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Accurate long-range coefficients for two excited like isotope He atoms: He($2\ ^1P$)–He($2\ ^1P$), He($2\ ^1P$)–He($2\ ^3P$), and He($2\ ^3P$)–He($2\ ^3P$)

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A general formalism is used to express the long-range potential energies in inverse powers of the separation distance between two like atomic or molecular systems with P symmetries. The long-range molecular interaction coefficients are calculated for the molecular symmetries Δ, Π, and Σ, arising from the following interactions: He($2\ ^1P$)–He($2\ ^1P$), He($2\ ^1P$)–He($2\ ^3P$), and He($2\ ^3P$)–He($2\ ^3P$). The electric quadrupole-quadrupole term C_5, the van der Waals (dispersion) term C_6, and higher-order terms C_8 and C_{10} are calculated *ab initio* using accurate variational wave functions in Hylleraas coordinates with finite nuclear mass effects. A comparison is made with previously published results where available.

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I. INTRODUCTION

An accurate description of the interactions between two excited atoms (or molecules) at long range is fundamentally important for studies of molecular excited-state spectroscopy [1,2], associative ionization [3,4], and other collisional processes [5], and is at the heart of several schemes for quantum computation [6,7]. At sufficiently large separations, the mutual electrostatic interaction energy between the two excited atoms can be accurately described using an expansion of the potential energy in inverse powers of the separation distance R. The terms describe the electric quadrupole-quadrupole interaction at order R^{-5}, the instantaneous dipole-dipole (e.g., dispersion) interaction at order R^{-6} [8], and higher-order instantaneous multipole-multipole interactions at orders R^{-8} and R^{-10}.

Long-range interactions involving few-electron atoms are the only interactions that presently can be rigorously calculated with high accuracy. Different levels of approximation are needed for the calculations of long-range forces for alkali- and alkaline-earth-metal atoms [5,9,10]. Sizable discrepancies between various calculations in the literature can occur, as illustrated in the comparisons of C_6 coefficients, for example, given by Zhang *et al.* [12] for Li($2p$)–Li($2p$) and by Yurova [13] for Na($3p$)–Na($3p$). For helium, it is possible to perform a highly accurate *ab initio* calculation of atomic properties and long-range interaction coefficients. Such results could become benchmarks for eventual *ab initio* calculations of alkaline-earth-metal atomic interactions. Alkaline-earth and other two-electron excited P atoms are currently being studied as the optimal candidates for frequency-based standards and optical clock experiments [14].

We had previously studied the long-range interaction coefficients C_n (with $n \leqslant 10$) for all He($n\ ^\lambda S$)–He($n'\ ^{\lambda'} S$) and He($n\ ^\lambda S$)–He($n'\ ^{\lambda'} P$) systems of the energetically lowest five states: He($1\ ^1S$), He($2\ ^3S$), He($2\ ^1S$), He($2\ ^3P$), and He($2\ ^1P$) and the finite nuclear mass effects for like isotopes [15–17]. In this work, we present results for a more complicated set of interactions between two like isotope helium atoms with P symmetries. Degenerate perturbation theory is needed to derive the interaction terms for some of the terms. Section II introduces a general formalism for calculating dispersion coefficients between two like atomic or molecular systems of P symmetry. Section III presents numerical results of dispersion coefficients C_5, C_6, C_8, and C_{10} for the following three systems: He($2\ ^1P$)–He($2\ ^1P$), He($2\ ^1P$)–He($2\ ^3P$), and He($2\ ^3P$)–He($2\ ^3P$).

II. FORMULATION

In this work, atomic units are used throughout. At large distances R between two atoms a and b, the Coulomb interaction [18], treated as a perturbation to the two isolated atoms, is

$$V = \sum_{\ell=0}^{\infty} \sum_{L=0}^{\infty} \frac{V_{\ell L}}{R^{\ell+L+1}}, \tag{1}$$

where

$$V_{\ell L} = 4\pi(-1)^L (\ell,L)^{-1/2} \sum_{\mu} K^{\mu}_{\ell L} T^{(\ell)}_{\mu}(\boldsymbol{\sigma}) T^{(L)}_{-\mu}(\boldsymbol{\rho}). \tag{2}$$

In the above, $T^{(\ell)}_{\mu}(\boldsymbol{\sigma})$ and $T^{(L)}_{-\mu}(\boldsymbol{\rho})$ are the atomic multipole tensor operators defined by

$$T^{(\ell)}_{\mu}(\boldsymbol{\sigma}) = \sum_i Q_i \sigma_i^{\ell} Y_{\ell\mu}(\hat{\boldsymbol{\sigma}}_i) \tag{3}$$

and

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TABLE I. Convergence study for the nonrelativistic energy of He($2\,^3P$) with infinite nuclear mass. N denotes the number of terms in the basis set. Units are atomic units.

Ω	N	$E(\Omega)$
12	910	−2.133 164 190 779 194
13	1120	−2.133 164 190 779 246
14	1360	−2.133 164 190 779 279
15	1632	−2.133 164 190 779 281 2
16	1892	−2.133 164 190 779 282 6
Drake [20]		−2.133 164 190 779 283 202(5)

$$T^{(L)}_{-\mu}(\boldsymbol{\rho}) = \sum_j q_j \rho_j^L Y_{L-\mu}(\hat{\boldsymbol{\rho}}_j), \tag{4}$$

and Q_i and $\boldsymbol{\sigma}_i$ are the charge and the position vector of the ith particle in atom a, respectively. Similarly, q_j and $\boldsymbol{\rho}_j$ are for the jth particle in atom b. The coefficient $K^{\mu}_{\ell L}$ in Eq. (2) is

$$K^{\mu}_{\ell L} = \left[\begin{pmatrix} \ell + L \\ \ell + \mu \end{pmatrix}\begin{pmatrix} \ell + L \\ L + \mu \end{pmatrix}\right]^{1/2} \tag{5}$$

and $(\ell, L, \ldots) = (2\ell+1)(2L+1)\cdots$.

Since the Coulomb interaction V is cylindrically symmetric about the molecular axis $\mathbf{R}$ or the z axis [6,10], the projection of the total angular momentum of the combined system a-b along the z axis (with magnetic quantum number M), is conserved. Therefore, states with $M=\pm 2$, ±1, and 0 are not mixed with each other, corresponding to the Δ, Π, and Σ molecular states, respectively. The Δ and Π states are degenerate with respect to the sign of M, and the degeneracy cannot be removed physically in the free combined system a-b. Therefore, we study only the states with positive M in this work.

A. Δ state

For two like isotope atoms a and b in P symmetry, the zeroth-order wave function for the Δ state of the combined system a-b can be written in the form

$$\Psi^{(0)}(\Delta,\beta) = \frac{\alpha}{\sqrt{2}}[\Psi_{n_{\mathrm{a}}}(M_a;\boldsymbol{\sigma})\Psi_{n_{\mathrm{b}}}(M_b;\boldsymbol{\rho}) + \beta\Psi_{n_{\mathrm{a}}}(M_a;\boldsymbol{\rho})\Psi_{n_{\mathrm{b}}}(M_b;\boldsymbol{\sigma})], \tag{6}$$

where $M_a = M_b = 1$ are the magnetic quantum numbers, α is the normalization factor, and β describes the symmetry due to the exchange of two initial states $\Psi_{n_{\mathrm{a}}}$ and $\Psi_{n_{\mathrm{b}}}$. If two atoms are both in the same P state, then $\alpha=\sqrt{2}$ and $\beta=0$; if they are in different P states, then $\alpha=1$ and $\beta=\pm 1$ [10].

According to perturbation theory, the first-order energy is

$$V^{(1)} = \langle \Psi^{(0)}(\Delta,\beta)|V|\Psi^{(0)}(\Delta,\beta)\rangle = -\frac{C_5(\Delta,\beta)}{R^5}, \tag{7}$$

where, after some angular momentum algebra, one gets (see also Ref. [11]),

$$C_5(\Delta,\beta) = -A_1 + \beta A_2, \tag{8}$$

$$A_1 = \frac{4\pi}{25}\langle \Psi_{n_a}(\boldsymbol{\sigma})\|\sum_i Q_i\sigma_i^2 Y_2(\hat{\boldsymbol{\sigma}}_i)\|\Psi_{n_a}(\boldsymbol{\sigma})\rangle \times \langle \Psi_{n_b}(\boldsymbol{\rho})\|\sum_j q_j\rho_j^2 Y_2(\hat{\boldsymbol{\rho}}_j)\|\Psi_{n_b}(\boldsymbol{\rho})\rangle, \tag{9}$$

$$A_2 = \frac{4\pi}{25}|\langle \Psi_{n_a}(\boldsymbol{\sigma})\|\sum_i Q_i\sigma_i^2 Y_2(\hat{\boldsymbol{\sigma}}_i)\|\Psi_{n_b}(\boldsymbol{\sigma})\rangle|^2. \tag{10}$$

The second-order energy is

$$V^{(2)} = -\sum_{n_s n_t}{}' \sum_{L_s M_s}\sum_{L_t M_t} \frac{|\langle \Psi^{(0)}(\Delta)|V|\chi_{n_s}(L_s M_s;\boldsymbol{\sigma})\omega_{n_t}(L_t M_t;\boldsymbol{\rho})\rangle|^2}{E_{n_s n_t} - E^{(0)}_{n_a n_b}}, \tag{11}$$

where $\chi_{n_s}(L_s M_s;\boldsymbol{\sigma})\omega_{n_t}(L_t M_t;\boldsymbol{\rho})$ is an allowed intermediate state with the energy eigenvalue $E_{n_s n_t} = E_{n_s} + E_{n_t}$, and the prime in the summation indicates that the terms with $E_{n_s n_t} = E^{(0)}_{n_a n_b}$ should be excluded. Substituting Eqs. (1) and (6) into Eq. (11), we obtain

$$V^{(2)} = -\sum_{n_s n_t}{}' \sum_{L_s M_s}\sum_{L_t M_t} \frac{B_1 + \beta B_2}{E_{n_s n_t} - E^{(0)}_{n_a n_b}}, \tag{12}$$

with

$$B_1 = |\langle \Psi_{n_a}(M_a;\boldsymbol{\sigma})\Psi_{n_b}(M_b;\boldsymbol{\rho})|V|\chi_{n_s}(L_s M_s;\boldsymbol{\sigma})\omega_{n_t}(L_t M_t;\boldsymbol{\rho})\rangle|^2, \tag{13}$$

$$B_2 = \langle \Psi_{n_a}(M_a;\boldsymbol{\sigma})\Psi_{n_b}(M_b;\boldsymbol{\rho})|V|\chi_{n_s}(L_s M_s;\boldsymbol{\sigma})\omega_{n_t}(L_t M_t;\boldsymbol{\rho})\rangle \times \langle \Psi_{n_a}(M_a;\boldsymbol{\rho})\Psi_{n_b}(M_b;\boldsymbol{\sigma})|V|\chi_{n_s}(L_s M_s;\boldsymbol{\sigma})\omega_{n_t}(L_t M_t;\boldsymbol{\rho})\rangle. \tag{14}$$

After applying the Wigner-Eckart theorem, we have

TABLE II. Convergence study of $C_6(\Delta,0)$, $C_6(\Pi,+,0)$, and $C_6(\Sigma,0;\lambda_1)$, in atomic units, for $^{\infty}\mathrm{He}(2\,^3P)$–$^{\infty}\mathrm{He}(2\,^3P)$. $N_{2\,^3P}$, $N_{^3S}$, $N_{(pp)\,^3P}$, and $N_{^3D}$ denote, respectively, the sizes of bases for the initial state and the three intermediate states of symmetries ^3S, $(pp)\,^3P$, and ^3D.

$N_{2\,^3P}$	$N_{^3S}$	$N_{(pp)\,^3P}$	$N_{^3D}$	$C_6(\Delta,0)$	$C_6(\Pi,+,0)$	$C_6(\Sigma,0;\lambda_1)$
1360	560	1230	853	4083.026 993 80	2324.937 567 24	7296.821 324 76
1632	680	1430	1071	4083.026 997 99	2324.937 572 24	7296.821 330 48
1938	816	1650	1323	4083.026 998 66	2324.937 572 91	7296.821 331 49

$$\sum_{n_s n_t}{}' \sum_{L_s M_s} \sum_{L_t M_t} \frac{B_1}{E_{n_s n_t} - E^{(0)}_{n_a n_b}} = \sum_{\ell \ell' L L'} \frac{D_1(\ell,L,\ell',L')}{R^{\ell+L+\ell'+L'+2}}, \quad (15)$$

with

$$D_1(\ell,L,\ell',L') = \frac{1}{2\pi} \sum_{L_s L_t} G_1(\ell,L,\ell',L',L_s,L_t) F_1(\ell,L,\ell',L',L_s,L_t). \quad (16)$$

In Eq. (16), G_1 is the angular-momentum part and F_1 is the oscillator strength part. Their expressions are

$$G_1(\ell,L,\ell',L',L_s,L_t) = (-1)^{L+L'} (\ell,L,\ell',L')^{1/2} \sum_{\mu} K^{\mu}_{\ell L} K^{\mu}_{\ell' L'} \times \begin{pmatrix} L_a & \ell & L_s \\ -M_a & \mu & M_a-\mu \end{pmatrix} \begin{pmatrix} 1 & L & L_t \\ -M_b & -\mu & M_b+\mu \end{pmatrix} \times \begin{pmatrix} 1 & \ell' & L_s \\ -M_a & \mu & M_a-\mu \end{pmatrix} \begin{pmatrix} 1 & L' & L_t \\ -M_b & -\mu & M_b+\mu \end{pmatrix} \quad (17)$$

and

$$F_1(\ell,L,\ell',L',L_s,L_t) = \frac{9\pi}{2} \sum_{n_s n_t} \frac{\bar{g}_{n_s;n_a n_a}(L_s,1,1,\ell,\ell') \bar{g}_{n_t;n_b n_b}(L_t,1,1,L,L')}{(\Delta E_{n_s,n_a} + \Delta E_{n_t,n_b}) |\Delta E_{n_s,n_a} \Delta E_{n_t,b}|}, \quad (18)$$

with

$$\bar{g}_{n_s;n_a n_b}(L_s,L_1,L_2,\ell,\ell') = \frac{8\pi}{(\ell,\ell')} \frac{\sqrt{|\Delta E_{n_s n_a} \Delta E_{n_s n_b}|}}{\sqrt{(2L_1+1)(2L_2+1)}} \times \langle \Psi_{n_a}(L_1;\boldsymbol{\sigma}) \| \sum_i Q_i \sigma_i^{\ell} Y_{\ell}(\hat{\boldsymbol{\sigma}}_i) \| \chi_{n_s}(L_s;\boldsymbol{\sigma}) \rangle \times \langle \Psi_{n_b}(L_2;\boldsymbol{\sigma}) \| \sum_i Q_i \sigma_i^{\ell'} Y_{\ell'}(\hat{\boldsymbol{\sigma}}_i) \| \chi_{n_s}(L_s;\boldsymbol{\sigma}) \rangle, \quad (19)$$

and $\Delta E_{n_s n_a} = E_{n_s} - E_{n_a}$, etc. For the special case where the two initial states Ψ_{n_a} and Ψ_{n_b} are the same and $\ell = \ell'$, $\bar{g}_{n_s;n_a n_a}$ reduces to the absolute value of the 2^{ℓ}-pole oscillator strength,

TABLE III. Long-range interaction coefficients, in atomic units, for the He$(2\,^1P)$–He$(2\,^1P)$ system.

C_n	$^{\infty}$He$(2\,^1P)$–$^{\infty}$He$(2\,^1P)$	^{4}He$(2\,^1P)$–^{4}He$(2\,^1P)$	^{3}He$(2\,^1P)$–^{3}He$(2\,^1P)$
$C_5(\Delta,0)$	−227.26160604(2)	−227.31888382(1)	−227.33762037(2)
$C_5(\Pi,+,0)$	909.04642409(1)	909.27553527(2)	909.35048146(3)
$C_5(\Pi,-,0)$	0	0	0
$C_5(\Sigma,0;\lambda_1)$	0	0	0
$C_5(\Sigma,0;\lambda_2)$	−1363.56963613(1)	−1363.91330289(1)	−1364.02572224(5)
$C_5(\Sigma,0;\lambda_3)$	0	0	0
$C_6(\Delta,0)$	5578.63(2)	5584.99(1)	5587.07(1)
$C_6(\Pi,+,0)$	3606.63(2)	3610.56(2)	3611.84(1)
$C_6(\Pi,-,0)$	10831.74(2)	10844.25(2)	10848.35(2)
$C_6(\Sigma,0;\lambda_1)$	9682.78(1)	9693.98(2)	9697.63(2)
$C_6(\Sigma,0;\lambda_2)$	1025.14(2)	1032.23(2)	1034.58(3)
$C_6(\Sigma,0;\lambda_3)$	1966.062(1)	1968.141(1)	1968.821(1)
$C_8(\Delta,0)$	1556.9(6)	1458.9(7)	1426.6(6)
$C_8(\Pi,+,0)$	−170489.4(5)	−170548.7(5)	−170567.9(3)
$C_8(\Pi,-,0)$	1315208(3)	1316393(2)	1316781(2)
$C_8(\Sigma,0;\lambda_1)$	1106570(2)	1107553(2)	1107874(2)
$C_8(\Sigma,0;\lambda_2)$	1788288(2)	1790861(2)	1791704(2)
$C_8(\Sigma,0;\lambda_3)$	−16971.98(4)	−17030.68(3)	−17049.91(3)
$C_{10}(\Delta,0)$	$3.61343(3)\times10^6$	$3.61541(2)\times10^6$	$3.61607(3)\times10^6$
$C_{10}(\Pi,+,0)$	$5.163864(4)\times10^7$	$5.168052(3)\times10^7$	$5.169423(3)\times10^7$
$C_{10}(\Pi,-,0)$	$1.7334869(4)\times10^8$	$1.7349273(2)\times10^8$	$1.7353990(4)\times10^8$
$C_{10}(\Sigma,0;\lambda_1)$	$2.0453997(5)\times10^8$	$2.0471586(3)\times10^8$	$2.0477345(5)\times10^8$
$C_{10}(\Sigma,0;\lambda_2)$	$7.6324701(1)\times10^8$	$7.6394035(3)\times10^8$	$7.6416728(2)\times10^8$
$C_{10}(\Sigma,0;\lambda_3)$	$-2.992224(2)\times10^6$	$-2.996113(3)\times10^6$	$-2.997383(2)\times10^6$

TABLE IV. Long-range interaction coefficients, in atomic units, for the He($2\,^1P$)–He($2\,^3P$) system.

Mass	$^\infty$He($2\,^1P$)–$^\infty$He($2\,^3P$)	^{4}He($2\,^1P$)–^{4}He($2\,^3P$)	^{3}He($2\,^1P$)–^{3}He($2\,^3P$)
$C_5(\Delta,\pm)$	−189.519232605(3)	−189.513470009(3)	−189.511579458(2)
$C_5(\Pi,+,\pm)$	758.07693042(3)	758.05388004(2)	758.04631785(3)
$C_5(\Pi,-,\pm)$	0	0	0
$C_5(\Sigma,\pm;\lambda_1)$	0	0	0
$C_5(\Sigma,\pm;\lambda_2)$	−1137.11539564(3)	−1137.08082006(2)	−1137.06947676(2)
$C_5(\Sigma,\pm;\lambda_3)$	0	0	0
$C_6(\Delta,\pm)$	5186.93(2)	5190.06(3)	5191.91(2)
$C_6(\Pi,+,\pm)$	2990.19(1)	2992.03(2)	2992.640(2)
$C_6(\Pi,-,\pm)$	10353.76(2)	10359.97(5)	10362.05(2)
$C_6(\Sigma,\pm;\lambda_1)$	9245.11(2)	9250.65(3)	9252.52(3)
$C_6(\Sigma,\pm;\lambda_2)$	6162.84(4)	6165.27(3)	6166.13(4)
$C_6(\Sigma,\pm;\lambda_3)$	1505.135(1)	1506.081(1)	1506.390(1)
$C_8(\Delta,\pm)$	−41757.6(6)	−41832.7(4)	−41856.3(4)
$C_8(\Pi,+,\pm)$	−88728.8(2)	−88801.9(1)	−88825.1(2)
$C_8(\Pi,-,\pm)$	993884(3)	994253(2)	994375(2)
$C_8(\Sigma,\pm;\lambda_1)$	843530(3)	843832(2)	843931(2)
$C_8(\Sigma,\pm;\lambda_2)$	2139396(4)	2140392(3)	2140712(2)
$C_8(\Sigma,\pm;\lambda_3)$	−11571.12(3)	−11605.17(2)	−11616.32(3)
$C_{10}(\Delta,\pm)$	$2.32333(4)\times 10^6$	$2.32313(3)\times 10^6$	$2.32312(1)\times 10^6$
$C_{10}(\Pi,+,\pm)$	$5.236817(3)\times 10^7$	$5.238065(4)\times 10^7$	$5.238463(1)\times 10^7$
$C_{10}(\Pi,-,\pm)$	$1.224688(2)\times 10^8$	$1.224994(2)\times 10^8$	$1.225094(1)\times 10^8$
$C_{10}(\Sigma,\pm;\lambda_1)$	$1.435423(2)\times 10^8$	$1.435806(2)\times 10^8$	$1.435933(1)\times 10^8$
$C_{10}(\Sigma,\pm;\lambda_2)$	$5.737754(2)\times 10^8$	$5.739452(2)\times 10^8$	$5.740007(2)\times 10^8$
$C_{10}(\Sigma,\pm;\lambda_3)$	$-2.018823(3)\times 10^6$	$-2.020165(2)\times 10^6$	$-2.020604(2)\times 10^6$

$$\bar{f}^{\ell}_{n_s n_a} = \frac{8\pi\Delta E_{n_s n_a}}{(2\ell+1)^2(2L_1+1)} \left|\langle \Psi_{n_a}(L_1;\boldsymbol{\sigma}) \| \sum_i Q_i \sigma_i^{\ell} Y_{\ell}(\hat{\boldsymbol{\sigma}}_i) \| \chi_{n_s}(L_s;\boldsymbol{\sigma})\rangle\right|^2. \tag{20}$$

Similarly, we have

$$\sum_{n_s n_t}{}' \sum_{L_s M_s} \sum_{L_t M_t} \frac{B_2}{E_{n_s n_t} - E^{(0)}_{n_a n_b}} = \sum_{\ell \ell' L L'} \frac{D_2(\ell, L, \ell', L')}{R^{\ell+L+\ell'+L'+2}}, \tag{21}$$

$$D_2(\ell, L, \ell', L') = \frac{1}{2\pi} \sum_{L_s L_t} G_2(\ell, L, \ell', L', L_s, L_t) F_2(\ell, L, \ell', L', L_s, L_t), \tag{22}$$

with

$$\begin{aligned} G_2(\ell, L, \ell', L', L_s, L_t) = {} & (-1)^{L+L'} (\ell, L, \ell', L')^{1/2} \sum_{\mu} K^{\mu}_{\ell L} K^{M_b - M_a + \mu}_{\ell' L'} \begin{pmatrix} 1 & \ell & L_s \\ -M_a & \mu & M_a - \mu \end{pmatrix} \begin{pmatrix} 1 & L' & L_t \\ -M_a & M_a - M_b - \mu & M_b + \mu \end{pmatrix} \\ & \times \begin{pmatrix} 1 & L & L_t \\ -M_b & -\mu & M_b + \mu \end{pmatrix} \begin{pmatrix} 1 & \ell' & L_s \\ -M_b & M_b - M_a + \mu & M_a - \mu \end{pmatrix}, \end{aligned} \tag{23}$$

$$F_2(\ell, L, \ell', L', L_a, L_b, L_s, L_t) = \frac{9\pi}{2} \sum_{n_s n_t} \frac{\bar{g}_{n_s; n_a n_b}(L_s, 1, 1, \ell, \ell')\, \bar{g}_{n_t; n_a n_b}(L_t, 1, 1, L', L)}{(\Delta E_{n_s, n_a} + \Delta E_{n_t, n_b}) \sqrt{|\Delta E_{n_s, n_a} \Delta E_{n_s, n_b} \Delta E_{n_t, n_a} \Delta E_{n_t, n_b}|}}. \tag{24}$$

TABLE V. Long-range interaction coefficients, in atomic units, for the He(2 ^3P)–He(2 ^3P) system.

Mass	$^{\infty}$He(2 ^3P)–$^{\infty}$He(2 ^3P)	^{4}He(2 ^3P)–^{4}He(2 ^3P)	^{3}He(2 ^3P)–^{3}He(2 ^3P)
$C_5(\Delta,0)$	−158.044 907 607 9(7)	−157.995 476 272 6(5)	−157.979 302 728 9(2)
$C_5(\Pi,+,0)$	632.179 630 432(3)	631.981 905 089(1)	631.917 210 917(2)
$C_5(\Pi,-,0)$	0	0	0
$C_5(\Sigma,0;\lambda_1)$	0	0	0
$C_5(\Sigma,0;\lambda_2)$	−948.269 445 647(4)	−947.972 857 636(3)	−947.875 816 375(3)
$C_5(\Sigma,0;\lambda_3)$	0	0	0
$C_6(\Delta,0)$	4083.026 998 9(3)	4082.935 140 9(1)	4082.904 962 9(7)
$C_6(\Pi,+,0)$	2324.937 573 2(4)	2325.200 148 8(4)	2325.285 984 8(3)
$C_6(\Pi,-,0)$	8172.742842(3)	8172.314300(1)	8172.173845(3)
$C_6(\Sigma,0;\lambda_1)$	7296.821 336(5)	7296.447 426(2)	7296.324 875(5)
$C_6(\Sigma,0;\lambda_2)$	8367.590 5(5)	8361.204 8(2)	8359.115 7(4)
$C_6(\Sigma,0;\lambda_3)$	1159.124 365 8(5)	1159.378 065 7(5)	1159.461 033 6(4)
$C_8(\Delta,0)$	−30170.71(6)	−30168.72(8)	−30168.10(6)
$C_8(\Pi,+,0)$	17083.8(2)	17044.4(2)	17031.5(3)
$C_8(\Pi,-,0)$	726869.3(2)	726728.9(2)	726682.8(1)
$C_8(\Sigma,0;\lambda_1)$	618334.9(1)	618201.6(2)	618157.8(1)
$C_8(\Sigma,0;\lambda_2)$	1835912.3(2)	1835108.6(4)	1834846(1)
$C_8(\Sigma,0;\lambda_3)$	−8209.2(2)	−8229.3(3)	−8236.16(8)
$C_{10}(\Delta,0)$	1537493(3)	1536725(3)	1536474(3)
$C_{10}(\Pi,+,0)$	$3.656172(2)\times 10^7$	$3.653559(2)\times 10^7$	$3.652704(2)\times 10^7$
$C_{10}(\Pi,-,0)$	$8.4139100(8)\times 10^7$	$8.410605(1)\times 10^7$	$8.409524(2)\times 10^7$
$C_{10}(\Sigma,0;\lambda_1)$	$9.846488(2)\times 10^7$	$9.842827(2)\times 10^7$	$9.841629(2)\times 10^7$
$C_{10}(\Sigma,0;\lambda_2)$	$3.9464965(4)\times 10^8$	$3.94483100(3)\times 10^8$	$3.9442865(4)\times 10^8$
$C_{10}(\Sigma,0;\lambda_3)$	$-1.378107(3)\times 10^6$	$-1.378199(2)\times 10^6$	$-1.378225(5)\times 10^6$

Finally, the second-order energy $V^{(2)}$ is

$$V^{(2)} = -\sum_{n\geqslant 3} \frac{C_{2n}(\Delta,\beta)}{R^{2n}}, \tag{25}$$

where the dispersion coefficients $C_{2n}(\Delta,\beta)$ are defined by

$$C_{2n}(\Delta,\beta) = \sum_{\substack{\ell,L,\ell',L'\geqslant 1\\ \ell+L+\ell'+L'+2=2n}} [D_1(\ell,L,\ell',L') + \beta D_2(\ell,L,\ell',L')]. \tag{26}$$

B. Π state

For the Π state, the zeroth-order wave function is in the following form:

$$\begin{aligned}\Psi^{(0)}(\Pi,\beta,\gamma) = {} & \frac{\alpha}{2}[\Psi_{n_a}(M_a;\boldsymbol{\sigma})\Psi_{n_b}(M_b;\boldsymbol{\rho}) \\ & + \gamma\Psi_{n_a}(M_b;\boldsymbol{\sigma})\Psi_{n_b}(M_a;\boldsymbol{\rho})] \\ & + \frac{\alpha\beta}{2}[\Psi_{n_a}(M_a;\boldsymbol{\rho})\Psi_{n_b}(M_b;\boldsymbol{\sigma}) \\ & + \gamma\Psi_{n_a}(M_b;\boldsymbol{\rho})\Psi_{n_b}(M_a;\boldsymbol{\sigma})],\end{aligned} \tag{27}$$

where $\beta=\pm 1$, $M_a=0$, and $M_b=1$. If $n_a=n_b$, $\alpha=\sqrt{2}$ and $\gamma=0$. If $n_a\neq n_b$, then $\alpha=1$ and $\gamma=\pm 1$. The first-order energy correction yields

$$C_5(\Pi,\beta,\gamma) = -\alpha^2(1+2\gamma+\gamma^2)C_5(\Delta,\beta). \tag{28}$$

The second-order energy correction is

$$V^{(2)}(\Pi,\beta,\gamma) = -\sum_{n_s n_t}{}' \sum_{L_s M_s} \sum_{L_t M_t} \frac{|\langle\Psi^{(0)}(\Pi,\beta,\gamma)|V|\chi_{n_s}(L_s M_s;\mathbf{r})\omega_{n_t}(L_t M_t;\rho)\rangle|^2}{E_{n_s n_t} - E^{(0)}_{n_a n_b}}. \tag{29}$$

Introducing a function g_o defined by

$$
\begin{aligned}
g_o(M_a,M_b,M_c,M_d,\ell,L,L_s,L_t,\ell',L') = (-1)^{L+L'}(\ell,L,\ell',L')^{1/2} \sum_{\mu\mu' M_s M_t} K^{\mu}_{\ell L} K^{\mu'}_{\ell' L'} \begin{pmatrix} 1 & \ell & L_s \\ -M_a & \mu & M_s \end{pmatrix} \begin{pmatrix} 1 & L & L_t \\ -M_b & -\mu & M_t \end{pmatrix} \\
\times \begin{pmatrix} 1 & \ell' & L_s \\ -M_c & \mu' & M_s \end{pmatrix} \begin{pmatrix} 1 & L' & L_t \\ -M_d & -\mu' & M_t \end{pmatrix},
\end{aligned} \tag{30}
$$

one can write $V^{(2)}(\Pi,\beta,\gamma)$ as

$$
V^{(2)}(\Pi,\beta,\gamma) = -\sum_{n \geqslant 3} \frac{C_{2n}(\Pi,\beta,\gamma)}{R^{2n}}, \tag{31}
$$

where

$$
C_{2n}(\Pi,\beta,\gamma) = \sum_{\substack{\ell,L,\ell',L' \geqslant 1 \\ \ell+L+\ell'+L'+2=2n}} D_{\beta\gamma}(\ell,L,\ell',L'), \tag{32}
$$

$$
\begin{aligned}
D_{\beta\gamma}(\ell,L,\ell',L') = \frac{9\alpha^2}{16} \sum_{L_s L_t} [& f_{1\gamma}(\ell,L,L_s,L_t,\ell',L') G_1 \\
& + f_{2\gamma}(\ell,L,L_s,L_t,\ell',L') G_2],
\end{aligned} \tag{33}
$$

$$
\begin{aligned}
& f_{1\gamma}(\ell,L,L_s,L_t,\ell',L') \\
& \quad = \frac{1}{2}(1+\gamma^2)[g_o(0,1,0,1,\ell,L,L_s,L_t,\ell',L') \\
& \qquad + g_o(1,0,1,0,\ell,L,L_s,L_t,\ell',L')] \\
& \qquad + \gamma g_o(0,1,1,0,\ell,L,L_s,L_t,\ell',L') \\
& \qquad + \gamma g_o(1,0,0,1,\ell,L,L_s,L_t,\ell',L'),
\end{aligned} \tag{34}
$$

$$
\begin{aligned}
& f_{2\gamma}(\ell,L,L_s,L_t,\ell',L') \\
& \quad = \frac{1}{2}(1+\gamma^2)[g_o(0,1,1,0,\ell,L,L_s,L_t,\ell',L') \\
& \qquad + g_o(1,0,0,1,\ell,L,L_s,L_t,\ell',L')] \\
& \qquad + \gamma g_o(0,1,0,1,\ell,L,L_s,L_t,\ell',L') \\
& \qquad + \gamma g_o(1,0,1,0,\ell,L,L_s,L_t,\ell',L'),
\end{aligned} \tag{35}
$$

$$
\begin{aligned}
G_1 = \sum_{n_s n_t}{}' \Bigg(& \frac{\bar{g}_{n_s;n_a n_a}(L_s,1,1,\ell,\ell')\bar{g}_{n_t;n_b n_b}(L_t,1,1,L,L')}{(\Delta E_{n_s,n_a} + \Delta E_{n_t,n_b})|\Delta E_{n_s,n_a}\Delta E_{n_t,n_b}|} \\
& + \frac{\bar{g}_{n_s;n_b n_b}(L_s,1,1,\ell,\ell')\bar{g}_{n_t;n_a n_a}(L_t,1,1,L,L')}{(\Delta E_{n_s,n_a} + \Delta E_{n_t,n_b})|\Delta E_{n_s,n_a}\Delta E_{n_t,n_b}|} \Bigg),
\end{aligned} \tag{36}
$$

and

$$
G_2 = \beta \sum_{n_s n_t}{}' \left(\frac{\bar{g}_{n_s;n_a n_b}(L_s,1,1,\ell,\ell')\bar{g}_{n_t;n_b n_a}(L_t,1,1,L,L')}{(\Delta E_{n_s,n_a} + \Delta E_{n_t,n_b})\sqrt{|\Delta E_{n_s,n_a}\Delta E_{n_s,n_b}\Delta E_{n_t,n_a}\Delta E_{n_t,n_b}|}} + \frac{\bar{g}_{n_s;n_b n_a}(L_s,1,1,\ell,\ell')\bar{g}_{n_t;n_a n_b}(L_t,1,1,L,L')}{(\Delta E_{n_s,n_a} + \Delta E_{n_t,n_b})\sqrt{|\Delta E_{n_s,n_a}\Delta E_{n_s,n_b}\Delta E_{n_t,n_a}\Delta E_{n_t,n_b}|}} \right). \tag{37}
$$

From the above expressions, it is clear that $f_{1\gamma} = \gamma f_{2\gamma}$ when $\gamma = \pm 1$ and $G_2 = \beta G_1$ when $\gamma = 0$.

C. Σ state

For the Σ state, the possible zeroth-order wave functions for the combined system *a*-*b* are

$$
\begin{aligned}
\Psi^{(0)}(\Sigma,\beta) = \frac{\alpha}{\sqrt{2}} [& \Psi_{n_a}(M_a;\boldsymbol{\sigma})\Psi_{n_b}(M_b;\rho) \\
& + \beta \Psi_{n_a}(M_a;\rho)\Psi_{n_b}(M_b;\boldsymbol{\sigma})]
\end{aligned} \tag{38}
$$

and

$$
\begin{aligned}
\Psi^{(0)}(\Sigma,\beta,\gamma) = \frac{\alpha}{2} [& \Psi_{n_a}(M_a;\boldsymbol{\sigma})\Psi_{n_b}(M_b;\rho) \\
& + \gamma \Psi_{n_a}(M_b;\boldsymbol{\sigma})\Psi_{n_b}(M_a;\rho)] \\
& + \frac{\alpha\beta}{2} [\Psi_{n_a}(M_a;\rho)\Psi_{n_b}(M_b;\boldsymbol{\sigma}) \\
& + \gamma \Psi_{n_a}(M_b;\rho)\Psi_{n_b}(M_a;\boldsymbol{\sigma})].
\end{aligned} \tag{39}
$$

In the $\Psi^{(0)}(\Sigma,\beta)$ state we have $M_a = M_b = 0$, while in the $\Psi^{(0)}(\Sigma,\beta,\gamma)$ state, $M_a = -M_b = 1$, and $\gamma = \pm 1$. When $n_a = n_b$, $\beta = 0$ and $\alpha = \sqrt{2}$, while otherwise $\beta = \pm 1$ and $\alpha = 1$. For the Σ state, there is an additional symmetry with respect to the reflection of the wave function on a plane containing the molecular axis. If Q is the reflection operator [10],

$$
Q\Psi_{n_a}(M_a;\mathbf{r}) = (-1)^{M_a}\Psi_{n_a}(-M_a;\mathbf{r}), \tag{40}
$$

then

TABLE VI. Comparison of the present results with the available results of Ref. [9] for the C_6 coefficients of He($2\,^3P_2$)–He($2\,^3P_2$) with infinite nuclear mass. The relation between the present results [left-hand side (LHS)] and the results from Ref. [9] (RHS) is given in the first column. The symbols for the dispersion coefficients on the RHS represent values $C_6(M_A,M_B)$ for two atoms in the total angular momentum states $J_A=J_B=2$ and quantization axis along the internuclear axis.

Terms	Present	Ref. [9]
$C_6(\Delta,0)=C_6(2,2)$	4083	4056
$\frac{1}{2}[C_6(\Pi,+,0)+C_6(\Pi,-,0)]=2C_6(1,2)-C_6(2,2)$	4666	4645
$\frac{1}{3}\sum_{i=1}^{3}C_6(\Sigma,0;\lambda_i)=4C_6(0,2)+\frac{4}{3}C_6(1,1)-\frac{20}{3}C_6(1,2)+\frac{7}{3}C_6(2,2)$	5608	7026

$$Q\Psi^{(0)}(\Sigma,\beta)=\Psi^{(0)}(\Sigma,\beta) \tag{41}$$

and

$$Q\Psi^{(0)}(\Sigma,\beta,\gamma)=\gamma\Psi^{(0)}(\Sigma,\beta,\gamma). \tag{42}$$

Due to this symmetry, the state $\Psi^{(0)}(\Sigma,\beta,-1)$ cannot be mixed with the other two states by the Coulomb interaction V. However, degenerate perturbation theory is required to remove the degeneracy between $\Psi^{(0)}(\Sigma,\beta)$ and $\Psi^{(0)}(\Sigma,\beta,1)$.

1. The first-order energy

For the $\Psi^{(0)}(\Sigma,\beta,-1)$ state, the first-order energy is

$$\langle\Psi^{(0)}(\Sigma,\beta,-1)|V|\Psi^{(0)}(\Sigma,\beta,-1)\rangle=0. \tag{43}$$

For $\Psi^{(0)}(\Sigma,\beta)$ and $\Psi^{(0)}(\Sigma,\beta,1)$, the matrix elements of the Coulomb interaction V are

$$\langle\Psi^{(0)}(\Sigma,\beta)|V|\Psi^{(0)}(\Sigma,\beta)\rangle=-\frac{4C_5(\Delta,\beta)}{R^5}, \tag{44}$$

$$\langle\Psi^{(0)}(\Sigma,\beta)|V|\Psi^{(0)}(\Sigma,\beta,1)\rangle=-\frac{2\sqrt{2}C_5(\Delta,\beta)}{R^5}, \tag{45}$$

and

$$\langle\Psi^{(0)}(\Sigma,\beta,1)|V|\Psi^{(0)}(\Sigma,\beta,1)\rangle=-\frac{2C_5(\Delta,\beta)}{R^5}. \tag{46}$$

The first-order energies are obtained by the diagonalization of the following matrix:

$$-\frac{4C_5(\Delta,\beta)}{R^5}\begin{bmatrix}1 & 1/\sqrt{2}\\ 1/\sqrt{2} & 1/2\end{bmatrix}. \tag{47}$$

They are

$$\lambda_1=0, \tag{48}$$

$$\lambda_2=-\frac{6C_5(\Delta,\beta)}{R^5}. \tag{49}$$

Their corresponding normalized eigenvectors are

$$\Psi^{(0)}(\Sigma,\beta;\lambda_1)=-\frac{1}{\sqrt{3}}\Psi^{(0)}(\Sigma,\beta)+\sqrt{\frac{2}{3}}\Psi^{(0)}(\Sigma,\beta,1), \tag{50}$$

$$\Psi^{(0)}(\Sigma,\beta;\lambda_2)=\sqrt{\frac{2}{3}}\Psi^{(0)}(\Sigma,\beta)+\sqrt{\frac{1}{3}}\Psi^{(0)}(\Sigma,\beta,1), \tag{51}$$

where we introduce the semicolon to denote the use of the label λ now. Thus, C_5 for $\Psi^{(0)}(\Sigma,\beta;\lambda_1)$ is zero and C_5 for $\Psi^{(0)}(\Sigma,\beta;\lambda_2)$ is

$$C_5(\Sigma,\beta;\lambda_2)=6C_5(\Delta,\beta). \tag{52}$$

2. The second-order energy

For convenience, we use the expression $\Psi^{(0)}(\Sigma,\beta;\lambda_3)$ instead of $\Psi^{(0)}(\Sigma,\beta,-1)$. For the state $\Psi^{(0)}(\Sigma,\beta;\lambda_i)$, the second-order energy correction can be written in the form

$$V^{(2)}(\Sigma,\beta;\lambda_i)=-\sum_{n\geqslant 3}\frac{C_{2n}(\Sigma,\beta;\lambda_i)}{R^{2n}}, \tag{53}$$

where

$$C_{2n}(\Sigma,\beta;\lambda_i)=\sum_{\substack{\ell,L,\ell',L'\geqslant 1\\ \ell+L+\ell'+L'+2=2n}}D_{\lambda_i}(\ell,L,\ell',L'), \tag{54}$$

$$D_{\lambda_i}(\ell,L,\ell',L')=\frac{3\alpha^2}{8}\sum_{L_sL_t}f_{\lambda_i}(\ell,L,L_s,L_t,\ell',L')\times(G_1+(2-i)^{(2-i)}G_2), \tag{55}$$

and f_{λ_i} are

$$\begin{aligned}f_{\lambda_1}(\ell,L,L_s,L_t,\ell',L') = {}& g_o(0,0,0,0,\ell,L,L_s,L_t,\ell',L') - g_o(0,0,-1,1,\ell,L,L_s,L_t,\ell',L') - g_o(0,0,1,-1,\ell,L,L_s,L_t,\ell',L') \\ & - g_o(-1,1,0,0,\ell,L,L_s,L_t,\ell',L') + g_o(-1,1,-1,1,\ell,L,L_s,L_t,\ell',L') + g_o(-1,1,1,-1,\ell,L,L_s,L_t,\ell',L') \\ & - g_o(1,-1,0,0,\ell,L,L_s,L_t,\ell',L') + g_o(1,-1,-1,1,\ell,L,L_s,L_t,\ell',L') + g_o(1,-1,1,-1,\ell,L,L_s,L_t,\ell',L'),\end{aligned} \tag{56}$$

$$\begin{aligned}f_{\lambda_2}(\ell,L,L_s,L_t,\ell',L') = {}& g_o(0,0,0,0,\ell,L,L_s,L_t,\ell',L') + 2g_o(0,0,-1,1,\ell,L,L_s,L_t,\ell',L') + g_o(0,0,1,-1,\ell,L,L_s,L_t,\ell',L') \\ & + g_o(-1,1,0,0,\ell,L,L_s,L_t,\ell',L') + \frac{1}{2}g_o(-1,1,-1,1,\ell,L,L_s,L_t,\ell',L') + \frac{1}{2}g_o(-1,1,1,-1,\ell,L,L_s,L_t,\ell',L') \\ & + g_o(1,-1,0,0,\ell,L,L_s,L_t,\ell',L') + \frac{1}{2}g_o(1,-1,-1,1,\ell,L,L_s,L_t,\ell',L') \\ & + \frac{1}{2}g_o(1,-1,1,-1,\ell,L,L_s,L_t,\ell',L'),\end{aligned} \tag{57}$$

and

$$\begin{aligned}f_{\lambda_3}(\ell,L,L_s,L_t,\ell',L') = {}& \frac{3}{2}[g_o(-1,1,-1,1,\ell,L,L_s,L_t,\ell',L') - g_o(-1,1,1,-1,\ell,L,L_s,L_t,\ell',L') - g_o(1,-1,-1,1,\ell,L,L_s,L_t,\ell',L') \\ & + g_o(1,-1,1,-1,\ell,L,L_s,L_t,\ell',L')].\end{aligned} \tag{58}$$

III. CALCULATIONS AND RESULTS

In the center-of-mass frame, the Hamiltonian of a helium atom can be written in the form

$$H = -\frac{1}{2\mu_e}\nabla^2_{\mathbf{r}_1} - \frac{1}{2\mu_e}\nabla^2_{\mathbf{r}_2} - \frac{1}{m_n}\nabla_{\mathbf{r}_1}\cdot\nabla_{\mathbf{r}_2} - \frac{2}{r_1} - \frac{2}{r_2} + \frac{1}{r_{12}}, \tag{59}$$

where m_n is the nucleus mass, μ_e is the reduced mass between the electron and the nucleus, $\mathbf{r}_1$ and $\mathbf{r}_2$ are the position vectors of the two electrons relative to the nucleus, and r_{12} is the distance between them. To calculate the dispersion coefficients C_n, we variationally evaluate the energy eigenvalues and corresponding eigenfunctions of the initial states He($2\,^1P$) and He($2\,^3P$) with the correlated Hylleraas basis set

$$\{r_1^i r_2^j r_{12}^k e^{-\alpha r_1-\beta r_2}\mathcal{Y}^{LM}_{\ell_1\ell_2}(\hat{\mathbf{r}}_1,\hat{\mathbf{r}}_2)\}, \tag{60}$$

where $\mathcal{Y}^{LM}_{\ell_1\ell_2}(\hat{\mathbf{r}}_1,\hat{\mathbf{r}}_2)$ is the coupled spherical harmonics for the two electrons forming a common eigenstate of $\mathbf{L}^2$ and L_z, and α and β are two nonlinear parameters, which are optimized by first calculating analytically the first-order derivatives of the variation energy with respect to these parameters and then using Newton's method to find their roots. The basis set includes all combinations of $i \geqslant \ell_1$, $j \geqslant \ell_2$, and $k \geqslant 0$ with $i+j+k \leqslant \Omega$, where Ω is an integer controlling the size of the basis set. Then we generate the spectra of the intermediate states for the S, P, D, F, and G symmetries by diagonalizing directly the Hamiltonian of the helium atom in chosen basis sets. In addition, we need to transform the 2^ℓ-pole transition operator $T^\ell_\mu(\sigma)$, defined in Eq. (3), into the center-of-mass coordinates and calculate the reduced matrix elements of dipole, quadrupole, octupole, and hexapole transition operators (for details, refer to Ref. [19]).

Table I shows the convergence study of the nonrelativistic energy of the $^\infty$He($2\,^3P$) state with increase of the size of the basis set. Compared to the value of Drake [20], our result is accurate to about 15 digits. Table II gives the convergence pattern of $C_6(\Delta,0)$, $C_6(\Pi,+,0)$, and $C_6(\Sigma,0;\lambda_1)$ for $^\infty$He($2\,^3P$)$-^\infty$He($2\,^3P$) as the sizes of the basis sets, including the initial state and the three intermediate states, increase progressively.

Table III presents the long-range interaction coefficients C_5, C_6, C_8, and C_{10} for the He($2\,^1P$)–He($2\,^1P$) system. Table IV shows C_5, C_6, C_8, and C_{10} for the He($2\,^1P$)–He($2\,^3P$) system. Table V lists C_5, C_6, C_8, and C_{10} for the He($2\,^3P$)–He($2\,^3P$) system. We note that, for the three He($n\,P$)–He($n'\,P$) systems, $C_5(\Pi,-,\beta)$, $C_5(\Sigma,\beta;\lambda_1)$, and $C_5(\Sigma,\beta;\lambda_3)$ are zero, $C_5(\Pi,+,\beta)$ and C_6 are positive, and both $C_5(\Delta,\beta)$ and $C_5(\Sigma,\beta;\lambda_2)$ are negative. For the $\Psi^{(0)}(\Sigma,\beta;\lambda_3)$ states, C_8 and C_{10} are negative in Tables III–V.

Ovsyannikov obtained expressions for the C_6 (dispersion) coefficients between two excited atoms [9] and evaluated the He($2\,^3P_2$)–He($2\,^3P_2$) coefficients using the atomic dynamic polarizability obtained with a model potential for the He($2\,^3P$) atom. The diagonal elements of the long-range interaction were given in the *jj* representation; after transformation to the *LS* representation [13] the results of Ref. [9] can be compared with ours. The one significant discrepancy is between our results for the summed $C_6(\Sigma,0;\lambda)$ and that of Ref. [9]. In Table VI we compare the transformed coefficients of Ref. [9] with the present calculations.

To the best of our knowledge, there are no other published results for the dispersion coefficients for interaction between He($2\ ^1P$)–He($2\ ^1P$) and He($2\ ^1P$)–He($2\ ^3P$).

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