# Electron capture in $C^{6+}$ + He and $O^{8+}$ + He collisions at intermediate energies in the atomic-orbital-expansion method

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A multistate two-center atomic-orbital-expansion method is applied to study the subshell capture cross sections from helium atoms in collisions with bare C<sup>6+</sup> and O<sup>8+</sup> ions. The energy dependence of subshell capture cross sections, i.e., the n, nl, and nlm distribution, is examined. In view of the lack of detailed subshell cross section measurements, we compare our calculations with experimental total capture cross sections and with polarization fraction for the 2p-1s transition in O<sup>8+</sup>-He collisions. For the latter process, the cascade effect must be included in the theoretical analysis. We show that our results are in good agreement with existing experimental data.

# I. INTRODUCTION

The electron-capture process in the collision of multiply charged ions with atoms and molecules has been studied extensively in the last decade both theoretically and experimentally. In the late 1970's most of the experimental studies were carried out in heavy-ion accelerator laboratories where the heavy ions are generally in the energy range of a few MeV to hundreds of MeV. These earlier studies had spurred the renewed interest in the theory of electron capture in ion-atom collisions. In the last few years, with the advent of highly charged recoil ions<sup>2</sup> and the availability of different ion sources such as the electron-cyclotron resonance (ECR) and electron-beam ion source (EBIS), experimental efforts appear to have been shifted to the lower-energy region (from a few tenths of one keV to several tens of keV).3-6 Meanwhile, theoretical efforts have been concentrated also in the lower-energy region in the last few years with the aim of understanding experimental results.<sup>7-8</sup>

For collisions in the low-energy region involving highly charged ions with neutral atoms, electron capture to the excited states of the projectile is the dominant inelastic process and transition occurs primarily at large internuclear separations. Although there are a number of simple classical models and a few quantum-mechanical models aiming at describing these processes, most of these models can only explain qualitatively the total capture cross sections. These models are useful in understanding the "first-generation" experiments. With the advance in energy-loss spectroscopy9 and the introduction of the detection of the light emission from the decay of the excited states after the capture, partial cross sections to individual final states have been reported. 10 Theoretical models proposed for understanding these measurements are mostly based on the close-coupling method in which the time-dependent electronic wave function is expanded in terms of convenient basis functions. For the lowenergy region, both traveling atomic orbitals (AO) and

traveling molecular orbitals8 (MO), as well as a combination of atomic and molecular orbitals have been employed.<sup>11</sup> Total cross sections obtained from these calculations are generally in good agreement with the experimental data. Extensive comparison for partial cross sections calculated based upon atomic-orbital expansion have been shown in reasonable agreement with measurements for a number of collision systems.<sup>12</sup> Current work in the AO-expansion method aims at the development of a general AO-expansion code for two-electron (or manyelectron) collision systems where electron correlation effects can be included in the theoretical study.

In this paper we apply the AO-expansion method to study the electron-capture process in the higher-energy region. We have specifically chosen collisions of bare carbon and bare oxygen ions with helium atoms. We calculate the partial cross sections for each system from about 10 keV/amu to about 2 MeV/amu, or in terms of the relative collision speed v with respect to the orbital speed  $v_{e}$ of the electron in helium,  $v/v_e$ , from 0.8 to about 10.0. At the low-energy end reported here, we overlap with the high-energy end of some earlier more sophisticated calculations<sup>13</sup> to check the validity of some of the assumptions used in the present calculation. In the higher-energy region, we can compare our calculations with the measurement of total capture cross sections by Dillingham et al. 14 Our calculations provide detailed information on the cross section to each individual nlm subshell of the projectile, but no such measurements on the partial cross sections are available at present. In the absence of these data, we compare our theoretical results with the measured polarization of Lyman- $\alpha$  spectra for bare oxygen with helium at 16 MeV by Ellsworth et al. 15 Since capture to the n=3 and 4 states of the hydrogenlike oxygen ion is quite important at this energy, cascade effects from n = 3 and 4 shells to the 2p shell must be included in the calculation of polarization for comparison with experimental data. At this energy point, we found that our calculation is in good agreement with the experimental value.

There are at least two reasons for carrying out this study. First, the range of the validity of the AOexpansion model has not been tested in detail for the highor the intermediate-energy regions for collisions involving multiply charged heavy ions (for lighter ions, see the work of Bransden and co-workers<sup>16</sup>). Because of the large positive charge carried by the projectile into the collision, electron capture is still dominant over the direct excitation or ionization for  $v/v_e = 1-4$  for the present systems. This is different from near-symmetric singly charged collision systems where the ionization channel becomes important over other inelastic processes at  $v/v_e > 1$ . For asymmetric collisions such as the capture by protons from the inner shells of atoms, the ionization process is dominant even for  $v/v_e < 1$ . It is known from the strong potential Born (SPB) approximation<sup>17</sup> in recent years that the coupling of capture channels with the ionization channels must be included for the later systems. For near-symmetric systems at velocities in the range  $v/v_e = 1-2$ , it has been shown that effects due to ionization channels can be included by pseudostates. 18 By comparing the AO calculations with experimental results, it is hoped that we can establish the range of validity of the model for collisions involving multiply charged ions.

Another reason to carry out the present study is that we want to examine the evolution of the relative importance of the individual nlm subshell population as the collision energy increases. It is desirable to see how good the prediction of the simple Oppenheimer-Brinkman-Kramer (OBK) model<sup>19</sup> is as compared with the present model. By examining parameters such as the polarization of the 2p-1s and 3p-1s transitions, we wish to stimulate experimentalists into carrying out this type of measurement. The results of such predictions are given in Sec. III.

The rest of this paper is organized as follows. In Sec. II we briefly review the theoretical methods used in the present calculations and discuss some numerical problems encountered. The results from this investigation are shown in Sec. III and compared with experimental data whenever possible. The *nlm* distribution and its variation with collision energies are also discussed in this section. A brief summary and some concluding remarks are given in Sec. IV.

# II. THEORETICAL AND COMPUTATIONAL METHODS

We adopt the semiclassical impact-parameter formulation of the close-coupling method with straight-line trajectories for the heavy particles. Traveling atomic orbitals are used as basis sets. In the present study, we employ a single-electron approximation for describing the helium atom. In this simple model, we consider the two electrons in helium as independent, one a passive electron and the other an active electron. The passive electron does not participate in the collision except to screen the active electron. For the active electron, the time-dependent Hamiltonian is given by

$$H = -\frac{1}{2}\nabla^2 - \frac{Z_p}{r_p} + V(\mathbf{r}_t) , \qquad (1)$$

where  $\mathbf{r}_t$  and  $\mathbf{r}_p$  are the distances of the active electron

from the target and the projectile nuclei, respectively,  $Z_p$  is the projectile nuclear charge, and  $V(\mathbf{r}_t)$  is a model potential for the active electron in helium. The model potential is taken from the work of Opradolce *et al.*<sup>20</sup> It reads as follows:

$$V(r) = -\frac{1}{r} - \frac{1}{r} [(1 + 1.665r)\exp(-3.36r)].$$
 (2)

By expressing the ground-state wave functions of the helium atom as the linear combination of 1s Slater orbitals with exponents 1.453 and 2.78, this model potential gives a binding energy of -0.9041 a.u. which is to be compared with the experimental value, -0.90356 a.u.

With these assumptions we then solve the timedependent Schrödinger equation

$$(H - i\partial/\partial t)\Psi = 0 \tag{3}$$

for the active electron by expanding  $\Psi$  as

$$\Psi = \sum_{n} a_{n} \widetilde{\phi}_{n}(\mathbf{r}_{t}) + \sum_{m} b_{m} \widetilde{\phi}_{m}(\mathbf{r}_{p}) , \qquad (4)$$

where  $\widetilde{\phi}_m(\mathbf{r}_p)$  and  $\widetilde{\phi}_n(\mathbf{r}_t)$  are, respectively, the traveling target and traveling projectile atomic states with appropriate plane-wave translational factors. Substitution of Eq. (4) into (3) and following a standard procedure results in a set of first-order coupled differential equations for  $a_m$ 's and  $b_m$ 's, which are solved numerically with proper initial conditions for each impact parameter b. The capture probability P(b) to a specific individual state i is  $|b_i(+\infty)|^2$  for a given impact parameter b. In order to obtain partial cross section to any substate i, we need to evaluate

$$\sigma_i = 4\pi \int_0^\infty P(b)b \ db \ , \tag{5}$$

where the additional factor of 2 comes from the fact that there are two equivalent active electrons, one for spin up and the other spin down. It should be mentioned that Eq. (5) involves a number of additional approximations such as the neglect of exchange correlation<sup>21</sup> and the correlation between the two electrons. In the energy region studied here, the neglect of these correlation effects is not a severe handicap.

The major approximation in the solution of Eq. (3) is the truncation of basis functions included in the expansion (4). What basis functions are to be included is suggested by the nature of the collision system and the collision conditions as well as by practical considerations. Obviously all the important physical channels at the end of the collision have to be included in the expansion (4). In the low-energy regime (10-100 keV/amu) of the present collision systems, electron capture to the excited states of the projectile is the dominant process; thus only these important final states and the initial state need to be included in the expansion [Eq. (4)]. For collisions at higher velocities, ionization becomes dominant. In a close-coupling calculation for the electron-capture process, it would be desirable to incorporate the effects due to these continuum channels. This has been done for several limited nearsymmetric collision systems by representing the continuum channels using pseudostates. <sup>18</sup> In this study, however, we do not include any ionization channels as this would require very large basis sets. The precise basis functions used in the expansion for each collision system will be discussed in Sec. III.

In the higher-energy region studied here, extra care is needed in the calculation of exchange matrix elements. Because of the plane-wave translational factor  $e^{i\mathbf{v}\cdot\mathbf{r}}$ , the integrand in the two-center exchange matrix elements oscillates rapidly. We evaluate these integrals by integrating over the spheroidal coordinates,  $\lambda$ ,  $\mu$ , and  $\phi$ . Integration over  $\phi$  gives a Bessel function and the two other integrals are evaluated numerically using Gauss-Legendre quadrature for  $\mu$  and Gauss-Laguerre quadrature for  $\lambda$ . For  $v/v_e \gg 1$ , quadrature points up to 40 for Gauss-Legendre and 30 for Gauss-Laguerre are used. These number of points are about a factor of 2-3 more than needed for the  $v/v_e \sim 1$  region and is the source of major CPU usage in the present calculation (a typical calculation including 20 states needs about two minutes on the Cray X-MP computer per impact parameter).

# III. RESULTS AND DISCUSSION

We discuss here our calculations for  $C^{6+}$  and  $O^{8+}$  collisions with He. There have been a number of calculations on these systems: Suzuki et al.22 applied a unitarized distorted-wave approximation (UDWA) to these systems over a range of energies (1-4 MeV/amu); a classical trajectory Monte Carlo (CTMC) approach has been applied by Olson<sup>23</sup> from 100 to 500 keV/amu. In the lowenergy region (E < 20 keV/amu), Kimura and Olson<sup>8</sup> have carried out two-electron MO calculations for total and partial cross sections for O<sup>8+</sup> on He and Fritsch and Lin<sup>13</sup> have carried out an extensive two-electron AO expansion for  $C^{6+}$  on He for 0.1 < E < 20 keV/amu. Less extensive MO calculations by Bliman et al.3 for O8+ on He have also been reported. Several partial cross section measurements have been carried out in the low-energy region.<sup>10</sup> In this paper, our attention is directed at the higher-energy region.

In the following subsections we discuss the results for  $C^{6+}$  on He and  $O^{8+}$  on He separately, and in Sec. III C we address the polarization of the 2p-1s and 3p-1s transitions after capture.

# A. C<sup>6+</sup> on He

In Fig. 1 we show total capture cross sections and the ndistribution  $(\sigma_n)$  in the energy range from 1-25.5 MeV, along with the total capture cross sections measured by Dillingham et al. 14 Our calculated total cross sections are in good agreement with experimental data except for a systematic overestimate at the higher-energy end. In this calculation we include the ground state of helium atom and all the n = 1, 2, and 3 channels of  $C^{5+}$  in the expansion of Eq. (4), resulting in a 12-state calculation (since the ground state of He is represented as a linear combination of two Slater orbitals, there are actually two target states in He included). (We estimate the contribution from all the n > 4 shells to be about 10% of the calculated cross sections.) The n distribution is also shown in Fig. 1. We note that for E < 4 MeV, the n = 3 is dominant. For energy between 4 and 25 MeV, the capture to n=2 is

dominant. For higher energies, capture to the 1s state becomes dominant. No measurements on n distribution (or the nlm) is available in this energy region (however, below v=0.5 a.u.,  $\sigma_n$  cross sections have been measured; see Dijkkamp et al.<sup>5(b)</sup> and references therein).

The discrepancy between the present calculations and the experimental total cross sections at higher energies is not unexpected. It is partly due to the neglect of ionization channels in the present close-coupling method. For example, at 12 MeV, the total ionization cross section has been measured<sup>24</sup> to be  $6 \times 10^{-16}$  cm<sup>2</sup>: this is much higher than the total capture cross section, which is about  $2\times10^{-18}$  cm<sup>2</sup>. In fact, it is surprising that the present calculations still give such a good agreement. To account for this discrepancy, it is in principle possible to include some pseudostates in the expansion (4). To pursue such a higher degree of accuracy using the present model, one may need to include some pseudostates on the projectile and on the target as well. However, the inclusion of pseudostates in the present systems makes the calculation computationally impractical.

In Fig. 2 we show the nl distribution and the total capture cross sections over a larger energy region, from 10 to 500 keV/amu. In the low-energy region we compare with the calculations by Fritsch and Lin, which in turn compare very well with available experimental data at even lower energy  $E \sim 1$  keV/amu. In this latter model, a two-electron AO expansion was adopted such that exchange correlation between the two electrons is properly included. Such an effect is expected to be more important

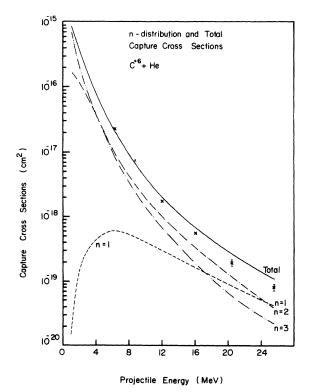


FIG. 1. Total and n-distribution capture cross sections in  $C^{6+}$  + He collisions. Results from the present calculations are shown by various curves. Experimental points of Dillingham et al. (Ref. 14) are indicated by crosses.

for the low-energy region. In Fig. 2 we indicate the results for Fritsch and Lin at 15, 25, and 40 keV/amu in symbols. Except for the 3d subshell, the present calculations are in good agreement with the more accurate ones by Fritsch and Lin. For the total capture cross section, the present calculation is about 30% higher. The dominant nl subshell at each energy and the energy dependence of  $\sigma_{nl}$  from the two calculation as are all in accord. At the highest energy,  $E \sim 500 \text{ keV/amu}$ , the calculated total transfer cross section is lower than the available experimental data point; <sup>14</sup> again given the simplicity and the restrictions of the model calculations as pointed out above, we consider the agreement is still satisfactory.

The agreement of our low-energy calculations with the more accurate ones and the general agreement of our calculated total capture cross sections for energies above 500 keV/amu with experimental data indicate that our results should be quite accurate in the energy region from 1.0 to 500 keV/amu where there are no experimental data available. For energies between 1.0 and 30 keV/amu, these data can be taken with ECR ion sources. For energies below 500 keV/amu, these ions can be produced by deaccelerating heavy ions after foil stripping. This latter type of experiment have been performed by Schuch and coworkers for sulfur ions but not for lighter ions. <sup>26</sup>

To get a general idea about the m distribution as a function of collision energy, we show the nlm-subshell cross sections in Fig. 3. In the low-energy region, the difference between m=0 and |m|=1 is small, with

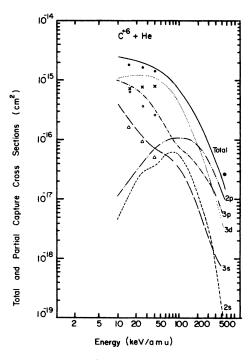


FIG. 2. Total and *nl*-distribution capture cross sections in  $C^{6+}$  + He collisions in the 10-500-kev/amu energy range. Present results are shown by various labeled curves. Results of the calculations by Fritsch and Lin (Ref. 13) are plotted for the total (solid circle), 3s (triangles), 3p (open circles), and 3d (crosses) capture cross sections. At 500 kev/amu, the experimental value of Ref. 13 is indicted by  $\otimes$ .

small contribution from m=2. At higher energies, the m=0 component is clearly dominant. This variation in the m distribution would be reflected in the polarization of the radiations emitted after the capture. We will address this problem in Sec. III C.

For the purpose of illustrating the relative nl distribution in the very-high-energy region, we display our calculated results from 1 to 25 MeV in Fig. 4. No experimental data are available for comparison. At even high energies ( $E \ge 100$  MeV) relativistic kinematics may be required. In this region the role of correlation due to continuum is not known.

We conclude from Figs. 1—4 that the AO method is quite successful up to about 1-MeV/amu energies and probably even beyond that region. The simple active one-electron approximation for helium does not pose any severe problem and the neglect of many small channels does not create significant discrepancy with experimental total capture cross sections.

# B. O<sup>8+</sup> on He

We present our AO results for this system in the MeV energy region only. Figure 5 displays the experimental total capture cross sections. If along with the present theoretical total and n-distribution capture cross sections. The agreement with experiment is quite good except at the high-energy and where the discrepancy is mainly attributed (see Sec. III A) to the neglect of ionization channels, which are important in this energy region (for example, at 16.8 MeV the ionization cross section<sup>24</sup> is  $10^{-15}$  cm<sup>2</sup> while the capture cross section is only  $4 \times 10^{-18}$  cm<sup>2</sup>). For the

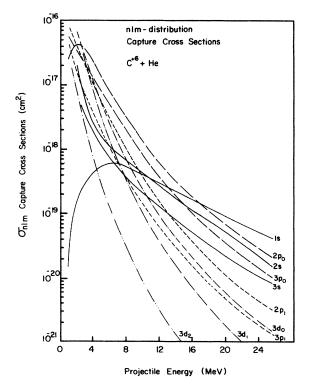


FIG. 3. *nlm*-distribution capture cross sections for the  $C^{6+}$  + He collisions in the 1-25.5-MeV energy region.

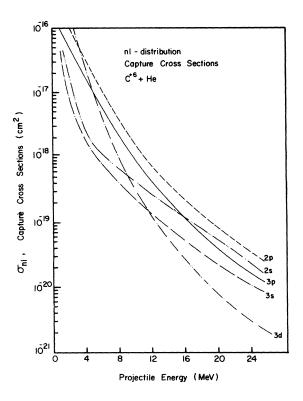


FIG. 4. nl-distribution of the capture cross sections in the  $C^{6+}$  + He collisions in the 1-25.5-MeV energy region.

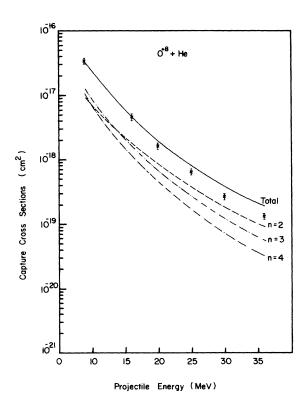


FIG. 5. Same as in Fig. 1 but for  $O^{8+}$  + He collisions.

n distribution, n=4 is dominant at low energies (E < 30 keV/amu), n=3 is dominant until at about 15 MeV. For energies between 15 and 35 MeV, n=2 is dominant. In this regime, n=1 is not important.

For comparison, we show in Fig. 6 the nl distribution and in Fig. 7 the nlm distribution for this system. No experimental data are available on the subshell capture cross sections in this energy range (however, very recently there have been several measurements on the nl populations following electron capture by low energy O<sup>8+</sup> ions from helium; see Politis et al.<sup>27</sup> and references therein). We note that although the cross sections for each subshell drop rapidly with energy, the rate of decrease is larger for  $m \neq 0$  states. This can be understood easily from the momentum distribution of the electron in each nlm state. For m = 0 states, it has a larger momentum component along the z direction (the incident direction). For the electron to be captured in a fast collision, it needs to acquire a large momentum along the z direction. The m = 0 states tend to have larger momentum along this axis. Similarly, at higher energies, capture tend to go into smaller n subshells since smaller n subshells have higher probability for larger momentum. This behavior can be easily understood even in the simple but unrealistic OBK model, 19 which predicts the high-energy dependence to be  $v^{-2l-12}$  for a given n and  $\sigma_n$  goes to  $v^{-12}$ .

# C. Polarization

Collisions between multiply charged ions with neutral atoms in the keV and MeV energy regions usually result

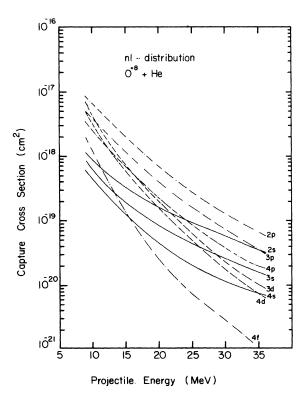


FIG. 6. nl-distribution capture cross sections for  $O^{8+}$  + He collisions.

in capture to excited states. From Figs. 3 and 7 it is obvious that capture cross sections to these excited states are not distributed statistically. At higher energies, capture is primarily to m=0 states. Radiation from the deexcitation of these excited atoms is polarized. Measurements on the polarization of the emitted radiation after electron capture have been performed for proton collisions on rare-gas atoms since the early 1970's. <sup>28</sup> Similar experiments <sup>16</sup> for collisions of multiply charged ions with atoms are more scarce since the emitted radiation is usually in the x-ray or far-uv region.

In comparing the theoretically calculated polarization with the measured value for a specific transition, it is important to include cascading effects from higher states. In the collision system  $O^{8+}$  + He, the polarization of the 2p-1s transition in  $O^{7+}$  after the capture process at 16 MeV has been measured by Ellsworth et al. From Fig. 5, it is clear that capture to the n=3 and n=4 shells at this energy is not small in comparison with capture to the n=2 shells. To compare with experimental results, we used the calculated capture cross sections to each individual nlm (n=3 and 4) state and examined the cascade of each state to the  $2p_0$  and  $2p_{+1}$  states. Contribution from the cascading are added to the direct capture to  $2p_0$  and  $2p_1$  subshells. The polarization fraction P is defined as  $2p_1$  subshells.

$$P = (\sigma_{2p_0} - \sigma_{2p_{\pm 1}})/(2.375\sigma_{2p_0} + 3.749\sigma_{2p_{\pm 1}})$$
 (6)

in which proper account of spin-orbit coupling has been taken. In the present calculations, the depolarization of the upper states (n=3,4) due to spin-orbit coupling has not been considered. The result of this analysis for the

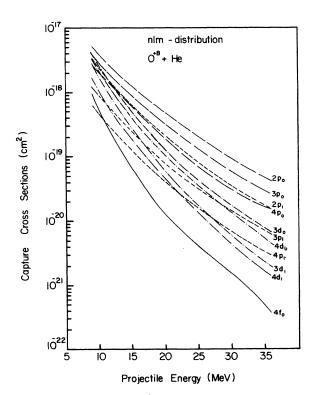


FIG. 7. Capture cross sections into nlm subshells for  $O^{8+}$  + He collisions.

polarization fraction from the calculated nlm distribution is shown in Fig. 8 from 5 to 40 MeV for the  $O^{8+}+He$  system. Over the energy region  $E \ge 16$  MeV, the polarization fraction does not show any significant variation but drops rapidly to low energies. Our calculated result at 16 MeV is in good agreement with the measured value,  $(17.6\pm3)\%$ , of Ellsworth  $et~al.^{16}$ 

In Fig. 8 we also indicate the calculated 2p-1s polarization if the cascade effect is not included. We note that the cascade has the effect of decreasing the value of the polarization fraction (i.e., a depolarization effect).

In Fig. 8 we also show the polarization fraction for the 3p-1s transition. The cascade effect has been included in this calculation too. We note that the variation of the polarization fraction with energy is larger for this transition as compared to the 2p-1s case.

To show the general feature of the predicted polarization fraction P over a larger energy range, in Fig. 9 we display the polarization of the 2p-1s transition for  $C^{6+}$  on He, including cascade effects, from 0.3-30 MeV. We note that P drops rapidly to about 10% or less for carbon energy of less than 2 MeV. For collision at lower energies, the m=0 and |m|=1 components are nearly equally populated for capture to n=3 and n=2 such that the total polarization fraction is nearly zero. For collisions at higher energies, P is large and positive, indicating that capture to m = 0 states is dominant. The hump at about 50 keV/amu and any structure below that energy may be associated with the peak in transfer cross sections at its low-energy side. Details of the molecular energy diagram become important and exclude any simple interpretation.

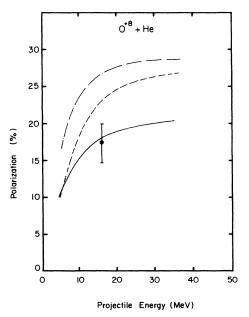


FIG. 8. Polarization percentage P [Eq. (6)] in case of  $O^{8+}$  + He collisions. Present calculations: solid curve, 2p-1s transitions including cascade effects from n=3 and 4 subshells; dashed curve, 2p-1s transitions without cascade effects; dash-dotted curve, 3p-1s transitions including cascade effects from n=4 subshells. The experimental value for the 2p-1s transition from Ref. 16 is indicated by solid circle with error bars.

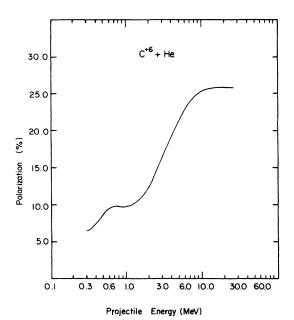


FIG. 9. Polarization fractions P [Eq. (6)] for the 2p-1s transition (including cascade effects) for  $C^{6+}$  + He collision in the range 0.3-30 MeV.

This dependence of P with energy is also true for p-He collisions<sup>27</sup> in the few keV to 100 keV region where the polarization [or the alignment parameter  $A_{20}$ , where  $A_{20}$  is given by  $(\sigma_{p_0} - \sigma_{p_1})/(\sigma_{p_0} + \sigma_{p_1})$ ] of the 2p-1s transition after capture has been measured to be nearly zero. At higher energies, m=0 component has been shown to be dominant such that a positive P is expected (or negative  $A_{20}$ ). We expect that this behavior of P with energy is generally true for all capture processes. Negative fractions P, corresponding to the dominance of capture into

|m|=1 slots are expected if rotational coupling is an important mechanism for the population of 2p states. This is the case for 2p excitation or for capture in p-H collisions below 10 keV.<sup>28</sup> Negative fractions P have been predicted but experimental data are still inconclusive.<sup>30</sup>

# IV. CONCLUSIONS

In this paper we apply the two-center AO-expansion method in a study of electron capture in the collision systems  $C^{6+}$  and  $O^{8+}$  + He at "high" energies. We discuss partial transfer cross sections for capture into individual nlm subshells and examine their variation with energy. There is no experimental data for subshell cross sections for comparison with our calculations. We compared however, our calculated total capture cross sections with the measurement of Dillingham  $et\ al.^{14}$  and found good agreement.

In the absence of experimental subshell cross sections, we derived the polarization fraction of the 2*p*-1*s* transition in O<sup>7+</sup> after capture. By including the effect of cascading from higher channels, we found that our predicted polarization fraction is in good accord with the measurement of Ellsworth *et al.*<sup>16</sup> We conclude that the multistate two-center AO-expansion method along with a one-electron description, appears to be adequate for describing details of the electron-capture process in collision system involving multiply charged ions in the energy region studied. More detailed experiments are needed in order to further assess the limitation of the multistate two-center AO-expansion model.

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