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TWO-ELECTRON CAPTURE CROSS SECTIONS INTO GROUND STATE IN COLLISION OF BARE PROJECTILE IONS WITH HELIUM ATOM

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Double charge-transfer cross-sections from ground state of helium atoms by multiply-charged bare ions have been studied in the energy range 50 − 200 keV/amu to investigate the dependence of cross-sections on the charge state of different ions (He^{2+}, Li^{3+}, Be^{4+}, B^{5+}, C^{6+}, N^{7+} and O^{8+}). In our calculation, we have employed the four-body boundary-corrected continuum intermediate state (BCCIS-4B) approximation. The variation of double charge transfer cross sections of bare ions into the ground state is displayed versus the incident projectile energy. Due to the non-availability of any theoretical and experimental findings in that energy range for collision systems under study (Be^{4+}, B^{5+}, C^{6+}, N^{7+} and O^{8+} + He), we can not compare the present results with other data. We have also analysed differential double-capture cross sections for the collision of α-particle with helium atom at 1500 keV. The obtained results for the differential double-capture cross sections into the ground state are compared with the experimental data and a satisfactory agreement has been obtained.

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Keywords: double capture cross sections, differential cross section, continuum state wavefunction, bare ions

1. Introduction

Theoretical and experimental investigations on double charge transfer cross sections of helium atoms by multi-charged bare ions are still in full expansion due to their connection with the practical aspects of controlled thermo-nuclear fusion development as well as astrophysics, ion-penetration in solids and also in radiation

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physics. Different theories such as continuum distorted wave (CDW) method by Gayet et al. [1] and Ghosh et al. [2], continuum distorted wave – eikonal initial state (CDW-EIS) by Gayet et al. [3], the impulse approximation by Gravielle and Miraglia [4] and classical trajectory Monte Carlo method by Olson [5] have been used to study the two-electron transfer by the independent event model (IEM) and the independent particle model (IPM).

Belkić and Mancev [6] proposed the full quantum-mechanical four-body formalism of two-electron capture cross sections in proton-helium collisions using CDW approximation (CDW-4B). The results are in good agreement with the existing experimental data. Double charge exchange in fast collisions of He^{2+} and Li^{3+} ions with helium atoms have been investigated by Belkić [7, 8] by the method of boundary-corrected first Born (CB1) approximation. The calculated results are in excellent agreement with the experimental observations. Later, Belkić himself and his collaborators [9, 10] developed the four-body formalism of boundary-corrected continuum intermediate state (BCIS-4B) approximation and the second-order Born distorted wave (BDW-4B) approximation to calculate the two electron capture cross sections in the high-energy region. The CB1 method [7, 8] is the simplified version of the boundary-corrected continuum intermediate state (BCIS-4B) approximation [9]. The simplification is the replacement of the full two-electron Coulomb wave functions from the BCIS method by the corresponding long-range logarithmic phase factor [7, 8] that have been defined in terms of the inter-aggregate separation. Gayet et al. [11] studied two-electron captures in the framework of the CDW-4B theory in the energy range 400 keV – 30 MeV. They have calculated the double electron capture cross sections into the ground state, singly excited state and doubly excited states from He atom by the impact of He^{2+}, Li^{3+} and B^{5+} ions, respectively. Purkait et al. [12] also investigated the double charge transfer cross sections into the same states (ground, singly and doubly excited states) for the collisions of α-particles with helium atoms in the energy range 50 – 500 keV/amu and studied the double electron capture cross sections into the ground states in collisions of $^{7}Li^{3+}$ and $^{10}B^{5+}$ with helium atoms. Purkait et al. [12] formulated the problem using the prior form of four-body boundary-corrected continuum intermediate state (BCCIS-4B) approximation. The total double electron capture cross sections in collisions of α-particle and Li^{3+} with helium atoms are well reproduced in comparison to the experimental results in the collision energy range 50 – 500 keV/amu. An extensive review of such investigations by Belkić et al. [13] is worth mentioning.

In our present work, we employed the prior and the post form of BCCIS-4B approximation to determine the double charge transfer cross sections into the ground state in the collision of bare projectile ions (He^{2+}, Li^{3+}, Be^{4+}, B^{5+}, C^{6+}, N^{7+} and O^{8+}) with helium atom in the energy range 50 – 200 keV/amu and also investigated the dependence of cross sections on the charge state of different bare ions. Viewing on the success of earlier investigation [12], we are motivated to build up the data bank in the specified energy range.

The organization of the paper is as follows. Section 2 contains the theoretical formulation of the problem. Results and discussion are presented in Section 3. Finally, in Section 4 conclusions are given.

2. Theory

The double electron capture from helium atom by the fully stripped projectile ions ($^4He^{2+}$, $^7Li^{3+}$, $^9Be^{4+}$, $^{10}B^{5+}$, $^{12}C^{6+}$, $^{14}N^{7+}$ and $^{16}O^{8+}$) may be represented by

$$Z_P + (Z_T; e_1, e_2)_i \to (Z_P; e_1, e_2)_f + Z_T \,, \tag{1}$$

where Z_P and Z_T are, respectively, the nuclear charges of the projectile and the target, e_1 and e_2 are the two electrons initially bound to the target nucleus and finally bound to the projectile. $\vec{s}_{1,2}$ and $\vec{x}_{1,2}$ have been labelled as the position vectors of the electrons $e_{1,2}$ relative to Z_P and Z_T, respectively. In terms of these vectors, the inter-electron distance $\vec{r}_{1,2}$ is given by $\vec{r}_{1,2} = |\vec{s}_1 - \vec{s}_2| = \vec{s}_{1,2} = |\vec{x}_1 - \vec{x}_2| = \vec{x}_{1,2}$. Let $\vec{R}$ be the position vector of the projectile (P) relative to the target (T) nucleus. In the entrance channel, it is convenient to introduce $\vec{R}_T$ as the relative vector of the projectile with respect to the center of mass of $(Z_T; e_1, e_2)_i$. Symmetrically, we denote by $\vec{R}_P$ the relative vector of the target with respect to the center of mass of $(Z_P; e_1, e_2)_f$ in the exit channel.

The "prior" and "post" total cross sections in the BCCIS-4B method are given by

$$Q_{if}^{\mp} = \frac{\mu_i \mu_f}{4\pi^2} \frac{k_f}{k_i} \int \left| T_{if}^{\mathrm{BCCIS}(\mp)} \right|^2 \mathrm{d}\Omega \,, \tag{2}$$

where μ_i and μ_f are the initial and final reduced masses, k_i and k_f are the initial and final relative momenta of the colliding systems and Ω is the solid angle around k_i.

The prior form of the transition amplitude in the BCCIS-4B method may be written as

$$\begin{aligned} T_{if}^{\mathrm{BCCIS}(-)} = N \iiint & \mathrm{d}\vec{x}_1 \mathrm{d}\vec{x}_2 \mathrm{d}\vec{R}\ \mathrm{e}^{-\mathrm{i}\vec{k}_f \cdot \vec{R}_P} \varphi_f^*(\vec{s}_1, \vec{s}_2)\ {}_1F_1(\mathrm{i}\alpha_1; 1; z_1)\ {}_1F_1(\mathrm{i}\alpha_2; 1; z_2) \\ & \times {}_1F_1(-\mathrm{i}\alpha_3; 1; z_3) \varphi_i(\vec{x}_1, \vec{x}_2) \left(\frac{Z_P Z_T}{R} - \frac{Z_P}{s_1} - \frac{Z_P}{s_2} \right) \mathrm{e}^{\mathrm{i}\vec{k}_i \cdot \vec{R}_T} \,, \end{aligned} \tag{3}$$

where

$$z_1 = \mathrm{i}(v_f x_1 + \vec{v}_f \cdot \vec{x}_1), \quad z_2 = \mathrm{i}(v_f x_2 + \vec{v}_f \cdot \vec{x}_2), \quad z_3 = \mathrm{i}(k_f R_T + \vec{k}_f \cdot \vec{R}_T), \quad \alpha_1 = \alpha_2 = \frac{Z_T}{v_f},$$

$$\alpha_3 = \frac{Z_P Z_T}{v_f}, \quad N = \mathrm{e}^{(\pi/2)(\alpha_1 + \alpha_2 - \alpha_3)} \Gamma(1 + \mathrm{i}\alpha_1) \Gamma(1 + \mathrm{i}\alpha_2) \Gamma(1 - \mathrm{i}\alpha_3) \,,$$

and the integral representation of the hypergeometric function is given by

$${}_1F_1(\mathrm{i}\alpha; 1; z) = \frac{1}{2\pi\mathrm{i}} \oint \mathrm{d}t\, (t-1)^{-\mathrm{i}\alpha}\, t^{\mathrm{i}\alpha - 1}\, \mathrm{e}^{tz} \,.$$

The post form of the transition amplitude can be written as

$$T_{if}^{\mathrm{BCCIS}(+)} = N \iiint \mathrm{d}\vec{s}_1 \mathrm{d}\vec{s}_2 \mathrm{d}\vec{R}\, \mathrm{e}^{-\mathrm{i}\vec{k}_f\cdot\vec{R}_P} \varphi_f^*(\vec{s}_1,\vec{s}_2)\ {}_1F_1(\mathrm{i}\alpha_1;1;z_1)\ {}_1F_1(\mathrm{i}\alpha_2;1;z_2)$$
$$\times\ {}_1F_1(-\mathrm{i}\alpha_3;1;z_3)\, {}_1F_1(-\mathrm{i}\alpha_4;1;z_4) \left(\frac{2Z_T}{R} - \frac{Z_T}{x_1} - \frac{Z_T}{x_2}\right) \varphi_i(\vec{x}_1,\vec{x}_2) \mathrm{e}^{\mathrm{i}\vec{k}_i\cdot\vec{R}_T}\,, \qquad (4)$$

where

$$z_1 = \mathrm{i}b_1(v_i s_1 + \vec{v}_i\cdot\vec{s}_1),\ z_2 = \mathrm{i}b_1(v_i s_2 + \vec{v}_i\cdot\vec{s}_2),\ z_3 = \mathrm{i}(k_f R_P + \vec{k}_f\cdot\vec{R}_P),\ z_4 = \mathrm{i}(k_i R_P - \vec{k}_i\cdot\vec{R}_P),$$

$$\alpha_1 = \alpha_2 = \frac{Z_P}{v_i}, \quad \alpha_3 = \frac{Z_P Z_T}{b_1 v_i}, \quad \alpha_4 = \frac{Z_T(Z_P-2)}{v_f}, \quad b_1 = \frac{M_P}{2+M_P}\,,$$

$$N = \mathrm{e}^{(\pi/2)(\alpha_1+\alpha_2-\alpha_3-\alpha_4)}\Gamma(1-\mathrm{i}\alpha_1)\Gamma(1-\mathrm{i}\alpha_2)\Gamma(1+\mathrm{i}\alpha_3)\Gamma(1+\mathrm{i}\alpha_4)\,.$$

In both the cases, $\varphi_i(\vec{x}_1,\vec{x}_2)$ and $\varphi_i(\vec{s}_1,\vec{s}_2)$ are the uncorrelated one-parameter orbital-type wavefunctions with effective charges $Z_{\mathrm{eff}} = Z_i - 0.3125$, $(i = P, T)$ and Z_i is the nuclear charge.

The "prior" form of the transition amplitude contains three-dimensional integrals such as Lewis, Feynmann and a complex contour integration, but the "post" form of the transition amplitude contains four-dimensional integrals such as Lewis, Feynmann and two complex contour integrations. The complex contour integration is changed into real integral from 0 to 1 which has been sub-divided into several parts and each sub-division is integrated using Gauss-Laguerre quadrature method. The Lewis and Feynmann integrals have been performed numerically by the Gauss-Legendre quadrature method. The Lewis integral and the Feynmann integral are evaluated numerically with the 60-point and 48-point Gauss-Legendre quadrature method, respectively. Finally, integration over the scattering angles has been performed with the 44-point Gauss-Legendre quadrature method.

3. *Results and discussion*

The double electron capture cross section into ground state in collisions of different fully stripped ions with helium atoms in the energy range 50 – 200 keV/amu are plotted in Fig. 1 by using the post form of BCCIS-4B approximation and are also displayed in Table 1 by using the prior and the post form of BCCIS-4B approximation. Variation of double capture cross sections with charge states at different energies are displayed in Fig. 2. The results of differential double capture cross sections for He^{2+} + He collisions is shown in Fig. 3 and in Table 2 at incident projectile energy 1500 keV.

In Fig. 1 we display the double electron capture cross sections into ground state for He^{2+} + He symmetric collisions along with some asymmetric collisions

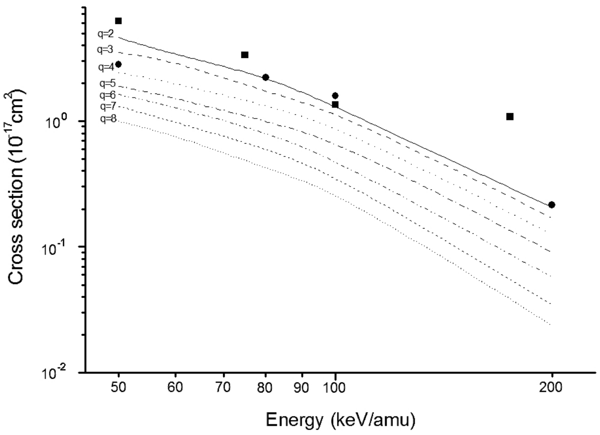

Fig. 1. Variation of double charge transfer cross sections into ground state as a function of projectile energy for the interaction of bare projectiles (X^{q+}; $q = 2-8$) *with helium atom. Theory: Present BCCIS-4B results in post form: solid line,* $q = 2$*; dash,* $q = 3$*; dot,* $q = 4$*, dash-dot,* $q = 5$*; dash-dot-dot,* $q = 6$*; short dash,* $q = 7$*; short-dot,* $q = 8$*. Experiments: Filled square, results of DuBois [14] for* He^{2+} *impact; filled circle, results of Shah and Gilbody [15] for* Li^{3+} *impact.*

TABLE 1. The present double electron ground state capture cross sections $Q_{if}^{\mathrm{BCCIS-4B}(\mp)}$ *for different bare ions as a function of the incident energy* E_{lab} (keV/amu)*. The numbers in the brackets denote multiplicative powers of ten.*

Energy	He^{2+}		Li^{3+}		Be^{4+}	
(keV/amu)	Prior	Post	Prior	Post	Prior	Post
50	3.32(-1)	4.55(-1)	2.35(-1)	3.48(-1)	1.61(-1)	2.43(-1)
60	2.89(-1)	3.35(-1)	2.25(-1)	3.00(-1)	1.47(-1)	2.01(-1)
80	2.00(-1)	2.28(-1)	1.75(-1)	1.70(-1)	1.09(-1)	1.32(-1)
100	1.15(-1)	1.30(-1)	1.00(-1)	1.21(-1)	7.60(-2)	9.28(-2)
200	2.05(-1)	2.06(-2)	1.82(-2)	1.70(-2)	1.72(-2)	1.25(-2)

Energy	B^{5+}		C^{6+}		N^{7+}		O^{8+}	
$\left(\frac{\mathrm{keV}}{\mathrm{amu}}\right)$	Prior	Post	Prior	Post	Prior	Post	Prior	Post
50	1.22(-1)	1.87(-1)	1.05(-1)	1.64(-1)	9.24(-2)	1.31(-1)	6.90(-2)	1.00(-1)
60	1.14(-1)	1.54(-1)	9.40(-2)	1.29(-1)	6.96(-2)	9.79(-2)	5.50(-2)	7.77(-2)
80	7.00(-2)	9.90(-2)	6.20(-2)	8.24(-2)	4.50(-2)	6.10(-2)	2.90(-2)	4.20(-2)
100	5.02(-2)	7.13(-2)	3.79(-2)	4.93(-2)	3.00(-2)	3.78(-2)	1.55(-2)	2.84(-2)
200	7.75(-3)	9.01(-3)	4.70(-3)	5.76(-3)	2.75(-3)	3.46(-3)	1.60(-3)	2.35(-3)

TABLE 2. Differential cross sections $\left(\mathrm{d}Q^{\pm}_{if}/\mathrm{d}\Omega\right)_{\mathrm{lab}}$ ($\mathrm{cm}^2/\mathrm{sr}$) *as a function of the scattering angle* $\theta \equiv \theta_{\mathrm{lab}}$ (mrad) *at the incident energy* $E_{\mathrm{lab}} = 1500$ keV *for the double charge exchange reaction* ${}^4\mathrm{He}^{2+} + {}^4\mathrm{He}(1\mathrm{s}^2) \rightarrow {}^4\mathrm{He}(1\mathrm{s}^2) + {}^4\mathrm{He}^{2+}$. *The numbers in the brackets denote multiplicative powers of ten.*

	$\left(\mathrm{d}Q^{\pm}_{if}/\mathrm{d}\Omega\right)_{\mathrm{lab}}$			$\left(\mathrm{d}Q^{\pm}_{if}/\mathrm{d}\Omega\right)_{\mathrm{lab}}$	
θ (mrad)	Prior	Post	θ (mrad)	Prior	Post
0.0000	5.55(-13)	5.88(-13)	0.2100	1.60(-14)	1.74(-14)
0.0125	5.00(-13)	5.24(-13)	0.2250	1.58(-14)	1.77(-14)
0.0250	4.21(-13)	4.40(-13)	0.2300	1.56(-14)	1.75(-14)
0.0375	3.00(-13)	3.14(-13)	0.2400	1.53(-14)	1.69(-14)
0.0500	2.20(-13)	2.38(-13)	0.2500	1.49(-14)	1.57(-14)
0.0625	1.38(-13)	1.58(-13)	0.2750	1.38(-14)	1.48(-14)
0.0750	5.80(-14)	6.02(-14)	0.3000	1.19(-14)	1.28(-14)
0.0875	3.45(-14)	3.55(-14)	0.4000	5.11(-15)	5.41(-15)
0.1000	2.48(-14)	2.49(-14)	0.4250	4.50(-15)	4.52(-15)
0.1050	1.97(-14)	2.20(-14)	0.4500	4.00(-15)	4.11(-15)
0.1100	1.75(-14)	1.86(-14)	0.5000	3.00(-15)	3.02(-15)
0.1200	1.46(-14)	1.53(-14)	0.5250	2.45(-15)	2.50(-15)
0.1300	1.30(-14)	1.38(-14)	0.5500	2.19(-15)	2.22(-15)
0.1400	1.28(-14)	1.34(-14)	0.6000	1.50(-15)	1.61(-15)
0.1500	1.32(-14)	1.34(-14)	0.6250	1.31(-15)	1.35(-15)
0.1550	1.28(-14)	1.38(-14)	0.6500	1.09(-15)	1.16(-15)
0.1600	1.30(-14)	1.40(-14)	0.7000	8.59(-16)	9.00(-16)
0.1750	1.40(-14)	1.54(-14)	0.7500	6.50(-16)	7.03(-16)
0.1800	1.48(-14)	1.61(-14)	0.8000	5.27(-16)	5.31(-16)
0.1850	1.51(-14)	1.64(-14)	0.8250	4.61(-16)	4.75(-16)
0.1900	1.53(-14)	1.67(-14)	0.8500	4.27(-16)	4.32(-16)
0.1950	1.55(-14)	1.70(-14)	0.9000	3.15(-16)	3.28(-16)
0.2000	1.58(-14)	1.73(-14)			

like $X^{q+} + He(1s^2) \rightarrow X^{(q-2)+}(1s^2) + He^{2+}$, where $q = 3, 4, 5, 6, 7$ and 8 by using the post form of BCCIS-4B approximation. The present BCCIS-4B results in collisions of He^{2+}/Li^{3+} ions with He atom are in good agreement with the experimental observations in the collision energy range $50-200$ keV/amu. We have only displayed the experimental results of DuBois [14] in the case of $He^{2+} + He$ collision and experimental results of Shah and Gilbody [15] have been shown for comparison with the present results for the $Li^{3+} + He$ collision. Ground to ground state capture is dominant in the case of $He^{2+} + He$ collision. This feature can be explained as follows: The ground state is a resonating state and the capture takes place predominantly to the nucleus where high energy electron momentum components are appreciable for symmetric and near symmetric collisions. But in the case of projectile ions Be^{4+}, B^{5+}, C^{6+}, N^{7+} and O^{8+}, the ground state capture contributes little. It is expected that contributions from excited states may be significant in the case of asymmetric collision. In the prior form of BCCIS-4B approximation, we look at charge transfer as the target ionization averaged over final state momentum distribution and inclusion of target continuum states is essential where $Z_P < Z_T$. In Fig. 2, variations of ground state capture cross sections from the post form of BCCIS-4B method with charge state for different ions at different energies are displayed. It has been found that the charge state increases from 2 to 8, the variation of ground state capture cross sections at different energies 50, 100 and 200 keV/amu diminishes very slowly. Here the post-prior discrepancy is well within 25% for symmetric collisions and within 35% for asymmetric collisions in the entire energy region.

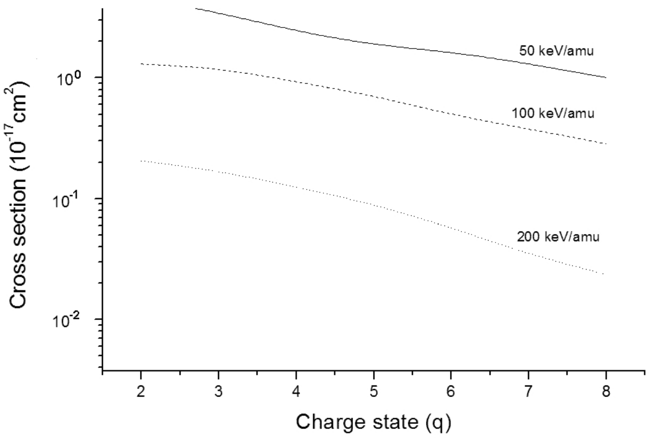

Fig. 2. Variation of double charge transfer cross sections into ground state as a function of charge state ($q = 2 - 8$) of different bare projectile ions at different energies. Theory: Present BCCIS-4B results in post form: solid line represents the results at 50 keV/amu*; dash, at 100* keV/amu*; dot, at 200* keV/amu.

The differential double electron capture cross sections both in prior and post results are shown in Fig. 3 at incident energy 1500 keV and compared with other

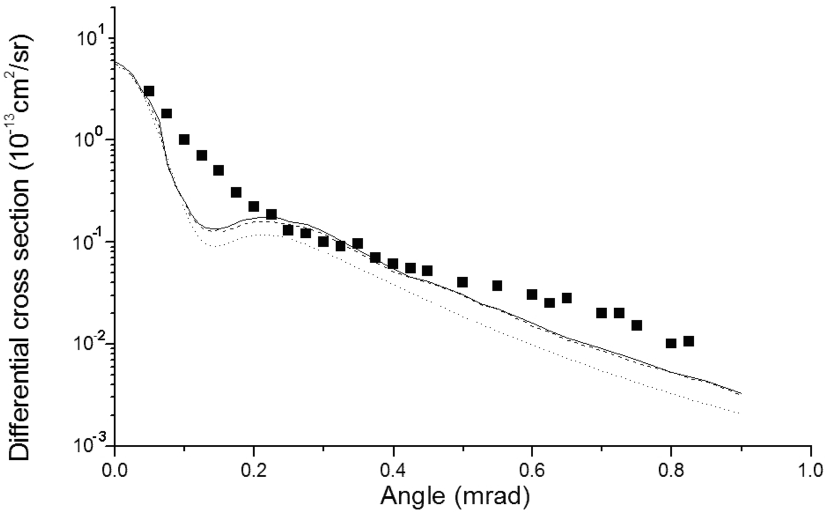

Fig. 3. Differential double capture cross sections in $He^{2+} + He$ *collisions for projectile energy 1500* keV*. Theory: Solid line, present BCCIS-4B results in post form; dash, results of BCCIS-4B in prior form [12]; dot, BCIS-4B results of Belkić [9]. Experiment: Filled square, results of Schuch et al. [16].*

theoretical results of Belkić [9] and experimental results of Schuch et al. [16] in connection with α-particle impact with helium atom. From this graph, we observe the Thomas peak at the energy 1500 keV around the critical angle 0.225 mrad which has already been observed in the calculation of Belkić [9]. But above 0.3 mrad, our results overestimate the results of Belkić and are in good agreement with experimental results of Schuch et al. Below 0.15 mrad, our BCCIS-4B results are in excellent agreement with the results of Belkić and experimental results of Schuch et al. [16].

4. *Conclusions*

Present calculation incorporates target continuum states in the framework of prior form of BCCIS-4B approximation. But in the case of asymmetric collision where $Z_P > Z_T$, post form of BCCIS-4B approximation is appropriate as projectile continuum states are to be taken into account. Double electron transfer cross sections into singly and doubly excited states are also calculated for asymmetric collision systems in order to complete present data bank. In the initial and final states, only static correlation of the electrons has been included and dynamic correlation effect is absent in our calculation. For a two electron transfer process in an asymmetric collision, dynamic correlation is important to test the validity of BCCIS-4B approximation. We observe that the post-prior discrepancies increase with increasing charge state. Experimental results for two electron capture cross sections for asymmetric collision in the intermediate energy region are scarce. More refined experiments regarding two electron transfers are much needed to sort out the discrepancies.

Acknowledgements

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UDARNI PRESJECI DVOELEKTRONSKOG UHVATA IZ HELIJEVIH ATOMA U OSNOVNO STANJE GOLIH UPADNIH IONA

Proučavamo udarne presjeke za prijelaz dvaju elektrona u osnovnom stanju helija u upadne potpuno gole ione energije $50-200$ keV/amu radi istraživanja ovisnosti udarnih presjeka o višestrukosti ionizacije upadnih iona (He^{2+}, Li^{3+}, Be^{4+}, B^{5+}, C^{6+}, N^{7+} i O^{8+}). Primijenili smo približenje međustanja u kontinuumu s graničnom popravkom za četiri tijela (BCCIS-4B). Predstavljamo energijsku ovisnost udarnih presjeka za prijelaz dvaju elektrona u osnovnom stanju helija u upadne potpuno gole ione. Zbog manjka teorijskih i eksperimentalnih podataka o proučavanim sustavima (Be^{4+}, B^{5+}, C^{6+}, N^{7+} and O^{8+} + He) u tom području energije nismo u mogućnosti načiniti usporedbe s drugim podacima. Također smo analizirali diferencijalne udarne presjeke za dvostruki uhvat u sudaru α-čestice s helijevim atomom na 1500 keV. Postignuti ishodi za diferencijalne udarne presjeke dvojnog uhvata se uspoređuju s eksperimentalnim podacima i postignuto je dobro slaganje.