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Citation: *The Journal of Chemical Physics* **138**, 134317 (2013); doi: 10.1063/1.4794048

View online: <http://dx.doi.org/10.1063/1.4794048>

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Long-range interactions of excited He atoms with the alkaline earth atoms Mg, Ca, and Sr

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(Received 6 December 2012; accepted 18 February 2013; published online 5 April 2013)

Dispersion coefficients for the long-range interactions of the first four excited states of He, i.e., He($2\ 1,3S$) and He($2\ 1,3P$), with the low-lying states of the alkaline earth atoms Mg, Ca, and Sr are calculated by summing over the reduced matrix elements of multipole transition operators.

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I. INTRODUCTION

The collisional deexcitation and Penning ionization processes have been an interesting topic for a long time, because they are of great importance in both fundamental and applied sciences. For example, the excitation-transfer collisions between metastable He atoms and Ne atoms underly the operation of the helium-neon gas laser.¹ Furthermore, metastable atom electron spectroscopy is a powerful technique widely used to study the electronic characteristics of various surfaces and interfaces.²⁻⁶ The basic principles of this technique are that a slow, long-lived, rare gas metastable atom is introduced onto a surface of condensed matter, where most of its excitation energy is used to eject electrons from the surface, and that the resultant spectrum of ejected electrons describes the electronic state of the surface.

In fundamental science, a large amount of experimental and theoretical work has been done to study the interactions of excited rare gas atoms with atomic and molecular targets and the collision characteristics of the corresponding processes.⁷⁻¹⁶ The excited rare gas atoms can be metastable atoms, optically allowed excited atoms,¹⁶ or even highly excited Rydberg atoms.¹⁷⁻²⁰ Most Penning ionization experiments involved the long-lived metastable species He($2\ 3S$) and He($2\ 1S$), since the excitation energies $E(2\ 3S) = 19.8$ eV and $E(2\ 1S) = 20.6$ eV are larger than the lowest ionization energies of almost all atoms and molecules except for He and Ne. For the calculations, reliable model potentials are important as they directly impact on the accuracy of estimated collision characteristics such as the total ionization cross sections and their collisional-energy dependence. For the case of the deexcitation of optically allowed excited atoms such as He($2\ 1P$), Ne[$2p^5(2P_{1/2})3s\ 1P_1$], and Ar[$3p^5(2P_{1/2})4s\ 1P_1$],¹⁶

the long-range parts of the potentials are much stronger than for the case of the deexcitation of metastable atoms. The long-range interaction between the involved atoms or molecules determines the rate coefficient for close collisions so that it has an important influence on the rate coefficient for Penning ionization.^{9,10}

In this work, we compute the dispersion coefficients for long-range interactions of the first four excited states of He, i.e., He($2\ 1,3S$) and He($2\ 1,3P$), with the low-lying states of the alkaline earth atoms Mg, Ca, and Sr by the sum over the reduced matrix elements of multipole transition operators.²¹⁻²³ For the symmetries of diatomic molecules, we adopt the notations of Ref. 23. Atomic units are used throughout.

II. CALCULATION OF DISPERSION COEFFICIENTS

The long-range interaction between two atoms is treated as a perturbation to the isolated atoms. For a system A - B involving one S -symmetry atom (say A), for example, the zero-order wavefunction is simply a product of two atomic wave functions

$$\Psi^{(0)}(M_B) = \psi_{0A}^{00}(\mathbf{r}_A)\psi_{0B}^{L_B M_B}(\boldsymbol{\xi}_B), \quad (1)$$

where L_B represents the orbital angular momentum quantum number of atom B , M_B is its corresponding magnetic quantum number, $\mathbf{r}_A = \{\mathbf{r}_1, \dots, \mathbf{r}_{N_A}\}$ denotes a set of coordinates of electrons in atom A , and $\boldsymbol{\xi}_B = \{\boldsymbol{\xi}_1, \dots, \boldsymbol{\xi}_{N_B}\}$ has the analogous meaning for atom B .

According to the non-degenerate perturbation theory, for the above-mentioned system, the first-order correction to the energy vanishes and the second-order correction can be written in the form

$$V(R) = -\frac{C_6}{R^6} - \frac{C_8}{R^8} - \frac{C_{10}}{R^{10}} - \dots, \quad (2)$$

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where C_n are the dispersion coefficients and R is the interatomic distance. The coefficients C_n can be calculated by summing over the reduced matrix elements of multipole transition operators. For the simplest case where $L_B = M_B = 0$, for example, C_6 can be represented in the form

$$C_6 = \frac{2}{3} \sum_{n_A n_B} \left| \langle \psi_{0_A}^{00} \parallel \sum_{i=1}^{N_A} r_i \mathbf{C}^1(\hat{\mathbf{r}}_i) \parallel \psi_{n_A} \rangle \right|^2 \times \frac{\left| \langle \psi_{0_B}^{00} \parallel \sum_{j=1}^{N_B} \xi_j \mathbf{C}^1(\hat{\xi}_j) \parallel \psi_{n_B} \rangle \right|^2}{E_{n_A} + E_{n_B} - E_{0_A} - E_{0_B}}, \quad (3)$$

where $\mathbf{C}^1(\hat{\mathbf{r}}_i)$ and $\mathbf{C}^1(\hat{\xi}_j)$ are the spherical tensors of rank 1, ψ_{n_A} and ψ_{n_B} are the n_A th and n_B th intermediate eigenfunctions for atom A and atom B , respectively, and E_{n_A} and E_{n_B} are their corresponding eigenenergies.

For two P-symmetry atoms, there are one Δ molecular state, two Π states and three Σ states, according to the projection of the total angular momentum along the internuclear axis. The first-order correction to the energy can be expressed in the form $-C_5/R^5$, where C_5 is the first-order interaction coefficient. For details on the calculation of dispersion coefficients for two different atoms in arbitrary atomic states, the reader is referred to the comprehensive paper Ref. 23.

III. REPRESENTATION OF ATOMIC STRUCTURE

A. Transition spectra of helium atoms

For a He atom, the energy spectra and reduced matrix elements of the multipole transition operators are the same as those used for calculating the dispersion coefficients for the low-lying states.^{24–28} The wavefunction can be expanded in terms of the Hylleraas-type basis functions

$$r_1^i r_2^j r_{12}^k e^{-\alpha r_1 - \beta r_2} \mathcal{Y}_{\ell_1 \ell_2}^{LM}(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2), \quad (4)$$

where $\mathcal{Y}_{\ell_1 \ell_2}^{LM}(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2)$ is the coupled spherical harmonic forming a common eigenstate of L^2 and L_z . Except for some truncations made to avoid near linear dependence, all terms with $i + j + k \leq \Omega$ are included, where Ω is an integer. The nonlinear parameters α and β are variationally optimized by the power method.

B. Transition spectra of alkaline earth atoms

The reduced matrix elements of the transition operators and energy spectra for the alkaline earth atoms have been used to calculate the dispersion coefficients for the low-lying states of Mg, Ca, and Sr atoms.^{29–31} Details on calculations of atomic spectra of alkaline earth atoms may be found in Refs. 29–36. Accordingly, only a brief description is presented here. The spectra of the valence electrons have been generated by the configuration-interaction plus core-polarization (CICP) method with large mixed Laguerre-type and Slater-type orbital basis sets.^{32,33,35} Moreover, the core effects on the valence electrons have been represented by semiempirical polarization potentials in which the cutoff parameters have been obtained by reproducing the experimental

energies of the low-lying states of positive ions of the alkaline earth atoms.

For Sr atoms, the calculated energies of the singlet states $5s^2 \ ^1S$, $5s5p \ ^1P$, $5s6s \ ^1S$, and $5s4d \ ^1D$ were replaced with the corresponding experimental values, whereas the energies of the triplet states $5s5p \ ^3P$, $5s6s \ ^3S$, and $5s4d \ ^3D$ were changed to the J -weighted experimental values, see Table I in Ref. 31. In addition, the reduced matrix element for the $5s^2 \ ^1S$ – $5s5p \ ^1P$ resonance transition, namely $5.309 a_0$, was changed to the experimental value $5.249 a_0$ obtained from the photoassociation experiment.^{37,38} This matrix element list will be termed the empirically adjusted set and is used for the calculations of the C_n coefficients reported here.

IV. RESULTS AND DISCUSSION

For the He atom, the sufficient completeness of Hylleraas-type basis sets and the accuracy of reduced matrix elements of multipole transition operators have been well demonstrated by the accurate dispersion coefficients calculated for different combinations of low-lying states.^{24–27} Hence, the uncertainties of the dispersion coefficients reported in our paper are mainly determined by the completeness of the basis sets and the effectiveness of the model Hamiltonians for the alkaline earth atoms. The uncertainties of the present calculations can be estimated from the uncertainties of the dispersion coefficients for interactions of the alkaline earth atoms with the ground states of H and He.^{29–31} Generally, the long-range interactions of He($2 \ ^1S$) with other atoms are stronger than the long-range interactions of He($2 \ ^3S$) with the same atoms for the same molecular symmetry, because the polarizabilities of He($2 \ ^1S$) are larger than the polarizabilities of He($2 \ ^3S$). This rule does not always hold for He($2 \ ^1P$) and He($2 \ ^3P$), due to the complexity of the interactions with atoms of nonzero angular momentum.

Table I lists the dispersion coefficients for interaction of He($2 \ ^1,^3S$) with the ground-state alkaline earth atoms Mg($3s^2 \ ^1S$), Ca($4s^2 \ ^1S$), and Sr($5s^2 \ ^1S$). For systems involving

TABLE I. Dispersion coefficients for the He($2 \ ^1,^3S$) states with Mg($3s^2 \ ^1S$), Ca($4s^2 \ ^1S$), and Sr($5s^2 \ ^1S$). The numbers in square brackets denote powers of ten.

System	C_6 (a.u.)	C_8 (a.u.)	C_{10} (a.u.)
MgHe($2 \ ^1S$) $^1\Sigma$	1.835[3]	1.670[5]	1.895[7]
Ref. 39 SKA	2.506(50)[3]		
CaHe($2 \ ^1S$) $^1\Sigma$	3.835[3]	4.069[5]	4.866[7]
Ref. 39 CISCF	3.818[3]	3.974[5]	
Ref. 39 SKA	5.133(46)[3]		
SrHe($2 \ ^1S$) $^1\Sigma$	4.680[3]	5.392[5]	6.654[7]
Ref. 39 SKA	5.898(418)[3]		
MgHe($2 \ ^3S$) $^3\Sigma$	1.188[3]	8.765[4]	7.967[6]
Ref. 39 SKA	1.426(28)[3]		
CaHe($2 \ ^3S$) $^3\Sigma$	2.411[3]	2.179[5]	2.147[7]
Ref. 39 CISCF	2.398[3]	3.174[5]	
Ref. 39 SKA	2.821(24)[3]		
SrHe($2 \ ^3S$) $^3\Sigma$	2.923[3]	2.914[5]	3.000[7]
Ref. 39 SKA	3.217(209)[3]		

TABLE II. Dispersion coefficients for the interactions of He($2^1,^3P$) with Mg($3s^2^1S$), Ca($4s^2^1S$), and Sr($5s^2^1S$). The numbers in the square brackets denote powers of ten.

System	C_6 (a.u.)	C_8 (a.u.)	C_{10} (a.u.)
MgHe(2^1P) $^1\Sigma$	2.643[3]	4.538[5]	6.395[7]
MgHe(2^1P) $^1\Pi$	1.331[3]	4.657[4]	2.690[6]
CaHe(2^1P) $^1\Sigma$	5.819[3]	1.032[6]	1.570[8]
CaHe(2^1P) $^1\Pi$	2.768[3]	1.564[5]	1.018[7]
SrHe(2^1P) $^1\Sigma$	7.222[3]	1.327[6]	2.098[8]
SrHe(2^1P) $^1\Pi$	3.387[3]	2.287[5]	1.596[7]
MgHe(2^3P) $^3\Sigma$	2.294[3]	3.285[5]	4.182[7]
MgHe(2^3P) $^3\Pi$	1.102[3]	3.803[4]	2.037[6]
CaHe(2^3P) $^3\Sigma$	5.357[3]	7.724[5]	1.044[8]
CaHe(2^3P) $^3\Pi$	2.362[3]	1.331[5]	7.953[6]
SrHe(2^3P) $^3\Sigma$	6.792[3]	1.014[6]	1.407[8]
SrHe(2^3P) $^3\Pi$	2.927[3]	1.984[5]	1.258[7]

Mg($3s^2^1S$) and Ca($4s^2^1S$), the uncertainties in C_6 are about 2% and the uncertainties in C_8 and C_{10} slightly larger. For systems involving Sr, the uncertainties are larger than those involving Mg and Ca.

We also list in Table I the values of C_6 and C_8 which have been used by Ruf *et al.* to study Penning ionization collisions of state-selected metastable He($2^1,^3S$) atoms with the ground state alkaline earth atoms Mg, Ca, Sr, and Ba.³⁹ Ruf *et al.*³⁹ have calculated the coefficients C_6 for the systems He($2^1,^3S$)-Ca($4s^2^1S$) with the so-called configuration interaction plus core self consistent field method (CISCF), which is similar to the CICIP. Our C_6 values for these two systems are in agreement with those obtained by Ruf *et al.*³⁹ within 0.5%. Their estimated uncertainty (2%) is also consistent with our calculations. Ruf *et al.*³⁹ have estimated the coefficients C_8 for the above two systems by fitting their experimental parameters. Their C_8 for the He(2^1S)-Ca($4s^2^1S$) interaction is about 2% smaller than our value, while their C_8 for the He(2^3S)-Ca($4s^2^1S$) interaction is about 46% larger than our result. The causes for this large difference are unknown. When studying the Penning ionization involving the systems He($2^1,^3S$)-X (X=Mg, Sr, and Ba), Ruf *et al.*³⁹ have used the coefficients C_6 determined from the atomic static dipole polarizabilities

TABLE III. Dispersion coefficients for the interactions of He($2^1,^3S$) with Mg($3s^2^1S$), Ca($4s^2^1S$), and Sr($5s^2^1S$) except for the system Mg($3s^2^1S$)-He(2^1S). The numbers in square brackets denote powers of ten.

System	C_6 (a.u.)	C_8 (a.u.)	C_{10} (a.u.)
CaHe(2^1S) $^1\Sigma$	6.638[3]	1.886[6]	6.746[8]
CaHe(2^1S) $^1\Pi$	5.734[3]	1.988[5]	1.489[8]
SrHe(2^1S) $^1\Sigma$	5.959[3]	1.402[6]	8.183[8]
SrHe(2^1S) $^1\Pi$	6.955[3]	-3.148[5]	1.407[8]
MgHe(2^3S) $^3\Sigma$	4.356[3]	1.121[6]	1.960[8]
MgHe(2^3S) $^3\Pi$	2.931[3]	1.273[5]	1.934[7]
CaHe(2^3S) $^3\Sigma$	3.833[3]	2.326[6]	2.514[8]
CaHe(2^3S) $^3\Pi$	3.346[3]	5.643[5]	3.418[7]
SrHe(2^3S) $^3\Sigma$	3.851[3]	2.612[6]	3.671[8]
SrHe(2^3S) $^3\Pi$	3.992[3]	5.266[5]	4.335[7]

TABLE IV. Dispersion coefficients for the interactions of He($2^1,^3S$) with Mg($3s^2^1S$), Ca($4s^2^1S$), and Sr($5s^2^1S$) except for the system Mg($3s^2^1S$)-He(2^1S). The numbers in square brackets denote powers of ten.

System	C_6 (a.u.)	C_8 (a.u.)	C_{10} (a.u.)
MgHe(2^1S) $^3\Sigma$	2.803[3]	8.493[5]	8.382[7]
MgHe(2^1S) $^3\Pi$	2.346[3]	2.531[5]	1.973[7]
CaHe(2^1S) $^3\Sigma$	6.014[3]	2.102[6]	2.223[8]
CaHe(2^1S) $^3\Pi$	5.304[3]	4.984[5]	4.286[7]
SrHe(2^1S) $^3\Sigma$	8.690[3]	3.183[6]	3.566[8]
SrHe(2^1S) $^3\Pi$	7.473[3]	6.339[5]	5.959[7]
MgHe(2^3S) $^{1,3,5}\Sigma$	1.769[3]	4.191[5]	3.969[7]
MgHe(2^3S) $^{1,3,5}\Pi$	1.497[3]	1.064[5]	7.358[6]
CaHe(2^3S) $^{1,3,5}\Sigma$	3.490[3]	1.025[6]	1.079[8]
CaHe(2^3S) $^{1,3,5}\Pi$	3.101[3]	2.110[5]	1.658[7]
SrHe(2^3S) $^{1,3,5}\Sigma$	4.839[3]	1.540[6]	1.752[8]
SrHe(2^3S) $^{1,3,5}\Pi$	4.191[3]	2.711[5]	2.330[7]

in the Slater-Kirkwood approximation (SKA).⁴⁰ From Table I, it is noted that the SKA results are 10%–37% larger than our values, which should be more accurate. Accurate dispersion coefficients, especially C_6 , are essential to precisely determine the close collision cross sections and ionization cross sections at low collision energies.

Table II lists the dispersion coefficients for interactions of He($2^1,^3P$) with Mg($3s^2^1S$), Ca($4s^2^1S$), and Sr($5s^2^1S$). The dispersion coefficients C_6 for the Σ symmetry of diatomic molecules are at least 99% larger than for the Π symmetry of the same diatomic molecules. The differences of C_8 and C_{10} spread widely from 5 to 24 fold between the Σ and Π symmetries of the same diatomic molecules. Tables III–XII give dispersion coefficients obtained for the interactions described in the captions. Since the excitation energy of Mg($3s^2^1S$) is larger than the ionization energies of He(2^1S), He(2^3P), and He(2^1P), we can not get the converged C_n values for the systems Mg($3s^2^1S$)-He(2^1S), Mg($3s^2^1S$)-He(2^3P), and Mg($3s^2^1S$)-He(2^1P) using

TABLE V. Dispersion coefficients for the interactions of He(2^1P) with Ca($4s^2^1S$) and Sr($5s^2^1S$). The numbers in square brackets denote powers of ten.

Symmetry	C_5 (a.u.)	C_6 (a.u.)	C_8 (a.u.)	C_{10} (a.u.)
Ca(4^1P)-He(2^1P)				
$^1\Delta$	-2.039[2]	3.031[3]	2.961[5]	8.118[7]
(1) $^1\Pi$	8.156[2]	4.117[3]	9.204[5]	1.120[8]
(2) $^1\Pi$	0	4.237[3]	1.471[6]	3.466[8]
$^1\Sigma^-$	0	2.971[3]	1.350[5]	5.308[6]
(1) $^1\Sigma^+$	0	3.845[3]	1.178[6]	3.670[8]
(2) $^1\Sigma^+$	-1.223[3]	1.419[4]	1.378[6]	6.711[8]
Sr(5^1P)-He(2^1P)				
$^1\Delta$	-2.423[2]	2.952[3]	3.780[5]	1.272[8]
(1) $^1\Pi$	9.691[2]	4.883[3]	1.239[6]	1.598[8]
(2) $^1\Pi$	0	3.451[3]	1.827[6]	4.955[8]
$^1\Sigma^-$	0	3.669[3]	1.753[5]	8.194[6]
(1) $^1\Sigma^+$	0	3.165[3]	1.442[6]	5.275[8]
(2) $^1\Sigma^+$	-1.454[3]	1.736[4]	1.487[6]	9.137[8]

TABLE VI. Dispersion coefficients for the interactions of He(2^1P) with Mg($3s\ 3p^3P$), Ca($4s\ 4p^3P$), and Sr($5s\ 5p^3P$). The numbers in square brackets denote powers of ten.

Symmetry	C_5 (a.u.)	C_6 (a.u.)	C_8 (a.u.)	C_{10} (a.u.)
Mg(3^3P)–He(2^1P)				
$^3\Delta$	–1.553[2]	1.770[3]	4.312[4]	1.689[6]
(1) $^3\Pi$	6.213[2]	2.312[3]	1.960[5]	2.081[7]
(2) $^3\Pi$	0	2.797[3]	4.714[5]	5.725[7]
$^3\Sigma^-$	0	1.527[3]	1.860[4]	3.535[5]
(1) $^3\Sigma^+$	0	2.495[3]	3.665[5]	5.981[7]
(2) $^3\Sigma^+$	–9.319[2]	4.237[3]	4.222[5]	1.854[8]
Ca(4^3P)–He(2^1P)				
$^3\Delta$	–2.382[2]	2.798[4]	–7.178[5]	1.111[7]
(1) $^3\Pi$	9.529[2]	1.100[4]	–1.324[6]	1.624[8]
(2) $^3\Pi$	0	6.068[4]	1.174[6]	1.391[8]
$^3\Sigma^-$	0	3.140[3]	6.247[4]	1.766[6]
(1) $^3\Sigma^+$	0	5.392[4]	9.396[5]	1.505[8]
(2) $^3\Sigma^+$	–1.429[3]	3.235[4]	6.143[6]	7.562[8]
Sr(5^3P)–He(2^1P)				
$^3\Delta$	–2.862[2]	–2.885[3]	5.721[5]	–1.327[6]
(1) $^3\Pi$	1.145[3]	4.502[3]	1.192[6]	–4.500[6]
(2) $^3\Pi$	0	–9.448[3]	1.789[6]	2.095[8]
$^3\Sigma^-$	0	4.090[3]	9.779[4]	2.770[6]
(1) $^3\Sigma^+$	0	–8.423[3]	1.459[6]	2.314[8]
(2) $^3\Sigma^+$	–1.717[3]	3.809[3]	–4.512[5]	6.432[8]

the basis sets optimized for bound states of helium atoms. It is noted that only C_8 for the $^1\Pi$ symmetry of the Sr($5s\ 5p^1P$)–He(2^1S) system is negative in Table III. The reason is that the negative contribution of -1.818×10^6 a.u. mainly from the transition pairs He(2^1S)–He(3^1D) and Sr($5s\ 5p^1P$)–Sr($5s^2\ 1S$) as well as He(2^1S)–He(2^1P) and Sr($5s\ 5p^1P$)–Sr($5s\ nd^1D$), $4 \leq n \leq 7$, is larger than the positive contribution of 1.503×10^6 a.u. of all other transition pairs. For heteronuclear molecular states, comprised of two $^1,^3P$ atoms, due to the symmetries of the zero-order wave functions, C_5 is always negative for Δ and the second Σ^+

TABLE VII. Dispersion coefficients for the interaction of He(2^3P) with Ca($4s\ 4p^1P$) and Sr($5s\ 5p^1P$). The numbers in square brackets denote powers of ten.

Symmetry	C_5 (a.u.)	C_6 (a.u.)	C_8 (a.u.)	C_{10} (a.u.)
Ca(4^1P)–He(2^3P)				
$^3\Delta$	–1.700[2]	2.826[3]	2.273[5]	5.758[7]
(1) $^3\Pi$	6.802[2]	3.305[3]	8.927[5]	1.113[8]
(2) $^3\Pi$	0	4.373[3]	1.167[6]	2.480[8]
$^3\Sigma^-$	0	2.293[3]	1.738[5]	4.444[6]
(1) $^3\Sigma^+$	0	3.946[3]	9.344[5]	2.615[8]
(2) $^3\Sigma^+$	–1.020[3]	1.151[5]	2.003[6]	5.567[8]
Sr(5^1P)–He(2^3P)				
$^3\Delta$	–2.020[2]	7.436[3]	1.078[6]	–7.532[7]
(1) $^3\Pi$	8.082[2]	5.042[3]	1.443[6]	2.184[7]
(2) $^3\Pi$	0	1.429[4]	3.560[6]	3.158[8]
$^3\Sigma^-$	0	2.812[3]	2.458[5]	6.853[6]
(1) $^3\Sigma^+$	0	1.278[4]	3.249[6]	3.334[8]
(2) $^3\Sigma^+$	–1.212[3]	–1.128[5]	4.206[6]	1.389[9]

TABLE VIII. Dispersion coefficients for the interactions of He(2^3P) with Mg($3s\ 3p^3P$), Ca($4s\ 4p^3P$), and Sr($5s\ 5p^3P$). The numbers in square brackets denote powers of ten.

Symmetry	C_5 (a.u.)	C_6 (a.u.)	C_8 (a.u.)	C_{10} (a.u.)
Mg(3^3P)–He(2^3P)				
$1,^3,^5\Delta$	–1.295[2]	1.495[3]	2.979[4]	1.267[6]
(1) $1,^3,^5\Pi$	5.181[2]	1.956[3]	1.796[5]	1.431[7]
(2) $1,^3,^5\Pi$	0	2.446[3]	3.487[5]	3.857[7]
$1,^3,^5\Sigma^-$	0	1.250[3]	1.439[4]	2.470[5]
(1) $1,^3,^5\Sigma^+$	0	2.170[3]	2.731[5]	4.074[7]
(2) $1,^3,^5\Sigma^+$	–7.771[2]	4.074[3]	4.853[5]	1.293[8]
Ca(4^3P)–He(2^3P)				
$1,^3,^5\Delta$	–1.987[2]	1.317[3]	1.719[5]	1.852[6]
(1) $1,^3,^5\Pi$	7.947[2]	3.857[3]	4.984[5]	2.195[7]
(2) $1,^3,^5\Pi$	0	1.265[3]	8.868[5]	9.593[7]
$1\Sigma^-$	0	2.613[3]	5.169[4]	1.401[6]
(1) $1,^3,^5\Sigma^+$	0	1.066[3]	7.198[5]	1.040[8]
(2) $1,^3,^5\Sigma^+$	–1.192[3]	6.241[3]	7.854[5]	3.230[8]
Sr(5^3P)–He(2^3P)				
$1,^3,^5\Delta$	–2.387[2]	1.933[3]	2.821[5]	7.689[4]
(1) $1,^3,^5\Pi$	9.547[2]	5.129[3]	6.931[5]	2.695[7]
(2) $1,^3,^5\Pi$	0	2.172[3]	1.368[6]	1.468[8]
$1\Sigma^-$	0	3.412[3]	8.194[4]	2.265[6]
(1) $1,^3,^5\Sigma^+$	0	1.845[3]	1.132[6]	1.616[8]
(2) $1,^3,^5\Sigma^+$	–1.432[3]	1.038[4]	1.239[6]	5.200[8]

symmetries; C_5 for the first Π symmetry is always positive and for the second Π and other two Σ symmetries it is exactly zero, as presented in Tables V–VIII. Details about the symmetries of the zero-order wave functions were presented in Ref. 23.

Generally speaking, the uncertainties in the dispersion coefficients for the excited states of the alkaline earth atoms are larger than those for the ground states, since the CICP energy differences between the excited states are more susceptible to individual errors in the excited state energies than energy differences involving the ground state.

TABLE IX. Dispersion coefficients for the interactions of He($2^1,^3S$) with Mg($3s\ 3d^1D$) and Ca($4s\ 3d^1D$). The numbers in square brackets denote powers of ten.

System	C_6 (a.u.)	C_8 (a.u.)	C_{10} (a.u.)
MgHe(2^1S) $^1\Sigma$	1.946[4]	2.051[7]	5.288[9]
MgHe(2^1S) $^1\Pi$	1.749[4]	7.575[6]	2.743[8]
MgHe(2^1S) $^1\Delta$	1.159[4]	8.810[5]	–2.510[7]
CaHe(2^1S) $^1\Sigma$	3.871[3]	6.351[5]	4.268[7]
CaHe(2^1S) $^1\Pi$	4.053[3]	4.665[5]	1.882[7]
CaHe(2^1S) $^1\Delta$	4.600[3]	4.384[5]	4.522[7]
MgHe(2^3S) $^3\Sigma$	3.351[3]	6.373[6]	2.464[9]
MgHe(2^3S) $^3\Pi$	3.526[3]	3.339[6]	4.858[7]
MgHe(2^3S) $^3\Delta$	4.048[3]	3.628[5]	–9.356[6]
CaHe(2^3S) $^3\Sigma$	2.349[3]	3.494[5]	9.236[7]
CaHe(2^3S) $^3\Pi$	2.455[3]	2.542[5]	3.770[7]
CaHe(2^3S) $^3\Delta$	2.773[3]	2.181[5]	2.171[7]

TABLE X. Dispersion coefficients for the interactions of He($2\ 1,3S$) with Mg($3s\ 3d\ 3D$) and Ca($4s\ 3d\ 3D$). The numbers in square brackets denote powers of ten.

System	C_6 (a.u.)	C_8 (a.u.)	C_{10} (a.u.)
MgHe($2\ 1S$) $^3\Sigma$	5.444[4]	1.695[7]	1.281[10]
MgHe($2\ 1S$) $^3\Pi$	4.751[4]	3.181[6]	1.559[9]
MgHe($2\ 1S$) $^3\Delta$	2.673[4]	-8.035[4]	-2.573[8]
CaHe($2\ 1S$) $^3\Sigma$	-7.066[4]	-4.679[6]	-1.676[8]
CaHe($2\ 1S$) $^3\Pi$	-5.822[4]	2.317[6]	-7.497[7]
CaHe($2\ 1S$) $^3\Delta$	-2.090[4]	1.347[6]	3.561[7]
MgHe($2\ 3S$) $^{1,3,5}\Sigma$	2.153[4]	2.498[7]	6.790[9]
MgHe($2\ 3S$) $^{1,3,5}\Pi$	1.912[4]	1.051[7]	5.896[8]
MgHe($2\ 3S$) $^{1,3,5}\Delta$	1.190[4]	1.750[6]	-2.503[8]
CaHe($2\ 3S$) $^{1,3,5}\Sigma$	5.988[3]	5.533[5]	6.650[7]
CaHe($2\ 3S$) $^{1,3,5}\Pi$	5.397[3]	1.893[5]	2.661[7]
CaHe($2\ 3S$) $^{1,3,5}\Delta$	3.623[3]	1.815[5]	1.881[7]

TABLE XI. Dispersion coefficients for the interactions of He($2\ 1,3S$) with Mg($3s\ 4s\ 1,3S$) and Ca($4s\ 5s\ 1,3S$). The numbers in square brackets denote powers of ten.

System	C_6 (a.u.)	C_8 (a.u.)	C_{10} (a.u.)
$ns\ (n+1)s\ 1S$ state			
MgHe($2\ 1S$) $^1\Sigma$	9.532[3]	9.275[6]	2.056[9]
CaHe($2\ 1S$) $^1\Sigma$	3.789[4]	1.537[7]	4.441[9]
MgHe($2\ 3S$) $^3\Sigma$	7.469[4]	4.580[6]	1.061[9]
CaHe($2\ 3S$) $^3\Sigma$	-8.674[4]	7.142[6]	2.291[9]
$ns\ (n+1)s\ 3S$ state			
MgHe($2\ 1S$) $^3\Sigma$	2.631[4]	9.444[6]	1.112[9]
CaHe($2\ 1S$) $^3\Sigma$	3.511[4]	1.058[7]	2.573[9]
MgHe($2\ 3S$) $^{1,3,5}\Sigma$	1.113[4]	2.918[6]	5.629[8]
CaHe($2\ 3S$) $^{1,3,5}\Sigma$	1.556[4]	4.733[6]	1.321[9]

TABLE XII. Dispersion coefficients for the interactions of He($2\ 1,3P$) with Mg($3s\ 4s\ 1,3S$) and Ca($4s\ 5s\ 1,3S$). The numbers in square brackets denote powers of ten.

System	C_6 (a.u.)	C_8 (a.u.)	C_{10} (a.u.)
$ns\ (n+1)s\ 1S$ state			
MgHe($2\ 1P$) $^1\Sigma$	1.867[5]	6.366[6]	5.670[9]
MgHe($2\ 1P$) $^1\Pi$	5.821[4]	1.225[6]	1.597[9]
CaHe($2\ 1P$) $^1\Sigma$	-1.391[5]	-3.921[7]	1.277[10]
CaHe($2\ 1P$) $^1\Pi$	-2.028[4]	-1.321[7]	4.041[9]
MgHe($2\ 3P$) $^3\Sigma$	-2.371[4]	4.967[7]	6.988[9]
MgHe($2\ 3P$) $^3\Pi$	2.028[3]	1.624[7]	2.322[9]
CaHe($2\ 3P$) $^3\Sigma$	-1.939[4]	1.180[7]	-2.717[11]
CaHe($2\ 3P$) $^3\Pi$	5.207[3]	4.188[6]	-1.023[11]
$ns\ (n+1)s\ 3S$ state			
MgHe($2\ 1P$) $^3\Sigma$	1.015[5]	1.898[7]	3.088[9]
MgHe($2\ 1P$) $^3\Pi$	3.051[4]	7.269[6]	5.299[8]
CaHe($2\ 1P$) $^3\Sigma$	4.321[6]	4.453[7]	6.566[9]
CaHe($2\ 1P$) $^3\Pi$	1.078[6]	1.879[7]	1.775[9]
MgHe($2\ 3P$) $^{1,3,5}\Sigma$	-4.252[4]	-2.505[6]	2.539[9]
MgHe($2\ 3P$) $^{1,3,5}\Pi$	-9.140[3]	2.440[5]	6.802[8]
CaHe($2\ 3P$) $^{1,3,5}\Sigma$	-9.945[2]	6.283[6]	1.190[10]
CaHe($2\ 3P$) $^{1,3,5}\Pi$	2.183[4]	-1.888[6]	4.098[9]

V. CONCLUSION

Dispersion coefficients have been calculated for the long-range interactions of the first four excited states of He, i.e., He($2\ 1,3S$) and He($2\ 1,3P$), with the low-lying states of Mg, Ca, and Sr by summing over the reduced matrix elements of the multipole transition operators.^{21–23} For the systems He($2\ 1,3S$)–Mg($3s^2\ 1S$) and He($2\ 1,3S$)–Sr($5s^2\ 1S$), our values of C_6 are significantly more accurate than the SKA values. Dispersion coefficients for systems involving a He($2\ 1,3P$) state or excited states of Mg, Ca, and Sr have been computed for the first time. Therefore, the present set of dispersion coefficients will be highly valuable in *ab initio* calculations of potential curves. The main limitation of the present calculations is the absence of spin–orbit interaction, which can affect the atomic properties that are sensitive to a small difference in transition energies.

ACKNOWLEDGMENTS

Z.-C. Yan was supported by the NSERC of Canada, by the Canadian computing facilities of SHARCnet and ACEnet, and in part by the Chinese Academy of Sciences CAS/SAFEA International Partnership Program for Creative Research Teams. J. F. Babb and H. R. Sadeghpour were supported by the National Science Foundation through a grant for the Institute of Theoretical Atomic, Molecular, and Optical Physics at Harvard University and Smithsonian Astrophysical Observatory.

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