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Electron capture and excitation in low-energy collisions of He^{2+} with metastable $2\,^1S$ and $2\,^3S$ He

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Electron capture and excitation process in collisions of doubly charged ions of He^{2+} with neutral He in either a metastable ^1S or ^3S state are investigated using a theoretical model based on the adiabatic representation of the collision complex. Both *ab initio* and model potential calculations are used to treat the adiabatic states of the $He_2{}^{2+}$ molecular ion. A fully quantum mechanical treatment of the dynamics is adopted. Cross sections are calculated for energies ranging from 10^{-2} to 400 eV/amu. The singlet and triplet metastable states exhibit very pronounced differences in the low eV energy range. Whereas, electron capture and excitation occur simultaneously in collisions with $2\,^1S$ metastable He, electron capture is dominant in collisions with $2\,^3S$ metastable He.

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I. INTRODUCTION

Electron capture by multiply charged ions from neutral atoms can lead to the selective population of specific excited states, which may be used as a diagnostic in both laboratory and astrophysical plasmas. This is of special importance in ECR plasma sources, where there is a continuous injection of neutral gas interacting with the multicharged ions of the plasmas. An interesting case is the conversion of He^{2+} to He^{+} by charge exchange in collisions of He^{2+} with He. For He in the ground state, there is general agreement (both theoretical [1–8] and experimental [9]) that the single electron capture cross section is very small for energies less than 10 keV/amu. At low energies, the most favorable reaction involving ground state He is double electron capture, which of course leads to no net change in the ionic abundances. On the other hand, it is expected that He^{2+} can easily capture an electron from metastable He, leading to the production of two singly charged He^{+} ions. Calculations by Fritsch [7] suggest that the cross section for single electron capture from He in the metastable $(2\,^1S)$ state attains a value of the order of 10^{-14} cm^2 at an energy of 4 keV/amu. But there seems to have been little work on such processes at lower energies.

The aim of the present work is to investigate electron capture involving collisions of He^{2+} with metastable He in either the $2\,^3S$ or $2\,^1S$ state. An adiabatic representation of the molecular ion provides the simplest way to study such reactions at low collision energies (less than a few keV/amu). From the network of avoided crossings of the adiabatic potential energy curves, it is clear that the most likely avoided crossings are those leading to capture in excited $n=3$ Rydberg states of He^{+}:

$$He(1s2s)^1S+He^{2+}\rightarrow He^{+}(1s)^2S+He^{+}(n=3,l), \quad (1)$$

$$He(1s2s)^3S+He^{2+}\rightarrow He^{+}(1s)^2S+He^{+}(n=3,l). \quad (2)$$

Of course, detailed calculations are required to ascertain which crossings are the most effective for electron capture. Because of the proximity of the excitation channels correlated to the $(1s2p)$ configuration of He, it is also necessary to take into account the possibility of the following excitation processes:

$$He(1s2s)^1S+He^{2+}\rightarrow He(1s,2p)^1P+He^{2+}, \quad (3)$$

$$He(1s2s)^3S+He^{2+}\rightarrow He(1s,2p)^3P+He^{2+}. \quad (4)$$

II. METHOD

The first stage of the calculations is to determine the adiabatic energies and nonadiabatic couplings of the molecular ion. Both *ab initio* and model potential methods are used.

In view of the fact that the electron capture and excitation processes (1)–(4) involve only singly excited states of the $He_2{}^{2+}$ molecular ion, the core $1s$ orbital of He plays a purely passive role. We may then expect a model potential method to provide a satisfactory description of both the electron capture and excitation processes. It may be remarked that in this model no account is taken of g,u symmetry. Since there is no significant overlap between the $1s$ orbitals centered on different nuclei for internuclear distances greater than about $2a_0$ and since the processes (1)–(4) are governed by internuclear distances greater than about $5a_0$, the lack of g,u symmetry in the model potential method should not introduce any serious error.

In any case, the assumption of the model potential method can be tested by *ab initio* calculations. As we shall see, the g,u states are degenerate for all internuclear distances of interest.

A. Model potential method

The first step is to construct a model potential to describe the electron interaction with the helium core. Since metastable He has an open shell configuration, two different sets of parameters are used, one for the triplet and the other for

TABLE I. Model potential parameters.

Symmetry	a_1	b_1	a_2	b_2	a_3	b_3	a_4	b_4
Singlet	2.1929	3.426	-20.42	7.4538	8.9981	2.849	-2.117	2.216
Triplet	5.175	5.3732	1.6788	2.1266				

the singlet manifold. Following the method proposed by Valiron [10] and Valiron *et al.* [11], we have used model potentials expressed in the form

$$V(r) = -\frac{1}{r} - \frac{1}{r}\sum_i G_i(a_i,r)\exp(-b_i r), \tag{5}$$

where the G_i expressions are defined by

$$G_1(a_1,r) = 1 + a_1 r, \tag{6}$$

$$G_2(a_2,r) = a_2 r, \tag{7}$$

$$G_3(a_3,r) = a_3 r^2, \tag{8}$$

$$G_4(a_4,r) = a_4 r^3. \tag{9}$$

The a_i and b_i parameters are listed in Table I, and the eigenvalues of the corresponding model atomic Hamiltonian are compared with the experimental energy values of the neutral helium atom in Table II. The precision of the computed energy levels is adequate for the particular applications of this work.

The $He_2{}^{2+}$ molecular ion is treated as a single active electron system. Taking the He^+ core at *A* and the He^{2+} nucleus at *B*, the model Hamiltonian may be written as

$$H_{model} = T + V_{He^+}(r_A) - \frac{2}{r_B} + U_{core}, \tag{10}$$

where T is the electronic kinetic energy, and r_A and r_B are, respectively, the electron position with respect to the $He^+(1s)$ core and the He^{2+} nucleus. The He^{2+}-core interaction is designated in expression (10) by U_{core}. Since the core polarization is relatively unimportant for the charge transfer process, it is sufficient to consider U_{core} as the nuclear Coulomb repulsion.

$$U_{core} = \frac{2}{R}. \tag{11}$$

TABLE II. Comparison of calculated and experimental energy levels in a.u. (omitting the He^+ core energy) of the singlet and triplet series of helium.

Symmetry	nl	Model potential	Moore [12]
Singlet	$1s^2$	-0.8989	-0.9033
	$1s2s$	-0.1462	-0.1459
	$1s2p$	-0.1239	-0.1238
	$1s3s$	-0.0614	-0.0613
	$1s3p$	-0.0559	-0.0551
	$1s3d$	-0.0552	-0.0556
Triplet	$1s2s$	-0.1749	-0.1752
	$1s2p$	-0.1331	-0.1332
	$1s3s$	-0.0687	-0.0687
	$1s3p$	-0.0581	-0.0581
	$1s3d$	-0.0556	-0.0556

The spectrum of the model Hamiltonian (10) is determined by a standard variational method using a set of monoelectronic Slater orbitals. We present in Figs. 1 and 2 the corresponding potential energy curves.

In the singlet manifold, we observe two major avoided crossings, both of which have a direct influence on the excitation and charge transfer processes: one around $11.45a_0$, the other around $18.38a_0$. Identification of the channels affected by these crossings requires a calculation of the nonadiabatic radial coupling matrix. By this means, we are able to identify the $11.45a_0$ avoided crossing (energy separation 0.58 eV) with the interaction of the Σ_4 and Σ_5 channels and the other around $18.38a_0$ (energy separation 0.85 eV) with the interaction of the Σ_1 and Σ_4 channels. The inner $11.45a_0$ avoided crossing leads to excitation of the $He(1s2p)^1P$ state, while the outer $18.38a_0$ avoided crossing leads to charge transfer to He^+ in the excited channel $n=3$ state. We can deduce using a simple Landeau-Zener model that excitation is likely to dominate over charge transfer process at low energies. From

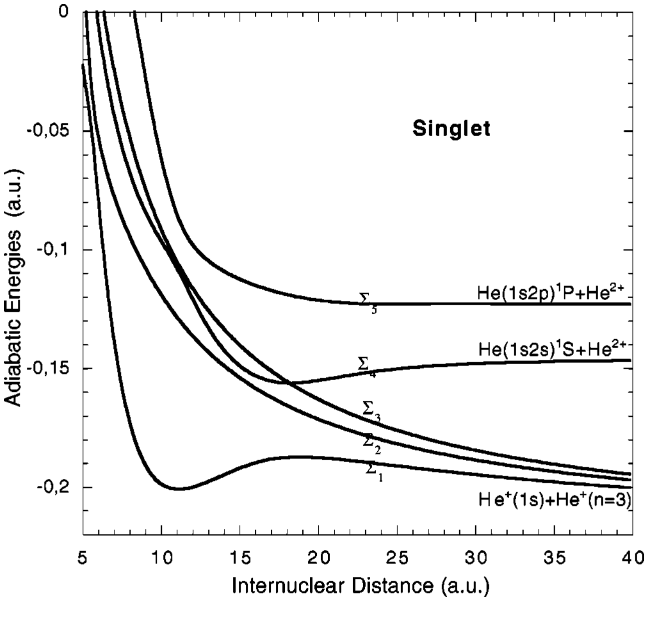

FIG. 1. Model potential method: He/He^{2+} singlet adiabatic potential energies (omitting the He^+ core potential) as a function of internuclear distance. Σ_1, $He^+(1s)+He^+(n=3)$; Σ_2, $He^+(1s)+He^+(n=3)$; Σ_3, $He^+(1s)+He^+(n=3)$; Σ_4, $He(1s2s)^1S+He^{2+}$; Σ_5, $He(1s2p)^1P+He^{2+}$.

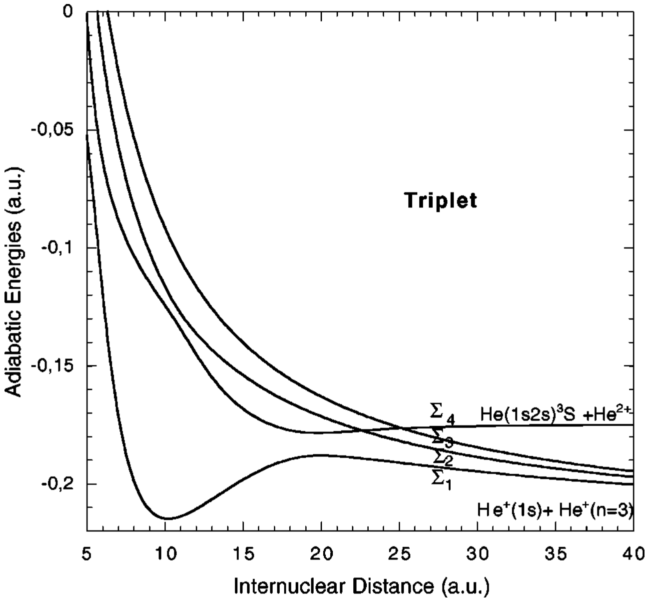

FIG. 2. Model potential method: He/He^{2+} triplet adiabatic potential energies (omitting the He$^+$ core potential) as a function of internuclear distance. Σ_1, He$^+(1s)+$He$^+(n=3)$; Σ_2, He$^+(1s)+$He$^+(n=3)$; Σ_3, He$^+(1s)+$He$^+(n=3)$; Σ_4, He$(1s2s)^3S+$He^{2+}.

Fig. 1 we can easily see that other long range crossings are all diabatic. A set of avoided crossings is also observed at short internuclear distances around $5a_0$. These have only a secondary influence on excitation and charge transfer.

In the triplet manifold, the principal feature is the presence of an isolated avoided crossing at $R_x = 19.93a_0$ (energy separation 0.26 eV) involving the Σ_1 and Σ_4 channels. The Σ_2 channel is subject to two avoided crossings: an outer unimportant diabatic one at $R_x = 22.5a_0$ and a more important inner one at $R_x = 10.83a_0$ (energy separation 0.18 eV). From the calculated energy separations at the crossings and the nonadiabatic coupling matrix, it can easily be deduced that both the $19.9a_o$ and the $10.8a_0$ avoided crossings lead to charge transfer processes. Contrary to the singlet manifold, it is observed that there are no avoided crossings leading to excitation in the triplet manifold.

B. Identification of the molecular states at the dissociation limit

It may be remarked that all three adiabatic states Σ_1, Σ_2, and Σ_3 lead to electron capture in the He$^+(n=3)$ state. It is obvious from Figs. 1 and 2 that their interactions with the initial and excitation channels differ markedly from each other. Their asymptotic behavior can easily be obtained by considering the perturbation of a He$^+(n=3)$ atom by the long range interaction due to the He$^+(1s)$ ion.

The perturbation is diagonal in the representation of the parabolic quantum numbers n_1, n_2, and m. The principal quantum number n is deduced from the relation [13]

$$n = n_1 + n_2 + |m| + 1. \tag{12}$$

The $\Sigma_1,\Sigma_2,\Sigma_3$ states can therefore be labeled by n,n_1,n_2, and m and their asymptotic energies vary with R according to

$$E(n,n_1,n_2) = -\frac{2}{n^2} - \frac{3}{2R^2} n(n_1 - n_2). \tag{13}$$

For $n=3$, a comparison of the energy values according to formula (13) with the adiabatic energies allows us to identify the Σ_j ($j=1,2,3$) molecular states with the atomic states, at the dissociation limit, as follows:

$$\Sigma_1 = |m=0, n_1=0, n_2=2\rangle, \tag{14}$$

$$\Sigma_2 = |m=0, n_1=1, n_2=1\rangle, \tag{15}$$

$$\Sigma_3 = |m=0, n_1=2, n_2=0\rangle. \tag{16}$$

C. *Ab initio* method

To test the accuracy of the model potential calculations described in Sec. II A, we have calculated the adiabatic energies of the molecular ion by a standard configuration interaction method using the total Hamiltonian

$$H_{total} = h_1 + h_2 + \frac{1}{r_{12}} + \frac{4}{R}, \tag{17}$$

where h_i ($i=1,2$) is the single electron Hamiltonian defined by

$$h_i = T_i - \frac{2}{r_{A_i}} - \frac{2}{r_{B_i}}. \tag{18}$$

T_i denotes the kinetic energy of the electron i, r_{A_i}, and r_{B_i} being, respectively, its radial distance with respect to centers A and B.

The spectrum of the total Hamiltonian is determined by conventional variational techniques using a basis set of Slater-type orbitals expressed in prolate spheroidal coordinates $(\lambda_i, \mu_i, \phi_i)$ where

$$\lambda_i = \frac{r_{Ai} + r_{Bi}}{R}, \quad \mu_i = \frac{r_{Ai} - r_{Bi}}{R}, \tag{19}$$

and ϕ_i is the azimuthal coordinate. The $\psi(1,2)$ basis functions are expressed in the form of an antisymmetrized product of monoelectronic Slater orbitals as

$$\psi_{a,b}(1,2) = \{f_a(1)f_b(2) \pm f_b(1)f_a(2)\}\chi(1,2), \tag{20}$$

where $f_\beta(i) = f_\beta(\lambda_i,\mu_i)e^{im_\beta\phi_i}$ ($\beta=a,b$ and $i=1,2$) is a function that generally is not separable in λ_i and μ_i, m_β is the projection ($\pm\Lambda$) of the electronic angular momentum on the internuclear axis, and $\chi(1,2)$ is the singlet or triplet spin function.

In practice, we have used, respectively, 155 and 53 basis function for the singlet and triplet manifolds, with the parameters as given in Table III.

In determining the Hamiltonian matrix elements, the main difficulty concerns the evaluation of the bielectronic integral

TABLE III. Slater-type-orbital basis.

n	l	m	α
1	0	0	2.00
1	0	0	1.34
2	0	0	1.00
2	1	0	1.00
2	1	0	0.54
2	1	± 1	1.00
2	1	± 1	2.20
2	1	± 1	0.54
3	0	0	0.67
3	1	± 1	0.67
3	2	± 1	0.67

$\langle \psi_{a,b}(1,2) | 1/r_{12} | \psi_{c,d}(1,2) \rangle$. The method used in the present work is based on the work of Henriet *et al.* [14], details of which can be found in the Appendix. We just mention here that for a given set of $(\lambda_i, \mu_i, \phi_i)$ coordinates integrals over the variables ϕ_1 and ϕ_2 can be carried out analytically in terms of elliptic integrals. Then the integrals involving the (λ_i, μ_i) coordinates are computed using a Gauss-Laguerre quadrature.

The computed adiabatic energies confirm that, for the range of internuclear distances given in Figs. 3 and 4, the adiabatic energies of the g,u states are essentially degenerate. It is therefore legitimate to assume that the $1s$ orbital is simply a spectator in the collision processes and that we need not take account of exchange processes involving the $1s$ electron.

By and large, the *ab initio* and model potential calculations are in excellent agreement for both the positions and energy separations of the avoided crossings (Table IV). The largest apparent difference concerns the location of the long distance singlet avoided crossing. It is seen from Table V that the error of the *ab initio* calculation for the dissociation limit is about 0.25% in the singlet case and 0.05% in the triplet case. This is sufficient to explain the differences between the *ab initio* and model potential determinations of the crossing radii. Since the model potential parameters are chosen to give the correct dissociation limit it is probable that the model potential results are more precise than the *ab initio* results for both the position and energy separation of the avoided crossings. In any case, even without any adjustment of the dissociation limit, both the *ab initio* and model potential calculations will yield very similar results for the collision process.

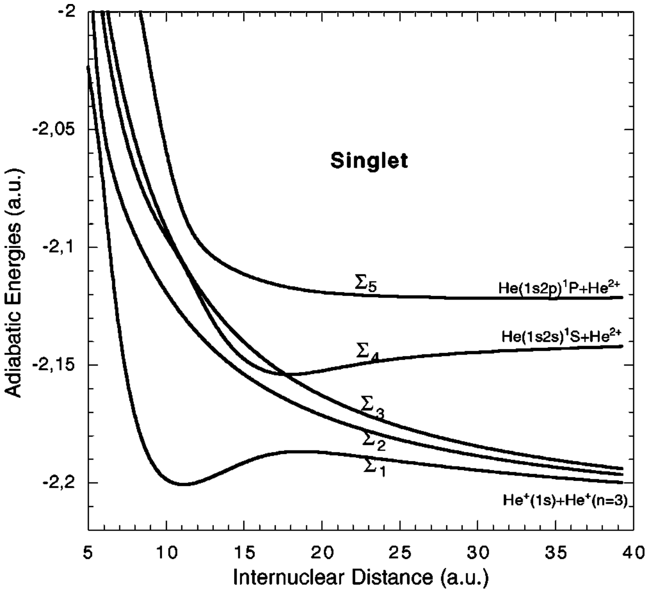

FIG. 3. *Ab initio* method: He/He^{2+} singlet adiabatic potential energies. Σ_1, He$^+(1s)+$He$^+(n=3)$; Σ_2, He$^+(1s)+$He$^+(n=3)$; Σ_3, He$^+(1s)+$He$^+(n=3)$; Σ_4, He$(1s2s)^1S+$He^{2+}; Σ_5, He$(1s2p)^1P+$He^{2+}.

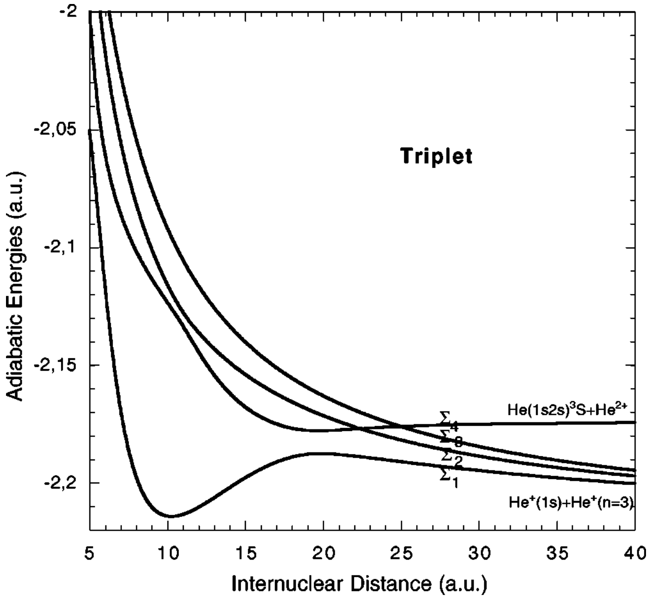

FIG. 4. *Ab initio* method: He/He^{2+} triplet adiabatic potential energies. Σ_1, He$^+(1s)+$He$^+(n=3)$; Σ_2, He$^+(1s)+$He$^+(n=3)$; Σ_3, He$^+(1s)+$He$^+(n=3)$; Σ_4, He$(1s2s)^3S+$He^{2+}.

III. NONADIABATIC COUPLING

In view of the excellent agreement of the model potential adiabatic energies with the *ab initio* calculations, we have chosen to calculate the nonadiabatic matrix elements using model potential wave functions. This choice was not dictated only by the desire to simplify the calculations. The main

TABLE IV. Comparison of *ab initio* and model potential avoided crossing parameters.

		Model potential		*Ab initio*	
Symmetry	Crossing	R_x (a_0)	Δ_x (eV)	R_x (a_0)	Δ_x (eV)
Singlet	Σ_1-Σ_4	18.38	0.85	18.17	0.89
	Σ4-Σ_5	11.45	0.58	11.55	0.57
Triplet	Σ_1-Σ_4	19.93	0.26	19.77	0.27
	Σ_2-Σ_4	10.83	0.18	10.84	0.16

TABLE V. Asymptotic separated-atom ionization potentials in a.u.

Asymptotic atomic states	Model potential	Moore [12]	*Ab initio*
$\mathrm{He}(1s2s)^1S+\mathrm{He}^{2+}$	0.1462	0.1459	0.1409
$\mathrm{He}(1s2s)^3S+\mathrm{He}^{2+}$	0.1749	0.1752	0.1742

reason is that reactions (1)–(3) are governed by very long range avoided crossings [crossing radii in the range $(10-20)a_0$]. Past experience with such calculations indicates that, under such conditions, model potential techniques have the advantage, in that they guarantee the numerical accuracy of the matrix elements (within the physical limitations of the method). Another reason was the need to modify the adiabatic basis to take account of the lack of Galilean invariance of standard scattering equations. One way is to introduce appropriate reaction coordinates [15] such that all nonadiabatic coupling terms vanish in the asymptotic limit. This procedure has given satisfactory results and we have been able to use the program developed by Gargaud *et al.* [16] without any major modification. Of course, other procedures exist [17,18], but for the energy range of interest in this work, such methods should yield very similar results.

In practice, the radial coupling elements have been determined using the finite difference technique. Translation effects have been taken into account using reaction coordinates [19]. In Figs. 5 and 6, we present the radial coupling matrix elements susceptible to inducing transitions between different molecular states and whose different peaks correspond to the avoided crossings cited above. The elements that are not illustrated here either have a weak magnitude or manifest at short internuclear distance highly peaked elements whose influence will be negligible for the dynamics.

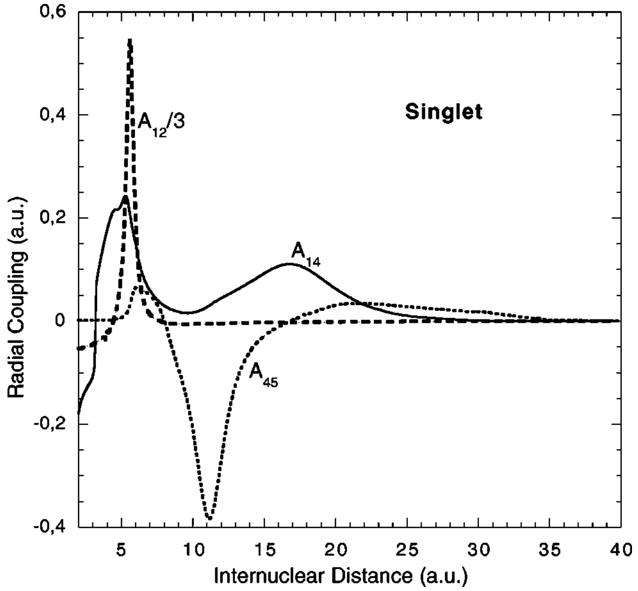

FIG. 5. He/He^{2+} radial coupling matrix elements for singlet manifold. $A_{12}=\langle\Sigma_1|\partial/\partial R|\Sigma_2\rangle$, $A_{14}=\langle\Sigma_1|\partial/\partial R|\Sigma_4\rangle$, $A_{45}=\langle\Sigma_4|\partial/\partial R|\Sigma_5\rangle$.

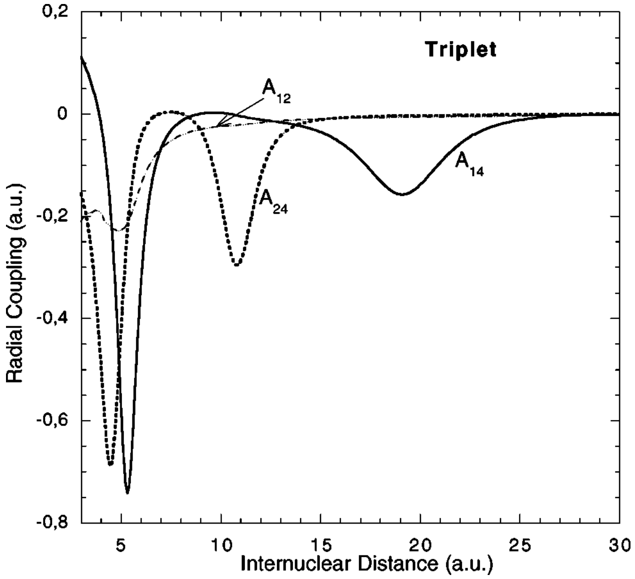

FIG. 6. He/He^{2+} radial coupling matrix elements for triplet manifold. $A_{12}=\langle\Sigma_1|\partial/\partial R|\Sigma_2\rangle$, $A_{14}=\langle\Sigma_1|\partial/\partial R|\Sigma_4\rangle$, $A_{24}=\langle\Sigma_2|\partial/\partial R|\Sigma_4\rangle$.

For the singlet case, it should be remarked that the A_{14} radial coupling element matrix responsible for the electronic capture is smaller than the A_{45} element that leads to excitation of the $\mathrm{He}(1s2p)^1P$ state. We therefore conclude that excitation accompanies capture for the singlet manifold.

From our calculations, it is seen that electron capture principally populates the Stark state $\Sigma_1(n_1=0,n_2=2)$ of He$^+$. Of course rotational (Coriolis) coupling will lead to a mixing of this state with Σ and Π states. But this will not affect the total electron capture cross section to the $n=3$ state. Rotational coupling need only be introduced if information on the population of the sub-m levels is required.

IV. RESULTS

The electron capture and excitation cross sections have been calculated by a quantum mechanical coupled state program as described by Gargaud *et al.* [16]. Account has been taken of all the Σ states involved in the crossing network.

Results are presented, respectively, for the singlet and triplet systems in TablesVI and VII. A graphical presentation of the results is given in Figs. 7 and 8.

The most striking aspect of the results concerns the very different behavior of the singlet and triplet systems. The onset of electron capture by He^{2+} from $\mathrm{He}(2\,^1S)$ occurs at about 30 eV/amu and the cross section rises uniformly with increasing energy, attaining a value of about 5×10^{-15} cm^2 at 400 eV/amu. Above 400 eV/amu, the cross section begins to level off. So we have reason to expect that our calculations are consistent with those of Fritsch [7] at energies above 4 keV/amu. The onset of electron capture by He^{2+} from $\mathrm{He}(2\,^3S)$ occurs at much lower energies (about 1 eV/amu) and the cross section rises to a maximum of about 2×10^{-14} cm^2 at a collision energy of 350 eV/amu.

One other notable feature concerns the excitation chan-

TABLE VI. Cross sections in units of 10^{-16} cm^2 for electron capture and excitation in collisions of He^{2+} with He($2\,^1S$). The quantities σ_1, σ_2, and σ_3 refer to electron capture into the individual Stark states (see text) of He$^+(n=3)$, σ_{total} designates the electron capture cross section summed over all of the Stark states, and $\sigma_{excitation}$ designates the cross section for excitation of the $2\,^1P$ state of He.

E_{lab} (eV/amu)	σ_1	σ_2	σ_3	σ_{total}	$\sigma_{excitation}$
06.80	4.740×10^{-3}	1.200×10^{-2}	1.740×10^{-3}	1.850×10^{-2}	02.258
13.60	4.720×10^{-2}	8.960×10^{-2}	1.530×10^{-2}	1.520×10^{-1}	11.938
27.20	1.810×10^{-1}	1.890×10^{-1}	2.920×10^{-2}	3.990×10^{-1}	25.618
54.40	2.070	1.107	1.660×10^{-1}	3.382	46.179
108.80	5.856	1.238	3.130×10^{-1}	7.407	48.708
163.20	14.466	2.370	1.690×10^{-1}	16.994	53.933
204.00	16.854	1.915	2.310×10^{-1}	19.101	51.966
272.00	25.843	2.205	5.390×10^{-1}	28.651	61.798
408.00	43.371	4.516	1.159	49.213	68.539

nels. The cross section for excitation of He$(1s,2p)^1P$ in the singlet system is much larger than the electron capture cross section, ranging from 5×10^{-15} cm^2 at 60 eV/amu to a maximum of nearly 8×10^{-15} cm^2 at 350 eV/amu. The dominance of the excitation channel is also found in the calculations of Fritsch. On the other hand, excitation of He$(1s,2p)^3P$ in the triplet system is negligible.

The dominant electron capture channel for both the singlet and triplet systems is the Stark Σ state $(n_1=0,n_2=2)$. The cross section for electron capture to the Stark Σ state $(n_1=0,n_2=1)$ is an order of magnitude smaller than the cross section for the dominant channel. Electron capture to the Stark Σ state $(n_1=2,n_2=0)$ is negligible.

It would be of great interest to have some experimental measurements on this relatively simple system involving collisions of He^{2+} with metastable He. The electron capture and excitation mechanisms are highly selective in the energy range below 1 keV/amu.

ACKNOWLEDGMENTS

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APPENDIX

For a two-electron system, the $\psi_{a,b}(1,2)$ basis functions used in variational calculations to solve the total Schrödinger equation are taken to be antisymmetrized:

TABLE VII. Cross sections in units of 10^{-16} cm^2 for electron capture in collisions of He^{2+} with He($2\,^3S$). The quantities σ_1, σ_2 and σ_3 refer to electron capture into the individual Stark states (see text) of He$^+ n=3$, σ_{total} designates the electron capture cross section summed over all of the Stark states.

E_{lab}(eV/amu)	σ_1	σ_2	σ_3	σ_{total}
1.36×10^{-2}	1.190×10^{-4}	2.970×10^{-2}	7.700×10^{-12}	2.980×10^{-2}
6.80×10^{-2}	5.990×10^{-5}	1.920×10^{-2}	3.440×10^{-12}	1.920×10^{-2}
6.80×10^{-1}	9.900×10^{-2}	7.180×10^{-2}	2.130×10^{-9}	1.710×10^{-1}
1.36	8.620×10^{-1}	3.792	1.030×10^{-8}	4.635
2.72	4.223	15.082	2.860×10^{-8}	19.304
4.08	8.498	21.094	3.960×10^{-8}	29.593
5.44	14.241	25.891	5.130×10^{-8}	40.132
6.80	19.523	30.618	5.670×10^{-8}	50.001
13.60	43.259	34.832	6.540×10^{-8}	78.287
27.20	79.038	34.072	6.140×10^{-8}	113.111
40.80	101.583	39.072	5.360×10^{-8}	140.655
54.40	115.730	34.832	4.640×10^{-8}	150.001
108.80	144.102	30.160	2.940×10^{-8}	174.439
163.20	160.112	26.824	2.210×10^{-7}	186.798
204.00	161.517	26.545	1.790×10^{-8}	188.203
272.00	167.135	29.635	1.370×10^{-8}	196.629
408.00	165.393	22.921	9.010×10^{-9}	188.315

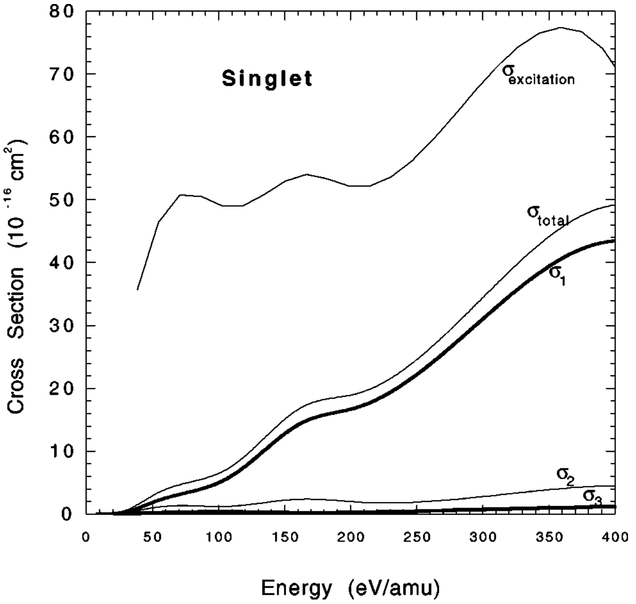

FIG. 7. Cross sections in units of 10^{-16} cm^2 for electron capture and excitation in collisions of He^{2+} with He$(2\ {}^1S)$. The quantities σ_1, σ_2, and σ_3 refer to electron capture into the individual Stark states (see text) of He$^+(n=3)$, σ_{total} designates the electron capture cross section summed over all of the Stark states, and $\sigma_{excitation}$ designates the cross section for excitation of the $(2\ {}^1P)$ state of He.

$$\psi_{a,b}(1,2)=\frac{1}{\sqrt{2}}[g_a(1)g_b(2)\pm g_a(2)g_b(1)]\chi(1,2), \tag{A1}$$

where $\chi(1,2)$ is the total singlet or triplet spin function and g the monoelectronic spatial orbital, which may be expressed in prolate spheroidal coordinates (λ,μ,ϕ), in the form

$$\begin{aligned}g_a(j)&=N[(\lambda_j^2-1)(1-\mu_j^2)]^{|m_a/2|}\lambda_j^{p_a}\mu_j^{q_a}\\&\quad\times\exp\left[-\frac{\alpha R}{2}(\lambda_j+\epsilon_a\mu_j)\right]\exp(im_a\phi_j)\\&=f_a(j)\exp(im_a\phi_j),\end{aligned}\tag{A2}$$

where N designates a normalization coefficient, (p_a,q_a) is an entire set, α is a positive variational parameter, $\epsilon_a=\pm1$ depending on the limit of dissociation of the function $g_a(j)$, and m_a is the projection $(\pm\Lambda)$ of the electronic angular momentum on the internuclear axis.

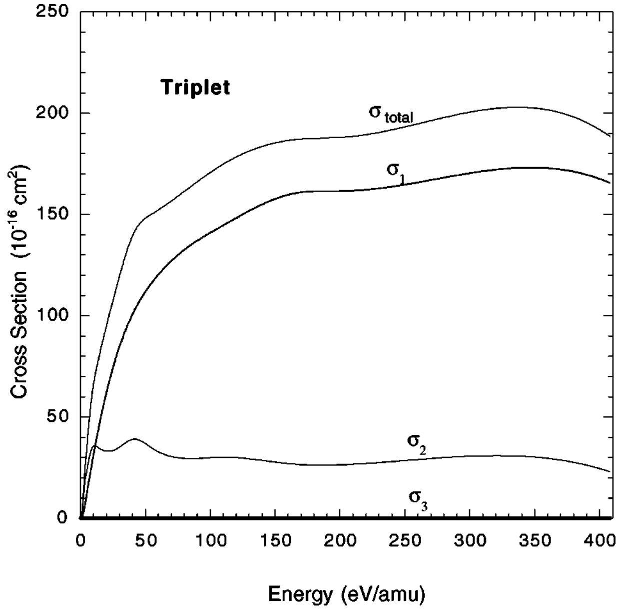

FIG. 8. Cross sections in units of 10^{-16} cm^2 for electron capture in collisions of He^{2+} with He$(2\ {}^3S)$. The quantities σ_1, σ_2, and σ_3 refer to electron capture into the individual Stark states (see text) of He$^+(n=3)$ and σ_{total} designates the electron capture cross section summed over all of the Stark states.

We show in this Appendix how to calculate the integral analytically over the ϕ_1 and ϕ_2 coordinates involved in the bielectronic matrix element calculations,

$$I=\left\langle\psi_{a,b}(1,2)\left|\frac{1}{|\vec{r}_1-\vec{r}_2|}\right|\psi_{c,d}(1,2)\right\rangle, \tag{A3}$$

where $|\vec{r}_1-\vec{r}_2|$ can be expressed in prolate spheroidal coordinates as

$$|\vec{r}_1-\vec{r}_2|=\sqrt{A-B}\sqrt{1-k^2\sin^2[(\phi_2-\phi_1)/2]} \tag{A4}$$

with

$$A=\frac{R^2}{4}[(\lambda_1+\mu_1)^2+(\lambda_2+\mu_2)^2-2(\lambda_1\mu_1+1)(\lambda_2\mu_2+1)], \tag{A5}$$

$$B=\frac{R^2}{2}\sqrt{(\lambda_1^2-1)(1-\mu_1^2)}\sqrt{(\lambda_2^2-1)(1-\mu_2^2)}, \tag{A6}$$

and

$$k^2=k^2(\lambda_1,\mu_1,\lambda_2,\mu_2)=\frac{2B}{B-A}. \tag{A7}$$

The bielectronic integral I in Eq. (A3) can be written as a sum or a difference $(I=I_{co}\pm I_{ex})$ of two terms I_{co} and I_{ex} called, respectively, the Coulomb and exchange integral, given by

$$\begin{aligned}I_{co}&=\int\int\frac{f_a(1)f_b(2)f_c(1)f_d(2)}{\sqrt{A-B}}\\&\quad\times\frac{e^{i(m_c-m_a)\phi_1}e^{i(m_d-m_b)\phi_2}}{\sqrt{1-k^2\sin^2[(\phi_2-\phi_1)/2]}}d\tau_1 d\tau_2\end{aligned}\tag{A8}$$

and

$$I_{ex}=\int\int\frac{f_a(1)f_b(2)f_c(2)f_d(1)}{\sqrt{A-B}}\times\frac{e^{i(m_d-m_a)\phi_1}e^{i(m_c-m_b)\phi_2}}{\sqrt{1-k^2\sin^2[(\phi_2-\phi_1)/2]}}d\tau_1 d\tau_2. \tag{A9}$$

Here $d\tau_1$ and $d\tau_2$ are the volume elements.

For a given molecular symmetry, we have $\Lambda=|m_a+m_b|=|m_c+m_d|$. The above integrals I_{co} and I_{ex} can be expressed as follows:

$$I_{co}=\int\int\frac{f_a(1)f_b(2)f_c(1)f_d(2)}{\sqrt{A-B}}\times\frac{e^{im(\phi_2-\phi_1)}}{\sqrt{1-k^2\sin^2[(\phi_2-\phi_1)/2]}}d\tau_1 d\tau_2, \tag{A10}$$

$$I_{ex}=\int\int\frac{f_a(1)f_b(2)f_d(1)f_c(2)}{\sqrt{A-B}}\times\frac{e^{im'(\phi_2-\phi_1)}}{\sqrt{1-k^2\sin^2[(\phi_2-\phi_1)/2]}}d\tau_1 d\tau_2, \tag{A11}$$

with

$$m=m_a-m_c=m_d-m_b, \tag{A12}$$

$$m'=m_c-m_b=m_a-m_d. \tag{A13}$$

Following Herriet *et al.* [14], it is practical to make the change of variables

$$\{\phi_1,\phi_2\}\rightarrow\{\phi_1-\phi_2,\phi_2\}, \tag{A14}$$

$$d\phi_1 d\phi_2=d\phi_1 d|\phi_1-\phi_2|=d\phi_1 d\phi',\quad(\phi'=|\phi_1-\phi_2|), \tag{A15}$$

which allows us to express I_{co} as

$$I_{co}=\frac{R^6}{64}\int d\lambda_1\int d\lambda_2\int(\lambda_1^2-\mu_1^2)f_a(1)f_c(1)d\mu_1\times\int\frac{(\lambda_2^2-\mu_2^2)f_b(2)f_d(2)}{\sqrt{A-B}}d\mu_2 J_m(k), \tag{A16}$$

where $J_m(k)=J_{a,b,c,d}(k)$ is the integral defined by

$$J_m(k)=\int_0^{2\pi}d\phi_2\int_0^{2\pi}\frac{e^{im\phi'}}{\sqrt{1-k^2\sin^2(\phi'/2)}}d\phi' =2\pi\int_0^{2\pi}\frac{e^{im\phi'}}{\sqrt{1-k^2\sin^2(\phi'/2)}}d\phi'. \tag{A17}$$

For symmetry reasons, the imaginary part in Eq. (A17) vanishes and the above expression can be reduced to

$$J_m(k)=2\pi\int_0^{2\pi}\frac{\cos(m\phi')}{\sqrt{1-k^2\sin^2(\phi'/2)}}d\phi' =8\pi\int_0^{\pi/2}\frac{\cos(2m\phi')}{\sqrt{1-k^2\sin^2(\phi')}}d\phi'. \tag{A18}$$

For a given value of the set $(\lambda_1,\mu_1,\lambda_2,\mu_2)$, we fix the value of k according to the rule (A7), and the integral (A18) can be expressed in terms of the elliptic integrals F and E defined by

$$F(k)=\int_0^{\pi/2}\frac{dx}{\sqrt{1-k^2\sin^2 x}}, \tag{A19}$$

$$E(k)=\int_0^{\pi/2}\sqrt{1-k^2\sin^2 x}dx. \tag{A20}$$

In practice we have calculated the Σ $(\Lambda=0)$ molecular states of the $\mathrm{He_2}^{2+}$ system. We have taken $m_a=m_b=0$ and $m_a=-m_b=1$, which yield to two possible values of $|m|$ equal to 0 and 2, involving $J_0(k)$ and $J_2(k)$ expressions given by [20]

$$J_0(k)=F(k), \tag{A21}$$

$$J_2(k)=-F(k)+2\left[\frac{1}{k^2}E(k)-\frac{1-k^2}{k^2}F(k)\right]. \tag{A22}$$

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