-body boundary-corrected first Born (CB1-4B) method is applied to calculate the total cross sections for single electron capture from the K-shell of multi-electron atoms (C, N, O, Ar) by fast projectiles (H^+ , He^{2+} and Li^{3+}). All calculations are carried out for electron capture into the arbitrary n , l , and m final states of the projectiles. The present results are found to be in very good agreement with the available experimental data at intermediate and high impact energies.*

Keywords: ion-atom collisions, electron capture

1. INTRODUCTION

Single electron capture from multi-electron targets colliding with bare projectiles has attracted a great deal for decades. These processes are very important for understanding collisional interaction between fast ion and plasma in fusion experiments, or tissue in hadron therapy, or atomic systems from interstellar media in astrophysics. At low impact energies of projectiles, capture from the outer target shells is dominated. However, with the increasing incidence of energies single electron capture from inner shells has increasingly significant contributions and at high enough energies charge exchange from K-shell plays the main role. In the present work, the four-body boundary-corrected first Born (CB1-4B) approximation is used to investigate single electron capture from K-shell of the various multi-electron atomic systems into the final arbitrary shells (n , l , m) of the transferred electron, where are n , l , m principal, orbital and magnetic quantum numbers, respectively. The bound state wave functions for many-electron systems are not known exactly and this is one of the biggest problems in the calculations of the cross sections for many-electron atoms. In CB1-4B method, both of the K-shell electrons are considering as being active while the other electrons are considered as the passive. The passive electrons

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and the target nucleus form effective potential and the active electrons move in this potential. This is well known as frozen core approximation. Such an approximation is a reduction of the many-body problem to a four-body problem (two K-shell electrons, bare projectile, and effective target nucleus). The first Born approximation with the correct boundary conditions has been introduced within the three-body formalism (Belkić et al., 1979). On the other hand, the CB1-4B method was adapted and applied to single electron capture (Mančev and Milojević, 2010; Mančev et al., 2012; Mančev et al., 2013; Milojević, 2014). The CB1-4B method is a fully quantum-mechanical four-body formalism and strictly preserve the correct boundary conditions in both collisional channels. The correct Coulomb boundary conditions mean the simultaneous requirement for the correct asymptotic behaviors of the scattering wave functions in the entrance and exit channels and their proper connection with the corresponding perturbation interactions (Belkić et al., 1979; Belkić, 2004; Belkić, 2008; Belkić et al., 2008).

2. THEORY

We will examine single charge exchange between fast bare projectiles and multi-electron targets considering both K-shell electrons as active. The non-relativistic scattering theory does not count the spin effects and in this spin-independent formalism, the two active target electrons can be considered as distinguishable from each other. Accordingly, we shall consider that electron e_1 is captured, whereas electron e_2 will remain in the target rest. In such a case, e_1 and e_2 can be captured with equal probabilities and the total cross section for single electron capture should be multiplied by 2. This charge exchange process is symbolized as follows:

$$Z_p + (Z_T, e_1, e_2, \{e_3, e_4, \dots, e_N\}) \rightarrow (Z_p, e_1)_\Sigma + (Z_T, e_2, \{e_3, e_4, \dots, e_N\}), \quad (1)$$

where the set $\{e_3, e_4, \dots, e_N\}$ denotes the $N-2$ non-captured electrons which are considered as passive and Z_p and Z_T are the charge of the projectiles and target nuclei, respectively. The symbol Σ denotes the formation of the hydrogen-like systems $(Z_p, e_1)_\Sigma$ in any state. In frozen core approximation multi-electron problem (1) can be reduced to the four-body problem:

$$Z_p + (Z_T^{eff}, e_1, e_2)_{1s^2} \rightarrow (Z_p, e_1)_\Sigma + (Z_T^{eff}, e_2)_{1s}. \quad (2)$$

Where $Z_T^{eff} = Z_T - 5/16$ is the effective charge of the target nucleus, while $1s^2$ and $1s$ denote the ground states of helium-like atomic systems (Z_T^{eff}, e_1, e_2) and one-electron atomic systems (Z_T^{eff}, e_2) , respectively.

The prior form of the transition amplitude in the CB1-4B method for process (2) is given by (Mančev et al., 2012):

$$T_{if} = \iiint d\vec{x}_1 d\vec{x}_2 d\vec{R} \bar{\varphi}_{nlm}^*(\vec{s}_1) \varphi_T^*(\vec{x}_2) \left(\frac{2Z_p}{R} - \frac{Z_p}{s_1} - \frac{Z_p}{s_2} \right) \varphi_i(\vec{x}_1, \vec{x}_2) e^{-i\vec{a} \cdot \vec{R} - i\vec{v} \cdot \vec{x}_1} (vR + \vec{v} \cdot \vec{R})^{i\xi}. \quad (3)$$

Here, $\xi = (Z_p - Z_T^{eff} + 1)/v$ where v is the velocity of the projectile. The position vectors of the K-shell electrons e_1 and e_2 relative to the projectile (target nucleus) are

denoted by \vec{s}_1 and \vec{s}_2 (\vec{x}_1 and \vec{x}_2). Further, let \vec{R} be the position vector of Z_p with respect to Z_T^{eff} . The momentum transfers $\vec{\alpha}$ is defined by:

$$\vec{\alpha} = \vec{\eta} - \left(\frac{v}{2} - \frac{\Delta E}{v} \right) \vec{v} / v, \quad (4)$$

where $\Delta E = e_i - e_f$ with e_i being the binding energy of the two-electron target, $e_f = -Z_p^2 / (2n^2) - (Z_T^{eff})^2 / 2$ and the transverse component of the change in the relative linear momentum of a heavy particle is denoted by $\vec{\eta} = (\eta \cos \phi_\eta, \eta \sin \phi_\eta, 0)$ and has the property $\vec{\eta} \cdot \vec{v} = 0$. The one-electron wave functions $\varphi_{nlm}(\vec{s}_1)$ and $\varphi_T(\vec{x}_2)$ represent the bound-state wave functions of the hydrogen-like atomic systems $(Z_p, e_1)_{nlm}$ and $(Z_T^{eff}, e_2)_{1s}$, respectively. The wave function of the two-electron ground state of the atomic system $(Z_T^{eff}, e_1, e_2)_{1s^2}$ is denoted by $\varphi_i(\vec{x}_1, \vec{x}_2)$. In the present work, both of the K-shell target electrons are described by one-parameter Hylleraas wave function $\varphi_i(\vec{x}_1, \vec{x}_2) = (\beta^3 / \pi) e^{-\alpha(x_1+x_2)}$ with binding energies $e_i = -\beta^2$. We shall use two values of the parameter β and according to this, we have two different variants of the CB1-4B models. In the first case we set $\beta \equiv \beta_a = Z_T - 5/16$ obtained from a variational calculation, minimizing the binding energy for a two-electron target system with nuclear charge Z_T and this variant is labeled by CB1-4Ba. In the second case we have CB1-4Bb with $\beta \equiv \beta_b = Z_T^{eff} - 5/16$ obtained from a variational calculation, minimizing the binding energy for a two-electron atom with nuclear charge Z_T^{eff} .

After analytical calculations the original nine-dimensional integral for the transition amplitude T_{if} from Eq. (3) can be reduced to a two-dimensional integral over real variables t and t_1 . The total cross sections read:

$$Q_{if}(a_0^2) = \frac{1}{2\pi v^2} \int_0^\infty d\eta \int_0^\infty d\eta \eta |T_{if}(\vec{\eta})|^2, \quad (5)$$

where the angular integration of the orientation of vector $\vec{\eta}$ is performed analytically. The Gauss-Legendre quadrature is employed for numerical integration of this three-dimensional integral over t , t_1 and η . The integration over η is carried out after performing the change of variable $\eta = \sqrt{2(1+z)/(1-z)}$, where $z \in [-1, 1]$. This change of variable is important since it concentrates integration points near the forward cone, which provides the main contribution to the total cross sections. The numbers of integration points NGL for all calculations are varied until convergence to two decimal places and in the present calculation, their number is NGL=96. The total cross sections $Q_{tot} \equiv Q(\Sigma)$ for electron capture summed over the final states of hydrogen-like atomic systems according to the Oppenheimer n^{-3} scaling law (Oppenheimer, 1928):

$$Q_{tot} = Q_1 + Q_2 + Q_3 + 2.561Q_4. \quad (6)$$

This is justified because the contributions from the higher excited states are found to be negligible. The partial (state selective) cross sections are given by:

$$Q_n = \sum_{l=0}^{n-1} Q_{nl}, \quad Q_{nl} = \sum_{m=-l}^{+l} Q_{nlm}. \quad (7)$$

3. RESULTS AND DISCUSSIONS

In the present work, the total cross sections Q_{tot} are computed for the following single electron capture processes:

$$H^+ + C(1s^2 2s^2 2p^2) \rightarrow H(\Sigma) + C^+(1s^1 2s^2 2p^2), \quad (8)$$

$$H^+ + N(1s^2 2s^2 2p^3) \rightarrow H(\Sigma) + N^+(1s^1 2s^2 2p^3), \quad (9)$$

$$H^+ + O(1s^2 2s^2 2p^4) \rightarrow H(\Sigma) + O^+(1s^1 2s^2 2p^4), \quad (10)$$

$$H^+ + Ar(1s^2 2s^2 2p^6 3s^2 3p^6) \rightarrow H(\Sigma) + Ar^+(1s^1 2s^2 2p^6 3s^2 3p^6), \quad (11)$$

$${}^3He^{2+} + C(1s^2 2s^2 2p^2) \rightarrow {}^3He^+(\Sigma) + C^+(1s^1 2s^2 2p^2), \quad (12)$$

$${}^7Li^{3+} + C(1s^2 2s^2 2p^2) \rightarrow {}^7Li^{2+}(\Sigma) + C^+(1s^1 2s^2 2p^2). \quad (13)$$

The total cross sections from the CB1-4Ba and CB1-4Bb model for processes (8)-(11) are plotted in Figs. 1-4 by the dotted and solid lines, respectively. As can be seen from these figures at all energies the two lines display similar behavior. In Fig. 1 we can see in the case of electron capture by protons from the K-shell of the carbon the CB1-4Ba method gives good agreement with experimental results of Rødbro et al. (1979) at higher energies above 0.5 MeV and overestimate measurements at lower energies, whereas the CB1-4Bb results overestimate measurements at lower energies below 1.2 MeV but at higher energies these results are in good agreement with experimental results. At energies above 1.5 MeV, the CB1-4Bb underestimate CB1-4Ba results whereas at lower energies is opposite behaviors.

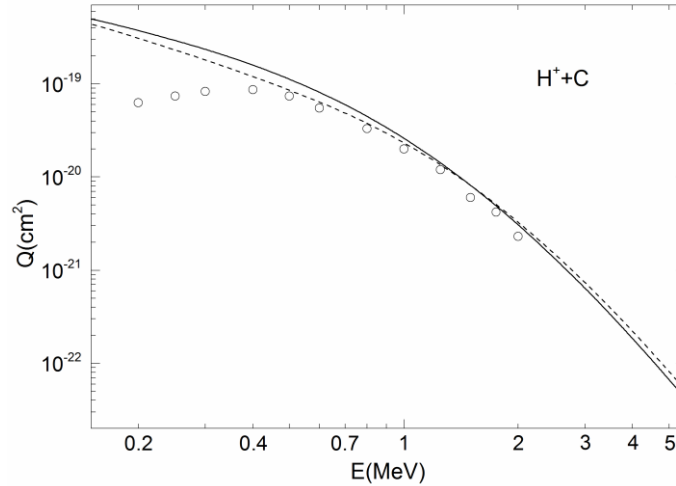


Fig. 1 Total cross sections $Q_{tot} \equiv Q(\Sigma) \equiv Q(\text{cm}^2)$ as a function of the laboratory incident energy $E(\text{MeV})$. The full curve represents CB1-4Bb results, whereas the dashed line represents the CB1-4Ba total cross sections. Experimental data: \circ Rødbro et al. (1979).

The cross sections for reactions (9) and (10) are given in Figs. 2 and 3, respectively. Both curves (CB14Ba and CB1-4Bb) describe measurements very good at a very wide interval incident energy of protons, 0.79-40 MeV for proton-nitrogen collision and 1.7-40 MeV for proton-oxygen interaction. At lower energies from 0.35 to 0.79 MeV for $H^+ - N$ collisions, the experimental results of Allison et al. (1958), Welsh et al. (1967) and Toburen et al. (1968) overestimate theoretical curves. Similarly, for $H^+ - O$ collisions at energies from 0.79 to 1.7 MeV the measurements of Varghese et al. (1983), Schryber et al. (1967) and Toburen et al. (1968) slightly overestimate our calculations. This slight disagreement between the experimental and the theory of lower energies can be explained by the fact that only the measurements of Cocke et al. (1977) correspond to electron capture from the K-shell of nitrogen and oxygen while other experiments did not isolate K-shell of the target. The contribution from the L-shell becomes significant at lower energies but at higher energies the contribution from the K-shell becomes dominant over that from the L-shell, so that in this high energy region our presented results are in very good agreement with measurements, especially is in excellent agreement with measurement of Acerbi et al. (1967;1969) at 24.7, 27.3, 32.5 and 37.7 MeV.

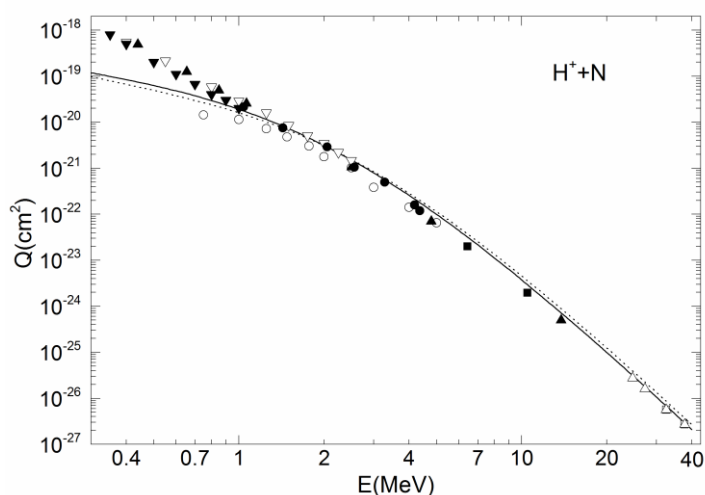


Fig. 2 The same as in Fig. 1. Experimental data: \circ Cocke et al. (1977), \blacksquare Berkner et al. (1965), \blacktriangledown Allison et al. (1958), \bullet Schryber et al. (1967), \square Acerbi et al. (1967), \triangle Acerbi et al. (1969), \blacktriangle Welsh et al. (1967), ∇ Toburen et al. (1968).

From Fig. 4 we can see that measurements of Horsdal-Pedersen et al. (1983), Macdonald et al. (1974) for single electron capture in $H^+ - Ar$ collisions underestimate both CB1-4Ba and CB1-4Bb curves, but also, in this case, excellent agreement with experimental data of Acerbi et al. (1967;1969) was observed. The theoretical curves cross each other at the energy around 10 MeV and at larger energies are very close to each other, while at lower energies CB1-4Bb slightly dominates with respect to CB1-4Ba.

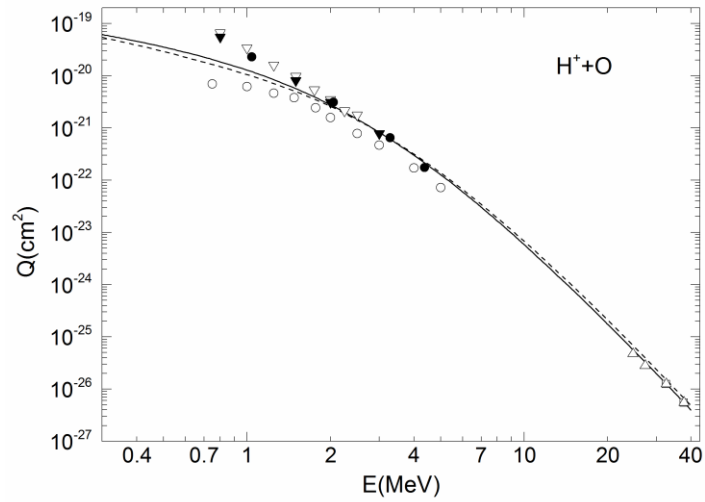


Fig. 3 The same as in Fig. 1. Experimental data: \circ Cocke et al. (1977), \blacktriangledown Varghese et al. (1985), \bullet Schryber et al. (1967), \square Acerbi et al. (1967), Δ Acerbi et al. (1969), ∇ Toburen et al. (1968).

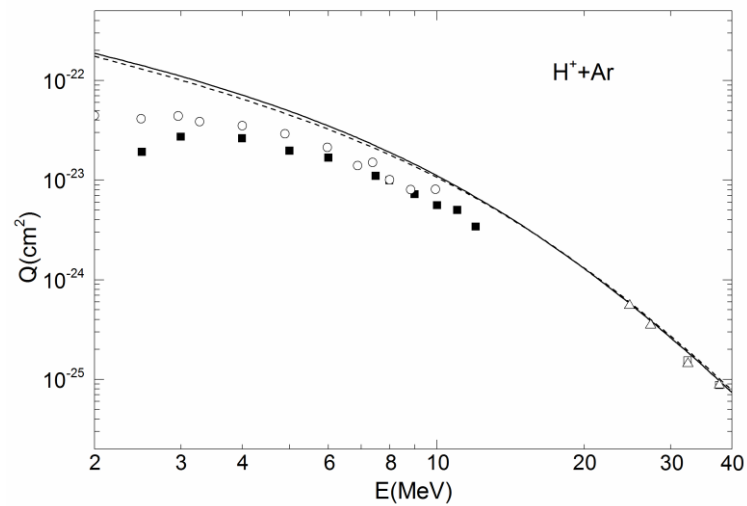


Fig. 4 The same as in Fig. 1. Experimental data: \circ Horsdal-Pedersen et al. (1983), \blacksquare Macdonald et al. (1974), \square Acerbi et al. (1967), Δ Acerbi et al. (1969).

The computed total cross sections for single electron capture from K-shell of carbon by alpha particles (${}^3\text{He}^{2+}$), process (12), are compared with available experimental data (Rødbrø et al., 1979) in Fig. 5. For this case, the present CB1-4Bb results are in a better agreement with

the measurements and at large impact energies above 1.8 MeV, this agreement is very good. The four-body CB1-4Ba and CB1-4Bb lines are significantly different, especially at lower energies.

Finally, the total cross sections for single K-shell electron capture from carbon by Li^{3+} are displayed in Fig. 6. Our CB1-4Ba and CB1-4Bb methods very well describe experimental results. Like as in all the previously discussed processes (8)-(12), in this process (13) the CB1-4Bb results dominate with respect to CB1-4Ba at lower energies, while at higher energies of CB1-4Ba total cross sections become dominant.

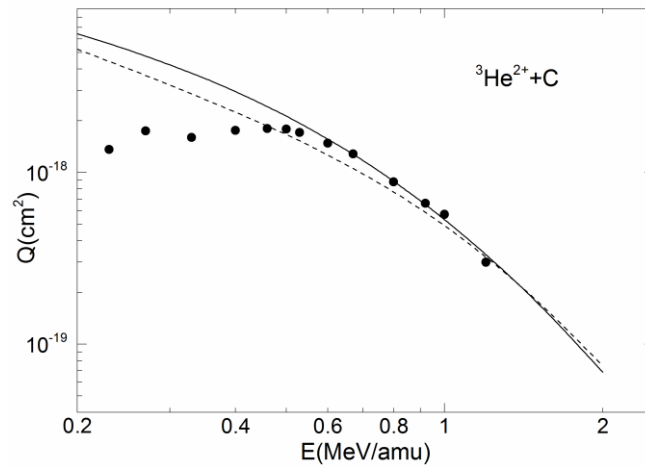


Fig. 5 The same as in Fig. 1. Experimental data: ○ Rødbro et al. (1979).

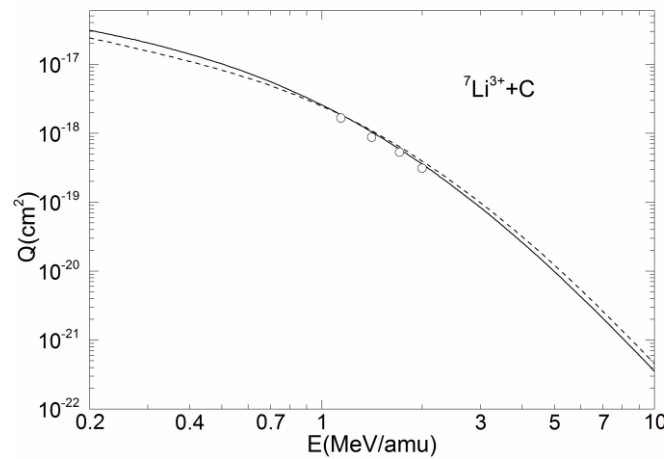


Fig. 6 The same as in Fig. 1. Experimental data: ○ Rødbro et al. (1979).

4. CONCLUSION

The high-energy prior form of the four-body first Born approximation with the correct boundary conditions (CB1-4B) was used for research single-electron capture from K-shell of neutrals atoms such as C, N, O, Ar by protons, alpha particles and nuclei of lithium. The partial cross sections are calculated for capture into the arbitrary n, l, m states of single electron projectiles in exit channels. The total cross sections $Q_{tot} \equiv Q(\Sigma)$ for electron capture summed over the final states of hydrogen-like atomic systems according to the Oppenheimer scaling law. Two variants CB1-4B (CB1-4Bb and CB1-4Ba) methods are applied and compared with existing experimental data. For $H^+ - C$, $H^+ - N$, $H^+ - O$, $H^+ - Ar$ and $Li^{3+} - C$ collisions the present CB1-4Ba and CB1-4Bb results are in very good agreement with measurements, especially at higher impact energies projectiles. On the other hand, for single electron capture in ${}^3He^{2+} - C$ collisions, only the CB1-4Bb method gives results witch in good agreement with available experimental data. In the all of the considered single electron capture processes, CB1-4Bb dominates in comparison with CB1-4Ba at lower energies, while the behavior at higher energies is the opposite.

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**JEDNOSTRUKI ZAHVAT ELEKTONA
IZ VIŠE-ELEKTRONSKIH META U PROIZVOLJNA STANJA
OGOLJENIH PROJEKTILA**

Prior forma četvoro-čestične granično korektna prva Born-ova aproksimacija je primenjena za izračunavanje totalnog efikasnog preseka za jednostruki elektronski zahvat iz K ljuske više-elektronskih atoma (C, N, O, Ar) od strane brzih projektila (H^+ , He^{2+} and Li^{3+}). Sva izračunavanja su sprovedena za elektronski zahvat u proizvoljna n , l , m konačna stanja projektila. Nađeno je da se prezentovani rezultati veoma dobro slažu sa dostupnim eksperimentalnim podacima na srednjim i visokim upadnim energijama.

Ključne reči: jon-atomski sudari, elektronski zahvat