Long-range interactions between a He($^2\!^3S$) atom and a He($^2\!^3P$) atom for like isotopes

J.-Y. Zhang\textsuperscript{1}, Z.-C. Yan\textsuperscript{1}, D. Vrinceanu\textsuperscript{2}, J. F. Babb\textsuperscript{3}, and H. R. Sadeghpour\textsuperscript{3}

\textsuperscript{1}Department of Physics, University of New Brunswick, Fredericton, New Brunswick, Canada E3B 5A3
\textsuperscript{2}T-4 Group, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA and
\textsuperscript{3}ITAMP, Harvard-Smithsonian Center for Astrophysics, Cambridge, Massachusetts 02138, USA

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Abstract

For the interactions between a He($^2\!^3S$) atom and a He($^2\!^3P$) atom for like isotopes, we report perturbation theoretic calculations using accurate variational wave functions in Hylleraas coordinates of the coefficients determining the potential energies at large internuclear separations. We evaluate the coefficient $C_3$ of the first order resonant dipole-dipole energy and the van der Waals coefficients $C_6$, $C_8$, and $C_{10}$ for the second order energies arising from the mutual perturbations of instantaneous electric dipole, quadrupole, and octupole interactions. We also evaluate the coefficient $C_9$ of the leading contribution to the third order energy. We establish definitive values including treatment of the finite nuclear mass for the $^3\!^3\text{He}(^2\!^3S)$–$^3\!^3\text{He}(^2\!^3P)$ and $^4\!^4\text{He}(^2\!^3S)$–$^4\!^4\text{He}(^2\!^3P)$ interactions.

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Recently, there has been considerable interest in the study of helium dimers and ultracold helium collisions associated with metastable helium atoms [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]. Molecular lines of the helium dimers associated with the He(2\(^3\)S)–He(2\(^3\)P) asymptotes have been produced by photoassociation of spin-polarized metastable helium atoms He(2\(^3\)S\(_1\)). In the purely long-range 0\(^+_u\) potential well (with a minimum internuclear distance reaching 150 bohr) associated with the He(2\(^3\)S\(_1\))–He(2\(^3\)P\(_0\)) asymptote, bound states of the helium dimer [1, 2, 5] can be used in measurements of the s-wave scattering length for collisions of two \(^4\)He(2\(^3\)S\(_1\)) atoms [4, 11]. Molecular lines to the red of the D\(_2\) atomic transition in helium dimers associated with the He(2\(^3\)S)–He(2\(^3\)P\(_2\)) asymptote are of interest for control of the scattering length using an “optical Feshbach resonance” [4, 6]. Published data are scarce on the long-range part of the He(2\(^3\)S)–He(2\(^3\)P) potential energies, which determine the energy level structures of the ultralong-range dimers formed in photoassociation of ultracold metastable helium atoms.

In this paper, we present perturbation theoretic calculations of the coefficients determining the potential energies at large internuclear separations using accurate variational wave functions in Hylleraas coordinates. We evaluate the coefficient \(C_3\) of the first order resonant dipole-dipole energy, and the van der Waals coefficients \(C_6\), \(C_8\), and \(C_{10}\) of the second order energies arising from the mutual perturbations of instantaneous electric dipole, quadrupole, and octupole interactions. We also evaluate for the third order energy the coefficient \(C_9\) of the leading term. We establish definitive values including treatment of the finite nuclear mass for the \(^3\)He(2\(^3\)S)–\(^3\)He(2\(^3\)P) and \(^4\)He(2\(^3\)S)–\(^4\)He(2\(^3\)P) interactions. Definitive values for the \(C_6\), \(C_8\), \(C_9\), and \(C_{10}\) coefficients are established.

In this work, atomic units are used throughout. For the He(2\(^3\)S)–He(2\(^3\)P) system, the zeroth-order wave function appropriate for the perturbation calculation of the long-range interaction can be written in the form [12]:

\[
\Psi^{(0)}(M, \pm) = \frac{1}{\sqrt{2}}[\Psi_{n_a}(\sigma)\Psi_{n_b}(1M; \rho) \pm \Psi_{n_a}(\rho)\Psi_{n_b}(1M; \sigma)],
\]

where \(\Psi_{n_a}\) is the metastable He(2\(^3\)S) wave function, \(\Psi_{n_b}\) is the wave function for the He(2\(^3\)P) atom with magnetic quantum number \(M\), \(\sigma\) and \(\rho\) are the collection of coordinates of the two helium atoms in the laboratory reference frame, and the “\(\pm\)” sign indicates the gerade and ungerade states. The corresponding zeroth-order energy is \(E^{(0)}_{n_an_b} = E^{(0)}_{n_a} + E^{(0)}_{n_b}\). At large internuclear distances, the interaction potential between the two helium atoms can be
expanded as an infinite series in powers of $1/R$

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

(2)

where

\[ V_{\ell L} = 4\pi (-1)^L (\ell, L)^{-1/2} \sum_\mu K_{\ell L}^{\mu} T_\mu^{(\ell)}(\sigma) T_-^{(L)}(\rho). \]  

(3)

$T_\mu^{(\ell)}(\sigma)$ and $T_-^{(L)}(\rho)$ are the atomic multipole tensor operators defined as

\[ T_\mu^{(\ell)}(\sigma) = \sum_i Q_i \sigma_i Y_\ell(\hat{\sigma}_i), \]  

(4)

and

\[ T_-^{(L)}(\rho) = \sum_j q_j \rho_j Y_L(\hat{\rho}_j), \]  

(5)

where $Q_i$ and $q_j$ are the charges on particles $i$ and $j$. The coefficient $K_{\ell L}^{\mu}$ is

\[ K_{\ell L}^{\mu} = \left[ \frac{1}{2} \left( \frac{\ell + L}{\ell} \right) \left( L + M \right) \right]^{1/2} \]  

(6)

and $(\ell, L, \ldots) = (2\ell + 1)(2L + 1)\ldots$. According to the perturbation theory, the first-order energy \[12\] can be written as

\[ V^{(1)} = -\frac{C_3(M, \pm)}{R^3}, \]  

(7)

where

\[ C_3(0, \pm) = \pm \frac{8\pi}{9} |\langle \Psi_{na}(\sigma) | (\sum_i Q_i \sigma_i Y_1(\hat{\sigma}_i)) | \Psi_{nb}(1; \sigma) \rangle|^2, \]  

(8)

and

\[ C_3(\pm1, \pm) = \mp \frac{4\pi}{9} |\langle \Psi_{na}(\sigma) | (\sum_i Q_i \sigma_i Y_1(\hat{\sigma}_i)) | \Psi_{nb}(1; \sigma) \rangle|^2. \]  

(9)

The second-order energy is

\[ V^{(2)} = -\sum_{n_s n_t} \sum_{L_s M_s L_t M_t} \frac{|\langle \Psi^{(0)} | \Gamma(L_s M_s; \sigma) \omega_{n_s}(L_t M_t; \rho) \rangle|^2}{E_{n_s n_t} - E_{n_s n_t}^{(0)}}, \]  

(10)

where $\Gamma(L_s M_s; \sigma)\omega_{n_s}(L_t M_t; \rho)$ is one of the intermediate states with the energy eigenvalue $E_{n_s n_t} = E_{n_s}^{(0)} + E_{n_t}^{(0)}$, and the prime in the summation indicates that the terms with $E_{n_s n_t} = E_{n_s n_t}^{(0)}$ should be excluded. Substituting $2$ into $10$, we obtain

\[ V^{(2)} = -\sum_{n_s n_t} \sum_{L_s M_s L_t M_t} \frac{B_1 \pm B_2}{E_{n_s n_t} - E_{n_s n_t}^{(0)}}, \]  

(11)
with

$$B_1 = |\langle \Psi_{n_a}(\sigma)\Psi_{n_b}(1M;\rho)|V|\chi_{n_a}(L_sM_s;\sigma)\omega_{n_t}(L_tM_t;\rho)\rangle|^2,$$

(12)

and

$$B_2 = \langle \Psi_{n_a}(\sigma)\Psi_{n_b}(1M;\rho)|V|\chi_{n_a}(L_sM_s;\sigma)\omega_{n_t}(L_tM_t;\rho)\rangle$$

$$\times \langle \Psi_{n_a}(\rho)\Psi_{n_b}(1M;\sigma)|V|\chi_{n_a}(L_sM_s;\sigma)\omega_{n_t}(L_tM_t;\rho)\rangle.$$  

(13)

$B_2$ in Eq. (13) is the exchange interaction of the two states He(2$^3S$) and He(2$^3P$). After applying the Wigner-Eckart theorem, we have

$$\sum'_n \sum_{L_sM_s} \sum_{L_tM_t} \frac{B_1}{E_{n_a} - E_{n_b}} = \sum_{L'L_sL_t} \frac{C_1(L, L', L_s, L_t, M)}{R^{2L_s+L+L'+2}},$$

(14)

with

$$C_1(L, L', L_s, L_t, M) = \frac{1}{2\pi} G_1'(L, L', L_s, L_t, M) F^{(1)}(L, L', L_s, L_t).$$  

(15)

In Eq. (13), $G_1'$ is the angular-momentum part and $F^{(1)}$ is the oscillator strength part. Their expressions are

$$G_1'(L, L', L_s, L_t, M) = (-1)^{L+L'} (L, L')^{1/2} \sum_{M_sM_t} K^{-M_s}_{L_sL'} K^{-M_t}_{L_sL_t}$$

$$\times \left( \begin{array}{ccc}
1 & L & L_t \\
-M & M_s & M_t \\
1 & L' & L_t
\end{array} \right),$$

(16)

and

$$F^{(1)}(L, L', L_s, L_t) = \frac{3\pi}{2} \sum_{n_{aT}} |\tilde{g}_{n_{aT}n_{aT}}(L_s, 0, 0, L_s, L_s)\tilde{g}_{n_{bT}n_{bT}}(L_t, 1, 1, L, L')| \frac{\Delta E_{n_{aT}} + \Delta E_{n_{bT}}}{\Delta E_{n_{aT}} \Delta E_{n_{bT}}},$$

(17)

with

$$\tilde{g}_{n_{aT}n_{bT}}(L_s, L_t, L_{1T}, \ell, \ell') = \frac{8\pi}{(\ell, \ell')} \sqrt{|\Delta E_{n_{aT}} \Delta E_{n_{bT}}|}$$

$$\times \langle \Psi_{n_{aT}}(L_1; \sigma)\| \sum_i Q_i \sigma_i^L Y_1(\sigma_i)\| \chi_{n_{aT}}(L_s; \sigma) \rangle$$

$$\times \langle \Psi_{n_{bT}}(L_2; \sigma)\| \sum_i Q_i \sigma_i^L Y_1(\sigma_i)\| \chi_{n_{bT}}(L_s; \sigma) \rangle,$$

(18)

and $\Delta E_{n_{aT}} = E_{n_{aT}}^{(0)} - E_{n_{aT}}^{(0)}$, etc. For the special case when the two initial states $\Psi_{n_a}$ and $\Psi_{n_b}$ are the same and $\ell = \ell'$, $\tilde{g}_{n_{aT}n_{aT}}$ reduces to the absolute value of the $2\ell$-pole oscillator strength

$$\tilde{f}_{n_{aT}}^\ell = \frac{8\pi \Delta E_{n_{aT}}}{(2\ell+1)^2(2L_1+1)} |\langle \Psi_{n_a}(L_1; \sigma)\| \sum_i Q_i \sigma_i^L Y_1(\sigma_i)\| \chi_{n_a}(L_s; \sigma) \rangle|^2.$$

(19)
Finally, the second-order energy is

\[ C_2(L, L', L_s, L_t, M) = \frac{1}{2\pi} G_2'(L, L', L_s, L_t, M) F^{(2)}(L, L', L_s, L_t) , \]

with

\[ G_2'(L, L', L_s, L_t, M) = (-1)^{L+L_s+L'} \sum_{M_s M_t} (-1)^{M_s+M_t} K_{LsL_t}^s K_{L'^{L_t}}^t \]

\[ \times \begin{pmatrix} 1 & L & L_t \\ -M & M_s & M_t \end{pmatrix} \begin{pmatrix} 1 & L' & L_s \\ -M & M_t & M_s \end{pmatrix}, \]

\[ F^{(2)}(L, L', L_s, L_t) = \frac{3\pi}{2} \sum_{n_s n_t} \frac{\bar{g}_{n_s n_t n_b} (L_s, 0, 1, L_s, L') \bar{g}_{n_s n_t n_b} (L_t, 0, 1, L_t, L)}{\sqrt{\Delta E_{n_s n_b}^2 + \Delta E_{n_t n_b}^2 \Delta E_{n_s n_b} \Delta E_{n_t n_b}}} . \]

Finally, the second-order energy is

\[ V^{(2)} = -\sum_{n \geq 3} \frac{C_{2n}(M, \pm)}{R^{2n}} , \]

where \(C_{2n}(M, \pm)\) are the dispersion coefficients

\[ C_{2n}(M, \pm) = \sum_{L' L_s L_t \atop L+L'+2L_s+2=2n} C_1(L, L', L_s, L_t, M) \pm \sum_{L' L_s L_t \atop L+L'+2L_s+2=2n} C_2(L, L', L_s, L_t, M) . \]

According to third-order perturbation theory, the third-order energy correction is

\[ V^{(3)} = \sum_{n_u n_v \atop L_u L_t} \frac{D_1}{\sum_{n_s n_t} \sum_{L_s M_s} \sum_{L_t M_t} (E_{n_s n_t} - E_{n_s n_b}) (E_{n_u n_v} - E_{n_u n_b})^2} , \]

\[ \frac{D_2}{\sum_{n_s n_t} \sum_{L_s M_s} \sum_{L_t M_t} (E_{n_s n_t} - E_{n_s n_b})^2} , \]
For the He($2^3S$)–He($2^3P$) system, following a procedure similar to the second-order perturbation, the third-order energy correction can be expanded in terms of powers of $1/R$:

$$V^{(3)} = -\frac{C_9(M, \pm)}{R^9} - \frac{C_{11}(M, \pm)}{R^{11}} - \ldots.$$  \hspace{1cm} (29)

In this work, we do not present a complete third order calculation. We only consider the leading term $C_9(M, \pm)$ of $V^{(3)}$, which is comparable to the smallest term of $V^{(2)}$.

$$C_9(M, \pm) = C_9^{D_1}(M, \pm) + C_9^{D_2}(M, \pm),$$ \hspace{1cm} (30)

where

$$C_9^{D_1}(M, \pm) = \sum_{n_u, n_v, n_{nt}}' \sum_{L_u, L_v} \frac{\mp (4\pi)^3 G_{D_1}(L_t, L_u, M)}{(E_{n_u} - E_{n_{nt}})(E_{n_v} - E_{n_{nt}})} \times$$

$$\langle \Psi_{n_a}(\sigma) | \sum_i Q_i \sigma_i Y_1(\hat{\sigma}_i) | \chi_n(1; \sigma) \rangle \langle \Psi_{n_b}(1; \rho) | \sum_j Q_j \rho_j Y_1(\hat{\rho}_j) | \omega_{n_t}(L_t; \rho) \rangle \times$$

$$\langle \chi_n(1; \sigma) | \sum_i Q_i \sigma_i Y_1(\hat{\sigma}_i) | \chi_n(L_u; \sigma) \rangle \langle \omega_{n_t}(L_t; \rho) | \sum_j Q_j \rho_j Y_1(\hat{\rho}_j) | \omega_{n_v}(1; \rho) \rangle \times$$

$$\langle \chi_n(L_u; \sigma) | \sum_i Q_i \sigma_i Y_1(\hat{\sigma}_i) | \Psi_{n_b}(1; \sigma) \rangle \langle \omega_{n_v}(1; \rho) | \sum_j Q_j \rho_j Y_1(\hat{\rho}_j) | \Psi_{n_a}(\rho) \rangle,$$ \hspace{1cm} (31)

$$G_{D_1}(L_t, L_u, M) = \sum_{M_t, M_u, M_z} \frac{(-1)^{M_z + L_t + L_u - M_u}}{81} \begin{pmatrix} K_{11}^{-M_z} & K_{11}^{M_z - M_u} & K_{11}^{M_u - M} \\ 1 & 1 & L_t \\ -M & M_z & M_t \end{pmatrix} \begin{pmatrix} 1 & 1 & L_u \\ -M_z & M_z - M_u & M_u \\ M_t & M_u - M_z & M - M_u \end{pmatrix} (32)$$

$$C_9^{D_2}(M, \pm) = -\frac{C_3(M, \pm)}{2\pi} \sum_{L_t} C'_1(1, 1, 1, L_t, M) F^{D_2}(L_t),$$ \hspace{1cm} (33)

$$F^{D_2}(L_t) = \frac{3\pi}{2} \sum_{n_u, n_v} \frac{g_{n_u, n_v, n_{nt}}(1, 0, 0, 1, 1)g_{n_u, n_v, n_{nt}}(L_t, 1, 1, 1, 1)}{(\Delta E_{n_u} + \Delta E_{n_v})^2 |\Delta E_{n_u} \Delta E_{n_v}|},$$ \hspace{1cm} (34)

The nonrelativistic Hamiltonian for a helium atom in a laboratory frame is

$$H = -\frac{1}{2m_n} \nabla^2_{R_n} - \frac{1}{2m_e} \nabla^2_{R_1} - \frac{1}{2m_e} \nabla^2_{R_2} + \frac{q_n q_e}{|R_n - R_1|} + \frac{q_n q_e}{|R_n - R_2|} + \frac{q_e^2}{|R_1 - R_2|},$$ \hspace{1cm} (35)

where $m_n$ and $m_e$ are the masses of nucleus and electron respectively, $q_n$ and $q_e$ are their charges, and $R_n$, $R_1$, and $R_2$ are the corresponding position vectors relative to the laboratory.
frame. Introduce the following transformation

\[ r_1 = R_1 - R_n, \]
\[ r_2 = R_2 - R_n, \]
\[ X = \frac{1}{M_T} (m_n R_n + m_e R_1 + m_e R_2), \]

where \( M_T = m_n + 2m_e \) is the total mass of helium atom and \( X \) is the position vector for the center of mass of helium. In the center-of-mass frame, the Hamiltonian becomes

\[ H = -\frac{1}{2\mu_e} \nabla^2 r_1 - \frac{1}{2\mu_e} \nabla^2 r_2 - \frac{1}{m_n} \nabla r_1 \cdot \nabla r_2 + \frac{q_n q_e}{r_1} + \frac{q_o q_e}{r_2} + \frac{q_e^2}{r_{12}}, \]

where \( r_{12} = |r_1 - r_2| \) and \( \mu_e = m_e m_n / (m_e + m_n) \) is the reduced mass between the electron and the nucleus. The eigenvalue spectrum and corresponding eigenfunctions are obtained by diagonalizing the Hamiltonian \([39]\) in the correlated Hylleraas basis set \([12]\)

\[ \{ r_i^k r_j^k r_{12}^k e^{-\alpha r_1 - \beta r_2} \mathcal{Y}^{LM}_{\ell_1 \ell_2}(\hat{r}_1, \hat{r}_2) \}, \]

where \( \mathcal{Y}^{LM}_{\ell_1 \ell_2}(\hat{r}_1, \hat{r}_2) \) is the coupled spherical harmonics for the two electrons forming a common eigenstate of \( L^2 \) and \( L_z \). Except for some truncations, all terms are included in the basis such that

\[ i + j + k \leq \Omega, \]

with \( \Omega \) being an integer. As \( \Omega \) increases, the size of basis set is increased progressively.

It is necessary to transform the transition operator

\[ T_\ell = q_n R_n \ell Y_{\ell 0}(\hat{R}_n) + q_e R_1 \ell Y_{\ell 0}(\hat{R}_1) + q_e R_2 \ell Y_{\ell 0}(\hat{R}_2) \]

into the center-of-mass coordinates \([13]\). The transformed \( T_\ell \) with \( \ell = 1, 2, \) and \( 3 \) for the dipole, quadrupole, and octupole moments for a neutral helium are

\[ T_1 = -\sum_{j=1}^{2} r_j Y_{10}(\hat{r}_j), \]
\[ T_2 = -\left(1 - \frac{2m_e}{M_T}\right) \sum_{j=1}^{2} r_j^2 Y_{20}(\hat{r}_j) + \sqrt{\frac{30}{\pi}} \frac{m_e}{M_T} r_1 r_2 (\hat{r}_1 \otimes \hat{r}_2)_0^{(2)}, \]
\[ T_3 = -\left[1 - \frac{3m_e}{M_T} + 3 \left(\frac{m_e}{M_T}\right)^2\right] \sum_{j=1}^{2} r_j^3 Y_{30}(\hat{r}_j) \]
\[ + \frac{3}{2} \sqrt{\frac{35}{2\pi}} \frac{m_e}{M_T} - 3 \left(\frac{m_e}{M_T}\right)^2 \left[r_1^2 r_2 (\hat{r}_1 \otimes \hat{r}_1)_0^{(2)} \otimes \hat{r}_2)_0^{(2)} + r_2^2 r_1 (\hat{r}_2 \otimes \hat{r}_2)_0^{(2)} \otimes \hat{r}_1)_0^{(2)}\right] \]
It is noted that for the case of infinite nuclear mass, the above operators reduce to

\[ T_\ell^\infty = -\sum_{j=1}^{2} r_j^\ell Y_{00}(\hat{r}_j). \]  

(46)

For the finite nuclear mass case, however, \( T_\ell \) can not be obtained by a simple mass scaling from \( T_\ell^\infty \), except \( T_1 \) which does not contain \( m_e/M_T \) explicitly for a neutral system.

Table \[\text{I}\] gives the convergence pattern of \( C_6(M, \pm) \) for the case of infinite nuclear mass as the sizes of basis sets, including the two initial states and the four intermediate states, increase progressively. Table \[\text{II}\] lists the contributions to \( C_6(M, \pm) \) from three pairs of intermediate symmetries (\( ^3P, ^3S \)), (\( ^3P, (pp)^3P \)) doubly-excited states, and (\( ^3P, ^3D \)). Our final results for \( C_3(M, \pm) \), \( C_6(M, \pm) \), \( C_8(M, \pm) \), \( C_9(M, \pm) \), and \( C_{10}(M, \pm) \) are presented in Table \[\text{II}\]. To our knowledge, no definitive calculations have been reported for the dispersion coefficients \( C_6(M, \pm) \), \( C_8(M, \pm) \), \( C_9(M, \pm) \), and \( C_{10}(M, \pm) \). Table \[\text{IV}\] is a comparison with the existing values of \( C_3(M, \pm) \) and \( C_6(M, \pm) \). Our values for \( C_3(M, \pm) \) differ from those given in Refs. \[\text{2}\] and \[\text{5}\]. The origins of these discrepancies are uncertain. Drake \[\text{14}\] tabulated the oscillator strengths of helium, including \( ^3\text{He} \) and \( ^4\text{He} \). In order to extract the square of the transition matrix element connecting \( 2^3\text{S} \) and \( 2^3\text{P} \), besides some numerical constants, the tabulated value should be multiplied by \( 1 + 2m_e/m_n \) and divided by the transition energy corrected for the finite nuclear mass. Our results are in perfect agreement with Drake’s values such obtained. For \( C_6(M, \pm) \), our values differ from the values used in the work of Venturi \textit{et al.} \[\text{3}\] at the level of 0.8% and 0.9% respectively for \( C_6(0, \pm) \) and \( C_6(\pm 1, \pm) \).

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TABLE I: Convergence characteristics of $C_6(M, \pm)$, in atomic units, for the $\infty \text{He}(2^3S) - \infty \text{He}(2^3P)$ system. $N_{3S}$, $N_{3P}$, $N^*_{3S}$, $N^*_{3P}$, $N_{(pp)3P}$, and $N_{3D}$ denote respectively the sizes of bases for the two initial states and the four intermediate states of symmetries $^3S$, $^3P$, $(pp)^3P$, and $^3D$.

| $N_{3S}$ | $N_{3P}$ | $N^*_{3S}$ | $N^*_{3P}$ | $N_{(pp)3P}$ | $N_{3D}$ | $C_6(0, \pm)$ | $C_6(\pm1, \pm)$ |
|---|---|---|---|---|---|---|---|
| 1330 | 1360 | 560 | 1360 | 1230 | 853 | 2640.233 681 | 1862.572 368 |
| 1540 | 1632 | 680 | 1632 | 1430 | 1071 | 2640.233 694 | 1862.572 376 |
| 1771 | 1938 | 816 | 1938 | 1650 | 1323 | 2640.233 700 | 1862.572 380 |

TABLE II: Contributions to $C_6(M, \pm)$, in atomic units, for the $\infty \text{He}(2^3S) - \infty \text{He}(2^3P)$ system from $(^3P, ^3S)$, $(^3P, (pp)^3P)$, and $(^3P, ^3D)$ symmetries.

| Symmetries | $C_6(0, \pm)$ | $C_6(\pm1, \pm)$ |
|---|---|---|
| $(^3P, ^3S)$ | 684.091969(2) | 171.0229919(1) |
| $(^3P, (pp)^3P)$ | 1.31648932(2) | 3.29122329(3) |
| $(^3P, ^3D)$ | 1954.825248(4) | 1688.258168(3) |
TABLE III: $C_3(M, \pm), C_6(M, \pm), C_8(M, \pm), C_9(M, \pm), \text{ and } C_{10}(M, \pm)$, in atomic units, for the He(2$^3S$)–He(2$^3P$) system.

| Mass            | $\infty$He–$\infty$He | $^4$He–$^4$He | $^3$He–$^3$He |
|-----------------|------------------------|---------------|---------------|
| $C_3(0, \pm)$   | ±12.8154931075(4)      | ±12.8181751205(4) | ±12.8190526019(4) |
| $C_3(\pm1, \pm)$| ±6.4077465536(2)       | ±6.4090875603(2) | ±6.4095263011(2) |
| $C_6(0, \pm)$   | 2640.2338(1)           | 2641.5083(2)   | 2641.9255(3)  |
| $C_6(\pm1, \pm)$| 1862.5724(1)           | 1863.4726(2)   | 1863.7674(4)  |
| $C_8(0, +)$     | 311901.2(4)            | 311955.4(5)    | 311972.8(1)   |
| $C_8(0, -)$     | 1541993(2)             | 1542352(1)     | 1542470(1)    |
| $C_8(\pm1, +)$  | 168906.5(4)            | 168921.6(3)    | 168926.5(2)   |
| $C_8(\pm1, -)$  | 103017.3(3)            | 103039.5(4)    | 103046.7(3)   |
| $C_9(0, \pm)$   | ±512059.227(6)         | ±512572.343(6) | ±512740.318(6) |
| $C_9(\pm1, \pm)$| ±117073.536(2)         | ±117199.211(2) | ±117240.354(2) |
| $C_{10}(0, +)$  | 2.922482(3) $\times 10^7$ | 2.922304(5) $\times 10^7$ | 2.922244(3) $\times 10^7$ |
| $C_{10}(0, -)$  | 1.857456(3) $\times 10^8$ | 1.8574503(3) $\times 10^8$ | 1.8574492(3) $\times 10^8$ |
| $C_{10}(\pm1, +)$| 1.611301(3) $\times 10^7$ | 1.611325(3) $\times 10^7$ | 1.611334(5) $\times 10^7$ |
| $C_{10}(\pm1, -)$| 2.40597(3) $\times 10^6$ | 2.40608(1) $\times 10^6$ | 2.40613(2) $\times 10^6$ |

TABLE IV: Comparison of $C_3(M, \pm)$ and $C_6(M, \pm)$ for the $^4$He(2$^3S$)–$^4$He(2$^3P$) system.

| Author          | $C_3(0, \pm)$ | $C_3(\pm1, \pm)$ | $C_6(0, \pm)$ | $C_6(\pm1, \pm)$ |
|-----------------|---------------|-------------------|---------------|-------------------|
| Venturi et al. [5] | ±12.82044     | ±6.41022           | 2620.76       | 1846.60           |
| Léonard et al. [2] | ±12.810(6)     | ±6.405(3)          |               |                   |
| This work        | ±12.8181751205(4) | ±6.4090875603(2) | 2641.5083(2) | 1863.4726(2)     |