Single Electron Capture Cross-Sections in Ion-Helium Collisions

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Abstract: ***This research presents a calculation of single-electron capture cross-sections resulting from the collision of helium atoms with a variety of projectile ions-specifically He^{2+}, Li^{q+} (where q=1,2,3), C^{6+}, and O^{8+} over an incident energy spectrum ranging from 50 to 5000 keV/amu. We employed the four-body boundary corrected continuum intermediate state (BCCIS-4B) formalism, utilizing both the post and prior forms to ensure robust analysis. This theoretical framework is specifically designed to account for distortions in the final channel arising from Coulomb continuum states associated with the projectile ion and the active electron within the field of the residual target ion. By summing the contributions from shells and sub-shells up to n=3, we derived the total cross-sections for single-electron capture. Our findings suggest that while capture into excited states is a dominant factor in asymmetric collisions (where the projectile charge Z_P exceeds the target charge Z_T), it becomes negligible in symmetric collision systems. The numerical data obtained via the post-form approximation exhibits a high degree of consistency with established experimental data. Furthermore, the divergence between the post and prior forms is generally contained within 30%, with the notable exception of Li^{+}+He systems at energies below 150 keV/amu.***

Keywords: Charge Transfer, Ion-Atom Interaction, Theoretical Cross-sections, BCCIS-4B

1. Introduction

The mechanism by which multiply charged ions sequester single electrons from multi-electron atoms has remained a subject of intense scrutiny within the physics community. This interest spans both theoretical [1-23] and experimental [24-35] domains, driven by its critical implications for astrophysics, plasma physics, and the ongoing development of controlled nuclear fusion. A prime example is the capture of electrons by partially stripped ions within tokamak fusion plasmas, a fundamental process involving helium atoms [1].

From a theoretical standpoint, foundational work by Dewangan and Eichler [2] emphasized the critical importance of establishing accurate boundary conditions for scattering wavefunctions and transition potentials. Their work demonstrated that neglecting these conditions in higher-order calculations leads to singularities in the transition amplitude. Consequently, extensive research has been dedicated to resolving these anomalies.

In collision systems where partners possess multiple electrons, electron-electron interactions become a governing factor. Helium, being the simplest multi-electron atom, serves as an ideal candidate for examining these correlation effects. These correlations are generally classified into two types: static correlation, pertaining to the initial electron arrangement, and dynamic correlation, which governs the temporal evolution of the system post-collision. While previous methodologies, such as the independent-electron approximation (IEA) [8] and the continuum distorted wave (CDW-4B) framework [10, 11], have provided valuable insights, they often exhibit discrepancies with experimental data, particularly at lower energy thresholds (below 500 keV/amu). In light of these challenges, the present study adopts the BCCIS-4B approximation [36-37] to investigate single charge transfer in collisions involving fully stripped (He^{2+}, Li^{3+}, C^{6+}, O^{8+}) and partially stripped (Li^{+}, Li^{2+}) ions against helium targets. We focus on a broad energy window of 50 to 5000 keV/amu to evaluate the efficacy of this approximation where previous models have faltered.

The structure of the paper will be as follows. Section II lays out the theoretical calculations, Section III covers results and discussion, and Section IV with conclusions. We use atomic units throughout.

2. Theory

The interaction describing single-electron capture from a two-electron target by a projectile ion (P) can be formally expressed as:

$$P^{Z_P+} + T^{(Z_T-2)+}(e_1, e_2) \rightarrow P^{(Z_P-1)+}(e_1) + T^{(Z_T-1)+}(e_2) \quad (1)$$

Here, Z_P and Z_T denote the nuclear charges of the projectile and target, respectively. The system involves two electrons, e_1 and e_2, initially bound to the target, with one active electron transferring to the projectile in the final state.

The total Hamiltonian (H) for the collision system is defined by the sum of the channel Hamiltonian and the perturbation potential for both the entrance (i) and exit (f) channels:

$$H = H_i + V_i = H_f + V_f \quad (2)$$

In the initial channel, the Hamiltonian H_i and potential V_i account for the interactions between the target nucleus and the electrons, as well as the inter-electronic repulsion. In the final channel, the passive electron screens the target ion, while the active electron's interaction with the projectile is modeled using Coulomb continuum wavefunctions.

$$H_i = H_0 - \frac{Z_T}{x_1} - \frac{Z_T}{x_2} + \frac{1}{r_{12}},$$

$$V_i = \frac{Z_P Z_T}{R} - \frac{Z_P}{s_1} - \frac{Z_P}{s_2}$$

And $H_0 = -\frac{1}{2\mu_i}\nabla^2_{R_T} - \frac{1}{2a}\nabla^2_{x_1} - \frac{1}{2a}\nabla^2_{x_2}.$

In the final channel,

$$H_f = H_0 - \frac{Z_P}{s_1} - \frac{Z_T}{x_2} + \frac{(Z_P-1)(Z_T-1)}{R_P},$$

$$V_f = \frac{Z_P Z_T}{R} - \frac{Z_T}{x_1} - \frac{Z_P}{s_2} + \frac{1}{r_{12}} - \frac{(Z_P-1)(Z_T-1)}{R_P}.$$

Using $R_P \approx R$, we obtain the following approximate expression:

$$V_f = Z_T\left(\frac{1}{R} - \frac{1}{x_1}\right) + Z_P\left(\frac{1}{R} - \frac{1}{s_2}\right) + \left(\frac{1}{r_{12}} - \frac{1}{R}\right)$$

And $H_0 = -\frac{1}{2\mu_f}\nabla^2_{R_P} - \frac{1}{2b}\nabla^2_{s_1} - \frac{1}{2a}\nabla^2_{x_2}$,

$$\mu_i = \frac{M_P(2+M_T)}{2+M_P+M_T}, \quad \mu_f = \frac{(M_P+1)(M_T+1)}{2+M_P+M_T},$$

$$a = \frac{M_T}{1+M_T}, \quad b = \frac{M_P}{1+M_P}.$$

Here e,T and P denote active electron, target atom and projectile ion respectively. $\vec{R}$ means the position vector of the projectile (P) relative to the target (T) nucleus. $\vec{x}_j$ and $\vec{s}_j$ (j=1,2) are the electron co-ordinates measured from the target and projectile nuclei respectively. μ_i, μ_f, a and b are the reduced masses associated with the relative coordinates $\vec{R}_T$, $\vec{R}_P$, $\vec{x}_j$ (j=1,2), and $\vec{s}_j$ (j=1,2), respectively. The interelectronic co-ordinate is denoted by $\vec{r}_{12} = \vec{s}_1 - \vec{s}_2 = \vec{x}_1 - \vec{x}_2$.

The prior form of the scattering amplitude may be written in the form

$$T_{if}^{(-)} = \langle \psi_f^- \,|\, V_i \,|\, \psi_i \rangle, \qquad (3)$$

where $\psi_i(\vec{x}_1,\vec{x}_2) = e^{i\vec{k}.\vec{R}_T}\varphi_i(\vec{x}_1,\vec{x}_2)$. $\varphi_i(\vec{x}_1,\vec{x}_2)$ is the product of one-parameter orbitals for the initial bound state of helium atom with effective charge Z_{eff}=1.6875. $\psi_f^{(-)}$ is the distorted wave in the final channel. The final state wave function $\psi_f^{(-)}$ can be written as,

$$\psi_f^{(-)} = e^{\frac{\pi}{2}(\alpha_1-\alpha_2)}\Gamma(1+i\alpha_1)\Gamma(1-i\alpha_2)e^{i\vec{k}_f.\vec{R}_P}\,{}_1F_1\{-i\alpha_1;1;-i(v_f x_1 + \vec{v}_f.\vec{x}_1)\}\times$$
$${}_1F_1\{i\alpha_2;1;-ib(k_f R_T + \vec{k}_f.\vec{R}_T)\}\varphi_f(\vec{x}_2,\vec{s}_1) \qquad (4)$$

where $\alpha_1 = \frac{Z_T-1}{v_f}$, $\alpha_2 = \frac{Z_P(Z_T-1)}{v_f}$.

In post form the scattering amplitude may be written as

$$T_{if}^{(+)} = \langle \psi_f \,|\, V_f \,|\, \psi_i^+ \rangle. \qquad (5)$$

Here the wavefunction in the final channel is given by

$$\psi_f = \varphi_f(\vec{s}_1,\vec{x}_2)\chi_f^-(\vec{R}_P),$$

where $\varphi_f(\vec{s}_1,\vec{x}_2)$ is the final bound state wavefunction which is the product of hydrogen like wavefunctions and $\chi_f^-(\vec{R}_P)$ is the Coulomb distorted wave in the exit channel. Since both the target and the projectile are ionic in nature except for $Li^+ + He$ collision, their relative motion should be described by Coulomb continuum function $\chi_f^-(\vec{R}_P)$, which satisfies the equation

$$\left(-\frac{1}{2\mu_f}\nabla^2_{R_P} + \frac{(Z_P-1)(Z_T-1)}{R_P} - \frac{k_f^2}{2\mu_f}\right)\chi_f^-(\vec{R}_P) = 0.$$

However, in the construction of the above differential equation we have used the asymptotic form of the internuclear interaction to take account of the effect of core electron (s) in both the target and the projectile.

Solving this equation, we find

$$\chi_f^-(\vec{R}_P) = e^{-\frac{\pi}{2}\alpha_3}\Gamma(1-i\alpha_3)e^{i\vec{k}_i.\vec{R}_P}\,{}_1F_1\{i\alpha_3;1;-i(k_f R_P + \vec{k}_f.\vec{R}_P)\}, \qquad (6)$$

where $\alpha_3 = \frac{(Z_P-1)(Z_T-1)}{v_f}$ and $\vec{k}_f$ is the final wave vector. ψ_i^+, the Coulomb continuum wavefunction in the entrance channel, is given by

$$\psi_i^+ = e^{\frac{\pi}{2}(\alpha_1-\alpha_2)}\Gamma(1-i\alpha_1)\Gamma(1+i\alpha_2)e^{i\vec{k}_i.\vec{R}_T}\,{}_1F_1\{i\alpha_1;1;i(v_i s_1 + \vec{v}_i.\vec{s}_1)\}$$
$${}_1F_1\{-i\alpha_2;1;i(k_i R_P + \vec{k}_i.\vec{R}_P)\}\varphi_i(\vec{x}_1,\vec{x}_2), \qquad (7)$$

where $\alpha_1 = \frac{Z_P}{v_i}$, $\alpha_2 = \frac{Z_T(Z_P-1)}{v_i}$.

It is well known [36,37] that the post form of the BCCIS-4B method is suitable for asymmetric collision ($Z_P > Z_T$) and for symmetric collisions, either form of the transition matrix element may be used.

The transition amplitude in the prior and post forms for single capture in the BCCIS-4B method may be written as

$$T_{if}^{(-)} = N\iiint d\vec{x}_1 d\vec{x}_2 d\vec{R}\, e^{-i\vec{k}_f.\vec{R}_P + i\vec{k}_i.\vec{R}_T}\, \varphi_f^*(\vec{x}_2,\vec{s}_1)\, {}_1F_1\{i\alpha_1;1;i(v_f x_1 + \vec{v}_f.\vec{x}_1)\}\times$$
$${}_1F_1\{-i\alpha_2;1;ib(k_f R_T + \vec{k}_f.\vec{R}_T)\}\left(\frac{Z_P Z_T}{R} - \frac{Z_P}{s_1} - \frac{Z_P}{s_2}\right)\varphi_i(\vec{x}_1,\vec{x}_2), \quad (8)$$

where $N = e^{\frac{\pi}{2}(\alpha_1-\alpha_2)}\Gamma(1-i\alpha_1)\Gamma(1+i\alpha_2)$, $\alpha_1 = \dfrac{Z_T-1}{v_f}$ and $\alpha_2 = \dfrac{Z_P(Z_T-1)}{v_f}$

and
$$T_{if}^{(+)} = N\iiint d\vec{x}_1 d\vec{x}_2 d\vec{R}\, e^{-i\vec{k}_f.\vec{R}_P + i\vec{k}_i.\vec{R}_T}\, \varphi_f^*(\vec{x}_2,\vec{s}_1)\, {}_1F_1\{i\alpha_1;1;i(v_i s_1 + \vec{v}_i.\vec{s}_1)\}\times$$
$${}_1F_1\{-i\alpha_2;1;i(k_i R - \vec{k}_i.\vec{R})\}\left\{Z_T\left(\frac{1}{R}-\frac{1}{x_1}\right) + Z_P\left(\frac{1}{R}-\frac{1}{s_2}\right) + \left(\frac{1}{r_{12}}-\frac{1}{R}\right)\right\}\times \quad (9)$$
$${}_1F_1\{-i\alpha_3;1;i(k_f R + \vec{k}_f.\vec{R})\}\varphi_i(\vec{x}_1,\vec{x}_2),$$

where $N = e^{\frac{\pi}{2}(\alpha_1-\alpha_2-\alpha_3)}\Gamma(1-i\alpha_1)\Gamma(1+i\alpha_2)\Gamma(1+i\alpha_3)$, $\alpha_1 = \dfrac{Z_P}{v_i}$, $\alpha_2 = \dfrac{Z_T(Z_P-1)}{v_i}$,

and $\alpha_3 = \dfrac{(Z_P-1)(Z_T-1)}{R_P}$.

Using integral representation ${}_1F_1(i\alpha;1;z) = \dfrac{1}{2\pi i}\oint dt\,(t-1)^{-i\alpha}\, t^{i\alpha-1}\, e^{zt}$, the transition amplitude of equations (8) and (9) may be written as

$$T_{if}^{(-)} = \frac{AN}{(2\pi i)^2}\lim_{\varepsilon_1,\lambda_2\to 0} D(\delta_1,\gamma_2,\lambda_1,\lambda_2,\varepsilon_1)\oint dt_1 t_1^{i\alpha_1-1}(t_1-1)^{-i\alpha_1}\oint dt_2 t_2^{-i\alpha_2-1}(t_2-1)^{i\alpha_2}\, J \quad (10)$$

where
$$J = \iiint d\vec{x}_1 d\vec{x}_2\, d\vec{R}\, e^{i\vec{k}_i.\vec{R}_T - i\vec{k}_f.\vec{R}_P + i\vec{v}_f.\vec{x}_1 t_1 + ib\vec{k}_f.\vec{R}t_2}\, \frac{e^{-\beta_1 x_1}}{x_1}.\frac{e^{-\beta_2 x_2}}{x_2}.\frac{e^{-\lambda_1 s_1}}{s_1}.\frac{e^{-\lambda_2 s_2}}{s_2}.\frac{e^{-\varepsilon R}}{R}, \quad (11)$$

$$\beta_1 = \delta_1 - i v_f t_1,\ \beta_2 = \delta_1 + \gamma_2 \text{ and } \varepsilon = \varepsilon_1 - ibk_f t_2 .$$

and
$$T_{if}^{(+)} = \frac{NA}{(2\pi i)^3}\lim_{\lambda_2,\varepsilon_1\to 0} D(\delta_1,\gamma_2,\lambda_1,\lambda_2,\varepsilon_1)\oint dt_1 (t_1-1)^{-i\alpha_1} t_1^{i\alpha_1-1}\oint dt_2 (t_2-1)^{i\alpha_2} t_2^{-i\alpha_2-1}\times$$
$$\oint dt_3 (t_3-1)^{i\alpha_3} t_3^{-i\alpha_3-1}, \quad (12)$$

where
$$J = \iiint d\vec{x}_1 d\vec{x}_2\, d\vec{R}\, e^{i\vec{k}_i.\vec{R}_T - i\vec{k}_f.\vec{R}_P + i\vec{v}_f.\vec{x}_1 t_1 + ib\vec{k}_f.\vec{R}t_2}\, \frac{e^{-\beta_1 x_1}}{x_1}.\frac{e^{-\beta_2 x_2}}{x_2}.\frac{e^{-\lambda_1 s_1}}{s_1}.\frac{e^{-\lambda_2 r_{12}}}{r_{12}}.\frac{e^{-\varepsilon R}}{R}, \quad (13)$$

$$\beta_1 = \delta_1,\quad \beta_2 = \delta_1 + \gamma_2 \text{ and } \varepsilon = \varepsilon_1 - ik_i t_2 - ik_f t_3 .$$

Here the constant A originates from the initial and final bound state wave functions. $D(\delta_1,\gamma_2,\lambda_1,\lambda_2,\varepsilon_1)$ is a parametric differential operator used to generate the excited state wave functions. δ_1,γ_2 and λ_1 are the orbital component of the initial and final bound state wave functions. To obtain the perturbation potential term $\dfrac{1}{s_2}$ in the final channel, the term $\dfrac{e^{-\lambda_2 r_{12}}}{r_{12}}$ in equation (13) is replaced by $\dfrac{e^{-\lambda_2 s_2}}{s_2}$ and the parametric differential operator $D(\delta_1,\gamma_2,\lambda_1,\lambda_2,\varepsilon_1)$ should be changed accordingly.

Using the techniques of Fourier transform, Feynman parametric integral and the integral representation of three denominator integral of Lewis [38], equation (11) or (13) may be reduced following Sinha and Sil [39] as

$$J = 32\pi^3\int_0^1 \frac{dx}{\Delta}\int_0^\infty \frac{dy}{A + Bt_1 + Ct_2 + Dt_1t_2} \quad (14)$$

where

$$\Delta^2 = \left\{(1-a)\vec{k}_f - \frac{\vec{k}_i}{2+M_T}\right\}^2 (1-x) + \beta_2^2 x + \lambda_2^2(1-x)$$

for post form

and
$$\Delta^2 = \left\{\frac{\vec{k}_i}{2+M_T}\right\}^2 (1-x) + \beta_2^2 x + \lambda_2^2(1-x)$$

for prior form.

So the transition matrix element given by the equation (10) and (12) may be reduced as

$$T_{if}^{(-)} = 32\pi^3 A N \lim_{\varepsilon_1,\lambda_2\to 0} D(\delta_1,\gamma_2,\lambda_1,\lambda_2,\varepsilon_1)\int_0^1 \frac{dx}{\Delta}\int_0^\infty dy\, K \quad (15)$$

and $$T_{if}^{(+)} = 32\pi^3 \frac{AN}{(2\pi i)}\oint dt_3 t_3^{-i\alpha_3-1}(t_3-1)^{i\alpha_3} \lim_{\varepsilon_1,\lambda_2\to 0} D(\delta_1,\gamma_2,\lambda_1,\lambda_2,\varepsilon_1)\int_0^1 \frac{dx}{\Delta}\int_0^\infty dy\, K, \quad (16)$$

where $K = A^{i\alpha_1-i\alpha_2-1}(A+B)^{-i\alpha_1}(A+C)^{-i\alpha_2}\, {}_2F_1(i\alpha_1;-i\alpha_2;1;z)$ and $z = \frac{BC-AD}{(A+B)(A+C)}$.

The scattering amplitude is calculated using two distinct forms. In the Prior Form, This utilizes the product of one-parameter orbitals for the initial bound state of the helium atom (with an effective charge Z_{eff}=1.6875) and the distorted wave in the final channel. In the Post Form, This approach employs a final bound state wavefunction-composed of hydrogen-like wavefunctions- and the Coulomb distorted wave in the exit channel. It is well-established that the post form of the BCCIS-4B method yields superior results for asymmetric collisions (Z_P>Z_T), whereas symmetric collisions can be accurately described by either form. To ensure numerical precision, we employed Gauss-Laguerre and Gauss-Legendre quadrature methods for integration, achieving convergence accuracy within 0.1%.

3. Results and Discussion

To determine the total single-electron transfer cross-sections, we aggregated the contributions from all individual shells and sub-shells up to n=3. The derived data for collisions between helium atoms and various projectile ions across the 50–5000 keV/amu energy spectrum are presented in Figures 1 through 6. These figures contrast the results obtained from both the prior and post forms of the BCCIS-4B approximation.

A. Symmetric Collisions (He^{2+}+He) Figure 1 displays the data for symmetric collisions. A distinct observation is that the post-form results align more closely with experimental benchmarks-such as those by de Castro et al. [26] and Shah and Gilbody [24]- than the prior form results. This superior agreement is likely attributable to the post form's inclusion of dynamic electron correlation effects. In contrast, the prior form relies on an independent particle model with a frozen core, which oversimplifies static correlations. Theoretical comparisons show that our results surpass the accuracy of the CDW-4B approximation at lower energies.

B. Asymmetric Collisions For asymmetric systems, such as Li^{3+}+He (Figure 2), the BCCIS-4B post-form results demonstrate remarkable consistency with experimental measurements across the entire energy range, including the lower sector (<150 keV/amu) where other theories often underperform. This accuracy is credited to the inclusion of continuum interactions between the active electron and the highly charged projectile.

Similarly, in collisions involving heavier ions like C^{6+} (Figure 5) and O^{8+} (Figure 6), our calculations show strong agreement with available experimental data [31, 32] and other theoretical models like the Classical Trajectory Monte Carlo (CTMC) method. In these high-charge scenarios, the divergence between the post and prior forms is minimal, consistently remaining below 10%.

4. Conclusions

In this work, we extended the application of the BCCIS-4B approximation-previously utilized for double electron capture- to the domain of single-electron capture at intermediate and high collision energies. The results exhibit a high degree of concordance with experimental data throughout the examined energy spectrum. The success of this approach can be attributed to three primary factors: (i) the incorporation of the active electron's continuum state in the presence of the stronger charge, (ii) the adherence of the scattering wavefunction to correct boundary conditions, and (iii) the asymptotic behaviour of the transition potential, which decays more rapidly than the Coulomb potential. While the approximation still underestimates certain electron correlation effects, it proves to be a robust framework for analyzing asymmetric collisions in multi-electron systems.

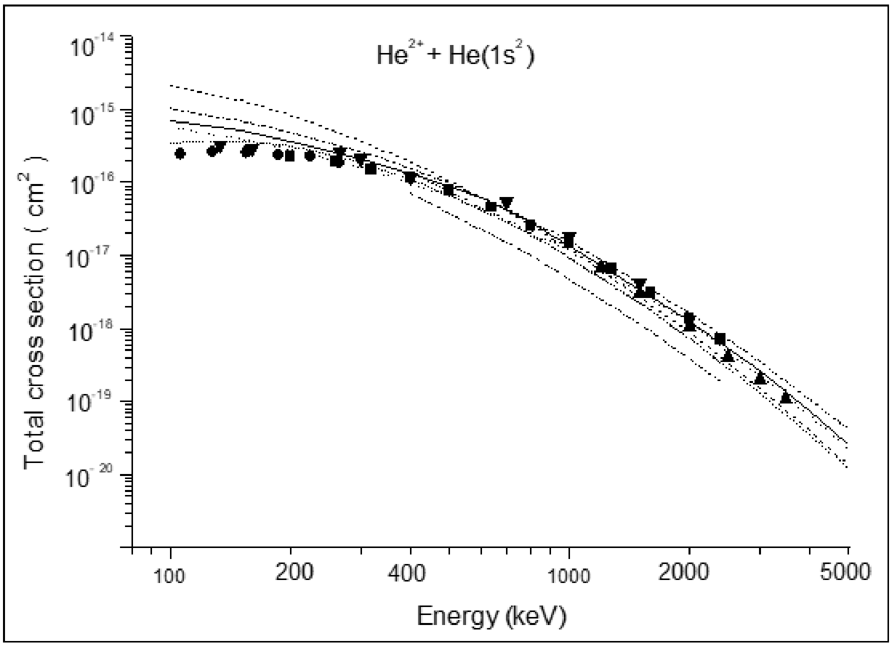

Figure 1: Total cross sections (in cm^2) as a function of the incident energy E (keV)
Theory: solid line, current results (post form BCCIS-4B); short dash-dotted line, current results (prior form BCCIS-4B); dashed line, results of Mancev [11]; dotted line, results of Mancev and Milojevic [14]; dash-dotted line, results of Dunseath and Crothers [16]; dash-dot-dotted line, results of Dunseath and Crothers [16]; dense dotted line, results of Mancev [13].
Experiments: ■, results of Shah and Gilbody [24]; ●, results of Shah et al [25]; ▲, results of de Castro et al [26]; ▼, results of DuBois [27].

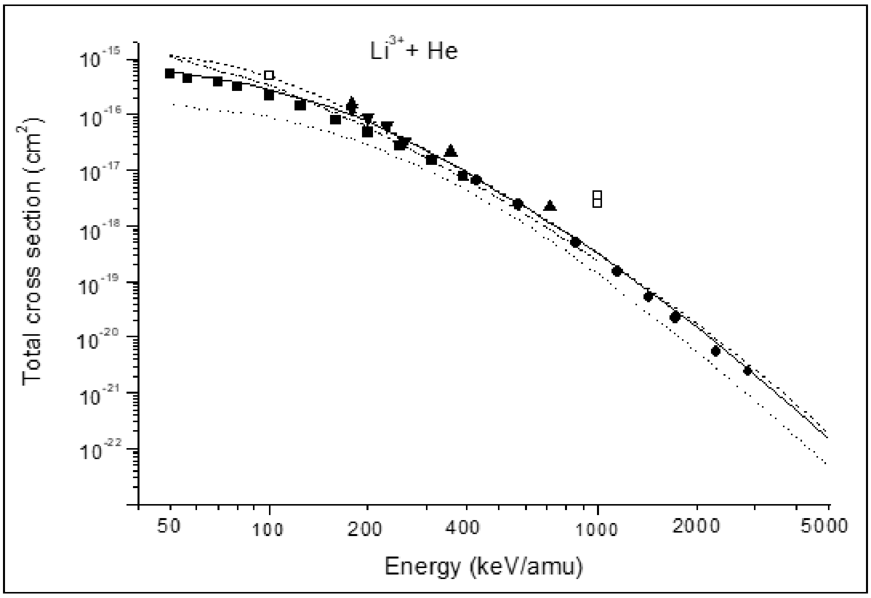

Figure 2: Total cross sections (in cm^2) as a function of the incident energy E (keV/amu).
Theory: solid line, current results (post form BCCIS-4B); dashed line, current results (prior form BCCIS-4B); dotted line, results of Mancev [12]; dash-dotted line, results of Belkic [17]; □, results of Sidorovich et al [8].
Experiments: ■, results of Shah and Gilbody [24]; ●, results of Woitke et al [30]; ▲, results of Nikolaev et al [28]; ▼, results of Pivovar et al [29].

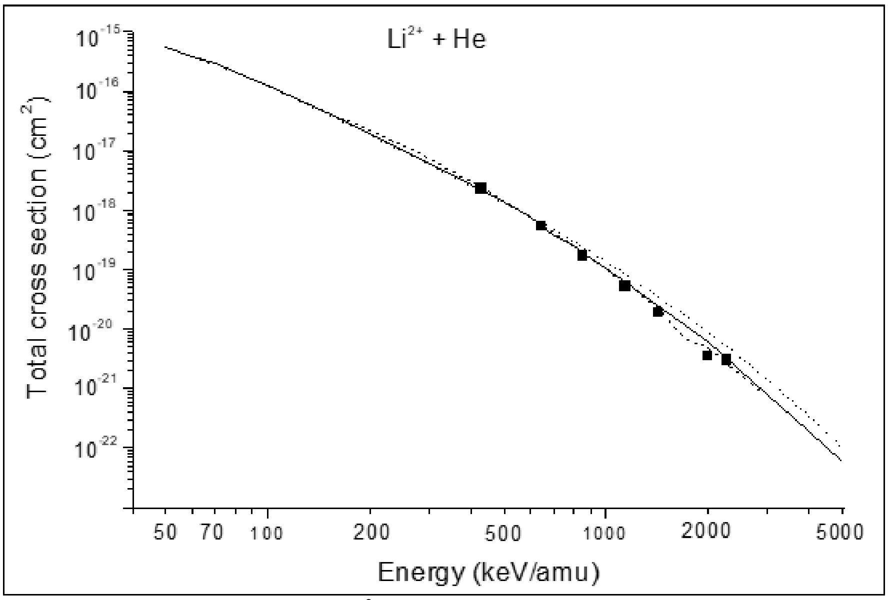

Figure 3: Total cross sections (in cm^2) as a function of the incident energy E (keV/amu).
Theory: solid line, current results (post form BCCIS-4B); dotted line, current results (prior form BCCIS-4B); dashed line, results of Mancev [18].
Experiment: ■, results of Woitke et al [30].

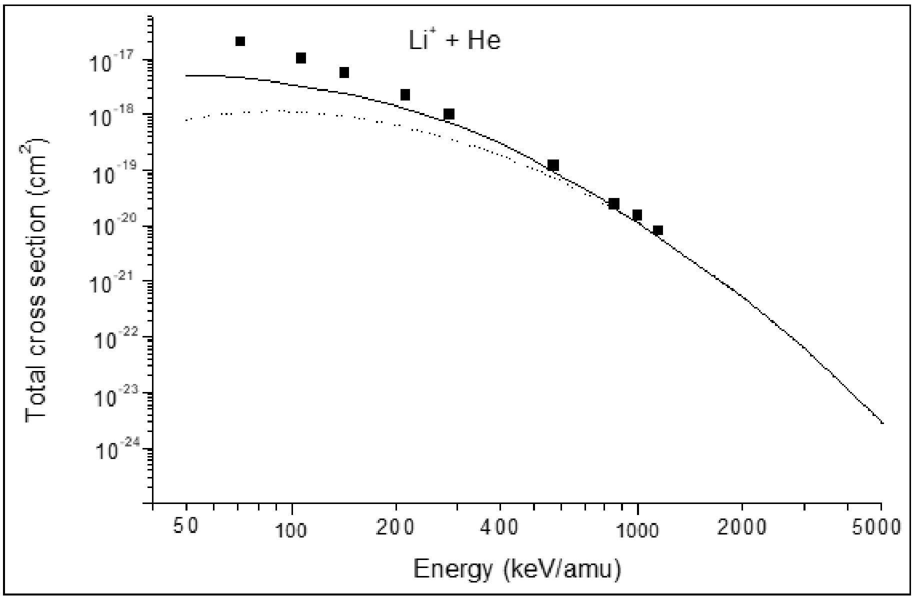

Figure 4: Total cross sections (in cm^2) as a function of the incident energy E (keV/amu). Theory: solid line, current results (Post form BCCIS-4B); dotted line, current results (Prior form BCCIS-4B).
Experiment: ■, results of Woitke et al [30].

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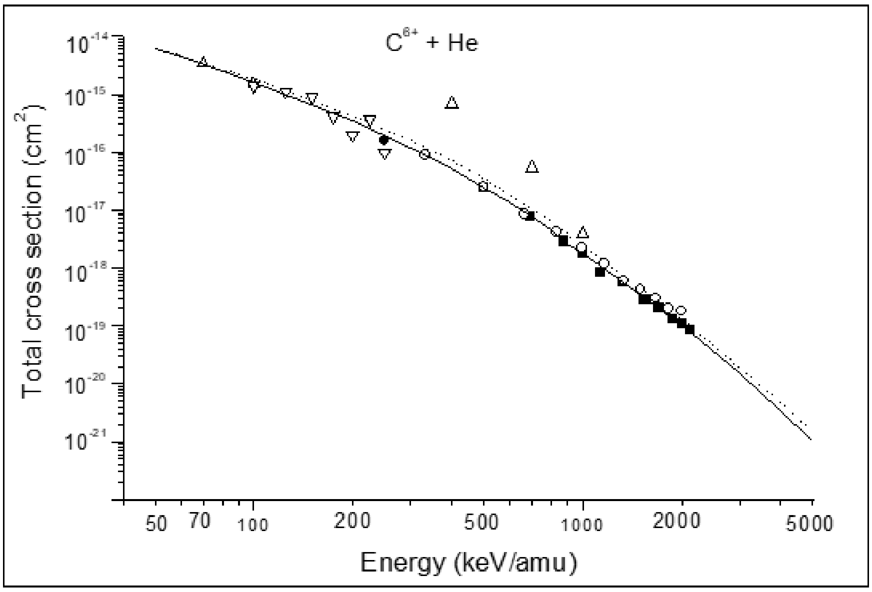

Figure 5: Total cross sections (in cm^2) as a function of the incident energy E (keV/amu). Theory: solid line, current results (post form BCCIS-4B); dashed line, current results (prior form BCCIS-4B); ○, results of Jain et al [9]; Δ, results of Suzuki et al [20]; ∇ , results of Olson [19].
Experiments: ■, results of Dillingham et al [31]; ●, results of Guffey et al [32].

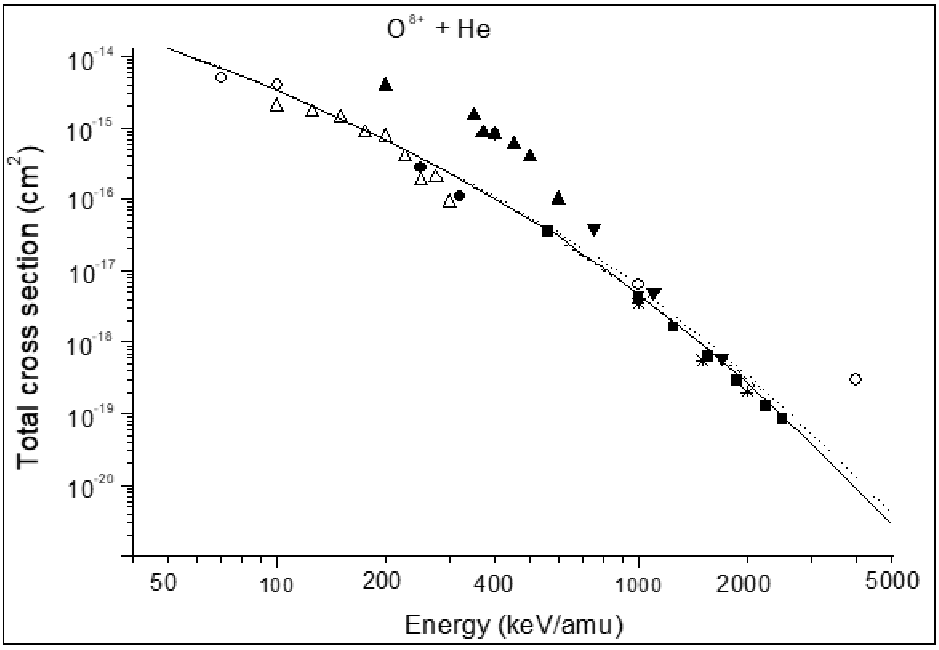

Figure 6: Total cross sections (in cm^2) as a function of the incident energy E (keV/amu). Theory: solid line, current results (post form BCCIS-4B); dotted line, current results (prior form BCCIS-4B); dashed line, results of Jain et al [9]; ○, results of Suzuki et al [20]; Δ, results of Olson [19].
Experiments: ■, results of Dillingham et al [31]; ●, results of Guffey et al [32]; ▼, results of Macdonald and Martin [34]; ▲, results of Afrosimov et al [33]; *, results of Hippler et al [35].

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