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Exponentially Correlated Hylleraas–Configuration Interaction Studies of Atomic Systems—IV: Energies for the Five Lowest ^1S and ^1P States of He and Oscillator Strengths, Including Bounds, for Their Allowed Transitions

James S. Sims [1,*], Bholanath Padhy [2] and María Belén Ruiz [3]

[1] National Institute of Standards and Technology, Gaithersburg, MD 20899, USA
[2] Department of Physics, Khallikote College, Brahmapur 760001, Odisha State, India; bholanath.padhy@gmail.com
[3] Computer Chemistry Center, Department of Chemistry and Pharmacy, Friedrich-Alexander-University Erlangen-Nürnberg, Nägelsbachstraße 25, 91052 Erlangen, Germany; maria.belen.ruiz@fau.de
* Correspondence: jim.sims@nist.gov

Abstract

The Exponentially Correlated Hylleraas–Configuration Interaction method (E-Hy-CI) is a generalization of the Hylleraas–Configuration Interaction method (Hy-CI), in which the single r_{ij} is generalized to a form of the generic type $r_{ij}^{\nu_{ij}} e^{-\omega_{ij} r_{ij}}$. This paper extends our earlier work of exploring whether wave functions containing both linear and exponential r_{ij} factors converge more rapidly. In the present study, we calculate the five lowest ^1S and ^1P states of He I in two wave functions. These two wave functions are used to calculate oscillator strengths, including upper and lower bounds, for the allowed transitions between these states. The results of this study are oscillator strengths for the $n\,^1S \rightarrow m\,^1P$ transitions for $n = 1-5$, $m = 2-6$ with rigorous upper and lower bounds, which in the best case ($1\,^1S \rightarrow 2\,^1P$) are 0.00000001% and probable precision ≤ 0.0000000001.

Keywords: atoms; excited states; Exponentially Correlated Hylleraas–Configuration Interaction; E-Hy-CI; f-values; Hy-CI; oscillator strengths; Slater-type orbitals (STOs); transition moments; upper and lower bounds

1. Introduction

The Hylleraas–Configuration Interaction (Hy-CI) technique (developed by Sims and Hagstrom (SH) [1] and also independently by Woźnicki [2]) is a hybrid approach which attempts to combine the high precision of explicitly correlated traditional Hylleraas (Hy) [3] methods with the analytical tractability of strictly orbital based Configuration Interaction (CI) methods [4]. The use of configurations wherever possible leads to less difficult integrals than in a purely Hy[1] approach whose progress beyond the three electron atomic level has been hindered by the intractability of integrals involving nonseparable products of factors of the form $r_{12}r_{23}r_{34}$. If one restricts the wave function to at most a single, linear interelectronic distance r_{ij} factor in each Configuration State Function (CSF), then the most difficult integrals are already dealt with at the four electron level and the calculation retains the precision of Hy techniques, but is greatly simplified by the use of CI basis sets. However, for $N_e \geq 4$, there exists an ultimately slowly convergent "$r_{ij}r_{kl}$" double cusp which is built into Hy-CI for four or more electrons. Consequently, methods which speed

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up the convergence of a single r_{ij} factor may facilitate the extension of Hy-CI to systems with $N_e > 4$, although a true test of this conjecture will require a calculation on a genuine multi-electron system ($N_e > 2$).

In this paper, we continue to explore[2] a generalization of the Hy-CI method first proposed by Wang et al. [9], the Exponentially Correlated Hylleraas–Configuration Interaction (E-Hy-CI) method,[3] in which the single r_{ij} of an Hy-CI wave function is generalized to a form of the generic type $r_{ij}^{\nu_{ij}} e^{-\omega_{ij} r_{ij}}$. Pairing an exponential r_{12} factor with linear r_{12} was first suggested for helium by Hirschfelder who, in 1963 [10], suggested that this type of correlation factor has the right behavior in the vicinity of the r_{12} cusp, and also has the right behavior as r_{12} goes to infinity, but he did no calculations. Whether functions having both linear and exponential r_{ij} factors might be more rapidly convergent than either one alone remained to be seen. The E-Hy-CI proposal has been followed by many papers discussing the integrals arising in E-Hy-CI [9,11–15], but there had been no atomic or molecular structure E-Hy-CI calculations other than an examination of optimized values of ω_{ij} for the E-Hy-CI wave function by Nakatsuji (which is referred to as unpublished in [9]) until our recent studies of the ground ^1S state of the helium atom [6], the ground $1\,^1S$ state through $6\,^1S$ excited states of the Li^+ ion (Li II) [7] and the calculation of wave functions and oscillator strengths, including upper and lower bounds, for the lowest $^1S \rightarrow {}^1P$ resonance transition of the He isoelectronic sequence [8][4].

One of the goals of this work is to explore whether lower bounds to non-relativistic energies can be obtained with the same level of accuracy as upper bounds. This is the subject of the Pollak–Martinazzo (PM) lower-bound theory [17], and Pollak and co-workers find that to get reasonably good results, they need to build wave functions which are optimized not just for one state but for excited states as well [18]. Hence, this research involves producing wave functions which are optimal for not only the ground state, but also the next four excited states. To facilitate this, E-Hy-CI wave functions are calculated for the five lowest ^{1}S states of He I all within one wave function and for the five lowest ^{1}P states of He I all within a second wave function.

One thought that has driven this project is that with all the effort being put into the wave function to achieve a good energy bound, *why not use it to compute properties in addition to the energy?* Hence, these wave functions are used to calculate oscillator strengths, including rigorous quantum mechanical upper and lower bounds, for the 25 lines arising from allowed transitions among these five ^1S and five ^1P states. The results of this study are oscillator strengths for the $1sns\ ^1S \rightarrow 1smp\ ^1P$ transitions for which n = 1–5, m = 2–6 with rigorous upper and lower bounds, which in the best case ($1sxs \rightarrow 1syp\ ^1P$) are 0.00000001% and probable precision $\leq$ 0.0000000001.

2. Variational Calculations

The calculations reported in this work were obtained by solving the non-relativistic Schrödinger equation. Chung et al. [19] discussed the relative importance of correlation effects versus relativistic effects and stated that, for $Z \leq 27$, correlation effects dominate relativistic effects. Consequently, one should start out with the best possible solutions to the non-relativistic Schrödinger equation and treat relativistic effects as a perturbation. Since this work considers only helium with $Z = 2$, solving the non-relativistic Schrödinger equation is meaningful.

For N_e electrons, the total non-relativistic, stationary-point-nucleus energy E_{NR} is defined as the exact solution (eigenvalue) of the time-independent, non-relativistic Schrödinger equation:

$$H_{NR}\Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots \mathbf{r}_{N_e}) = E_{NR}\Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots \mathbf{r}_{N_e}), \quad (1)$$

where the Hamiltonian H_{NR} is defined as (in hartree atomic units)

$$H_{NR} = \sum_{i=1}^{N_e} \mathcal{H}_i + \sum_{i<j}^{N_e} r_{ij}^{-1}. \quad (2)$$

Here, $\mathcal{H}_i = \mathcal{T}_i + \mathcal{V}_i$, $\mathcal{H}_i$ being a one-electron operator (electron i) consisting of a kinetic energy part $\mathcal{T}_i = -\frac{1}{2}\nabla_i^2$ and a nuclear attraction part $\mathcal{V}_i = -Z/r_i$. N_e denotes the number of electrons and Z the corresponding nuclear charge.

The E-Hy-CI wave function for N_e electron atomic states is

$$\Psi = \sum_{K=1}^{N} C_K \Phi_K, \quad (3)$$

where

$$\Phi_K = \Lambda(r_{ij}^{\nu_K} e^{-\omega_K r_{ij}} \prod_{s=1}^{N_e} \{\phi_{K_s}(\mathbf{r_s})\}\Theta_K) = O_{as} O_{L,M_L} O_{S,M_S} (r_{ij}^{\nu_K} e^{-\omega_K r_{ij}} \prod_{s=1}^{N_e} \{\phi_{K_s}(\mathbf{r_s})\}\Theta_K) \quad (4)$$

denotes the K-th antisymmetrized orbital and spin angular momentum projected explicitly correlated Configuration State Function (CSF). Λ is the symmetry adaptation operator that performs the projection and is a product of an idempotent projection operator that makes the state antisymmetric, O_{as}, and O_{L,M_L}, O_{S,M_S} which are idempotent orbital and spin angular momentum projection operators of the Löwdin type [20] for a state of total quantum numbers L, M_L, S, M_S (Russell–Saunders (LS) coupling is assumed). Each term K contains at most one explicitly correlated factor $r_{ij}^{\nu_K} e^{-\omega_K r_{ij}}$ that, in addition to the Hy-CI case with $\omega_K = 0$, can also have $\omega_K \neq 0$. In practice, it is sufficient to take ν_K equal to 0 or 1, with $\nu_K = 1, \omega_K = 0$ the Hy-CI case and $\nu_K = 0, \omega_K = 0$ the CI case[5]. Θ_K is a primitive spin product function for term K and $\phi_{K_s}(\mathbf{r_s})$ represents the s-th basis orbital in the K-th term.

The basis orbitals are unnormalized Slater-type orbitals (STOs) $\phi(\mathbf{r})$ that are defined as

$$\phi_i(\mathbf{r}) = [n_i, l_i, m_i]_{\zeta_i}^i = r^{n_i - 1} e^{-\zeta_i r} Y_{l_i}^{m_i}(\theta, \phi), \quad (5)$$

where $Y_l^m(\theta, \phi)$ is a normalized spherical harmonic in the Condon and Shortley phase convention [23]. With this choice of phase convention, the spherical harmonics satisfy

$$Y_l^{m*}(\theta, \phi) = (-1)^m Y_l^{-m}(\theta, \phi). \quad (6)$$

The coefficients C_K in Equation (3) were found in this work by solving the generalized eigenvalue problem

$$\mathbf{HC} = E\mathbf{SC}, \quad (7)$$

$$(\mathbf{H} - E_0\mathbf{S})\mathbf{C} = (E - E_0)\mathbf{SC}, \quad (8)$$

$$\mathbf{C} = (E - E_0)(\mathbf{H} - E_0\mathbf{S})^{-1}\mathbf{SC}, \quad (9)$$

where the matrix elements are given by $H_{KL} = \langle \Phi_K | \mathcal{H} | \Phi_L \rangle$ and $S_{KL} = \langle \Phi_K | \Phi_L \rangle$ with the Hamiltonian H given by Equation (2) and E_0 being some starting approximation for the eigenvalue E of interest.

The details of how the authors solve this real symmetric-definite eigenvalue problem are discussed in [24], including how to obtain a quadruple precision version of our computationally fast Fortran 90+ portable parallel package suitable for large (80,000 × 80,000 or greater) dense matrices. All results reported in this article were obtained using real*32 extended precision (quad-double-with exponent or QDE, 256-bit, ≈64 digits) floating point

arithmetic, and the Message-Passing Interface (MPI) standard [25] was used to parallelize the code.

Method of Calculation

For two electrons, spin can be eliminated and the E-Hy-CI wave function becomes [6,7]

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = \sum_{K=1}^{N} C_K \Phi_K(\mathbf{r}_1, \mathbf{r}_2), \tag{10}$$

where the terms Φ_K are specifically of the form

$$\Phi_K(\mathbf{r}_1, \mathbf{r}_2) = (1 \pm P_{12}) O_{L,M_L}(r_{12}^{\nu_K} e^{-\omega_K r_{12}} \phi_{K_1}(\mathbf{r_1}) \phi_{K_2}(\mathbf{r_2})). \tag{11}$$

P_{12} is the operator which permutes electrons 1 and 2, and the plus sign is for singlet states, the minus sign for triplet states[6]. Equation (2) becomes

$$H_{NR} = \mathcal{H}_1 + \mathcal{H}_2 + \mathcal{H}_{12}, \tag{12}$$

where $\mathcal{H}_{12} = r_{12}^{-1}$.

In the generalized eigenvalue problem $\mathbf{HC} = \lambda \mathbf{SC}$, matrix element H_{KL} is

$$H_{KL} = \langle \Phi_K | \mathcal{H} | \Phi_L \rangle = \langle \Lambda \Phi_K^P | \mathcal{H} | \Lambda \Phi_L^P \rangle, \tag{13}$$

where $\Phi_K^P = r_{12}^{\nu_K} e^{-\omega_K r_{12}} \phi_{K_1}(\mathbf{r_1}) \phi_{K_2}(\mathbf{r_2})$ denotes the K-th primitive (unprojected) function as given in Equation (11) above. S_{KL} is similar, with $\mathcal{H}$ replaced by the unit operator 1.

The projection reduction of these matrix elements has been discussed in Paper II [7] so just the result is given here, which is that H_{KL} is given by

$$H_{KL} = \langle g_K f_K | \mathcal{H} | O_{L,M_L} B(g_L f_L) \rangle, \tag{14}$$

where $g_K(r_{12}) = r_{12}^{\nu_K} e^{-\omega_K r_{12}}$ is the correlation factor and $f_K = \phi_{K_1}(\mathbf{r_1}) \phi_{K_2}(\mathbf{r_2})$ is a product of unnormalized STOs (Equation (5)).

In Equation (14), one can apply O_{L,M_L} either before or after applying $B = 1 \pm P_{12}$ (+ sign for singlet states, − sign for triplet states). The O_{L,M_L} projection is applied only on the orbital products since $g_L = r_{12}^{\nu_L} e^{-\omega_L r_{12}}$ commutes with O_{L,M_L} [1].

In generalizing Hy-CI to E-Hy-CI for the two electron He case, one merely has to take the correlation factor g_K to be $g_K = r_{12}^{\nu_K} e^{-\omega_K r_{12}}$ in the formulas above since $e^{-\omega_K r_{12}}$ has the same symmetry properties as r_{12}. Thus, H_{KL} becomes for singlet states

$$H_{KL} = \langle \phi_{K_1}(\mathbf{r}_1) \phi_{K_2}(\mathbf{r}_2) r_{12}^{\nu_K} e^{-\omega_K r_{12}} | \mathcal{H} | r_{12}^{\nu_L} e^{-\omega_L r_{12}} (1 + P_{12}) O_{L,M_L}(\phi_{L_1}(\mathbf{r}_1) \phi_{L_2}(\mathbf{r}_2)) \rangle. \tag{15}$$

A detailed discussion of the most general exponentially correlated integrals which have to be evaluated when using this wave function can be found in Section 3 of our recent study [6] of the ground state of helium.

3. Wave Functions

The basis set orbitals in Hy-CI and E-Hy-CI atomic calculations are STOs; see Equation (5). For the nonlinear orbital exponent parameters for ^{1}S states, the use of the "doubled" (orbital exponent) basis set E-Hy-CI introduced in paper I and continued in papers II and III is also continued here (see Note 2 below). In this treatment, the first set has an orbital with an orbital exponent ζ that makes it essentially a valence shell orbital, whereas for the second set, the orbital has a large exponent ζ' which brings it in closer

to the nucleus. This approach is due to Drake [26–28], who pointed out the need for "doubling" basis sets so there is a natural partition of the basis set into two distinct distance scales—one appropriate to the complex correlated motion near the nucleus, and the other appropriate further out. Results are very good for the ground 1 ^{1}S state of helium [6] and Li^+ ground and excited states [7] of ^{1}S symmetry; that approach is continued here in the treatment of excited states of He I with ^{1}S symmetry. However, our approach here is different in that we are interested in obtaining not only very precise variational upper bounds to the energies of these states, but also lower bounds to the energies which have precisions on par with calculated upper bounds [29]. Recently, Ronto et al. [18] have attained results for the lower bounds for He through Be atoms with a relative precision comparable to the corresponding upper bounds. To accomplish this, they needed to improve the description of excited states to get a better lower bound to the ground state. Thus, the final wave function expansion for ^{1}S will be a suitable description of the five lowest ^{1}S states of He I and the final wave function expansion for ^{1}P will be a suitable description of the five lowest ^{1}P states. What follows is a discussion of how we obtain these final wave functions.

3.1. He ^{1}S

In paper I [6] of this series, we developed an 8568 term expansion for the ground state of He I to 20 decimal place precision. This wave function is presented in Table 1, where each line in the table (and in subsequent tables) as in previous work specifies the {outer,outer} and {inner,inner} sets for each l quantum number. In the table, only the minimum information needed to specify the basis set is listed, namely, an exponent ξ, the l quantum number for orbitals with that exponent, n_{orbs}, the number of orbitals with that exponent (the n in Equation (5) run from $l_i + 1$ to $l_i + n_{orbs}$), and ω_{12}, the exponent of the exponentially correlated r_{12} factor for these E-Hy-CI calculations. There is an outer n_{orbs} and inner n'_{orbs} basis set for these "doubled" basis sets. In all of the tables, N is used to refer to the number of terms in the wave function (see Equation (3)). Also included in Table 1 is the result of using this equation through $l = 3$ for the 2 ^{1}S and 3 ^{1}S states, which shows that a 5928 term expansion gives the 1 ^{1}S state to 20 decimal places, but for the 2 ^{1}S state to only 7 decimal places, and the precision for the 3 ^{1}S state is just 3 decimal places. Inspection of the ground state results also shows that truncating the number of orbitals for each l to 13 loses only 1 significant digit and significantly reduces the number of terms to 2912, so it seems reasonable to consider adding 2912 terms for the 2 ^{1}S and 3 ^{1}S expansions. In the table for 2 ^{1}S and 3 ^{1}S the last columns display the result of optimizing ξ and ξ' for $l = 0$ and then using just those two orbital exponents for the $n_{orbs} = 13$, $l_i \leq 3$, 2912 term expansion. Table 1 shows that, as was in the case of the Li^+ ion [7], the use of different orbital exponents for different l quantum numbers can be simplified by the use of just two orbital exponents, one for the {inner,inner} set and one for the {outer,outer} set, resulting in a 2912-term expansion good to 14 significant digits for He 2 ^{1}S and a 2912-term expansion good to 10 significant digits for He 3 ^{1}S.

Table 2 displays the result of truncating the number of orbitals for each l to 13 and adding the Table 1 2912-term expansion suitable for 2 ^{1}S to the Table 1 2912 1 ^{1}S expansion, giving the 4368-term wave function displayed in the table[7]. Note that the addition of terms suitable for the 2 ^{1}S state has improved the 2 ^{1}S energy to 15 decimal digits. To get an even better result and improve the treatment of the 3 ^{1}S state in the same wave function, we add the $n_{orbs} = 13$, $l_i \leq 1$, Table 1 1456-term 3 ^{1}S expansion to the 4368-term expansion, resulting in an 5824-term expansion suitable for the 1–3 S ^{1}S states of He. These results are also displayed in the table and it can be seen that not only is the ground 1 ^{1}S state precision 18–19 digits but so is the precision for the He 2 ^{1}S state. In addition, a 12 significant digit precision has been achieved for He 3 ^{1}S. Finally, terms with an orbital exponent ξ optimized

for the 4 and 5 ^{1}S states were added to the wave function, resulting in our final 8372-term ^{1}S wave function shown in Table 2, which improves the 3 ^{1}S precision to 14 decimal digits, and achieves 9 and 6 decimal digit precision for the 4 and 5 ^{1}S states of He, all within a single ^{1}S wave function.

Table 1. E-Hy-CI wave function He 1–3 ^{1}S non-relativistic energies (in hartrees using a doubled basis set of orbitals for each l-wave). N is the number of terms in the expansion.

State	l_{max}	n_{orbs}	ξ	n'_{orbs}	ξ'	ω_{12}	N	Energy (Hartree)
He I 1 ^{1}S	0	13	2.20	13	25.0	0.50	728	−2.9037 2435 3910 9601 8477 99
He I 1 ^{1}S	0	19	2.20	19	25.0	0.50	1520	−2.9037 2435 4275 7390 6714 30
He I 1 ^{1}S	1	13	3.05	13	40.5	0.50	1456	−2.9037 2437 7034 0679 8634 91
He I 1 ^{1}S	1	19	3.05	19	40.5	0.50	3040	−2.9037 2437 7034 1043 9282 03
He I 1 ^{1}S	2	13	3.50	13	40.5	0.50	2184	−2.9037 2437 7034 1195 0022 60
He I 1 ^{1}S	2	19	3.50	19	40.5	0.50	4560	−2.9037 2437 7034 1195 9808 72
He I 1 ^{1}S	3	13	3.90	13	40.5	0.50	2912	−2.9037 2437 7034 1195 9818 81
He I 1 ^{1}S	3	18	3.90	18	40.5	0.50	5928	−2.9037 2437 7034 1195 9830 82
He I 1 ^{1}S	4	15	4.50	15	40.5	0.50	6888	−2.9037 2437 7034 1195 9830 89
He I 1 ^{1}S	5	14	5.20	14	40.5	0.50	7728	−2.9037 2437 7034 1195 9830 92
He I 1 ^{1}S	6	14	6.00	14	40.5	0.50	8568	−2.9037 2437 7034 1195 9830 94
Nakashima and Nakatsuji [30]								−2.9037 2437 7034 1195 9831 12
He I 2 ^{1}S	0	13	2.20	13	25.0	0.50	728	−2.1458 1583 9153 1898 7651 82
He I 2 ^{1}S	0	19	2.20	19	25.0	0.50	1520	−2.1459 7296 0680 5517 9959 59
He I 2 ^{1}S	1	13	3.05	13	40.5	0.50	1456	−2.1459 3197 5645 6946 7331 15
He I 2 ^{1}S	1	19	3.05	19	40.5	0.50	3040	−2.1459 7401 7550 4907 4823 56
He I 2 ^{1}S	2	13	3.50	13	40.5	0.50	2184	−2.1459 6598 5199 9917 6833 04
He I 2 ^{1}S	2	19	3.50	19	40.5	0.50	4560	−2.1459 7401 7550 4910 6552 34
He I 2 ^{1}S	3	13	3.90	13	40.5	0.50	2912	−2.1459 7086 8075 0361 8372 68
He I 2 ^{1}S	3	18	3.90	18	40.5	0.50	5928	−2.1459 7403 8720 4416 5929 53
He I 2 ^{1}S	0	13	1.17			0.50	364	−2.1459 7404 0535 3097 7045 24
He I 2 ^{1}S	0	13	1.17	13	5.56	0.50	728	−2.1459 7404 3612 0913 5467 36
He I 2 ^{1}S	1	13	1.17			0.50	1092	−2.1459 7404 6047 0655 1270 05
He I 2 ^{1}S	1	13	1.17	13	5.56	0.50	1456	−2.1459 7404 6053 6944 5980 09
He I 2 ^{1}S	2	13	1.17			0.50	1820	−2.1459 7404 6054 3426 1444 65
He I 2 ^{1}S	2	13	1.17	13	5.56	0.50	2184	−2.1459 7404 6054 3850 4859 01
He I 2 ^{1}S	3	13	1.17			0.50	2548	−2.1459 7404 6054 4109 6097 06
He I 2 ^{1}S	3	13	1.17	13	5.56	0.50	2912	−2.1459 7404 6054 4135 1667 74
Aznabaev et al. [31]								−2.1459 7404 6054 4174 1580 50
He I 3 ^{1}S	0	13	2.20	13	25.0	0.50	728	−2.0394 7820 3129 3021 4438 46
He I 3 ^{1}S	0	19	2.20	19	25.0	0.50	1520	−2.0586 3637 1840 4908 5662 22
He I 3 ^{1}S	1	13	3.05	13	40.5	0.50	1456	−2.0490 5802 7440 5968 0929 88
He I 3 ^{1}S	1	19	3.05	19	40.5	0.50	3040	−2.0598 8919 9507 4808 5730 81
He I 3 ^{1}S	2	13	3.50	13	40.5	0.50	2184	−2.0551 8265 2157 6960 1278 68
He I 3 ^{1}S	2	19	3.50	19	40.5	0.50	4560	−2.0607 3742 6133 4576 7962 61
He I 3 ^{1}S	3	13	3.90	13	40.5	0.50	2912	−2.0571 5082 5105 6874 5756 65
He I 3 ^{1}S	3	18	3.90	18	40.5	0.50	5928	−2.0609 8367 8785 6767 0081 24
He I 3 ^{1}S	0	13	0.8768			0.50	364	−2.0612 7055 9011 4692 4364 54
He I 3 ^{1}S	0	13	0.8768	13	1.17	0.50	728	−2.0612 7198 8680 3101 7768 24

Table 1. *Cont.*

State	l_{max}	n_{orbs}	ξ	n'_{orbs}	ξ'	ω_{12}	N	Energy (Hartree)
He I 3 ^{1}S	1	13	0.8768			0.50	1092	−2.0612 7198 9532 0260 5098 95
He I 3 ^{1}S	1	13	0.8768	13	1.17	0.50	1456	−2.0612 7198 9690 7384 7505 05
He I 3 ^{1}S	2	13	0.8768			0.50	1820	−2.0612 7198 9702 6768 9462 55
He I 3 ^{1}S	2	13	0.8768	13	1.17	0.50	2184	−2.0612 7198 9724 6358 8091 24
He I 3 ^{1}S	3	13	0.8768			0.50	2548	−2.0612 7198 9727 5879 9975 38
He I 3 ^{1}S	3	13	0.8768	13	1.17	0.50	2912	−2.0612 7198 9731 7141 2421 45
He I 3 ^{1}S	3	13	0.8768	13	1.17	0.75	2912	−2.0612 7198 7799 2318 1864 21
He I 3 ^{1}S	3	13	0.8768	13	1.17	0.50	2912	−2.0612 7198 9297 0617 4478 12
He I 3 ^{1}S	3	13	0.8768	13	1.17	0.35	2912	−2.0612 7198 9605 6309 2694 83
He I 3 ^{1}S	3	13	0.8768	13	1.17	0.16	2912	−2.0612 7198 9721 2586 0712 01
He I 3 ^{1}S	3	13	0.8768	13	1.17	0.10	2912	−2.0612 7198 9732 2552 1696 89
He I 3 ^{1}S	3	13	0.8768	13	1.17	0.05	2912	−2.0612 7198 9736 8662 6585 57
He I 3 ^{1}S	3	13	0.8768	13	1.17	0.01	2912	−2.0612 7198 9731 0321 7216 75
Aznabaev et al. [31]								−2.0612 7198 9740 9086 5074 03

Table 2. E-Hy-CI wave function He 1–5 ^{1}S non-relativistic energies (in hartrees using a doubled basis set of orbitals for each *l*-wave). N is the number of terms in the expansion.

State	l_{max}	n_{orbs}	ξ	n'_{orbs}	ξ'	ω_{12}	N	Energy (Hartree)
He I 1 ^{1}S	0	13	2.20	13	25.0	0.5	728	−2.9037 2435 3910 9601 8477 99
He I 1 ^{1}S	1	13	3.05	13	40.5	0.5	1456	−2.9037 2437 7034 0679 8634 91
He I 1 ^{1}S	2	13	3.50	13	40.5	0.5	2184	−2.9037 2437 7034 1195 0022 60
He I 1 ^{1}S	3	13	3.90	13	40.5	0.5	2912	−2.9037 2437 7034 1195 9818 81
He I 1 ^{1}S	0	13	1.17			0.5	3276	−2.9037 2437 7034 1195 9821 90
He I 1 ^{1}S	0	13	1.17	13	5.56	0.5	3640	−2.9037 2437 7034 1195 9827 31
He I 1 ^{1}S	1	13	1.17			0.5	4004	−2.9037 2437 7034 1195 9827 51
He I 1 ^{1}S	1	13	1.17	13	5.56	0.5	4368	−2.9037 2437 7034 1195 9828 45
He I 1 ^{1}S	0	13	0.8768			0.5	4732	−2.9037 2437 7034 1195 9828 45
He I 1 ^{1}S	1	13	0.8768			0.5	5096	−2.9037 2437 7034 1195 9828 51
He I 1 ^{1}S	0	13	0.7635			0.05	5460	−2.9037 2437 7034 1195 9828 52
He I 1 ^{1}S	1	13	0.7635			0.05	5824	−2.9037 2437 7034 1195 9828 54
He I 1 ^{1}S	2	13	0.7635			0.05	6188	−2.9037 2437 7034 1195 9828 54
He I 1 ^{1}S	0	13	0.623			0.05	6552	−2.9037 2437 7034 1195 9828 55
He I 1 ^{1}S	1	13	0.623			0.05	6916	−2.9037 2437 7034 1195 9828 55
He I 1 ^{1}S	2	13	0.623			0.05	7280	−2.9037 2437 7034 1195 9828 56
He I 1 ^{1}S	0	13	0.53			0.05	7644	−2.9037 2437 7034 1195 9828 56
He I 1 ^{1}S	2	13	0.53			0.05	8008	−2.9037 2437 7034 1195 9828 56
He I 1 ^{1}S	2	13	0.53			0.05	8372	−2.9037 2437 7034 1195 9828 57
Nakashima and Nakatsuji [30]								−2.9037 2437 7034 1195 9831 12
He I 2 ^{1}S	0	13	2.20	13	25.0	0.5	728	−2.1458 1583 9153 1898 7651 82
He I 2 ^{1}S	1	13	3.05	13	40.5	0.5	1456	−2.1459 3197 5645 6946 7331 15
He I 2 ^{1}S	2	13	3.50	13	40.5	0.5	2184	−2.1459 6598 5199 9917 6833 04
He I 2 ^{1}S	3	13	3.90	13	40.5	0.5	2912	−2.1459 7086 8075 0361 8372 68
He I 2 ^{1}S	0	13	1.17			0.5	3276	−2.1459 7404 6054 4092 8533 86
He I 2 ^{1}S	0	13	1.17	13	5.56	0.5	3640	−2.1459 7404 6054 4133 7261 74

Table 2. *Cont.*

State	l_{max}	n_{orbs}	ξ	n'_{orbs}	ξ'	ω_{12}	N	Energy (Hartree)
He I 2 ^{1}S	1	13	1.17			0.5	4004	−2.1459 7404 6054 4168 5754 42
He I 2 ^{1}S	1	13	1.17	13	5.56	0.5	4368	−2.1459 7404 6054 4169 9326 43
He I 2 ^{1}S	0	13	0.8768			0.5	4732	−2.1459 7404 6054 4174 1565 80
He I 2 ^{1}S	1	13	0.8768			0.5	5096	−2.1459 7404 6054 4174 1578 46
He I 2 ^{1}S	0	13	0.7635			0.05	5460	−2.1459 7404 6054 4174 1579 66
He I 2 ^{1}S	1	13	0.7635			0.05	5824	−2.1459 7404 6054 4174 1579 88
He I 2 ^{1}S	2	13	0.7635			0.05	6188	−2.1459 7404 6054 4174 1580 21
He I 2 ^{1}S	0	13	0.623			0.05	6552	−2.1459 7404 6054 4174 1580 21
He I 2 ^{1}S	1	13	0.623			0.05	6916	−2.1459 7404 6054 4174 1580 22
He I 2 ^{1}S	2	13	0.623			0.05	7280	−2.1459 7404 6054 4174 1580 24
He I 2 ^{1}S	0	13	0.53			0.05	7644	−2.1459 7404 6054 4174 1580 24
He I 2 ^{1}S	2	13	0.53			0.05	8008	−2.1459 7404 6054 4174 1580 24
He I 2 ^{1}S	2	13	0.53			0.05	8372	−2.1459 7404 6054 4174 1580 24
Aznabaev et al. [31]								−2.1459 7404 6054 4174 1580 50
He I 3 ^{1}S	0	13	2.20	13	25.0	0.5	728	−2.0394 7820 3129 3021 4438 46
He I 3 ^{1}S	1	13	3.05	13	40.5	0.5	1456	−2.0490 5802 7440 5968 0929 88
He I 3 ^{1}S	2	13	3.50	13	40.5	0.5	2184	−2.0551 8265 2157 6960 1278 68
He I 3 ^{1}S	3	13	3.90	13	40.5	0.5	2912	−2.0571 5082 5105 6874 5756 65
He I 3 ^{1}S	0	13	1.17			0.5	3276	−2.0612 7180 2884 5812 3866 31
He I 3 ^{1}S	0	13	1.17	13	5.56	0.5	3640	−2.0612 7183 3107 1210 7617 29
He I 3 ^{1}S	1	13	1.17			0.5	4004	−2.0612 7189 2572 7594 0565 87
He I 3 ^{1}S	1	13	1.17	13	5.56	0.5	4368	−2.0612 7190 7217 2476 2465 64
He I 3 ^{1}S	0	13	0.8768			0.5	4732	−2.0612 7198 9685 3720 7713 92
He I 3 ^{1}S	1	13	0.8768			0.5	5096	−2.0612 7198 9730 8848 8878 49
He I 3 ^{1}S	0	13	0.7635			0.05	5460	−2.0612 7198 9740 3739 8201 46
He I 3 ^{1}S	1	13	0.7635			0.05	5824	−2.0612 7198 9740 6694 5016 03
He I 3 ^{1}S	2	13	0.7635			0.05	6188	−2.0612 7198 9740 8854 5669 77
He I 3 ^{1}S	0	13	0.623			0.05	6552	−2.0612 7198 9740 8882 5163 76
He I 3 ^{1}S	1	13	0.623			0.05	6916	−2.0612 7198 9740 8896 0853 78
He I 3 ^{1}S	2	13	0.623			0.05	7280	−2.0612 7198 9740 8978 7794 23
He I 3 ^{1}S	0	13	0.53			0.05	7644	−2.0612 7198 9740 8978 9667 65
He I 3 ^{1}S	1	13	0.53			0.05	8008	−2.0612 7198 9740 8979 7524 35
He I 3 ^{1}S	2	13	0.53			0.05	8372	−2.0612 7198 9740 8984 9048 81
Aznabaev et al. [31]								−2.0612 7198 9740 9086 5074 03
He I 4 ^{1}S	1	13	3.05	13	40.5	0.5	1456	−1.9976 6239 2700 2082 4570 52
He I 4 ^{1}S	3	13	3.90	13	40.5	0.5	2912	−2.0105 3191 2403 6325 8650 19
He I 4 ^{1}S	0	13	1.17			0.5	3276	−2.0332 5958 8508 1518 1492 46
He I 4 ^{1}S	0	13	1.17	13	5.56	0.5	3640	−2.0332 8931 7093 5158 7845 21
He I 4 ^{1}S	1	13	1.17			0.5	4004	−2.0333 5162 4496 3566 3580 82
He I 4 ^{1}S	1	13	1.17	13	5.56	0.5	4368	−2.0333 7111 4814 9961 0916 61
He I 4 ^{1}S	0	13	0.8768			0.5	4732	−2.0335 8336 0670 2166 8677 46
He I 4 ^{1}S	1	13	0.8768			0.5	5096	−2.0335 8541 4508 6363 5033 29
He I 4 ^{1}S	0	13	0.7635			0.05	5460	−2.0335 8663 6247 7125 3107 21
He I 4 ^{1}S	1	13	0.7635			0.05	5824	−2.0335 8669 2150 0956 8171 41
He I 4 ^{1}S	2	13	0.7635			0.05	6188	−2.0335 8671 0100 9427 2040 94

Table 2. *Cont.*

State	l_{max}	n_{orbs}	ξ	n'_{orbs}	ξ'	ω_{12}	N	Energy (Hartree)
He I 4 ^{1}S	0	13	0.623			0.05	6552	−2.0335 8671 5182 6200 6911 83
He I 4 ^{1}S	1	13	0.623			0.05	6916	−2.0335 8671 6097 7917 5860 95
He I 4 ^{1}S	2	13	0.623			0.05	7280	−2.0335 8671 6576 5463 7833 37
He I 4 ^{1}S	0	13	0.53			0.05	7644	−2.0335 8671 6587 4213 9070 62
He I 4 ^{1}S	1	13	0.53			0.05	8008	−2.0335 8671 6611 1351 4341 18
He I 4 ^{1}S	2	13	0.53			0.05	8372	−2.0335 8671 6646 1515 5575 70
Aznabaev et al. [31]								−2.0335 8671 7030 7254 4743 93
He I 5 ^{1}S	1	13	3.05	13	40.5	0.5	1456	−1.9968 8048 6541 5060 4620 06
He I 5 ^{1}S	3	13	3.90	13	40.5	0.5	2912	−2.0088 3402 8156 5823 7954 03
He I 5 ^{1}S	0	13	1.17			0.5	3276	−2.0145 9845 2315 1192 1420 73
He I 5 ^{1}S	0	13	1.17	13	5.56	0.5	3640	−2.0149 3322 7973 3784 9273 38
He I 5 ^{1}S	1	13	1.17			0.5	4004	−2.0156 4302 4203 0922 2695 48
He I 5 ^{1}S	1	13	1.17	13	5.56	0.5	4368	−2.0158 9180 6275 8008 6208 10
He I 5 ^{1}S	0	13	0.8768			0.5	4732	−2.0205 5903 8968 9575 6372 00
He I 5 ^{1}S	1	13	0.8768			0.5	5096	−2.0207 9539 0029 9299 0151 49
He I 5 ^{1}S	0	13	0.7635			0.05	5460	−2.0211 0657 5245 7647 6858 33
He I 5 ^{1}S	1	13	0.7635			0.05	5824	−2.0211 3894 5696 7931 3799 95
He I 5 ^{1}S	2	13	0.7635			0.05	6188	−2.0211 5799 0369 3487 8634 18
He I 5 ^{1}S	0	13	0.623			0.05	6552	−2.0211 7183 9914 3573 8483 67
He I 5 ^{1}S	1	13	0.623			0.05	6916	−2.0211 7496 0675 2167 7934 89
He I 5 ^{1}S	2	13	0.623			0.05	7280	−2.0211 7614 2072 1554 4086 17
He I 5 ^{1}S	0	13	0.53			0.05	7644	−2.0211 7625 2368 9962 4465 74
He I 5 ^{1}S	1	13	0.53			0.05	8008	−2.0211 7636 6093 8514 7908 44
He I 5 ^{1}S	2	13	0.53			0.05	8372	−2.0211 7648 1662 2560 6741 68
Nakashima and Nakatsuji [32]								−2.0211 7685 1574 3739 0280 37

Note: All energies are variational; all calculations were done in quadruple-double-with exponent (QDE) precision.

3.2. *He* ^{1}P

In paper III of this series [8], we developed a 7744-term expansion for lowest state of ^{1}P symmetry of He I, the 2 ^{1}P state, to 15 decimal place precision. This wave function is presented in Table 3, where in contrast to the ^{1}S states, each line specifies an inner set for the first electron and its associated l quantum number (=l_{max}), and an outer set with its associated $l' = l + 1$ quantum number for the second electron, but is otherwise the same. The steps leading to the final 7744-term 2 ^{1}P state wave function begin with a fixed $\xi, \xi' = 1.085$ for $l, l' = \{0,1\}$, i.e., a single orbital exponent was varied until the energy went through a minimum and there were enough data points to fit a smooth curve and yield an optimized $\xi = 2.272$. Next, ξ was fixed at 2.272 and ξ' was optimized in a similar fashion, yielding the optimized values of $\xi, \xi' = \{2.272,1.291\}$ for the $l, l' = \{0, 1\}$ 480-term wave function used in the optimization. n_{orbs} and n'_{orbs} are then extended to 19 for a $l, l' = \{0,1\}$ 722-term Hy-CI ($\omega_{12} = 0$) wave function of ≈0.015 millihartree precision. The effect of the exponential r_{12} on the precision of the calculation is clearly evident when adding to each term an exponentially correlated $e^{-\omega_{12} r_{12}}$ factor whose exponent ω_{12} is chosen to be the one (0.5) which satisfies the Kato cusp condition [33], yielding a 1444-term E-Hy-CI wave function of ≈15 microhartree precision.

This strategy was continued to the $l, l' = \{1,2\}$ block, yielding optimized values of $\xi, \xi' = \{1.955,2.25\}$ for both the 1444-term Hy-CI wave function and the 2888-term E-Hy-CI wave function; the precision of the 2888-term E-Hy-CI wave function is ≈picohartree.

Thanks to the very high precision Exponentially Correlated Hylleraas (E-Hy) calculation of Aznabaev et al. [31], it is clear that the l_{max} = 3 (*s*-, *p*-, *d*- and *f*- STO) E-Hy-CI precision is >13 decimal places, which is better than all previous calculations except for the Drake [27] and the Aznabaev et al. calculations. The results from continuing the comparison through l_{max} = 7 are tabulated in Table 3 for the 2 ^{1}P state.

Table 3. E-Hy-CI energies (in hartrees) for He 2 ^{1}P through 6 ^{1}P using two separate basis sets of orbitals ($\xi \neq \xi'$) for the inner and outer electrons. For each l_{max}, $l'_{max} = l_{max} + 1$. N is the number of terms in the expansion. Ellipses denote a continuation of the previous line's Energy value.

State	l_{max}	n_{orbs}	ξ	l'_{max}	n'_{orbs}	ξ'	ω_{12}	N	Energy (Hartree)
He I 2 ^{1}P	0	16	2.272	1	15	1.291		480	−2.1238 2780 3657 1217 9787
He I 2 ^{1}P	0	16	2.272	1	15	1.291	0.5	960	−2.1238 4308 3927 0924 8309
He I 2 ^{1}P	0	19	2.272	1	19	1.291		722	−2.1238 2782 6872 0251 1341
He I 2 ^{1}P	0	19	2.272	1	19	1.291	0.5	1444	−2.1238 4308 5062 4897 8422
He I 2 ^{1}P	1	15	1.955	2	14	2.25	0.5	1800	−2.1238 4308 6441 2634 4197
He I 2 ^{1}P	1	19	1.955	2	19	2.25	0.5	2888	−2.1238 4308 6497 9644 7703
Drake [27]								804	−2.1238 4308 6498 091
He I 2 ^{1}P	2	14	2.40	3	13	2.30	0.5	2528	−2.1238 4308 6441 6174 9409
He I 2 ^{1}P	2	19	2.40	3	18	2.30	0.5	4256	−2.1238 4308 6498 0912 9534
He I 2 ^{1}P	3	18	2.40	4	15	2.30	0.5	5336	−2.1238 4308 6498 0989 3227
He I 2 ^{1}P	4	15	2.40	5	14	2.30	0.5	6176	−2.1238 4308 6498 1004 0079
He I 2 ^{1}P	5	14	2.40	6	14	2.30	0.5	6960	−2.1238 4308 6498 1008 1958
He I 2 ^{1}P	6	14	2.40	7	14	2.30	0.5	7744	−2.1238 4308 6498 1009 6317
Aznabaev et al. [31]								22 000	−2.1238 4308 6498 1013 5924
									... 7333 1423 74
He I 3 ^{1}P	0	19	2.272	1	19	1.291		722	−2.0551 2957 2690 5521 6676
He I 3 ^{1}P	0	19	2.272	1	19	1.291	0.5	1444	−2.0551 4056 1426 0678 6679
He I 3 ^{1}P	1	19	1.955	2	19	2.25	0.5	2888	−2.0551 4532 9833 8593 9552
He I 3 ^{1}P	2	19	2.40	3	18	2.30	0.5	4256	−2.0551 4533 5705 9570 8050
Aznabaev et al. [31]								22 000	−2.0551 4636 2091 9435 3692
									... 8341 0921
He I 4 ^{1}P	0	19	2.272	1	19	1.291		722	−2.0288 0329 4116 3357 4602
He I 4 ^{1}P	0	19	2.272	1	19	1.291	0.5	1444	−2.0294 9904 5755 9157 9802
He I 4 ^{1}P	1	19	1.955	2	19	2.25	0.5	2888	−2.0303 9917 4851 1295 5260
He I 4 ^{1}P	2	19	2.40	3	18	2.30	0.5	4256	−2.0304 0108 8190 4879 3037
Aznabaev et al. [31]								22 000	−2.0310 6965 0450 2407 1475
									... 8931 4360 941
He I 5 ^{1}P	0	19	2.272	1	19	1.291		722	−2.0017 1464 6479 8943 9119
He I 5 ^{1}P	0	19	2.272	1	19	1.291	0.5	1444	−2.0052 6311 0797 7085 2680
He I 5 ^{1}P	1	19	1.955	2	19	2.25	0.5	2888	−2.0110 0135 5084 5148 9961
He I 5 ^{1}P	2	19	2.40	3	18	2.30	0.5	4256	−2.0110 0928 7598 8666 0232
Drake [28]									−2.0199 0598 9900 83
He I 6 ^{1}P	0	19	2.272	1	19	1.291		722	−2.0017 5741 1183 8565 3955
He I 6 ^{1}P	0	19	2.272	1	19	1.291	0.5	1444	−2.0052 6313 5624 4064 3461
He I 6 ^{1}P	1	19	1.955	2	19	2.25	0.5	2888	−2.0108 6708 7327 5707 8962
He I 6 ^{1}P	2	19	2.40	3	18	2.30	0.5	4256	−2.0108 8137 0863 3369 3933
Drake [28]									−2.0138 3397 9671 73

Note: All energies are variational; all calculations were done in quadruple-double-with exponent (QDE) precision.

Table 3 also displays the result of truncating the number of orbitals for l = 0–3 to 16, 15, 14, and 13 respectively, to form the 2528-term wave function which loses only 2 significant digits and, analogous to the ^{1}S case, becomes the wave function to which expansions suitable for the 3 ^{1}P, 4 ^{1}P and 5 ^{1}P are added.

In Table 4, the 2528-term wave function which yields 10 significant digit precision for the ground 2 ^{1}P is augmented with two blocks with ξ, ξ' = {2.402,0.625}, which were obtained by optimizing the wave function containing these terms for the 3 ^{1}P state. In optimization runs for 4 ^{1}P through 6 ^{1}P, the optimum value for the inner s orbital exponent does not vary much, so ξ = 2.402 is maintained for the inner s orbital in the remaining blocks. From Table 4, it can be seen that just adding these two blocks to the 2528-term wave function to create a 3880-term wave function on par with the 7744-term wave function previously obtained yields the same 14 significant digit accuracy for the 3 ^{1}P state as well. Adding two blocks with ξ, ξ' = {2.402,0.468} appropriate for the 4 ^{1}P state and another block with ξ, ξ' = {2.402,0.375} appropriate for the 5 ^{1}P state yields the final 5960-term wave function, which achieves 12–14 significant digit accuracy for He 2 through 6 ^{1}P, i.e, for not just the ground ^{1}P state but for 4 excited states as well. It is to be noted that the energy for the 5 and 6 ^{1}P states are of the same precision as the best result reported by Drake [28].

Table 4. E-Hy-CI energies (in hartrees) for He 2 ^{1}P through 6 ^{1}P using two separate basis sets of orbitals ($\xi \neq \xi'$) for the inner and outer electrons. For each l_{max}, $l'_{max} = l_{max} + 1$. N is the number of terms in the expansion. Ellipses denote a continuation of the previous line's Energy value.

State	l_{max}	n_{orbs}	ξ	l'_{max}	n'_{orbs}	ξ'	ω_{12}	N	Energy (Hartree)
He I 2 ^{1}P	0	16	2.272	1	15	1.291	0.5	960	−2.1238 4308 3927 0924 8309
He I 2 ^{1}P	1	15	1.955	2	14	2.25	0.5	1800	−2.1238 4308 6441 2634 4197
He I 2 ^{1}P	2	14	2.40	3	13	2.30	0.5	2528	−2.1238 4308 6441 6174 9409
He I 2 ^{1}P	0	14	2.402	1	13	0.625	0.5	3256	−2.1238 4308 6498 0901 3192
He I 2 ^{1}P	1	13	2.402	2	12	0.625	0.5	3880	−2.1238 4308 6498 0938 8692
He I 2 ^{1}P	0	14	2.402	1	13	0.468	0.5	4608	−2.1238 4308 6498 0961 4281
He I 2 ^{1}P	1	13	2.402	2	12	0.468	0.5	5232	−2.1238 4308 6498 0970 2959
He I 2 ^{1}P	0	14	2.402	1	13	0.375	0.5	5960	−2.1238 4308 6498 0973 9383
Aznabaev et al. [31]								22,000	−2.1238 4308 6498 1013 5924
									... 7333 1423 74
He I 3 ^{1}P	0	16	2.272	1	15	1.291	0.5	960	−2.0550 3873 3547 3086 1461
He I 3 ^{1}P	1	15	1.955	2	14	2.25	0.5	1800	−2.0551 2212 6152 8270 4161
He I 3 ^{1}P	2	14	2.40	3	13	2.30	0.5	2528	−2.0551 2220 3606 5331 6247
He I 3 ^{1}P	0	14	2.402	1	13	0.625	0.5	3256	−2.0551 4636 2091 7442 8817
He I 3 ^{1}P	1	13	2.402	2	12	0.625	0.5	3880	−2.0551 4636 2091 9398 9874
He I 3 ^{1}P	0	14	2.402	1	13	0.468	0.5	4608	−2.0551 4636 2091 9407 7473
He I 3 ^{1}P	1	13	2.402	2	12	0.468	0.5	5232	−2.0551 4636 2091 9415 9896
He I 3 ^{1}P	0	14	2.402	1	13	0.375	0.5	5960	−2.0551 4636 2091 9418 8216
Aznabaev et al. [31]								22,000	−2.0551 4636 2091 9435 3692
									... 8341 0921
He I 4 ^{1}P	0	16	2.272	1	15	1.291		960	−2.0246 5161 9219 8828 4956
He I 4 ^{1}P	1	15	1.955	2	14	2.25	0.5	1800	−2.0279 6692 3067 9451 6718
He I 4 ^{1}P	2	14	2.40	3	13	2.30	0.5	2528	−2.0279 7173 4168 2245 7269
He I 4 ^{1}P	0	14	2.402	1	13	0.625	0.5	3256	−2.0310 6964 9114 6071 9421
He I 4 ^{1}P	1	13	2.402	2	12	0.625	0.5	3880	−2.0310 6964 9345 5165 5835
He I 4 ^{1}P	0	14	2.402	1	13	0.468	0.5	4608	−2.0310 6965 0450 2299 1761

Table 4. *Cont.*

State	l_{max}	n_{orbs}	ξ	l'_{max}	n'_{orbs}	ξ'	ω_{12}	N	Energy (Hartree)
He I 4 ^{1}P	1	13	2.402	2	12	0.468	0.5	5232	−2.0310 6965 0450 2335 1293
He I 4 ^{1}P	0	14	2.402	1	13	0.375	0.5	5960	−2.0310 6965 0450 2337 6579
Aznabaev et al. [31]								22 000	−2.0310 6965 0450 2407 1475
									... 8931 4360 941
He I 5 ^{1}P	0	16	2.272	1	15	1.291		960	−1.9853 5119 3528 3878 1086
He I 5 ^{1}P	1	15	1.955	2	14	2.25	0.5	1800	−1.9980 9066 8533 4492 7952
He I 5 ^{1}P	2	14	2.40	3	13	2.30	0.5	2528	−1.9981 1138 8707 5396 3092
He I 5 ^{1}P	0	14	2.402	1	13	0.625	0.5	3256	−2.0198 9818 6800 0550 0090
He I 5 ^{1}P	1	13	2.402	2	12	0.625	0.5	3880	−2.0198 9905 0264 4541 9071
He I 5 ^{1}P	0	14	2.402	1	13	0.468	0.5	4608	−2.0199 0598 9900 7210 1999
He I 5 ^{1}P	1	13	2.402	2	12	0.468	0.5	5232	−2.0199 0598 9900 7494 3737
He I 5 ^{1}P	0	14	2.402	1	13	0.375	0.5	5960	−2.0199 0598 9900 8445 4576
Drake [28]									−2.0199 0598 9900 83
He I 6 ^{1}P	0	16	2.272	1	15	1.291		960	−1.9853 5151 8164 7987 2969
He I 6 ^{1}P	1	15	1.955	2	14	2.25	0.5	1800	−1.9980 9252 4185 4981 1386
He I 6 ^{1}P	2	14	2.40	3	13	2.30	0.5	2528	−1.9981 1317 0868 7386 7102
He I 6 ^{1}P	0	14	2.402	1	13	0.625	0.5	3256	−2.0132 6688 6192 4322 9000
He I 6 ^{1}P	1	13	2.402	2	12	0.625	0.5	3880	−2.0133 0161 2903 3736 2347
He I 6 ^{1}P	0	14	2.402	1	13	0.468	0.5	4608	−2.0138 3396 8157 9529 8369
He I 6 ^{1}P	1	13	2.402	2	12	0.468	0.5	5232	−2.0138 3397 8731 9136 7973
He I 6 ^{1}P	0	14	2.402	1	13	0.375	0.5	5960	−2.0138 3397 9671 6873 9539
Drake [28]									−2.0138 3397 9671 73

4. Oscillator Strengths

The basic theory of electric dipole radiation in atomic systems was given by Condon and Shortley [23][8]. Their terminology is followed closely herein. Assuming Russell–Saunders (LS) coupling and the non-relativistic many-electron Hamiltonian H_{NR} (Equation (2)), the energy states of an atom are characterized by the set of quantum numbers γLSM_LM_S (here, γ denotes the electronic configuration[9]). For an electric dipole transition connecting the terms (multiplets) γLS and $\gamma' L'S'$, Condon and Shortley introduced the quantity $S(\gamma LS;\gamma' L'S')$, called the absolute multiplet oscillator strength (line strength). It is defined in terms of the electric dipole moment operator

$$\vec{P} = \sum_{i=1}^{N_e} \vec{r}_i \tag{16}$$

by

$$S(\gamma LS;\gamma' L'S') = \sum_{M_L,M_S} \sum_{M'_L,M'_S} |\langle \gamma LSM_LM_S|\vec{P}|\gamma' L'S'M'_LM'_S\rangle|^2. \tag{17}$$

Method of Calculation

$S(\gamma LS \to \gamma' L'S')$ is shown in Section 3.0.1 of Paper III in this series [8] to be given by

$$S(\gamma\,{}^1S;\gamma'\,{}^1P) = 4\pi|\tilde{W}_0|^2, \tag{18}$$

where $|\tilde{W}_0|$, the non-vanishing component of the electronic dipole transition moment, is defined by

$$|\tilde{W}_0| = \left| \langle \gamma\ ^1S| \sum_{i=1}^{N_e} [2,1,0]_0^i | \gamma'\ ^1P, M_{L'} = 0 \rangle \right| \tag{19}$$

in terms of unnormalized STOs (Equation (5)).

To evaluate Equation (18), we use the fact that the wave functions employed to evaluate Equation (18) are given by Equations (3) and (4) and are linear combinations of antisymmetrized projected products of orbitals and at most one correlation factor of the form $r_{12}^{\nu_{12}} e^{-\omega_{12} r_{12}}$. Thus,

$$|\tilde{W}_0| = \sum_{K,L} C_K C_L |\tilde{W}_0|_{KL}, \tag{20}$$

where

$$|\tilde{W}_0|_{KL} = \left| \langle \Phi_K | \sum_{i=1}^{N_e} [2,1,0]_0^i | \Phi_L \rangle \right|. \tag{21}$$

In Equation (21), Φ_L is a linear combination of orbitals and at most one correlation factor, so Equation (21) can be evaluated by expanding the product of $[2,1,0]_0^i$ and the appropriate STO of Φ_L in terms of STOs by the formulas given in a previous paper [35]. Then, the integrals required to evaluate Equation (18) are similar in type to those required to calculate overlap matrix elements using these wave functions and can be evaluated as described in Section 3.0.2 (transition moment integrals) of Paper III in this series [8].

5. Upper and Lower Bounds to Oscillator Strengths

The f-value or multiplet oscillator strength is notoriously sensitive to the wave functions employed in computing S (S is used to compute f [36,37]), because significant contributions to the integral may arise from regions that do not significantly affect the energies of either state. To remedy this situation, Weinhold [38,39] showed how to calculate rigorous upper and lower bounds to f-values (dipole oscillator strengths) from non-relativistic quantum mechanical principles. While bounds were computed for a few atomic and molecular oscillator strengths [40–42], the rigorous bounds did not reflect the true precision of the computed oscillator strengths. To obtain good bounds, the calculations have to be of higher precision, as was the case in our two-electron helium atom E-Hy-CI wave functions which were precise enough energetically for us to use them to compute oscillator strengths and upper and lower bounds which provided rigorous estimates of the uncertainty in the computed f-values.

Method of Calculation

Weinhold's procedure for calculating rigorous upper and lower bounds to dipole strengths computes bounds to the transition moment

$$W_{ab} = \langle \Psi_a | W_l | \Psi_b \rangle, \tag{22}$$

where Ψ_a and Ψ_b are the approximate wave functions for states a and b, respectively, and W_l[10] is some particular Cartesian component of the vector operator $\vec{P}$ (which for us is the z component). As pointed out in Paper III, the calculation of error bounds requires the following additional quantities: the overlap integrals of the approximate wave functions ψ_a, ψ_b with the true wave functions Ψ_a, Ψ_b,

$$S_a \equiv \langle \psi_a | \Psi_a \rangle, S_b \equiv \langle \psi_b | \Psi_b \rangle, \tag{23}$$

the corresponding overlap errors ϵ_{a+}, ϵ_{b+},

$$\epsilon_{a+} \equiv (1 - S_{a-}^2)^{\frac{1}{2}},\ \epsilon_{b+} \equiv (1 - S_{b-}^2)^{\frac{1}{2}}, \tag{24}$$

and an uncertainty Δ_{ab} which is defined by

$$\Delta_{ab} \equiv (\langle \psi_b | W_l^2 | \psi_b \rangle - \tilde{W}_{ab}^2)^{1/2}. \tag{25}$$

Upper and lower bounds can now be calculated using Weinhold's inequalities,

$$W_{ab} \lessgtr S_{a\pm} S_{b\pm} \tilde{W}_{ab} \pm \epsilon_{a+} S_{b\pm} \Delta_{ab} \pm \epsilon_{b+} [\langle \Psi_a | W_l^2 | \Psi_a \rangle_+ - (S_{a-} \tilde{W}_{ab} - \epsilon_{a+} \Delta_{ab})^2]^{\frac{1}{2}}, \tag{26}$$

where the subscript $\pm$ signs mean the upper (+) or lower ($-$) bounds to the corresponding quantities.[11] With $|\tilde{W}|$'s defined by Equation (21), we have that

$$S(\gamma\ ^1S; \gamma'\ ^1P) = 4\pi |\tilde{W}_0|^2 = 3\tilde{W}_{ab}^2, \tag{27}$$

which relates upper and lower bounds to transition moments and oscillator strengths.

Weinhold's formula does require the calculation of $\langle \psi_b | W_l^2 | \psi_b \rangle$. With the aid of [35]

$$\begin{aligned} [2,1,j]_0^{i*} [2,1,j]_0^i &= \sum_{P_a=0}^{1} r_i^2 [\frac{(2l_1+1)}{(4\pi)}]^{\frac{1}{2}} C^{l_1}(1,j;1,j) Y_{l_1,0} \quad (l_1 = 2 - 2P_a) \\ &= \sum_{P_a=0}^{1} [\frac{(2l_1+1)}{(4\pi)}]^{\frac{1}{2}} C^{l_1}(1,j;1,j) [3,l_1,0]_0^i \end{aligned} \tag{28}$$

we obtain, for two electrons [40],

$$\begin{aligned} \langle \psi_b | (\frac{3}{4\pi}) X_0 X_0 | \psi_b \rangle &= \sum_{i=1}^{2} \sum_{P_a=0}^{1} [\frac{(2l_1+1)}{4\pi}]^{\frac{1}{2}} C^{l_1}(1,0;1,0) \langle \psi_b | [3,l_1,0]_0^i | \psi_b \rangle \\ &\quad + 2 \langle \psi_b | [2,1,0]_0^1 [2,1,0]_0^2 | \psi_b \rangle. \end{aligned} \tag{29}$$

Here $C^L(l', m'; l, m)$ is a Condon and Shortley coefficient (a so-called c^k [23,35,40]) and X_0 is the particular component of the dipole moment operator $\vec{P}$ (see Equation (16)) being chosen to calculate $\langle \psi_b | W_l^2 | \psi_b \rangle$.

6. *f*-Values and Bounds

As discussed in Section 5, theoretical upper and lower bounds to f-values (multiplet oscillator strengths[12]) can be computed from non-relativistic quantum mechanical principles. These bounds do not, however, reflect the true precision of the calculation and are usually too crude to provide useful error estimates, even with fairly high precision electronic wave functions. This has lead to efforts by Roginsky and co-workers [44,45] to tighten the error bounds. While these efforts have lead to improved results for the special cases of the hydrogen atom [44] and alkali atoms [45], it is not clear to what extent they will be effective in the more general case. However, in the case of the two-electron helium atom the E-Hy-CI wave functions are precise enough energetically to suggest using them to compute oscillator strengths with upper and lower bounds to provide rigorous estimates of the uncertainty in the computed f-values, and we have done so in Paper III in this series [8]. Here, we compute f-values[13] (multiplet oscillator strengths) along with rigorous non-relativistic quantum mechanical upper and lower bounds for the 25 lines arising from allowed transitions among these five ^1S and five ^1P states. The results are presented in Tables 5–9.

Froese Fischer [46] has presented some general variational methods that rely on precision indicators and discusses precision in a general way. She points out that for light atoms, (using C III as an example) the relativistic correction is important for a precise energy but the line strength (and hence, the oscillator strength) is close to the non-relativistic one. Helium is the simplest multi-electron atom and there exists a recent high precision multi-configuration Dirac–Hartree–Fock (MCDHF) calculation (using the GRASP2K [47–49] program[14]) of the $^1S \rightarrow {}^1P$ transition [51]. Two lines in the data for He I in the table (the MCHF and MCDHF lines [51]) are from this study and are included here to ascertain the magnitude of the relativistic effects for the He I transition, which turn out to be ≈0.00003 (≈0.01%) and indeed show relativistic effects to be small[15]. Note that all of the high precision studies (all correlated wave function calculations) are in agreement that the oscillator strength is 0.27616. Our results are in agreement and extend the precision of the non-relativistic (NR) oscillator strength by two orders of magnitude, based on the rigorous quantum mechanical upper and lower bounds. We note here that these results show that the Anderson and Weinhold [41] result is better than their bounds suggest, which is probably true for our results as well. Specifically, it is clear from the convergence of the oscillator strength that the 8732 × 5960 term results are good to the 10th decimal digit, but the bounds suggest that the results are only good to six decimal places. We recommend the NR oscillator strength to be 0.2761 6470 39(1) for He I (the Paper III [8] 7 decimal digit 3040 × 2888 result is included in the table as well), where the number of digits reported is indicative of how precise these calculations are.

These calculations are very much in the spirit of the Kono and Hattori [53] Hylleraas-type basis function calculations in 1984 and the Cann and Thakkar [54] exponentially correlated basis function calculations in 1992, which are in very good agreement with each other. Here, we have both types of correlation (linear and exponential) in our wave functions and extend their results by orders of magnitude.

Table 5. Non-relativistic multiplet oscillator strengths (f-values) with rigorous upper and lower bounds for the $1\,^1S \rightarrow 2\text{–}6\,^1P$ transitions of He I. Oscillator strengths computed by other authors are included for comparison.

States	Technique	Author	N (^{1}S)	E (^{1}S) (Hartree)	N (^{1}P)	E (^{1}P) (Hartree)	f-Value
$1\,^1S \rightarrow 2\,^1P$	E-Hy-CI	This work	1456	−2.9037 2437 7034 0679 8634 91	960	−2.1238 4308 3927 0924 8309	0.2761 6473 74 ± 0.0004 03
$1\,^1S \rightarrow 2\,^1P$	E-Hy-CI	This work	2912	−2.9037 2437 7034 1195 9818 81	1800	−2.1238 4308 6441 2634 4197	0.2761 6470 65 ± 0.0000 60
$1\,^1S \rightarrow 2\,^1P$	E-Hy-CI	Sims et al. [8]	3040	−2.9037 2437 7034 1043 9282 03	2888	−2.1238 4308 6497 9644 7703	0.2761 6470 03 ± 0.0000 03
$1\,^1S \rightarrow 2\,^1P$	E-Hy-CI	This work	4368	−2.9037 2437 7034 1195 9828 45	3256	−2.1238 4308 6498 0901 3192	0.2761 6470 39 ± 0.0000 21
$1\,^1S \rightarrow 2\,^1P$	E-Hy-CI	This work	5096	−2.9037 2437 7034 1195 9828 51	3880	−2.1238 4308 6498 0938 8692	0.2761 6470 39 ± 0.0000 02
$1\,^1S \rightarrow 2\,^1P$	E-Hy-CI	This work	5460	−2.9037 2437 7034 1195 9828 52	4608	−2.1238 4308 6498 0961 4281	0.2761 6470 39 ± 0.0000 01
$1\,^1S \rightarrow 2\,^1P$	E-Hy-CI	This work	6188	−2.9037 2437 7034 1195 9828 54	5232	−2.1238 4308 6498 0970 2959	0.2761 6470 39 ± 0.0000 01
$1\,^1S \rightarrow 2\,^1P$	E-Hy-CI	This work	6552	−2.9037 2437 7034 1195 9828 55	5232	−2.1238 4308 6498 0970 2959	0.2761 6470 39 ± 0.0000 01
$1\,^1S \rightarrow 2\,^1P$	E-Hy-CI	This work	7280	−2.9037 2437 7034 1195 9828 56	5960	−2.1238 4308 6498 0973 9383	0.2761 6470 39 ± 0.0000 01
$1\,^1S \rightarrow 2\,^1P$	E-Hy-CI	This work	8372	−2.9037 2437 7034 1195 9828 57	5960	−2.1238 4308 6498 0973 9383	0.2761 6470 39 ± 0.0000 01
$1\,^1S \rightarrow 2\,^1P$	E-Hy-CI	Recommended					0.2761 6470 39(1)
$1\,^1S \rightarrow 2\,^1P$	Hy	Schiff et al. [55]	1078	−2.9037 2437 48	364	−2.1238 4308 26	0.2761 6
$1\,^1S \rightarrow 2\,^1P$	Hy-CI	Anderson and Weinhold [41]	135	−2.9037 2436 62	137	−2.1238 4303 14	0.2761 ± 0.0014
$1\,^1S \rightarrow 2\,^1P$	Hy	Kono and Hattori [53]	138	−2.9037 2437 51	140	−2.1238 4308	0.2761 6
$1\,^1S \rightarrow 2\,^1P$	E-Hy	Cann and Thakkar [54]	100	−2.9037 2437 36	100	−2.1238 4308 02	0.2761 7
$1\,^1S \rightarrow 2\,^1P$	Hy	Drake and Morton [56]					0.2761 6
$1\,^1S \rightarrow 2\,^1P$	MCHF [1]	Liu et al. [51]					0.2762 9
$1\,^1S \rightarrow 2\,^1P$	MCDHF [2]	Liu et al. [51]					0.2763 2
$1\,^1S \rightarrow 2\,^1P$	Reference [3]	Wiese and Fuhr [57]					0.2762 5
$1\,^1S \rightarrow 3\,^1P$	E-Hy-CI	This work	1456	−2.9037 2437 7034 0679 8634 91	960	−2.0550 3873 3547 3086 1461	0.0748 3304 37 ± 0.0805 43

Table 5. *Cont.*

States	Technique	Author	N (^{1}S)	E (^{1}S) (Hartree)	N (^{1}P)	E (^{1}P) (Hartree)	f-Value
$1\,^1S \rightarrow 3\,^1P$	E-Hy-CI	This work	2912	−2.9037 2437 7034 1195 9818 81	1800	−2.0551 2212 6152 8270 4161	0.0738 0422 27 ± 0.0368 95
$1\,^1S \rightarrow 3\,^1P$	E-Hy-CI	This work	4368	−2.9037 2437 7034 1195 9828 45	3256	−2.0551 4636 2091 7442 8817	0.0734 3489 64 ± 0.0002 02
$1\,^1S \rightarrow 3\,^1P$	E-Hy-CI	This work	5096	−2.9037 2437 7034 1195 9828 51	3880	−2.0551 4636 2091 9398 9874	0.0734 3489 64 ± 0.0000 05
$1\,^1S \rightarrow 3\,^1P$	E-Hy-CI	This work	5460	−2.9037 2437 7034 1195 9828 52	4608	−2.0551 4636 2091 9407 7473	0.0734 3489 64 ± 0.0000 02
$1\,^1S \rightarrow 3\,^1P$	E-Hy-CI	This work	6188	−2.9037 2437 7034 1195 9828 54	5232	−2.0551 4636 2091 9415 9896	0.0734 3489 64 ± 0.0000 01
$1\,^1S \rightarrow 3\,^1P$	E-Hy-CI	This work	6552	−2.9037 2437 7034 1195 9828 55	5232	−2.0551 4636 2091 9415 9896	0.0734 3489 64 ± 0.0000 01
$1\,^1S \rightarrow 3\,^1P$	E-Hy-CI	This work	7280	−2.9037 2437 7034 1195 9828 56	5960	−2.0551 4636 2091 9418 8216	0.0734 3489 64 ± 0.0000 01
$1\,^1S \rightarrow 3\,^1P$	E-Hy-CI	This work	8372	−2.9037 2437 7034 1195 9828 57	5960	−2.0551 4636 2091 9418 8216	0.0734 3489 64 ± 0.0000 01
$1\,^1S \rightarrow 3\,^1P$	E-Hy-CI	Recommended					0.0734 3489 64(1)
$1\,^1S \rightarrow 3\,^1P$	Reference	Konno and Hattori [53]					0.0734 4
$1\,^1S \rightarrow 3\,^1P$	Reference	Cann and Thakkar [54]					0.0734 3
$1\,^1S \rightarrow 4\,^1P$	E-Hy-CI	This work	1456	−2.9037 2437 7034 0679 8634 91	960	−2.0246 5161 9219 8828 4956	0.0594 2736 60 ± 1.2645 81
$1\,^1S \rightarrow 4\,^1P$	E-Hy-CI	This work	2912	−2.9037 2437 7034 1195 9818 81	1800	−2.0279 6692 3067 9451 6718	0.0468 2614 43 ± 0.0249 63
$1\,^1S \rightarrow 4\,^1P$	E-Hy-CI	This work	4368	−2.9037 2437 7034 1195 9828 45	3256	−2.0310 6964 9114 6071 9421	0.0298 6287 75 ± 0.0022 41
$1\,^1S \rightarrow 4\,^1P$	E-Hy-CI	This work	5096	−2.9037 2437 7034 1195 9828 51	3880	−2.0310 6964 9345 5165 5835	0.0298 6287 75 ± 0.0002 18
$1\,^1S \rightarrow 4\,^1P$	E-Hy-CI	This work	5460	−2.9037 2437 7034 1195 9828 52	4608	−2.0310 6965 0450 2299 1761	0.0298 6285 25 ± 0.0000 21
$1\,^1S \rightarrow 4\,^1P$	E-Hy-CI	This work	6188	−2.9037 2437 7034 1195 9828 54	5232	−2.0310 6965 0450 2335 1293	0.0298 6285 25 ± 0.0000 04
$1\,^1S \rightarrow 4\,^1P$	E-Hy-CI	This work	6552	−2.9037 2437 7034 1195 9828 55	5232	−2.0310 6965 0450 2335 1293	0.0298 6285 25 ± 0.0000 02
$1\,^1S \rightarrow 4\,^1P$	E-Hy-CI	This work	7280	−2.9037 2437 7034 1195 9828 56	5960	−2.0310 6965 0450 2337 6579	0.0298 6285 25 ± 0.0000 01
$1\,^1S \rightarrow 4\,^1P$	E-Hy-CI	This work	8372	−2.9037 2437 7034 1195 9828 57	5960	−2.0310 6965 0450 2337 6579	0.0298 6285 25 ± 0.0000 01
$1\,^1S \rightarrow 4\,^1P$	E-Hy-CI	Recommended					0.0298 6285 25(1)
$1\,^1S \rightarrow 4\,^1P$	Reference	Kono and Hattori [53]					0.0298 63
$1\,^1S \rightarrow 4\,^1P$	Reference	Cann and Thakkar [54]					0.0298 61
$1\,^1S \rightarrow 5\,^1P$	E-Hy-CI	This work	1456	−2.9037 2437 7034 0679 8634 91	960	−1.9853 5119 3528 3878 1086	0.0594 2741 30 ± 0.6471 45
$1\,^1S \rightarrow 5\,^1P$	E-Hy-CI	This work	2912	−2.9037 2437 7034 1195 9818 81	1800	−1.9980 9066 8533 4492 7952	0.0168 1530 70 ± 0.0310 22
$1\,^1S \rightarrow 5\,^1P$	E-Hy-CI	This work	4368	−2.9037 2437 7034 1195 9828 45	3256	−2.0198 9818 6800 0550 0090	0.0151 2967 39 ± 0.0278 81
$1\,^1S \rightarrow 5\,^1P$	E-Hy-CI	This work	5096	−2.9037 2437 7034 1195 9828 51	3880	−2.0198 9905 0264 4541 9071	0.0151 2053 86 ± 0.0027 88
$1\,^1S \rightarrow 5\,^1P$	E-Hy-CI	This work	5460	−2.9037 2437 7034 1195 9828 52	4608	−2.0199 0598 9900 7210 1999	0.0150 3931 34 ± 0.0001 93
$1\,^1S \rightarrow 5\,^1P$	E-Hy-CI	This work	6188	−2.9037 2437 7034 1195 9828 54	5232	−2.0199 0598 9900 7494 3737	0.0150 3931 34 ± 0.0000 19
$1\,^1S \rightarrow 5\,^1P$	E-Hy-CI	This work	6552	−2.9037 2437 7034 1195 9828 55	5232	−2.0199 0598 9900 7494 3737	0.0150 3931 33 ± 0.0000 02
$1\,^1S \rightarrow 5\,^1P$	E-Hy-CI	This work	7280	−2.9037 2437 7034 1195 9828 56	5960	−2.0199 0598 9900 8445 4576	0.0150 3931 33 ± 0.0000 01
$1\,^1S \rightarrow 5\,^1P$	E-Hy-CI	This work	8372	−2.9037 2437 7034 1195 9828 57	5960	−2.0199 0598 9900 8445 4576	0.0150 3931 33 ± 0.0000 01
$1\,^1S \rightarrow 5\,^1P$	E-Hy-CI	Recommended					0.0150 3931 33(1)
$1\,^1S \rightarrow 5\,^1P$	Reference	Kono and Hattori [53]					0.0150 39
$1\,^1S \rightarrow 5\,^1P$	Reference	Cann and Thakkar [54]					0.0150 39
$1\,^1S \rightarrow 6\,^1P$	E-Hy-CI	This work	1456	−2.9037 2437 7034 0679 8634 91	960	−1.9853 5151 8164 7987 2969	0.0594 1057 58 ± 0.0297 08
$1\,^1S \rightarrow 6\,^1P$	E-Hy-CI	This work	2912	−2.9037 2437 7034 1195 9818 81	1800	−1.9980 9252 4185 4981 1386	0.0100 7807 28 ± 0.0057 70
$1\,^1S \rightarrow 6\,^1P$	E-Hy-CI	This work	4368	−2.9037 2437 7034 1195 9828 45	3256	−2.0132 6688 6192 4322 9000	0.0116 0471 85 ± 0.0045 76
$1\,^1S \rightarrow 6\,^1P$	E-Hy-CI	This work	5096	−2.9037 2437 7034 1195 9828 51	3880	−2.0133 0161 2903 3736 2347	0.0146 0952 19 ± 0.0036 36
$1\,^1S \rightarrow 6\,^1P$	E-Hy-CI	This work	5460	−2.9037 2437 7034 1195 9828 52	4608	−2.0138 3396 8157 9529 8369	0.0086 2787 14 ± 0.0002 17
$1\,^1S \rightarrow 6\,^1P$	E-Hy-CI	This work	6188	−2.9037 2437 7034 1195 9828 54	5232	−2.0138 3397 8731 9136 7973	0.0086 2771 10 ± 0.0000 21
$1\,^1S \rightarrow 6\,^1P$	E-Hy-CI	This work	6552	−2.9037 2437 7034 1195 9828 55	5232	−2.0138 3397 8731 9136 7973	0.0086 2771 10 ± 0.0000 02
$1\,^1S \rightarrow 6\,^1P$	E-Hy-CI	This work	7280	−2.9037 2437 7034 1195 9828 56	5960	−2.0138 3397 9671 6873 9539	0.0086 2769 11 ± 0.0000 01
$1\,^1S \rightarrow 6\,^1P$	E-Hy-CI	This work	8372	−2.9037 2437 7034 1195 9828 57	5960	−2.0138 3397 9671 6873 9539	0.0086 2769 11 ± 0.0000 01
$1\,^1S \rightarrow 6\,^1P$	E-Hy-CI	Recommended					0.0086 2769 11(20)
$1\,^1S \rightarrow 6\,^1P$	Reference	Kono and Hattori [53]					0.0086 28
$1\,^1S \rightarrow 6\,^1P$	Reference	Cann and Thakkar [54]					0.0086 27

Note: All energies in this work are variational except for the Recommended energy; all calculations were done in quadruple-double-with exponent (QDE) precision. [1] Multi-configuration Hartree–Fock [58]. [2] Multi-configuration Dirac–Hartree–Fock [49,59,60]. [3] Relativisitic effects included.

Table 6. Non-relativistic multiplet oscillator strengths (f-values) with rigorous upper and lower bounds for the $2\,^1S \rightarrow 2\text{–}6\,^1P$ transitions of He I. Oscillator strengths computed by other authors are included for comparison.

States	Technique	Author	N (^{1}S)	E (^{1}S) (Hartree)	N (^{1}P)	E (^{1}P) (Hartree)	f-Value
$2\,^1S \rightarrow 2\,^1P$	E-Hy-CI	This work	1456	−2.1459 3197 5645 6946 7331 15	960	−2.1238 4308 3927 0924 8309	0.3737 4897 56 ± 0.0281 52
$2\,^1S \rightarrow 2\,^1P$	E-Hy-CI	This work	2912	−2.1459 7086 8075 0361 8372 68	1800	−2.1238 4308 6441 2634 4197	0.3761 4515 34 ± 0.0169 25
$2\,^1S \rightarrow 2\,^1P$	E-Hy-CI	This work	4368	−2.1459 7404 6054 4169 9326 43	3256	−2.1238 4308 6498 0901 3192	0.3764 4028 80 ± 0.0015 09
$2\,^1S \rightarrow 2\,^1P$	E-Hy-CI	This work	5096	−2.1459 7404 6054 4174 1578 46	3880	−2.1238 4308 6498 0938 8692	0.3764 4028 80 ± 0.0001 64
$2\,^1S \rightarrow 2\,^1P$	E-Hy-CI	This work	5460	−2.1459 7404 6054 4174 1579 66	4608	−2.1238 4308 6498 0961 4281	0.3764 4028 80 ± 0.0000 01
$2\,^1S \rightarrow 2\,^1P$	E-Hy-CI	This work	6188	−2.1459 7404 6054 4174 1580 21	5232	−2.1238 4308 6498 0970 2959	0.3764 4028 80 ± 0.0000 01
$2\,^1S \rightarrow 2\,^1P$	E-Hy-CI	This work	6552	−2.1459 7404 6054 4174 1580 21	5232	−2.1238 4308 6498 0970 2959	0.3764 4028 80 ± 0.0000 01
$2\,^1S \rightarrow 2\,^1P$	E-Hy-CI	This work	7280	−2.1459 7404 6054 4174 1580 24	5960	−2.1238 4308 6498 0973 9383	0.3764 4028 80 ± 0.0000 01
$2\,^1S \rightarrow 2\,^1P$	E-Hy-CI	This work	8372	−2.1459 7404 6054 4174 1580 24	5960	−2.1238 4308 6498 0973 9383	0.3764 4028 80 ± 0.0000 01
$2\,^1S \rightarrow 2\,^1P$	E-Hy-CI	Recommended					0.3764 4028 80(1)
$2\,^1S \rightarrow 2\,^1P$	Reference	Kono and Hattori [53]					0.3764 4
$2\,^1S \rightarrow 2\,^1P$	Reference	Cann and Thakkar [54]					0.3764 8
$2\,^1S \rightarrow 3\,^1P$	E-Hy-CI	This work	1456	−2.1459 3197 5645 6946 7331 15	960	−2.0550 3873 3547 3086 1461	0.1225 5946 20 ± 0.0251 74
$2\,^1S \rightarrow 3\,^1P$	E-Hy-CI	This work	2912	−2.1459 7086 8075 0361 8372 68	1800	−2.0551 2212 6152 8270 4161	0.1448 9431 36 ± 0.0167 22
$2\,^1S \rightarrow 3\,^1P$	E-Hy-CI	This work	4368	−2.1459 7404 6054 4169 9326 43	3256	−2.0551 4636 2091 7442 8817	0.1513 4166 48 ± 0.0009 21
$2\,^1S \rightarrow 3\,^1P$	E-Hy-CI	This work	5096	−2.1459 7404 6054 4174 1578 46	3880	−2.0551 4636 2091 9398 9874	0.1513 4166 58 ± 0.0000 51
$2\,^1S \rightarrow 3\,^1P$	E-Hy-CI	This work	5460	−2.1459 7404 6054 4174 1579 66	4608	−2.0551 4636 2091 9407 7473	0.1513 4166 58 ± 0.0000 02
$2\,^1S \rightarrow 3\,^1P$	E-Hy-CI	This work	6188	−2.1459 7404 6054 4174 1580 21	5232	−2.0551 4636 2091 9415 9896	0.1513 4166 58 ± 0.0000 01
$2\,^1S \rightarrow 3\,^1P$	E-Hy-CI	This work	6552	−2.1459 7404 6054 4174 1580 21	5232	−2.0551 4636 2091 9415 9896	0.1513 4166 58 ± 0.0000 01
$2\,^1S \rightarrow 3\,^1P$	E-Hy-CI	This work	7280	−2.1459 7404 6054 4174 1580 24	5960	−2.0551 4636 2091 9418 8216	0.1513 4166 58 ± 0.0000 01
$2\,^1S \rightarrow 3\,^1P$	E-Hy-CI	This work	8372	−2.1459 7404 6054 4174 1580 24	5960	−2.0551 4636 2091 9418 8216	0.1513 4166 58 ± 0.0000 01
$2\,^1S \rightarrow 3\,^1P$	E-Hy-CI	Recommended					0.1513 4166 58(1)
$2\,^1S \rightarrow 3\,^1P$	Reference	Kono and Hattori [53]					0.1513 4
$2\,^1S \rightarrow 3\,^1P$	Reference	Cann and Thakkar [54]					0.1513 5
$2\,^1S \rightarrow 4\,^1P$	E-Hy-CI	This work	1456	−2.1459 3197 5645 6946 7331 15	960	−2.0246 5161 9219 8828 4956	0.1139 3425 33 ± 1.9829 07
$2\,^1S \rightarrow 4\,^1P$	E-Hy-CI	This work	2912	−2.1459 7086 8075 0361 8372 68	1800	−2.0279 6692 3067 9451 6718	0.0832 8038 34 ± 0.1250 67
$2\,^1S \rightarrow 4\,^1P$	E-Hy-CI	This work	4368	−2.1459 7404 6054 4169 9326 43	3256	−2.0310 6964 9114 6071 9421	0.0491 5497 05 ± 0.0073 76
$2\,^1S \rightarrow 4\,^1P$	E-Hy-CI	This work	5096	−2.1459 7404 6054 4174 1578 46	3880	−2.0310 6964 9345 5165 5835	0.0491 5493 57 ± 0.0003 04
$2\,^1S \rightarrow 4\,^1P$	E-Hy-CI	This work	5460	−2.1459 7404 6054 4174 1579 66	4608	−2.0310 6965 0450 2299 1761	0.0491 5489 50 ± 0.0000 38
$2\,^1S \rightarrow 4\,^1P$	E-Hy-CI	This work	6188	−2.1459 7404 6054 4174 1580 21	5232	−2.0310 6965 0450 2335 1293	0.0491 5489 50 ± 0.0000 11
$2\,^1S \rightarrow 4\,^1P$	E-Hy-CI	This work	6552	−2.1459 7404 6054 4174 1580 21	5232	−2.0310 6965 0450 2335 1293	0.0491 5489 50 ± 0.0000 02
$2\,^1S \rightarrow 4\,^1P$	E-Hy-CI	This work	7280	−2.1459 7404 6054 4174 1580 24	5960	−2.0310 6965 0450 2337 6579	0.0491 5489 50 ± 0.0000 01
$2\,^1S \rightarrow 4\,^1P$	E-Hy-CI	This work	8372	−2.1459 7404 6054 4174 1580 24	5960	−2.0310 6965 0450 2337 6579	0.0491 5489 50 ± 0.0000 01
$2\,^1S \rightarrow 4\,^1P$	E-Hy-CI	Recommended					0.0491 5489 50(1)
$2\,^1S \rightarrow 4\,^1P$	Reference	Kono and Hattori [53]					0.0491 6
$2\,^1S \rightarrow 4\,^1P$	Reference	Cann and Thakkar [54]					0.0491 5
$2\,^1S \rightarrow 5\,^1P$	E-Hy-CI	This work	1456	−2.1459 3197 5645 6946 7331 15	960	−1.9853 5119 3528 3878 1086	0.1139 3434 76 ± 1.8786 55
$2\,^1S \rightarrow 5\,^1P$	E-Hy-CI	This work	2912	−2.1459 7086 8075 0361 8372 68	1800	−1.9980 9066 8533 4492 7952	0.0832 6557 32 ± 0.0949 33
$2\,^1S \rightarrow 5\,^1P$	E-Hy-CI	This work	4368	−2.1459 7404 6054 4169 9326 43	3256	−2.0198 9818 6800 0550 0090	0.0224 7025 85 ± 0.0853 21
$2\,^1S \rightarrow 5\,^1P$	E-Hy-CI	This work	5096	−2.1459 7404 6054 4174 1578 46	3880	−2.0198 9905 0264 4541 9071	0.0224 5693 67 ± 0.0076 78
$2\,^1S \rightarrow 5\,^1P$	E-Hy-CI	This work	5460	−2.1459 7404 6054 4174 1579 66	4608	−2.0199 0598 9900 7210 1999	0.0223 3707 76 ± 0.0000 54
$2\,^1S \rightarrow 5\,^1P$	E-Hy-CI	This work	6188	−2.1459 7404 6054 4174 1580 21	5232	−2.0199 0598 9900 7494 3737	0.0223 3707 78 ± 0.0000 07
$2\,^1S \rightarrow 5\,^1P$	E-Hy-CI	This work	6552	−2.1459 7404 6054 4174 1580 21	5232	−2.0199 0598 9900 7494 3737	0.0223 3707 77 ± 0.0000 02
$2\,^1S \rightarrow 5\,^1P$	E-Hy-CI	This work	7280	−2.1459 7404 6054 4174 1580 24	5960	−2.0199 0598 9900 8445 4576	0.0223 3770 77 ± 0.0000 01
$2\,^1S \rightarrow 5\,^1P$	E-Hy-CI	This work	8372	−2.1459 7404 6054 4174 1580 24	5960	−2.0199 0598 9900 8445 4576	0.0223 3770 77 ± 0.0000 01
$2\,^1S \rightarrow 5\,^1P$	E-Hy-CI	Recommended					0.0223 3770 77(1)
$2\,^1S \rightarrow 5\,^1P$	Reference	Kono and Hattori [53]					0.0223 4
$2\,^1S \rightarrow 5\,^1P$	Reference	Cann and Thakkar [54]					0.0223 4

Table 6. *Cont.*

States	Technique	Author	N (^{1}S)	E (^{1}S) (Hartree)	N (^{1}P)	E (^{1}P) (Hartree)	f-Value
$2\,^1S \rightarrow 6\,^1P$	E-Hy-CI	This work	1456	−2.1459 3197 5645 6946 7331 15	960	−1.9853 5151 8164 7987 2969	0.1139 1028 48 ± 0.8788 30
$2\,^1S \rightarrow 6\,^1P$	E-Hy-CI	This work	2912	−2.1459 7086 8075 0361 8372 68	1800	−1.9980 9252 4185 4981 1386	0.0082 2609 02 ± 0.0407 33
$2\,^1S \rightarrow 6\,^1P$	E-Hy-CI	This work	4368	−2.1459 7404 6054 4169 9326 43	3256	−2.0132 6688 6192 4322 9000	0.0162 3873 08 ± 0.0077 47
$2\,^1S \rightarrow 6\,^1P$	E-Hy-CI	This work	5096	−2.1459 7404 6054 4174 1578 46	3880	−2.0133 0161 2903 3736 2347	0.0160 4249 85 ± 0.0069 71
$2\,^1S \rightarrow 6\,^1P$	E-Hy-CI	This work	5460	−2.1459 7404 6054 4174 1579 66	4608	−2.0138 3396 8157 9529 8369	0.0121 3420 69 ± 0.0004 90
$2\,^1S \rightarrow 6\,^1P$	E-Hy-CI	This work	6188	−2.1459 7404 6054 4174 1580 21	5232	−2.0138 3397 8731 9136 7973	0.0121 3398 25 ± 0.0000 64
$2\,^1S \rightarrow 6\,^1P$	E-Hy-CI	This work	6552	−2.1459 7404 6054 4174 1580 21	5232	−2.0138 3397 8731 9136 7973	0.0121 3398 25 ± 0.0000 18
$2\,^1S \rightarrow 6\,^1P$	E-Hy-CI	This work	7280	−2.1459 7404 6054 4174 1580 24	5960	−2.0138 3397 8731 9136 7973	0.0121 3399 55 ± 0.0000 08
$2\,^1S \rightarrow 6\,^1P$	E-Hy-CI	This work	8372	−2.1459 7404 6054 4174 1580 24	5960	−2.0138 3397 8731 9136 7973	0.0121 3395 46 ± 0.0000 08
$2\,^1S \rightarrow 6\,^1P$	E-Hy-CI	Recommended					0.0121 3395 5(5)
$2\,^1S \rightarrow 6\,^1P$	Reference	Kono and Hattori [53]					0.0121 3
$2\,^1S \rightarrow 6\,^1P$	Reference	Cann and Thakkar [54]					0.0121 36

Note: All energies in this work are variational except for the Recommended energy; all calculations were done in quadruple-double-with exponent (QDE) precision.

Table 7. Non-relativistic multiplet oscillator strengths (f-values) with rigorous upper and lower bounds for the $3\,^1S \rightarrow 2$–$6\,^1P$ transitions of He I. Oscillator strengths computed by other authors are included for comparison.

States	Technique	Author	N (^{1}S)	E (^{1}S) (Hartree)	N (^{1}P)	E (^{1}P) (Hartree)	f-Value
$3\,^1S \rightarrow 2\,^1P$	E-Hy-CI	This work	1456	−2.0490 5802 7440 5968 0929 88	960	−2.1238 4308 3927 0924 8309	0.2195 0657 57 ± 1.1141 84
$3\,^1S \rightarrow 2\,^1P$	E-Hy-CI	This work	2912	−2.0571 5082 5105 6874 5756 65	1800	−2.1238 4308 6441 2634 4197	0.1796 6125 79 ± 0.0516 11
$3\,^1S \rightarrow 2\,^1P$	E-Hy-CI	This work	4368	−2.0612 7190 7217 2476 2465 64	3256	−2.1238 4308 6498 0901 3192	0.1454 7312 14 ± 0.0002 83
$3\,^1S \rightarrow 2\,^1P$	E-Hy-CI	This work	5096	−2.0612 7198 9730 8848 8878 49	3880	−2.1238 4308 6498 0938 8692	0.1454 7029 11 ± 0.0000 33
$3\,^1S \rightarrow 2\,^1P$	E-Hy-CI	This work	5460	−2.0612 7198 9740 3739 8201 46	4608	−2.1238 4308 6498 0961 4281	0.1454 7028 78 ± 0.0000 02
$3\,^1S \rightarrow 2\,^1P$	E-Hy-CI	This work	6188	−2.0612 7198 9740 8854 5669 77	5232	−2.1238 4308 6498 0970 2959	0.1454 7028 78 ± 0.0000 01
$3\,^1S \rightarrow 2\,^1P$	E-Hy-CI	This work	6552	−2.0612 7198 9740 8882 5163 76	5232	−2.1238 4308 6498 0970 2959	0.1454 7028 78 ± 0.0000 01
$3\,^1S \rightarrow 2\,^1P$	E-Hy-CI	This work	7280	−2.0612 7198 9740 8978 7744 23	5960	−2.1238 4308 6498 0973 9383	0.1454 7028 78 ± 0.0000 01
$3\,^1S \rightarrow 2\,^1P$	E-Hy-CI	This work	8372	−2.0612 7198 9740 8984 9048 81	5960	−2.1238 4308 6498 0973 9383	0.1454 7028 78 ± 0.0000 01
$3\,^1S \rightarrow 2\,^1P$	E-Hy-CI	Recommended					0.1454 7028 78(1)
$3\,^1S \rightarrow 2\,^1P$	Reference	Kono and Hattori [53]					0.1454 7
$3\,^1S \rightarrow 2\,^1P$	Reference	Cann and Thakkar [54]					0.1454 60
$3\,^1S \rightarrow 3\,^1P$	E-Hy-CI	This work	1456	−2.0490 5802 7440 5968 0929 88	960	−2.0550 3873 3547 3086 1461	0.2855 2048 33 ± 1.4492 36
$3\,^1S \rightarrow 3\,^1P$	E-Hy-CI	This work	2912	−2.0571 5082 5105 6874 5756 65	1800	−2.0551 2212 6152 8270 4161	0.1442 6968 13 ± 0.7741 65
$3\,^1S \rightarrow 3\,^1P$	E-Hy-CI	This work	4368	−2.0612 7190 7217 2476 2465 64	3256	−2.0551 4636 2091 7442 8817	0.6261 5162 87 ± 0.0425 10
$3\,^1S \rightarrow 3\,^1P$	E-Hy-CI	This work	5096	−2.0612 7198 9730 8848 8878 49	3880	−2.0551 4636 2091 9398 9874	0.6261 9301 77 ± 0.0042 65
$3\,^1S \rightarrow 3\,^1P$	E-Hy-CI	This work	5460	−2.0612 7198 9740 3739 8201 46	4608	−2.0551 4636 2091 9407 7473	0.6261 9308 27 ± 0.0000 63
$3\,^1S \rightarrow 3\,^1P$	E-Hy-CI	This work	6188	−2.0612 7198 9740 8854 5669 77	5232	−2.0551 4636 2091 9415 9896	0.6261 9308 31 ± 0.0000 02
$3\,^1S \rightarrow 3\,^1P$	E-Hy-CI	This work	6552	−2.0612 7198 9740 8882 5163 76	5232	−2.0551 4636 2091 9415 9896	0.6261 9308 31 ± 0.0000 01
$3\,^1S \rightarrow 3\,^1P$	E-Hy-CI	This work	7280	−2.0612 7198 9740 8978 7744 23	5960	−2.0551 4636 2091 9418 8216	0.6261 9308 31 ± 0.0000 01
$3\,^1S \rightarrow 3\,^1P$	E-Hy-CI	This work	8372	−2.0612 7198 9740 8984 9048 81	5960	−2.0551 4636 2091 9418 8216	0.6261 9308 31 ± 0.0000 01
$3\,^1S \rightarrow 3\,^1P$	E-Hy-CI	Recommended					0.6261 9308 31(1)
$3\,^1S \rightarrow 3\,^1P$	Reference	Kono and Hattori [53]					0.6262
$3\,^1S \rightarrow 3\,^1P$	Reference	Cann and Thakkar [54]					0.6263
$3\,^1S \rightarrow 4\,^1P$	E-Hy-CI	This work	1456	−2.0490 5802 7440 5968 0929 88	960	−2.0246 5161 9219 8828 4956	0.2263 1088 86 ± 0.6458 79
$3\,^1S \rightarrow 4\,^1P$	E-Hy-CI	This work	2912	−2.0571 5082 5105 6874 5756 65	1800	−2.0279 6692 3067 9451 6718	0.0944 5981 02 ± 0.1140 18
$3\,^1S \rightarrow 4\,^1P$	E-Hy-CI	This work	4368	−2.0612 7190 7217 2476 2465 64	3256	−2.0310 6964 9114 6071 9421	0.1428 9023 39 ± 0.7601 20
$3\,^1S \rightarrow 4\,^1P$	E-Hy-CI	This work	5096	−2.0612 7198 9730 8848 8878 49	3880	−2.0310 6964 9345 5165 5835	0.1438 8341 12 ± 0.0377 87
$3\,^1S \rightarrow 4\,^1P$	E-Hy-CI	This work	5460	−2.0612 7198 9740 3739 8201 46	4608	−2.0310 6965 0450 2299 1761	0.1438 8890 73 ± 0.0004 08
$3\,^1S \rightarrow 4\,^1P$	E-Hy-CI	This work	6188	−2.0612 7198 9740 8854 5669 77	5232	−2.0310 6965 0450 2335 1293	0.1438 8894 33 ± 0.0000 11

Table 7. *Cont.*

States	Technique	Author	N (^{1}S)	E (^{1}S) (Hartree)	N (^{1}P)	E (^{1}P) (Hartree)	f-Value
$3\,^1S \rightarrow 4\,^1P$	E-Hy-CI	This work	6552	−2.0612 7198 9740 8882 5163 76	5232	−2.0310 6965 0450 2335 1293	0.1438 8894 44 ± 0.0000 10
$3\,^1S \rightarrow 4\,^1P$	E-Hy-CI	This work	7280	−2.0612 7198 9740 8978 7744 23	5960	−2.0310 6965 0450 2337 6579	0.1438 8894 48 ± 0.0000 10
$3\,^1S \rightarrow 4\,^1P$	E-Hy-CI	This work	8372	−2.0612 7198 9740 8984 9048 81	5960	−2.0310 6965 0450 2337 6579	0.1438 8894 48 ± 0.0000 01
$3\,^1S \rightarrow 4\,^1P$	E-Hy-CI	Recommended					0.1438 8894 48(1)
$3\,^1S \rightarrow 4\,^1P$	Reference	Kono and Hattori [53]					0.1439 0
$3\,^1S \rightarrow 4\,^1P$	Reference	Cann and Thakkar [54]					0.1439
$3\,^1S \rightarrow 5\,^1P$	E-Hy-CI	This work	1456	−2.0490 5802 7440 5968 0929 88	960	−1.9853 5119 3528 3878 1086	0.2263 1124 27 ± 0.7259 68
$3\,^1S \rightarrow 5\,^1P$	E-Hy-CI	This work	2912	−2.0571 5082 5105 6874 5756 65	1800	−1.9980 9066 8533 4492 7952	0.0944 7249 91 ± 0.1368 22
$3\,^1S \rightarrow 5\,^1P$	E-Hy-CI	This work	4368	−2.0612 7190 7217 2476 2465 64	3256	−2.0198 9818 6800 0550 0090	0.0529 9223 93 ± 0.0149 93
$3\,^1S \rightarrow 5\,^1P$	E-Hy-CI	This work	5096	−2.0612 7198 9730 8848 8878 49	3880	−2.0198 9905 0264 4541 9071	0.0507 7114 21 ± 0.0044 98
$3\,^1S \rightarrow 5\,^1P$	E-Hy-CI	This work	5460	−2.0612 7198 9740 3739 8201 46	4608	−2.0199 0598 9900 7210 1999	0.0504 7181 37 ± 0.0003 37
$3\,^1S \rightarrow 5\,^1P$	E-Hy-CI	This work	6188	−2.0612 7198 9740 8854 5669 77	5232	−2.0199 0598 9900 7494 3737	0.0504 7145 53 ± 0.0001 69
$3\,^1S \rightarrow 5\,^1P$	E-Hy-CI	This work	6552	−2.0612 7198 9740 8882 5163 76	5232	−2.0199 0598 9900 7494 3737	0.0504 7142 98 ± 0.0000 80
$3\,^1S \rightarrow 5\,^1P$	E-Hy-CI	This work	7280	−2.0612 7198 9740 8978 7744 23	5960	−2.0199 0598 9900 8445 4576	0.0504 7142 56 ± 0.0000 61
$3\,^1S \rightarrow 5\,^1P$	E-Hy-CI	This work	8372	−2.0612 7198 9740 8984 9048 81	5960	−2.0199 0598 9900 8445 4576	0.0504 7142 49 ± 0.0000 40
$3\,^1S \rightarrow 5\,^1P$	E-Hy-CI	Recommended					0.0504 7142 5(1)
$3\,^1S \rightarrow 5\,^1P$	Reference	Kono and Hattori [53]					0.0505
$3\,^1S \rightarrow 5\,^1P$	Reference	Cann and Thakkar [54]					0.0505
$3\,^1S \rightarrow 6\,^1P$	E-Hy-CI	This work	1456	−2.0490 5802 7440 5968 0929 88	960	−1.9853 5151 8164 7987 2969	0.2263 1183 58 ± 0.3125 96
$3\,^1S \rightarrow 6\,^1P$	E-Hy-CI	This work	2912	−2.0571 5082 5105 6874 5756 65	1800	−1.9980 9252 4185 4981 1386	0.0897 7848 60 ± 0.2569 26
$3\,^1S \rightarrow 6\,^1P$	E-Hy-CI	This work	4368	−2.0612 7190 7217 2476 2465 64	3256	−2.0132 6688 6192 4322 9000	0.0318 1529 56 ± 0.1998 33
$3\,^1S \rightarrow 6\,^1P$	E-Hy-CI	This work	5096	−2.0612 7198 9730 8848 8878 49	3880	−2.0133 0161 2903 3736 2347	0.0315 9009 54 ± 0.0829 18
$3\,^1S \rightarrow 6\,^1P$	E-Hy-CI	This work	5460	−2.0612 7198 9740 3739 8201 46	4608	−2.0138 3396 8157 9529 8369	0.0241 8313 89 ± 0.0244 98
$3\,^1S \rightarrow 6\,^1P$	E-Hy-CI	This work	6188	−2.0612 7198 9740 8854 5669 77	5232	−2.0138 3397 8731 9136 7973	0.0241 8344 01 ± 0.0072 38
$3\,^1S \rightarrow 6\,^1P$	E-Hy-CI	This work	6552	−2.0612 7198 9740 8882 5163 76	5232	−2.0138 3397 8731 9136 7973	0.0241 8354 68 ± 0.0003 18
$3\,^1S \rightarrow 6\,^1P$	E-Hy-CI	This work	7280	−2.0612 7198 9740 8978 7744 23	5960	−2.0138 3397 9671 6873 9539	0.0241 8350 24 ± 0.0001 31
$3\,^1S \rightarrow 6\,^1P$	E-Hy-CI	This work	8372	−2.0612 7198 9740 8984 9048 81	5960	−2.0138 3397 9671 6873 9539	0.0241 8350 44 ± 0.0001 11
$3\,^1S \rightarrow 6\,^1P$	E-Hy-CI	Recommended					0.0241 8350 5(2)
$3\,^1S \rightarrow 6\,^1P$	Reference	Kono and Hattori [53]					0.0241 9
$3\,^1S \rightarrow 6\,^1P$	Reference	Cann and Thakkar [54]					0.0241

Note: All energies in this work are variational except for the Recommended energy; all calculations were done in quadruple-double-with exponent (QDE) precision.

Table 8. Non-relativistic multiplet oscillator strengths (f-values) with rigorous upper and lower bounds for the $4\,^1S \rightarrow 2$–$6\,^1P$ transitions of He I. Oscillator strengths computed by other authors are included for comparison.

States	Technique	Author	N (^{1}S)	E (^{1}S) (Hartree)	N (^{1}P)	E (^{1}P) (Hartree)	f-Value
$4\,^1S \rightarrow 2\,^1P$	E-Hy-CI	This work	1456	−1.9976 6239 2700 2082 4570 52	960	−2.1238 4308 3927 0924 8309	0.0219 5065 69 ± 0.0439 95
$4\,^1S \rightarrow 2\,^1P$	E-Hy-CI	This work	2912	−2.0105 3191 2403 6325 8650 19	1800	−2.1238 4308 6441 2634 4197	0.0428 5496 50 ± 0.0329 00
$4\,^1S \rightarrow 2\,^1P$	E-Hy-CI	This work	4368	−2.0333 7111 4814 9961 0916 61	3256	−2.1238 4308 6498 0901 3192	0.0272 8170 14 ± 0.0351 12
$4\,^1S \rightarrow 2\,^1P$	E-Hy-CI	This work	5096	−2.0335 8541 4508 6363 5033 29	3880	−2.1238 4308 6498 0938 8692	0.0259 1811 44 ± 0.0035 12
$4\,^1S \rightarrow 2\,^1P$	E-Hy-CI	This work	5460	−2.0335 8663 6247 7125 3107 21	4608	−2.1238 4308 6498 0961 4281	0.0258 7131 85 ± 0.0003 33
$4\,^1S \rightarrow 2\,^1P$	E-Hy-CI	This work	6188	−2.0335 8671 0100 9427 2040 94	5232	−2.1238 4308 6498 0973 9383	0.0258 7036 92 ± 0.0004 60
$4\,^1S \rightarrow 2\,^1P$	E-Hy-CI	This work	6552	−2.0335 8671 5182 6200 6911 83	5232	−2.1238 4308 6498 0973 9383	0.0258 7029 15 ± 0.0002 66
$4\,^1S \rightarrow 2\,^1P$	E-Hy-CI	This work	7280	−2.0335 8671 6576 5463 7833 37	5960	−2.1238 4308 6498 0973 9383	0.0258 7027 23 ± 0.0002 10
$4\,^1S \rightarrow 2\,^1P$	E-Hy-CI	This work	8372	−2.0335 8671 6646 1515 5575 70	5960	−2.1238 4308 6498 0973 9383	0.0258 7026 97 ± 0.0001 37
$4\,^1S \rightarrow 2\,^1P$	E-Hy-CI	Recommended					0.0258 703(1)
$4\,^1S \rightarrow 2\,^1P$	Reference	Kono and Hattori [53]					0.0258 7
$4\,^1S \rightarrow 2\,^1P$	Reference	Cann and Thakkar [54]					0.0258 65

Table 8. *Cont.*

States	Technique	Author	N (^{1}S)	E (^{1}S) (Hartree)	N (^{1}P)	E (^{1}P) (Hartree)	f-Value
$4\,^1S \rightarrow 3\,^1P$	E-Hy-CI	This work	1456	−1.9976 6239 2700 2082 4570 52	960	−2.0550 3873 3547 3086 1461	0.2855 2050 59 ± 0.2686 64
$4\,^1S \rightarrow 3\,^1P$	E-Hy-CI	This work	2912	−2.0105 3191 2403 6325 8650 19	1800	−2.0551 2212 6152 8270 4161	1.1964 8207 43 ± 1.4483 20
$4\,^1S \rightarrow 3\,^1P$	E-Hy-CI	This work	4368	−2.0333 7111 4814 9961 0916 61	3256	−2.0551 4636 2091 7442 8817	0.3208 6887 67 ± 0.0537 73
$4\,^1S \rightarrow 3\,^1P$	E-Hy-CI	This work	5096	−2.0335 8541 4508 6363 5033 29	3880	−2.0551 4636 2091 9398 9874	0.3079 8068 94 ± 0.0061 21
$4\,^1S \rightarrow 3\,^1P$	E-Hy-CI	This work	5460	−2.0335 8663 6247 7125 3107 21	4608	−2.0551 4636 2091 9407 7473	0.3075 1809 63 ± 0.0002 72
$4\,^1S \rightarrow 3\,^1P$	E-Hy-CI	This work	6188	−2.0335 8671 0100 9427 2040 94	5232	−2.0551 4636 2091 9415 9896	0.3075 0842 53 ± 0.0001 68
$4\,^1S \rightarrow 3\,^1P$	E-Hy-CI	This work	6552	−2.0335 8671 5182 6200 6911 83	5232	−2.0551 4636 2091 9415 9896	0.3075 0761 73 ± 0.0001 52
$4\,^1S \rightarrow 3\,^1P$	E-Hy-CI	This work	7280	−2.0335 8671 6576 5463 7833 37	5960	−2.0551 4636 2091 9418 8216	0.3075 0740 61 ± 0.0001 48
$4\,^1S \rightarrow 3\,^1P$	E-Hy-CI	This work	8372	−2.0335 8671 6646 1515 5575 70	5960	−2.0551 4636 2091 9418 8216	0.3075 0739 59 ± 0.0001 25
$4\,^1S \rightarrow 3\,^1P$	E-Hy-CI	Recommended					0.3075 074(2)
$4\,^1S \rightarrow 3\,^1P$	Reference	Kono and Hattori [53]					0.3075
$4\,^1S \rightarrow 3\,^1P$	Reference	Cann and Thakkar [54]					0.3075 3
$4\,^1S \rightarrow 4\,^1P$	E-Hy-CI	This work	1456	−1.9976 6239 2700 2082 4570 52	960	−2.0246 5161 9219 8828 4956	0.2263 1087 75 ± 0.8580 02
$4\,^1S \rightarrow 4\,^1P$	E-Hy-CI	This work	2912	−2.0105 3191 2403 6325 8650 19	1800	−2.0279 6692 3067 9451 6718	0.4911 8753 52 ± 0.4030 94
$4\,^1S \rightarrow 4\,^1P$	E-Hy-CI	This work	4368	−2.0333 7111 4814 9961 0916 61	3256	−2.0310 6964 9114 6071 9421	0.7328 8149 25 ± 0.3461 87
$4\,^1S \rightarrow 4\,^1P$	E-Hy-CI	This work	5096	−2.0335 8541 4508 6363 5033 29	3880	−2.0310 6964 9345 5165 5835	0.8540 6756 77 ± 0.0683 72
$4\,^1S \rightarrow 4\,^1P$	E-Hy-CI	This work	5460	−2.0335 8663 6247 7125 3107 21	4608	−2.0310 6965 0450 2299 1761	0.8579 3246 09 ± 0.0101 51
$4\,^1S \rightarrow 4\,^1P$	E-Hy-CI	This work	6188	−2.0335 8671 0100 9427 2040 94	5232	−2.0310 6965 0450 2335 1293	0.8580 1178 95 ± 0.0016 48
$4\,^1S \rightarrow 4\,^1P$	E-Hy-CI	This work	6552	−2.0335 8671 5182 6200 6911 83	5232	−2.0310 6965 0450 2335 1293	0.8580 1913 40 ± 0.0003 18
$4\,^1S \rightarrow 4\,^1P$	E-Hy-CI	This work	7280	−2.0335 8671 6576 5463 7833 37	5960	−2.0310 6965 0450 2337 6579	0.8580 2095 89 ± 0.0001 56
$4\,^1S \rightarrow 4\,^1P$	E-Hy-CI	This work	8372	−2.0335 8671 6646 1515 5575 70	5960	−2.0310 6965 0450 2337 6579	0.8580 2104 60 ± 0.0001 16
$4\,^1S \rightarrow 4\,^1P$	E-Hy-CI	Recommended					0.8580 21(2)
$4\,^1S \rightarrow 4\,^1P$	Reference	Kono and Hattori [53]					0.858
$4\,^1S \rightarrow 4\,^1P$	Reference	Cann and Thakkar [54]					0.8581
$4\,^1S \rightarrow 5\,^1P$	E-Hy-CI	This work	1456	−1.9976 6239 2700 2082 4570 52	960	−1.9853 5119 3528 3878 1086	0.2237 7590 58 ± 0.2037 28
$4\,^1S \rightarrow 5\,^1P$	E-Hy-CI	This work	2912	−2.0105 3191 2403 6325 8650 19	1800	−1.9980 9066 8533 4492 7952	0.4910 0821 28 ± 0.6391 27
$4\,^1S \rightarrow 5\,^1P$	E-Hy-CI	This work	4368	−2.0333 7111 4814 9961 0916 61	3256	−2.0198 9818 6800 0550 0090	0.2233 7104 36 ± 0.3195 64
$4\,^1S \rightarrow 5\,^1P$	E-Hy-CI	This work	5096	−2.0335 8541 4508 6363 5033 2	3880	−2.0198 9905 0264 4541 9071	0.1240 7409 27 ± 0.0635 13
$4\,^1S \rightarrow 5\,^1P$	E-Hy-CI	This work	5460	−2.0335 8663 6247 7125 3107 21	4608	−2.0199 0598 9900 7210 1999	0.1452 1292 40 ± 0.0074 83
$4\,^1S \rightarrow 5\,^1P$	E-Hy-CI	This work	6188	−2.0335 8671 0100 9427 2040 94	5232	−2.0199 0598 9900 7494 3737	0.1460 9789 48 ± 0.0070 54
$4\,^1S \rightarrow 5\,^1P$	E-Hy-CI	This work	6552	−2.0335 8671 5182 6200 6911 83	5232	−2.0199 0598 9900 7494 3737	0.1462 4775 33 ± 0.0006 36
$4\,^1S \rightarrow 5\,^1P$	E-Hy-CI	This work	7280	−2.0335 8671 6576 5463 7833 37	5960	−2.0199 0598 9900 8445 4576	0.1462 8152 56 ± 0.0003 17
$4\,^1S \rightarrow 5\,^1P$	E-Hy-CI	This work	8372	−2.0335 8671 6646 1515 5575 70	5960	−2.0199 0598 9900 8445 4576	0.1462 8326 42 ± 0.0001 48
$4\,^1S \rightarrow 5\,^1P$	E-Hy-CI	Recommended					0.1462 82(1)
$4\,^1S \rightarrow 5\,^1P$	Reference	Kono and Hattori [53]					0.1463
$4\,^1S \rightarrow 5\,^1P$	Reference	Cann and Thakkar [54]					0.1462 8
$4\,^1S \rightarrow 6\,^1P$	E-Hy-CI	This work	1456	−1.9976 6239 2700 2082 4570 52	960	−1.9853 5151 8164 7987 2969	0.2237 7773 19 ± 0.3436 21
$4\,^1S \rightarrow 6\,^1P$	E-Hy-CI	This work	2912	−2.0105 3191 2403 6325 8650 19	1800	−1.9980 9252 4185 4981 1386	0.1232 6866 30 ± 0.0531 74
$4\,^1S \rightarrow 6\,^1P$	E-Hy-CI	This work	4368	−2.0333 7111 4814 9961 0916 61	3256	−2.0132 6688 6192 4322 9000	0.1060 0191 23 ± 0.0137 52
$4\,^1S \rightarrow 6\,^1P$	E-Hy-CI	This work	5096	−2.0335 8541 4508 6363 5033 2	3880	−2.0133 0161 2903 3736 2347	0.0975 8922 72 ± 0.0116 88
$4\,^1S \rightarrow 6\,^1P$	E-Hy-CI	This work	5460	−2.0335 8663 6247 7125 3107 21	4608	−2.0138 3396 8157 9529 8369	0.0551 3036 32 ± 0.0066 06
$4\,^1S \rightarrow 6\,^1P$	E-Hy-CI	This work	6188	−2.0335 8671 0100 9427 2040 94	5232	−2.0138 3397 8731 9136 7973	0.0534 1180 07 ± 0.0011 22
$4\,^1S \rightarrow 6\,^1P$	E-Hy-CI	This work	6552	−2.0335 8671 5182 6200 6911 83	5232	−2.0138 3397 8731 9136 7973	0.0528 9364 93 ± 0.0005 96
$4\,^1S \rightarrow 6\,^1P$	E-Hy-CI	This work	7280	−2.0335 8671 6576 5463 7833 37	5960	−2.0138 3397 9671 6873 9539	0.0527 7371 66 ± 0.0003 87
$4\,^1S \rightarrow 6\,^1P$	E-Hy-CI	This work	8372	−2.0335 8671 6646 1515 5575 70	5960	−2.0138 3397 9671 6873 9539	0.0527 6500 84 ± 0.0001 83
$4\,^1S \rightarrow 6\,^1P$	E-Hy-CI	Recommended					0.0527 65(3)
$4\,^1S \rightarrow 6\,^1P$	Reference	Kono and Hattori [53]					0.0528
$4\,^1S \rightarrow 6\,^1P$	Reference	Cann and Thakkar [54]					0.0528

Note: All energies in this work are variational except for the Recommended energy; all calculations were done in quadruple-double-with exponent (QDE) precision.

Table 9. Non-relativistic multiplet oscillator strengths (f-values) with rigorous upper and lower bounds for the 5 ^{1}S → 2–6 ^{1}P transitions of He I. Oscillator strengths computed by other authors are included for comparison.

States	Technique	Author	N (^{1}S)	E (^{1}S) (Hartree)	N (^{1}P)	E (^{1}P) (Hartree)	f-Value
5 ^{1}S → 2 ^{1}P	E-Hy-CI	This work	1456	−1.9968 8048 6541 5060 4620 06	960	−2.1238 4308 3927 0924 8309	0.0239 5066 69 ± 0.0078 79
5 ^{1}S → 2 ^{1}P	E-Hy-CI	This work	2912	−2.0088 3402 8156 5823 7954 03	1800	−2.1238 4308 6441 2634 4197	0.0228 9130 19 ± 0.0022 49
5 ^{1}S → 2 ^{1}P	E-Hy-CI	This work	4368	−2.0158 9180 6275 8008 6208 10	3256	−2.1238 4308 6498 0901 3192	0.0191 1693 54 ± 0.0041 80
5 ^{1}S → 2 ^{1}P	E-Hy-CI	This work	5096	−2.0207 9539 0029 9299 0151 49	3880	−2.1238 4308 6498 0938 8692	0.0121 1793 08 ± 0.0013 14
5 ^{1}S → 2 ^{1}P	E-Hy-CI	This work	5460	−2.0211 0657 5245 7647 6858 33	4608	−2.1238 4308 6498 0961 4281	0.0099 8882 16 ± 0.0011 94
5 ^{1}S → 2 ^{1}P	E-Hy-CI	This work	6188	−2.0211 5799 0369 3487 8634 18	5232	−2.1238 4308 6498 0970 2959	0.0097 6467 02 ± 0.0004 34
5 ^{1}S → 2 ^{1}P	E-Hy-CI	This work	6552	−2.0211 7183 9914 3573 8483 67	5232	−2.1238 4308 6498 0970 2959	0.0096 8431 32 ± 0.0003 57
5 ^{1}S → 2 ^{1}P	E-Hy-CI	This work	7280	−2.0211 7614 2072 1554 4086 17	5960	−2.1238 4308 6498 0973 9383	0.0096 5712 76 ± 0.0003 22
5 ^{1}S → 2 ^{1}P	E-Hy-CI	This work	8372	−2.0211 7648 1662 2560 6741 68	5960	−2.1238 4308 6498 0973 9383	0.0096 5455 72 ± 0.0001 39
5 ^{1}S → 2 ^{1}P	E-Hy-CI	Recommended					0.0096 55(2)
5 ^{1}S → 2 ^{1}P	Reference	Kono and Hattori [53]					0.0096 52
5 ^{1}S → 2 ^{1}P	Reference	Cann and Thakkar [54]					0.0096 6
5 ^{1}S → 3 ^{1}P	E-Hy-CI	This work	1456	−1.9968 8048 6541 5060 4620 06	960	−2.0550 3873 3547 3086 1461	0.0668 5981 26 ± 0.0236 37
5 ^{1}S → 3 ^{1}P	E-Hy-CI	This work	2912	−2.0088 3402 8156 5823 7954 03	1800	−2.0551 2212 6152 8270 4161	0.1195 7904 00 ± 0.0143 57
5 ^{1}S → 3 ^{1}P	E-Hy-CI	This work	4368	−2.0158 9180 6275 8008 6208 10	3256	−2.0551 4636 2091 7442 8817	0.0862 0625 76 ± 0.0084 77
5 ^{1}S → 3 ^{1}P	E-Hy-CI	This work	5096	−2.0207 9539 0029 9299 0151 49	3880	−2.0551 4636 2091 9398 9874	0.0673 6750 25 ± 0.0066 10
5 ^{1}S → 3 ^{1}P	E-Hy-CI	This work	5460	−2.0211 0657 5245 7647 6858 33	4608	−2.0551 4636 2091 9407 7473	0.0572 2653 11 ± 0.0034 98
5 ^{1}S → 3 ^{1}P	E-Hy-CI	This work	6188	−2.0211 5799 0369 3487 8634 18	5232	−2.0551 4636 2091 9415 9896	0.0560 8662 74 ± 0.0011 69
5 ^{1}S → 3 ^{1}P	E-Hy-CI	This work	6552	−2.0211 7183 9914 3573 8483 67	5232	−2.0551 4636 2091 9415 9896	0.0556 5930 41 ± 0.0005 82
5 ^{1}S → 3 ^{1}P	E-Hy-CI	This work	7280	−2.0211 7614 2072 1554 4086 17	5960	−2.0551 4636 2091 9418 8216	0.0555 1363 77 ± 0.0002 90
5 ^{1}S → 3 ^{1}P	E-Hy-CI	This work	8372	−2.0211 7648 1662 2560 6741 68	5960	−2.0551 4636 2091 9418 8216	0.0554 9972 12 ± 0.0001 46
5 ^{1}S → 3 ^{1}P	E-Hy-CI	Recommended					0.0555 00(15)
5 ^{1}S → 3 ^{1}P	Reference	Kono and Hattori [53]					0.0554 8
5 ^{1}S → 3 ^{1}P	Reference	Cann and Thakkar [54]					0.0555 0
5 ^{1}S → 4 ^{1}P	E-Hy-CI	This work	1456	−1.9968 8048 6541 5060 4620 06	960	−2.0246 5161 9219 8828 4956	0.2207 0848 77 ± 0.4106 20
5 ^{1}S → 4 ^{1}P	E-Hy-CI	This work	2912	−2.0088 3402 8156 5823 7954 03	1800	−2.0279 6692 3067 9451 6718	0.4912 6034 32 ± 0.5132 75
5 ^{1}S → 4 ^{1}P	E-Hy-CI	This work	4368	−2.0158 9180 6275 8008 6208 10	3256	−2.0310 6964 9114 6071 9421	0.9626 2459 46 ± 0.4259 09
5 ^{1}S → 4 ^{1}P	E-Hy-CI	This work	5096	−2.0207 9539 0029 9299 0151 49	3880	−2.0310 6964 9345 5165 5835	0.5699 1516 30 ± 0.0364 85
5 ^{1}S → 4 ^{1}P	E-Hy-CI	This work	5460	−2.0211 0657 5245 7647 6858 33	4608	−2.0310 6965 0450 2299 1761	0.4882 2927 40 ± 0.0312 55
5 ^{1}S → 4 ^{1}P	E-Hy-CI	This work	6188	−2.0211 5799 0369 3487 8634 18	5232	−2.0310 6965 0450 2335 1293	0.4800 4245 27 ± 0.0306 04
5 ^{1}S → 4 ^{1}P	E-Hy-CI	This work	6552	−2.0211 7183 9914 3573 8483 67	5232	−2.0310 6965 0450 2335 1293	0.4770 1644 78 ± 0.0016 82
5 ^{1}S → 4 ^{1}P	E-Hy-CI	This work	7280	−2.0211 7614 2072 1554 4086 17	5960	−2.0310 6965 0450 2335 6579	0.4759 6720 87 ± 0.0003 92
5 ^{1}S → 4 ^{1}P	E-Hy-CI	This work	8372	−2.0211 7648 1662 2560 6741 68	5960	−2.0310 6965 0450 2335 6579	0.4758 6677 83 ± 0.0002 27
5 ^{1}S → 4 ^{1}P	E-Hy-CI	Recommended					0.4758 67(2)
5 ^{1}S → 4 ^{1}P	Reference	Kono and Hattori [53]					0.476
5 ^{1}S → 4 ^{1}P	Reference	Cann and Thakkar [54]					0.4758 0
5 ^{1}S → 5 ^{1}P	E-Hy-CI	This work	1456	−1.9968 8048 6541 5060 4620 06	960	−1.9853 5119 3528 3878 1086	0.2262 9215 02 ± 0.4210 39
5 ^{1}S → 5 ^{1}P	E-Hy-CI	This work	2912	−2.0088 3402 8156 5823 7954 03	1800	−1.9980 9066 8533 4492 7952	0.4910 8101 24 ± 0.4739 69
5 ^{1}S → 5 ^{1}P	E-Hy-CI	This work	4368	−2.0158 9180 6275 8008 6208 10	3256	−2.0198 9818 6800 0550 0090	0.8889 7825 33 ± 0.6637 12
5 ^{1}S → 5 ^{1}P	E-Hy-CI	This work	5096	−2.0207 9539 0029 9299 0151 49	3880	−2.0198 9905 0264 4541 9071	0.3390 2507 68 ± 0.7338 25
5 ^{1}S → 5 ^{1}P	E-Hy-CI	This work	5460	−2.0211 0657 5245 7647 6858 33	4608	−2.0199 0598 9900 7210 1999	0.9828 7744 14 ± 0.4105 51
5 ^{1}S → 5 ^{1}P	E-Hy-CI	This work	6188	−2.0211 5799 0369 3487 8634 18	5232	−2.0199 0598 9900 7210 3737	1.0528 6040 23 ± 0.0439 79
5 ^{1}S → 5 ^{1}P	E-Hy-CI	This work	6552	−2.0211 7183 9914 3573 8483 67	5232	−2.0199 0598 9900 7210 3737	1.0750 4329 23 ± 0.0306 24
5 ^{1}S → 5 ^{1}P	E-Hy-CI	This work	7280	−2.0211 7614 2072 1554 4086 17	5960	−2.0199 0598 9900 8445 4576	1.0820 4156 69 ± 0.0302 57
5 ^{1}S → 5 ^{1}P	E-Hy-CI	This work	8372	−2.0211 7648 1662 2560 6741 68	5960	−2.0199 0598 9900 8445 4576	1.0827 0928 95 ± 0.0149 47
5 ^{1}S → 5 ^{1}P	E-Hy-CI	Recommended					1.0827 (15)
5 ^{1}S → 5 ^{1}P	Reference	Kono and Hattori [53]					1.083
5 ^{1}S → 5 ^{1}P	Reference	Cann and Thakkar [54]					1.0833

Table 9. *Cont.*

States	Technique	Author	N (^{1}S)	E (^{1}S) (Hartree)	N (^{1}P)	E (^{1}P) (Hartree)	f-Value
$5\,^1S \rightarrow 6\,^1P$	E-Hy-CI	This work	1456	−1.9968 8048 6541 5060 4620 06	960	−1.9853 5151 8164 7987 2969	0.2207 1190 06
$5\,^1S \rightarrow 6\,^1P$	E-Hy-CI	This work	2912	−2.0088 3402 8156 5823 7954 03	1800	−1.9980 9252 4185 4981 1386	0.0218 8915 37 ± 0.3350 23
$5\,^1S \rightarrow 6\,^1P$	E-Hy-CI	This work	4368	−2.0158 9180 6275 8008 6208 10	3256	−2.0132 6688 6192 4322 9000	0.3336 9857 76 ± 0.5064 06
$5\,^1S \rightarrow 6\,^1P$	E-Hy-CI	This work	5096	−2.0207 9539 0029 9299 0151 49	3880	−2.0133 0161 2903 3736 2347	0.1964 4991 49 ± 0.2526 97
$5\,^1S \rightarrow 6\,^1P$	E-Hy-CI	This work	5460	−2.0211 0657 5245 7647 6858 33	4608	−2.0138 3396 8157 9529 8369	0.0221 1297 41 ± 0.2843 48
$5\,^1S \rightarrow 6\,^1P$	E-Hy-CI	This work	6188	−2.0211 5799 0369 3487 8634 18	5232	−2.0138 3397 8731 9136 7973	0.0776 3701 86 ± 0.0938 35
$5\,^1S \rightarrow 6\,^1P$	E-Hy-CI	This work	6552	−2.0211 7183 9914 3573 8483 67	5232	−2.0138 3397 8731 9136 7973	0.1256 8994 77 ± 0.0528 25
$5\,^1S \rightarrow 6\,^1P$	E-Hy-CI	This work	7280	−2.0211 7614 2072 1554 4086 17	5960	−2.0138 3397 9671 6873 9639	0.1469 2739 16 ± 0.0234 41
$5\,^1S \rightarrow 6\,^1P$	E-Hy-CI	This work	8372	−2.0211 7648 1662 2560 6741 68	5960	−2.0138 3397 9671 6873 9639	0.1506 9782 45 ± 0.0184 74
$5\,^1S \rightarrow 6\,^1P$	E-Hy-CI	Recommended					0.1507(30)
$5\,^1S \rightarrow 6\,^1P$	Reference	Kono and Hattori [53]					0.1526
$5\,^1S \rightarrow 6\,^1P$	Reference	Cann and Thakkar [54]					0.1526 46

Note: All energies in this work are variational except for the Recommended energy; all calculations were done in quadruple-double-with exponent (QDE) precision.

Table 5 displays the results for the $1\,^1S \rightarrow 2$–$6\,^1P$ transitions, from which it can be seen that 10 decimal precision has been achieved for all but the $1\,^1S \rightarrow 6\,^1P$ transition, which has lost only a digit. Similar behavior is seen for the $2\,^1S \rightarrow 2$–$6\,^1P$ transitions, and continues for the first three $3\,^1S \rightarrow 2$–$6\,^1P$ transitions, with the $3\,^1S \rightarrow 5\,^1P$ transition showing similar behavior as the $3\,^1S \rightarrow 6\,^1P$ transition. For the $4\,^1S \rightarrow 2$–$6\,^1P$ transitions, the $4\,^1S$ wave function is of course not as accurate as the $1\,^1S$ wave function but the oscillator strengths are still accurate to 6–7 decimal digits. Finally, for the highest $5\,^1S \rightarrow 2$–$4\,^1P$ transitions, the precision is still 6 decimal digits; only the highest $5\,^1S \rightarrow 5$–$6\,^1P$ transitions are accurate to only 3–4 decimal digits. In summary, the precision is 7–10 decimal digits for the vast majority of these transitions.

7. Conclusions

Papers I [6] and II [7] of this series demonstrated that Hy-CI and E-Hy-CI are capable of greater than 20 digit precision for the ground state energy of helium, and Hy-CI has been utilized to produce high-precision results for not only ground states but excited states as well. In Paper II, non-S states are treated for the first time by carrying out calculations on the lowest helium ^{1}P state ($2\,^1P$) and then extending the He $2\,^1P$ state calculation to other members of the He $2\,^1P$ isoelectronic sequence. It has been shown that an $l = 7$ Hy-CI result can be improved on with just an $l = 3$ E-Hy-CI basis; this demonstrates that the E-Hy-CI speed up convergence over Hy-CI continues to non-S states as well. In Paper III [8], not only are high-precision $1s^2\,^1S$ and $1s2p\,^1P$ calculations performed for the He I, Li II, Be III, C V and O VII members of the He isoelectronic sequence, but the wave functions obtained are used to calculate oscillator strengths, including upper and lower bounds, for the lowest $^1S \rightarrow {}^1P$ transition. This work has been motivated not only by a desire to achieve high-precision variational upper bounds to energies, but also to use the high-precision wave functions to compute properties in addition to the energy. This is a logical extension of previous work by one of the authors in computing oscillator strengths [40,42] and electric polarizabilities [61].

Another motivation, as mentioned in the Introduction, has been to explore whether lower bounds to non-relativistic energies can be obtained with the same level of accuracy as upper bounds. Ronto et al. [18] find that to get reasonably good results, they need to build wave functions which are optimized not just for one state but for excited states as well. To facilitate this, E-Hy-CI wave functions are calculated for the five lowest ^{1}S states of He I all within one wave function and for the five lowest ^{1}P states of He I all within a

second wave function. These wave functions are suitable for calculating lower bounds to energies which have precisions on par with calculated upper bounds [29].

Here, the wave functions are used to calculate oscillator strengths, including upper and lower bounds, for the 25 lines arising from allowed transitions among these five ^{1}S and five ^{1}P states. The results of this study are oscillator strengths for the $n\ ^1\mathrm{S} \rightarrow m\ ^1\mathrm{P}$ transitions for which n = 1–5, m = 2–6, with rigorous upper and lower bounds which in the best case ($1\ ^1\mathrm{S} \rightarrow 2\ ^1\mathrm{P}$) are 0.00000001% and probable precision $\leq$ 0.0000000001.

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Notes

1 Some authors refer to this as fully correlated [5].
2 For our previous studies, papers I–III in this series, see [6–8].
3 In their paper, Wang et al. [9] refer to this as extended Hy-CI. The authors of this paper prefer Exponentially Correlated Hy-CI since there is more than one way Hy-CI could be extended and exponentially correlated makes clear that the extension is an exponential r_{ij} factor.
4 For a review of both Hy-CI and E-Hy-CI, see [16].
5 In the orthogonal Hy-CI of Zhang et al. [21] (see also Jiao et al. [22]) discussed later, ν_K can be 2 or 3.
6 It is worth noting that this research is focused solely on singlet states, as in the previous papers in this series, and has nothing at all to say about the behavior of triplet states, which would be expected to be different because the spatial wave function of singlet states in He is symmetric and the spatial wave function of triplet states is antisymmetric.
7 Table 2 displays the final ^{1}S wave function expansion along with the energies obtained from this single wave function for each n ^{1}S state (for various expansion lengths).
8 See also [34].
9 Actually, the configuration designation is rigorous only for Russell–Saunders (LS) coupling in a central field. We retain the terminology here to conform to standard spectroscopic notation with the understanding that, by $1s^2\ ^1S$ and $1s2p\ ^1P$, we mean the lowest terms of those respective symmetries (the He $1\ ^1S$ ground state and the $2\ ^1P$ lowest state of P symmetry, respectively).
10 The l here is because we are using the length formulation for the electric dipole transition.
11 $\langle\Psi_a|W_l^2|\Psi_a\rangle_+$ is computed by a formula of Rebane and Braun [43], see [38,39].
12 In this paper, we use f-value and oscillator strength interchangeably. High-precision f-values have applications ranging from astrophysical and stellar analysis to plasma diagnostics and fusion research to fundamental atomic physics.
13 Computed using truncations of our final non-relativistic ^{1}S and ^{1}P wave functions.
14 For an introduction to relativistic theory as implemented in GRASP, see [50].
15 For a detailed treatment of line strengths, see Morton et al. [52], where the corrections are shown to be less than 0.1% for helium.

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