

## Long-range interactions of excited He atoms with ground-state noble-gas atoms

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The dispersion coefficients  $C_6$ ,  $C_8$ , and  $C_{10}$  for long-range interactions of He( $n\ ^1S$ ) and He( $n\ ^1P$ ),  $2 \leq n \leq 10$ , with the ground-state noble-gas atoms Ne, Ar, Kr, and Xe are calculated by summing over the reduced matrix elements of multipole transition operators. The large- $n$  expansions for the sums over the He oscillator strength divided by the corresponding transition energy are presented for these series. Using the expansions, the  $C_6$  coefficients for the systems involving He( $13\ ^1S$ ) and He( $13\ ^1P$ ) are calculated and found to be in good agreement with directly calculated values.

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Collisions of excited noble-gas atoms with atoms and molecules have attracted considerable attention for a long time. The collision processes include Penning ionization [1–5], associative ionization [2], and the formation of quasimolecules [6–8], which are of great importance in many areas of physics, such as gaseous lasers, low-temperature plasmas, astrophysics, and radiation physics. The excited noble-gas atoms can be metastable atoms, optically allowed excited atoms [9], or Rydberg atoms [10–12] such as He( $14\ ^1P$ ,  $15\ ^1P$ ,  $16\ ^1P$ ) [10]. A large amount of experimental and theoretical work has been performed to study the collision processes. For theoretical calculations, reliable model potentials are important, as they directly impact the accuracy of the estimated collision characteristics, such as the ionization cross sections and their collisional energy dependences. The long-range part of a model potential plays a key role in determining the rate coefficients for close collision and Penning ionization [13,14]. In this work, the dispersion coefficients  $C_6$ ,  $C_8$ , and  $C_{10}$  are computed for interactions of the Rydberg series of He with the ground-state noble-gas atoms Ne, Ar, Kr, and Xe. Atomic units are used throughout the Brief Report.

The long-range interaction between two atoms is treated as a perturbation to the two isolated atoms. For the systems He-X ( $X$  = ground-state Ne, Ar, Kr, and Xe), the energy correction can be written in the form

$$V(R) = -\frac{C_6}{R^6} - \frac{C_8}{R^8} - \frac{C_{10}}{R^{10}} - \dots, \quad (1)$$

where  $C_k$  are the dispersion coefficients and  $R$  is the interatomic distance. The  $C_k$  can be calculated by summing over the reduced matrix elements of  $2^\ell$ -pole transition operators [15].  $C_6$  can also be represented in terms of products of oscillator strengths  $\bar{f}_{nm}^\ell$  for  $m \rightarrow n$  transitions. For the system He-X with an  $S$ -symmetry He,  $C_6$  is given by

$$C_6 = -\frac{3}{2} \sum_{nm} \frac{\bar{f}_{nX}^1 \bar{f}_{mm_0}^1}{\Delta E_{nX} \Delta E_{mm_0} (\Delta E_{nX} + \Delta E_{mm_0})}, \quad (2)$$

where  $\Delta E_{nX}$  is the energy difference between the  $n$ th state and the ground state of atom X, and  $\Delta E_{mm_0}$  is the energy difference between the  $m$ th intermediate state and the initial  $m_0$ th state of He.

For a highly excited  $S$ -symmetry He, the main contribution comes from transitions with very small energy spacings, which are compared with the energy spacings of atom X,  $|\Delta E_{mm_0}| \ll \Delta E_{nX}$  [16–18]. Therefore,  $C_6$  can be approximated by the product of the dipole polarizability  $\alpha_1^X$  of the noble-gas atom and the dipole sum  $S_{LLm_0}^1(-1)$  of He [17,18]. We thus have

$$C_6 \simeq -\frac{3\alpha_1^X}{2} S_{10}^1(-1), \quad (3)$$

$$S_{LLm_0}^1(-1) = \sum_m \frac{\bar{f}_{mm_0}^1 \delta_{LmL}}{(E_m - E_{m_0})},$$

where  $L_m$  represents the orbital angular momentum quantum number of the  $m$ th state. Similarly,  $C_6$  for a  $P$ -symmetry He can be approximately represented in the form [16]

$$C_6 \simeq -\frac{3\alpha_1^X}{4} \left\{ (4 - 3M^2) S_{01}^1(-1) + \frac{22 - 3M^2}{10} S_{21}^1(-1) \right\}, \quad (4)$$

where  $M = 0, \pm 1$  is the magnetic quantum number of the  $m_0$ th state of He.

For He, 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 [19–24] and the polarizabilities of Rydberg states [25]. The wave functions are expanded in terms of Hylleraas-type basis functions,

$$r_1^i r_2^j r_{12}^k e^{-\alpha r_1 - \beta r_2} \mathcal{Y}_{\ell_1 \ell_2}^{LM}(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2), \quad (5)$$

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  $\Omega$  is an integer. The nonlinear parameters  $\alpha$  and  $\beta$  are variationally optimized by the Newton method.

The transition arrays for Ne, Ar, Kr, and Xe are the same as those used for calculating the dispersion coefficients listed

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in Refs. [26–29]. The transition distributions are constrained to satisfy a variety of sum rules [15,30,31]. Moreover, the data employed for the dipole transitions are those previously published by Kumar and Meath [30,31]. Using these data sets, it is expected that the dispersion coefficients  $C_6$  are accurate within about 1%. The distributions of Mitroy and Zhang [26] are used for the quadrupole and octupole transitions. In addition, the initial sets of distributions are generated by Hartree-Fock calculations. They then are refined by adjusting the excitation energies to reproduce the accurate polarizabilities and dispersion constants computed by many-body perturbation theory [32,33]. Relativistic effects are taken into account for Kr and Xe during the adjustment.

Table I presents the coefficients  $C_6$ ,  $C_8$ , and  $C_{10}$  for interactions between He( $2^{1,3}S$ ) metastable states and the ground states of Ne, Ar, Kr, and Xe. Comparisons are made with the calculations performed by Bell *et al.* [34] and by Proctor and Stwalley [18]. Bell *et al.* have computed the  $C_6$  coefficients by means of the Casimir-Polder formula [34,35]. For the noble-gas atoms, they employ semiempirical representations of the dynamic dipole polarizabilities  $\alpha_1(\omega)$  [36,37]. Proctor and Stwalley have evaluated the coefficients  $C_6$ ,  $C_8$ , and  $C_{10}$  in terms of series of products of oscillator strength sums [17,18]. According to Table I, our  $C_6$  coefficients are in good agreement with previously published values [18,34]. On the other hand, our values of  $C_8$  and  $C_{10}$  are generally larger than those of Proctor and Stwalley, even when taking into account their typical uncertainty of 5%. Since the transition distributions used in our calculations are tuned to reproduce the quadrupole and octupole polarizabilities, which are more accurate than

those used by these authors (compare Table II in Ref. [15] and Table VIII in Ref. [17]), the present calculations should be more accurate.

The coefficients  $C_6$ ,  $C_8$ , and  $C_{10}$  for interactions between He( $2^1P$ ,  $3^1P$ ) and the ground states of Ne, Ar, Kr, and Xe are listed in Table II. Kohmoto and Watanabe [16] have estimated  $C_6$  for these systems using Eq. (4). For He( $2^1P$ )-Ne, He( $2^1P$ )-Ar, and He( $2^1P$ )-Kr, the present  $C_6$  coefficients are 2%–5% larger than the values calculated by Kohmoto and Watanabe, except for the  $\Sigma$  state of He( $2^1P$ )-Kr where our  $C_6$  value is about 15% larger than their result. For He( $2^1P$ )-Xe, our  $C_6$  values are 4%–5% smaller. For He( $3^1P$ )-Ne and He( $3^1P$ )-Ar, our values are 1%–2% larger, and for He( $3^1P$ )-Kr, ours are 0.4%–0.7% larger. Finally, for He( $3^1P$ )-Xe, the  $C_6$  coefficients determined by the two approaches are virtually the same. It is noted from the above-detailed comparison that, since the assumption  $|\Delta E_{mm_0}| \ll \Delta E_{nX}$  is more appropriate for He( $3^1P$ ) than for He( $2^1P$ ), the two kinds of calculations are in better agreement for He( $3^1P$ ) than for He( $2^1P$ ).

The coefficients  $C_6$ ,  $C_8$ , and  $C_{10}$  for He( $2^3P$ ) and He( $3^3P$ ) are listed in Table III, while the coefficients for He( $3^{1,3}S$ ,  $n^{1,3}S$ ,  $n^{1,3}P$ ),  $4 \leq n \leq 10$ , are presented in the Supplemental Material [38]. The uncertainties of all our  $C_6$  values are about 1%, mainly due to uncertain distributions of the dipole transitions of noble-gas atoms. The uncertainties in  $C_8$  and  $C_{10}$  are larger. As expected, the absolute contribution of the He continuum to the coefficients  $C_n$  becomes larger for a rising energy of the initial state. However, the relative contribution becomes significantly smaller, since the density of bound states is higher for an initial state of higher energy

TABLE I. Dispersion coefficients for interactions of He( $2^{1,3}S$ ) with the ground states of noble-gas atoms Ne, Ar, Kr, and Xe. The numbers in the square brackets denote powers of ten.

System	$C_6$ (a.u.)	$C_8$ (a.u.)	$C_{10}$ (a.u.)
NeHe( $2^1S$ ) $^1\Sigma$	8.109[1]	6.644[3]	7.132[5]
Ref. [18]	$7.752[1] \pm 4.191[-1]$	$6.281[3] \pm 4.032[1]$	$6.66[5] \pm 6.751[3]$
Ref. [34]	8.0[1]		
ArHe( $2^1S$ ) $^1\Sigma$	3.286[2]	2.797[4]	3.059[6]
Ref. [18]	$3.228[2] \pm 4.089[0]$	$2.695[4] \pm 4.123[2]$	$2.891[6] \pm 6.650[4]$
Ref. [34]	3.25[2]		
KrHe( $2^1S$ ) $^1\Sigma$	4.938[2]	4.305[4]	4.782[6]
Ref. [18]	$4.841[2] \pm 8.207[0]$	$4.038[4] \pm 8.303[2]$	$4.308[6] \pm 1.334[5]$
Ref. [34]	4.88[2]		
XeHe( $2^1S$ ) $^1\Sigma$	7.891[2]	7.206[4]	8.244[6]
Ref. [18]	$7.731[2] \pm 1.889[1]$	$6.343[4] \pm 1.911[3]$	$6.687[6] \pm 3.065[5]$
Ref. [34]	7.75[2]		
NeHe( $2^3S$ ) $^3\Sigma$	5.646[1]	3.459[3]	2.832[5]
Ref. [18]	$5.345[1] \pm 5.031[-1]$	$3.220[3] \pm 3.866[1]$	$2.592[5] \pm 4.642[3]$
Ref. [34]	5.6[1]		
ArHe( $2^3S$ ) $^3\Sigma$	2.266[2]	1.465[4]	1.236[6]
Ref. [18]	$2.209[2] \pm 4.909[0]$	$1.387[4] \pm 3.999[2]$	$1.138[6] \pm 4.606[4]$
Ref. [34]	2.26[2]		
KrHe( $2^3S$ ) $^3\Sigma$	3.392[2]	2.269[4]	1.958[6]
Ref. [18]	$3.304[2] \pm 9.852[0]$	$2.073[4] \pm 8.061[2]$	$1.690[6] \pm 9.240[4]$
Ref. [34]	3.37[2]		
XeHe( $2^3S$ ) $^3\Sigma$	5.394[2]	3.841[4]	3.457[6]
Ref. [18]	$5.260[2] \pm 2.268[1]$	$3.233[4] \pm 1.855[3]$	$2.599[6] \pm 2.125[5]$
Ref. [34]	5.33[2]		

TABLE II. Dispersion coefficients for interactions of He( $2^1P$ ,  $3^1P$ ) with the ground states of noble-gas atoms Ne, Ar, Kr, and Xe. The numbers in the square brackets denote powers of ten.

System	$C_6$ (a.u.)	$C_8$ (a.u.)	$C_{10}$ (a.u.)
NeHe( $2^1P$ ) $^1\Sigma$	1.134[2]	1.928[4]	2.503[6]
Ref. [16]	1.09[2]		
NeHe( $2^1P$ ) $^1\Pi$	6.322[1]	8.670[2]	4.637[4]
Ref. [16]	6.1[1]		
ArHe( $2^1P$ ) $^1\Sigma$	4.502[2]	7.993[4]	1.061[7]
Ref. [16]	4.43[2]		
ArHe( $2^1P$ ) $^1\Pi$	2.509[2]	4.723[3]	2.506[5]
Ref. [16]	2.43[2]		
KrHe( $2^1P$ ) $^1\Sigma$	7.844[2]	1.215[5]	1.641[7]
Ref. [16]	6.85[2]		
KrHe( $2^1P$ ) $^1\Pi$	4.023[2]	8.104[3]	4.479[5]
Ref. [16]	3.83[2]		
XeHe( $2^1P$ ) $^1\Sigma$	1.070[3]	1.960[5]	2.768[7]
Ref. [16]	1.113[3]		
XeHe( $2^1P$ ) $^1\Pi$	5.934[2]	1.521[4]	9.321[5]
Ref. [16]	6.22[2]		
NeHe( $3^1P$ ) $^1\Sigma$	6.797[2]	5.598[5]	2.792[8]
Ref. [16]	6.73[2]		
NeHe( $3^1P$ ) $^1\Pi$	3.875[2]	1.875[4]	4.618[6]
Ref. [16]	3.82[2]		
ArHe( $3^1P$ ) $^1\Sigma$	2.821[3]	2.319[6]	1.163[9]
Ref. [16]	2.797[3]		
ArHe( $3^1P$ ) $^1\Pi$	1.602[3]	8.324[4]	1.969[7]
Ref. [16]	1.587[3]		
KrHe( $3^1P$ ) $^1\Sigma$	4.257[3]	3.513[6]	1.769[9]
Ref. [16]	4.234[3]		
KrHe( $3^1P$ ) $^1\Pi$	2.419[3]	1.314[5]	3.064[7]
Ref. [16]	2.403[3]		
XeHe( $3^1P$ ) $^1\Sigma$	6.882[3]	5.689[6]	2.889[9]
Ref. [16]	6.880[3]		
XeHe( $3^1P$ ) $^1\Pi$	3.901[3]	2.293[5]	5.241[7]
Ref. [16]	3.904[3]		

TABLE III. Dispersion coefficients for interactions of He( $2^3P$  and  $3^3P$ ) with the ground states of noble-gas atoms Ne, Ar, Kr, and Xe. The numbers in the square brackets denote powers of ten.

System	$C_6$ (a.u.)	$C_8$ (a.u.)	$C_{10}$ (a.u.)
NeHe( $2^3P$ ) $^3\Sigma$	9.246[1]	1.407[4]	1.624[6]
NeHe( $2^3P$ ) $^3\Pi$	5.190[1]	6.967[2]	3.188[4]
ArHe( $2^3P$ ) $^3\Sigma$	3.763[2]	5.793[4]	6.899[6]
ArHe( $2^3P$ ) $^3\Pi$	2.074[2]	3.690[3]	1.754[5]
KrHe( $2^3P$ ) $^3\Sigma$	5.666[2]	8.800[4]	1.070[7]
KrHe( $2^3P$ ) $^3\Pi$	3.102[2]	6.348[3]	3.194[5]
XeHe( $2^3P$ ) $^3\Sigma$	9.086[2]	1.438[5]	1.818[7]
XeHe( $2^3P$ ) $^3\Pi$	4.925[2]	1.260[4]	6.906[5]
NeHe( $3^3P$ ) $^3\Sigma$	6.078[2]	4.517[5]	2.057[8]
NeHe( $3^3P$ ) $^3\Pi$	3.461[2]	1.529[4]	3.408[6]
ArHe( $3^3P$ ) $^3\Sigma$	2.515[3]	1.870[6]	8.568[8]
ArHe( $3^3P$ ) $^3\Pi$	1.428[3]	6.830[4]	1.459[7]
KrHe( $3^3P$ ) $^3\Sigma$	3.806[3]	2.834[6]	1.304[9]
KrHe( $3^3P$ ) $^3\Pi$	2.158[3]	1.082[5]	2.279[7]
XeHe( $3^3P$ ) $^3\Sigma$	6.145[3]	4.591[6]	2.132[9]
XeHe( $3^3P$ ) $^3\Pi$	3.479[3]	1.901[5]	3.925[7]

TABLE IV.  $S_{10}^1(-1)$  for He( $n^{1,3}S$ ) ( $2 \leq n \leq 10$ ).

	Singlet	Triplet
He(2 $S$ )	21.36970	15.20715
He(3 $S$ )	114.3326	91.41838
He(4 $S$ )	374.9145	317.7976
He(5 $S$ )	937.6301	822.5745
He(6 $S$ )	1976.811	1773.808
He(7 $S$ )	3706.856	3379.610
He(8 $S$ )	6382.174	5888.127
He(9 $S$ )	10297.18	9587.488
He(10 $S$ )	15786.26	14805.83
He(13 $S$ )	45642.24	43456.08
Extrapolated	45642.10	43456.21

such that they contribute relatively more than the continuum. For He( $2^3S$ )-Ne and He( $5^1S$ )-Ne, for example, the absolute contributions to  $C_6$  are 3.70 a.u. and 13.82 a.u., respectively, while the relative contributions are 6.6% and 0.4%. The calculated sums  $S_{LLm_0}^1(-1)$  for He( $n^{1,3}S$ ) and He( $n^{1,3}P$ ),  $2 \leq n \leq 10$ , are presented in Tables IV and V, respectively, where the uncertainties are of the order of  $10^{-7}$ . The  $C_6$  values estimated by Eq. (4) for He( $n^{1,3}S$ ) and He( $n^{1,3}P$ ),  $3 \leq n \leq 10$ , are presented in Tables VII and VIII, respectively, of the Supplemental Material [38]. For He( $3^{1,3}S$ ) and He( $3^{1,3}P$ ), the approximate  $C_6$  values are 1%–2% larger than those calculated directly. For He( $4^{1,3}S$ ) and He( $4^{1,3}P$ ), they are only up to 0.5% larger. Since the assumption  $|\Delta E_{mm_0}| \ll \Delta E_{nX}$  is more appropriate for  $n \geq 5$ , the approximate  $C_6$  values are more accurate.

$S_{LLm}^1(n^sL_n)$ , which is  $S_{LLm_0}^1(-1)$ , for states with  $n > 10$  is estimated by extrapolating the data in Tables IV and V. The employed polynomial expansions are

$$S_{10}^1(n^1S) = 1.6666643n^4 - 0.9322431n^3 + 0.5480992n^2 - 0.3483184n + 0.5353862, \quad (6)$$

$$S_{10}^1(n^3S) = 1.6668290n^4 - 1.9823311n^3 + 1.2688204n^2 - 0.7780914n + 0.7694470, \quad (7)$$

$$S_{01}^1(n^1P) = 0.5555488n^4 + 0.0270814n^3 - 0.5565529n^2 - 0.0148016n + 0.0383942, \quad (8)$$

TABLE V.  $S_{01}^1(-1)$  and  $S_{21}^1(-1)$  for He( $n^{1,3}P$ ) ( $2 \leq n \leq 10$ ).

	Singlet		Triplet	
	$S_{01}^1(-1)$	$S_{21}^1(-1)$	$S_{01}^1(-1)$	$S_{21}^1(-1)$
He(2 $P$ )	6.892639	13.93435	5.688321	11.57888
He(3 $P$ )	40.71569	81.58852	36.35748	72.89091
He(4 $P$ )	135.0280	270.1158	124.2924	248.7315
He(5 $P$ )	336.6538	673.3360	315.2755	630.5895
He(6 $P$ )	705.7546	1411.524	668.4010	1336.829
He(7 $P$ )	1315.825	2631.659	1256.093	2512.202
He(8 $P$ )	2253.694	4507.394	2164.108	4328.226
He(9 $P$ )	3619.523	7239.049	3491.536	6983.079
He(10 $P$ )	5526.804	11053.61	5350.800	10701.60
He(13 $P$ )	15832.33	31569.71	15443.83	30711.64
Extrapolated	15832.32	31664.72	15443.82	30887.00

TABLE VI. Comparison of  $C_6$  between the directly calculated values and the values predicted by the asymptotic formulas (the second entry) for He( $13^{1,3}S$ ) and He( $13^{1,3}P$ ). The numbers in the square brackets denote powers of ten.

	Ne	Ar	Kr	Xe
He( $13^1S$ ) $^1\Sigma$	1.827[5]	7.587[5]	1.150[6]	1.859[6]
Estimated	1.827[5]	7.587[5]	1.150[6]	1.859[6]
He( $13^3S$ ) $^3\Sigma$	1.740[5]	7.223[5]	1.094[6]	1.770[6]
Estimated	1.740[5]	7.223[5]	1.094[6]	1.770[6]
He( $13^1P$ ) $^1\Sigma$	2.658[5]	1.104[6]	1.672[6]	2.704[6]
Estimated	2.662[5]	1.105[6]	1.675[6]	2.709[6]
He( $13^1P$ ) $^1\Pi$	1.518[5]	6.301[5]	9.547[5]	1.544[6]
Estimated	1.521[5]	6.316[5]	9.570[5]	1.548[6]
He( $13^3P$ ) $^3\Sigma$	2.589[5]	1.075[6]	1.629[6]	2.634[6]
Estimated	2.597[5]	1.078[6]	1.634[6]	2.642[6]
He( $13^3P$ ) $^3\Pi$	1.477[5]	6.133[5]	9.289[5]	1.503[6]
Estimated	1.484[5]	6.162[5]	9.336[5]	1.510[6]

$$S_{21}^1(n^1P) = 1.1112357n^4 + 0.0497262n^3 - 1.0591460n^2 - 0.3263700n + 0.7087267, \quad (9)$$

$$S_{01}^1(n^3P) = 0.5555341n^4 - 0.1510907n^3 - 0.5480438n^2 + 0.1398819n - 0.0453181, \quad (10)$$

$$S_{21}^1(n^3P) = 1.1105700n^4 - 0.2897963n^3 - 1.1990566n^2 + 0.5772455n - 0.1748896. \quad (11)$$

Using the above expressions, we calculate  $S_{10}^1(13^{1,3}S)$ ,  $S_{01}^1(13^{1,3}P)$ , and  $S_{21}^1(13^{1,3}P)$  and give a comparison with the directly calculated values in the end of Tables IV and V. The agreement is excellent for  $S_{10}^1(13^{1,3}S)$  and  $S_{01}^1(13^{1,3}P)$ , while for  $S_{21}^1(13^1P)$  and  $S_{21}^1(13^3P)$ , there appear differences of 0.3% and 0.6%, respectively. Comparison is also made between the directly calculated  $C_6$  coefficients and those estimated with the extrapolated  $S_{LL_n}^1(n^sL_n)$  in Table VI. Overall, the agreement in  $C_6$  is on the same level as that in  $S_{LL_n}^1(n^sL_n)$ .

In summary, the dispersion coefficients  $C_6$ ,  $C_8$ , and  $C_{10}$  have been calculated for long-range interactions of He( $n^{1,3}S$ ) and He( $n^{1,3}P$ ),  $2 \leq n \leq 10$ , with the ground-state atoms Ne, Ar, Kr, and Xe by summing over the reduced matrix elements of multipole transition operators. The calculated  $C_8$  and  $C_{10}$  coefficients for He( $2^{1,3}S$ ) and  $C_6$  coefficients for He( $2^1P$ ) and He( $3^1P$ ) are more accurate than those reported previously. By fitting the sums  $S_{LL_n}^1(n^sL_n)$ ,  $3 \leq n \leq 10$ , we have obtained approximate polynomial expansions to predict the sums for  $n > 10$ . In addition, the reliability of the polynomial expansions and the predicted  $C_6$  values have been confirmed by direct calculations.

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