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Hylleraas-Configuration Interaction (Hy-CI) Non-Relativistic Energies for the 3 ^1S, 4 ^1S, 5 ^1S, 6 ^1S, and 7 ^1S Excited States of the Beryllium Atom

James S. Sims

National Institute of Standards and Technology,
Gaithersburg, MD 20899, USA

jim.sims@nist.gov

In a previous work Sims and Hagstrom [*J Chem Phys* 140,224312(2014)] reported Hylleraas-configuration interaction (Hy-CI) method variational calculations for the ^1S ground states of the beryllium isoelectronic sequence with an estimated accuracy of 10 to 20 nanohartrees (nHa). In this work the calculations have been extended to the five higher states of the neutral beryllium atom, 3 ^1S, 4 ^1S, 5 ^1S, 6 ^1S, and 7 ^1S. The best non-relativistic energies obtained for these states are -14.4182 4034 6, -14.3700 8789 0, -14.3515 1167 6, -14.3424 0357 8, and -14.3372 6649 96 Ha, respectively. The 6 ^1S result is superior to the known reference energy for that state, while for the 7 ^1S state there is no other comparable calculation.

Key words: beryllium atom excited states; Hylleraas-CI; Hy-CI; non-relativistic energies.

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1. Introduction

Variational methods based on explicitly correlated wave functions are known to give the most accurate upper bounds to energy states, and hence the inclusion of terms containing the interelectronic distance r_{ij} in the wave function has become increasingly common, at least for few-electron atomic systems ($N \leq 4$) (so common, in fact, that a book dealing entirely with explicitly correlated wave functions has been produced [1]). These wave functions, which are commonly referred to now as Hylleraas (Hy), follow the landmark calculation of Hylleraas [2] by employing powers of the interelectronic distance in the wave function. The Hylleraas-configuration interaction (Hy-CI) technique (developed by us [3] and also independently by Woźnicki [4]) differs from the traditional Hy development by employing at most a single, linear r_{ij} factor with traditional configuration interaction orbital bases. While the work of Hylleraas demonstrated that two-electron atoms could be calculated accurately (for that time) with powers of r_{12}, it was Handy [5] who demonstrated that linear terms alone were sufficient for high accuracy for He. Hy-CI in its current incantation utilizes only linear terms in r_{ij}, and so r_{12}/f_{12} [1, 6, 7] methods are related to Hy-CI but outside the scope of this study (but see Ruiz [8] for a discussion of CI-r_{12} and a comparison with Hy-CI in the two-electron He atom case). Recently, Nakatsuji and Nakashima introduced Hy-CI into their

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free-complement chemical formula theory (FC-CFT) [9, 10], and while their study is not nearly as extensive as the current study, this is an interesting new development. In contrast to Hy and Hy-CI wave functions, the other common explicitly correlated wave function, the explicitly correlated Gaussian (ECG) [1] wave function, has the r_{ij} correlation appear as Gaussian exponentials.

As a consequence of its formalism with an at most single r_{ij} factor per term, Hy-CI is unique (among the Hy methods) in that the mathematical problems for $N > 4$ can be reduced to problems with four electrons. Therefore, beryllium, with its four electrons and strong mixing of $1s^2\ 2s^2$ and $1s^2\ 2p^2$ configurations, is ideal for a test of the Hy-CI formalism. In paper I of this series, Hy-CI calculations were carried out on the ^1S ground states of the Be isoelectronic series from $Z = 4$ through 113 [11]. Li^- (with $Z = 3$) has a decidedly different electronic structure from the other members of the sequence, and so it was not until the second paper in this series that a large, comparable calculation for the Li^- ground state was completed, and the results of that calculation were discussed [12]. What distinguishes Li^- from other members of the sequence is its negative charge, which makes for a much more diffuse electronic charge distribution than ^1S ground states of the other members of the Be isoelectronic series. Specifically, the ground ^1S state of Li^- is the same type of problem as the first excited state of Be; it is like Be($2s3s$)[1], not Be($2s2s$). This work continues the work begun with Li^- in examining how well Hy-CI can treat states successively more diffuse than the ground state by examining successively higher states of beryllium of ^1S symmetry.

A comprehensive review of the earlier non-relativistic, infinite nuclear mass calculations on the Li anion can be found in the work of King [13]. More recently, three ECG calculations have been reported [14–16], the last of which is the most extensive calculation and the best to date. The recent calculations of Hussein [17] are notable for their exploration of large-scale CI for ground and core excited states of the anion. A standard Hy calculation of more limited scope is of note for its relatively compact basis sets and its study of how well the basis sets employed can describe the more diffuse region of configuration space for this species [18]. For Be, Adamowicz and co-workers [19] reported ECG results for the five lowest ^1S states of the Be atom, i.e., for ground and $2s \rightarrow ns$ (n = 3-6) Rydberg excited states[2]. In two recent papers ([20, 21]), Adamowicz and co-workers extended these calculations to include the lowest ten ^1P Rydberg states and re-examined the ground and $2s \rightarrow ns$ (n = 3-5) Rydberg excited states. In this work, we treat the same $2s \rightarrow ns$ (n = 3-6) Rydberg excited states and then use that methodology to extend the calculations to include the $7s$ Rydberg excited state of Be.

2. Variational Calculations

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 Schrodinger equation

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

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

$$H_{NR} = \sum_{i=1}^{N_e} \mathscr{H}_i + \sum_{i<j}^{N_e} r_{ij}^{-1}. \tag{2}$$

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

[1]The successive Be ^1S excited states 3 ^1S, 4 ^1S, *etc*., are referred to herein also as Be($2s3s$), Be($2s4s$), *etc*.
[2]Nakatsuji and Nakashima ([10]) also studied ground and $2s \rightarrow ns$ (n = 3-6) Rydberg excited states of Be.

The Hy-CI wave function for four-electron atomic states is

$$\Psi = \sum_{K=1}^{N} C_K \Phi_K, \tag{3}$$

where

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

denotes the Kth antisymmetrized spin and angular momentum projected configuration state function (CSF). O_{L,M_L} and O_{S,M_S} are idempotent orbital and spin angular momentum projection operators of the Löwdin type [22] for a state of total quantum numbers L, M_L, S, and M_S (Russell–Saunders LS coupling is assumed). In practice, it is sufficient to take ν_K equal to 0 or 1, with $\nu_K = 0$ being the CI case. Θ_K is a primitive spin product function for term K, and $\phi_{K_s}(\mathbf{r_s})$ represents the sth basis orbital in the Kth term.

The basis orbitals are un-normalized Slater-type orbitals (STOs), $\phi(\mathbf{r})$, which are defined as

$$\phi_i(\mathbf{r}) = r^{n_i - 1} \mathrm{e}^{-\alpha_i \mathrm{r}} \mathrm{Y}_{\mathrm{l_i}}^{\mathrm{m_i}}(\theta, \phi), \tag{5}$$

where $Y_l^m(\theta, \phi)$ is a normalized spherical harmonic in the Condon and Shortley phase convention [23]. O_{as} is the idempotent antisymmetry projection operator. For four-electron singlet states, there exist two linearly independent primitive spin functions, $\Theta_1 = \alpha\beta\alpha\beta$ and $\Theta_2 = \alpha\alpha\beta\beta$. Cencek and Rychlewski [24] have given the general proof that only one primitive spin function is needed to ensure convergence of eigenvalues to the exact root of the Hamiltonian. Here, the Θ_1 spin function is used.

The coefficients C_K in Eq.(3) are found in this work by solving the generalized eigenvalue problem

$$\mathbf{HC} = E\mathbf{SC}, \tag{6}$$

$$(\mathbf{H} - E_0\mathbf{S})\mathbf{C} = (E - E_0)\mathbf{SC}, \tag{7}$$

$$\mathbf{C} = (E - E_0)(\mathbf{H} - E_0\mathbf{S})^{-1}\mathbf{SC}, \tag{8}$$

where the matrix elements are given by $\mathscr{H}_{KL} = <\Phi_K|\mathscr{H}|\Phi_L>$ and $\mathscr{S}_{KL} = <\Phi_K|\Phi_L>$, the Hamiltonian H is given by Eq.(2), and E_0 is some starting approximation for the eigenvalue E of interest.

(Shifted) inverse iteration [25] is the application of the power method [26] to $\mathbf{A}^{-1} = (\mathbf{H} - E_0\mathbf{S})^{-1}$ in the solution process used for solving for $\mathbf{C}$ in Eq.(8) and leads to the iteration formula

$$\mathbf{v}_{k+1} = \mathbf{A}^{-1}\mathbf{S}\mathbf{v}_k, \; k = 0, 1, 2, \ldots \tag{9}$$

with a convergence criterion for E, computed from

$$E_k = E_0 + \frac{\mathbf{v}_{k+1} \cdot \mathbf{S}\mathbf{v}_k}{\mathbf{v}_{k+1} \cdot \mathbf{S}\mathbf{v}_{k+1}}, \; k = 0, 1, 2, \ldots \tag{10}$$

which converges rapidly to E provided that the trial E_0 is sufficiently close to the desired eigenvalue, which turned out to be five digit accuracy in these calculations. In addition to a suitable E_0, shifted inverse iteration requires a starting vector $\mathbf{v}_0$ (which was usually taken to be a vector of all 1s) and an efficient factorization for $\mathbf{A}^{-1}$ in Eq.(9), which, for this calculation, is

$$\mathbf{A}^{-1} = \mathbf{L}^T\mathbf{D}^{-1}\mathbf{L}, \tag{11}$$

where $\mathbf{D}$ is a diagonal matrix, and $\mathbf{L}$ is the implicit representation of the lower triangular matrix $\mathbf{L}$ in terms of Gaussian transformations [27]. Quadruple precision was used in this work, and the Message Passing Interface (MPI) Standard [28] was used to parallelize the code.

3. Methodology

Excited states have a more diffuse electronic charge distribution than the ground state. Atomic anions also have a more diffuse electronic charge distribution than the neutral atom of the same charge. Hence, the first excited ^1S state of Be, Be($2s3s$), is the same type of problem as the Li^- S ground ^1S state previously treated [12] and can be treated using the same basic expansion philosophy as was used previously for Be($2s2s$) [11] as modified for Li^- [12]. This expansion philosophy is one in which the bulk of the computing involves development of a base expansion (which we refer to as the CORE), the purpose of which is to define the STO basis and the CSF basis for the most important term types, and most importantly to calculate STO orbital exponents with a reasonable amount of effort. Our first attempt at a core for Be($2s3s$) is listed in Table 1 and consists of 25 blocks (9803 terms) and gives a reasonably good energy (approximately 28 μHa accuracy) for this expansion size. Table 1 and other tables of Hy-CI expansions list energy results (column 5) for various expansion lengths, N_{tot}, shown in column 4. Column 2 lists the basis orbitals that are used to generate the CSFs (terms) for each block type in the order electron 1 (α spin), electron 2 (β spin), electron 3 (α spin), electron 4 (β spin). For example, in the first line 1:9s_K for the first electron means the basis orbitals are $1s_K$ through $9s_K$ orbitals (where K indicates an orbital exponent appropriate for a K shell electron). Products of four orbital types are built up by taking one pair of orbital types from the K-shell set and the other pair from the L-shell set. All the orbital promotions are within the shell, not between shells. This leaves out a substantial number of CSFs that turn out to be of no importance in this work. The number of CSFs in a block can be computed from the listed basis orbitals and the value of r-sum, which is the sum of the powers of r for each Hartree orbital product of four basis orbitals [11, 29]. Column 3 gives the number of CSFs added for the block or blocks shown in column 2. In Table 1 and elsewhere, ΔE is the energy improvement for the blocks shown in column 1 and is shown in column 6. In Table 1 and elsewhere, for $pppp$, there are degenerate S states listed. One of these states is (10, 10, 10, 10), where only the l and m orbital numbers are listed. For configurations with degeneracies, $m = 0$, unless otherwise noted. In this case, both the (10, 10, 10, 10) and the (11, 11, 1-1, 1-1) configurations contribute substantially and hence are included in the CORE. The term types are what one would expect from adding correlation to a typical closed K shell Be CI expansion using an s, p STO basis.

Table 1. 9,803 term $s,p\ r_{ij}$ Hy-CI expansion (the CORE) for the Be 3 ^1S state (in Ha). In the table, R_1 = {1,r_{12},r_{34}}, R_2 = {r_{13},r_{14}}, R = {1,r_{12},r_{34},r_{13},r_{14}}, N is the number of terms added and N_{tot} is the cumulative number of terms. All terms are r-sum filtered using N_{max} = 16 (see text). Orbital exponents and energies are for the final wave functions.

Block(s)	Terms Added[ab]	N	N_{tot}	$E(N_{tot})$ (Ha)	$-\Delta E$ (μHa)
1-3	1:9s_K 1:9s_K 1:9s_L 1:9s_L R_1	3255	3255	-14.4161 5696 0961	
4-5	1:6s_K 1:6s_K 1:6s_L 1:6s_L R_2	850	4105	-14.4163 5910 4230	202.1432 69
6	2:7p_{Kp} 2:7p_{Kp} 1:9s_L 1:9s_L	588	4693	-14.4171 5989 3091	800.7888 60
7	2:7p_{Kp} 2:7p_{Kp} 1:6s_L 1:6s_L r_{12}	391	5084	-14.4171 8833 1956	28.4388 65
8	2:7p_{Kp} 2:7p_{Kp} 1:9s_L 1:9s_L r_{34}	588	5672	-14.4177 3945 9519	551.1275 63
9-10	2:7p_{Kp} 2:7p_{Kp} 1:6s_L 1:6s_L R_2	782	6454	-14.4178 1074 0571	71.2810 52
11	1:9s_K 1:9s_K 2:7p_{L_p} 2:7p_{L_p}	588	7042	-14.4180 6071 2053	249.9714 82
12	1:9s_K 1:9s_K 2:7p_{L_p} 2:7p_{L_p} r_{12}	588	7630	-14.4181 5705 6807	96.3447 54
13	1:6s_K 1:6s_K 2:7p_{L_p} 2:7p_{L_p} r_{34}	391	8021	-14.4181 6034 4723	3.2879 17
14-15	1:6s_K 1:6s_K 2:7p_{L_p} 2:7p_{L_p} R_2	782	8803	-14.4182 0230 9844	42.7634 88
16-20	2:5p_{Kp} 2:5p_{Kp} 2:5p_{L_p} 2:5p_{L_p} R	500	9303	-14.4182 0771 9054	4.6108 43
21-25	2:5p_{1Kp} 2:5p_{1Kp} 2:5p_{-1L_p} 2:5p_{-1L_p} R	500	9803	-14.4182 1289 1914	5.1728 60

[a] K-shell orbital exponents are $K = 3.5, K_p = 4.1$; [b] L-shell orbital exponents are $L = 0.78237, L_p = 1.0375$.

In Table 1 and elsewhere only the orbital type for each electron is shown, and terms of each orbital type are combined with 1-5 of the five different r_{ij} types as noted. The terms in the CORE are what one would expect from adding explicit correlation to a typical Be expansion (cf. the Be($2s2s$) expansion in [11]) using an $s,p\ r_{ij}$ basis. Starting from a 10 block $s_Ks_Ks_Ls_L\times$ R (R = {1,r_{12},r_{34},r_{13},r_{14}}) + $s_{K_p}s_{K_p}s_Ls_L\times$ R pre-CORE, $L = L_s$ and $K = K_s$ are optimized to self-consistency, and then $p_{Kp}p_{Kp}s_Ls_L\times$ R blocks are added, and K_p is optimized. This unsplit L-shell representation, with its approximately 28 μHa accuracy, turned out to be inferior to a more natural representation for a pair of non-identical electrons in the L-shell. Starting from the unsplit L-shell (*e.g.*, 1:ms 1:ms), as in Li^-, L was split symmetrically into inner and outer electrons L_1 and L_2 (*e.g.* 1:ms_{L_1} 1:ms_{L_2}, where L_1 and L_2 are different L-shell orbital exponents), more representative of an excited Be($2s3s$) state, and then L_1 and L_2 were varied. The split Ls can be thought of as a symmetrical split of L into a higher inner L orbital exponent (less diffuse) and a lower L outer orbital exponent (more diffuse). In Table 2, this split shell 25 block (15,957 terms) CORE can be thought of as a base "state" of five decimal place accuracy using a correlated s,p STO basis, which is then augmented with enough correlated s,p,d,f basis blocks to achieve six decimal place accuracy. For Be($2s2s$) [11], Li^- [12], and Be($2s3s$), six decimal place accuracy is achieved with approximately 20,000 Hy-CI CSFs. For the more diffuse Li^- and the Be($2sns$) states, the split shell representation ultimately gives a better energy with fewer terms in the expansion. There was considerable experimentation to determine both the size of the inner and outer pair s and p orbital exponents as well as their optimization. Note that the L_1 and L_2 exponents are for a $2s3s$ excited state, with the $3s$ orbital tending to a hydrogenic L_s orbital with an exponent of -2.0/3 ≈ -0.67, where 2.0 is a guess for the effective nuclear charge (Z_{eff}) that the $3s$ electron sees. Similar considerations are valid for the L_3 and L_4 pair for the L_p orbitals.

Tables 2 and A1 (Appendix) give an overall picture of the Be(2s3s) ^1S energy convergence with an 82,807 term expansion using an $s,p,d,f\,r_{ij}$ STO[3] basis for the CSFs. The expansion beyond the CORE was obtained by expanding the basis to $s,p,d,f\,r_{ij}$ in a series of steps. The $spps$, $spsp$, and $ddss\times$ R additions to the CORE were tested, keeping blocks that contributed ≥ 1 μHa, resulting in a 40 block, 21,187 CSF expansion utilized for the second orbital optimization. This expansion was used to systematically try adding

[3] The STOs (Slater-type orbitals) we use were defined fully in Ref. [30]. An s STO has $l = 0$, a p STO has $l = 1$, a d STO has $l = 2$, *etc.*

ssdd, *sdds*, and *sdsd* and then different *sppd* + permutation blocks, keeping all blocks that contributed $\geq$ 0.5 μHa to form a 76 block, 33,596 CSF "expanded CORE" utilized for the final orbital optimization. This "expanded CORE" was then expanded further by adding $ffss$ [4], $ssff$, $sffs$, and selecting $sffs$, $sfsf$, $ppdd$, $p_1p_1d_{-1}d_{-1}$, $ddpp$, $d_1d_1p_{-1}p_{-1}$, $sppd$, and $s_{L1}s_{L2}$ blocks to form a 113 block, 42,139 term expansion of 0.25 μHa accuracy which formed the basis for final adjustments. A cutoff of 0.1 μHa was used in forming this expansion as well as previous experience, including the use of the Legendre expansion of possible Hy-CI term types to try [29].

The first set of adjustments[5] included r-sum and other adjustments to the CORE (r-sum, the sum of the powers of r for the four orbitals in a term, has to be $\leq$ 16 by default), starting with the first five blocks. The idea here is to look at the biggest energy contributors for the biggest adjustments to the 42,139 term energy, and this is done by allowing for higher powers of r to be included in the orbital products. Blocks 114-137 contain these adjustments where the added CSFs are obtained by taking the difference between the block listed and the block for which the block number is the number following the trailing "$-$#"[6]. Doing this for all blocks in the CORE improves the result by 0.197 μHa and results in a 137 block, 62,566 term expansion accurate to 0.1 μHa (seven decimal places).

The post-CORE analysis is presented next. Up to this point, the cutoff for including blocks in the expansion has been 0.025 μHa. After lowering the cutoff to 0.4 nanohartrees (nHa), next add *pssp*+*psps* to this 137 block, 62,566 term expansion, and then add *dssd*+*dsds* and $dpdp$ to form a 157 block, 70,084 term expansion. Then, test $dppd$, $pdpd$, and $pddp$. In each case (except no r_{12} block for $pdpd$) KKLL(1+r_{12}) + $K_1K_1L_{-1}L_{-1}$ (CI block) passes the - 0.4 nHa test to give a 163 block, 71,590 term expansion with seven decimal place accuracy. The next step is to add in the remaining *sppd* and permutation contributing blocks, where keeping only blocks that contribute $>$ 0.4 nHa leads to a 181 block, 77,092 term expansion. Then, $dddd, ddsd, ddds, ppff, ffpp$, $fssf$, and $fsfs$ blocks that contribute more than the final 0.25 nHa cutoff are added. Finally, all $spdf$ and permutation blocks and $s_{K_1}s_{K_1}s_{L_1}s_{L_2}$ blocks contributing more than that cutoff are considered, and only blocks that contribute $>$ 0.25 nHa are kept, which leads to our final 82,807 block, 203 block expansion with eight decimal place accuracy, given in Table 2 (overall_picture) and Table A1 of the Appendix (full_expansion).

In arriving at the final wave function, all possible blocks of s, p, d type were tried, keeping all blocks that contributed $>$ 0.25 nHa. For s, p, d, f types, most blocks were tried, and the ones not tried were deemed unimportant at this level.

Final orbital optimization was done at the N = 35,678 level (33,596 term expansion in Table A1 [Appendix] plus $ffss + ssff$ blocks). Due to program limitations, it was not possible to give every orbital type its own orbital exponent.

For estimating the convergence error, a record was kept of all blocks dropped and their energy contributions. For s, p, d orbitals, for which all blocks were tested, the sum of all the dropped blocks was 6.502 nHa. These contributions will be less sensitive when added to the final expansion than they were earlier on. Similar considerations apply for s, p, d, f, where there are many more blocks, and the sum of all dropped blocks adds up to 15 nHa, for a total of 22 nHa. To estimate how much less these contributions would be if added at the end of the expansion, we tested a few of them, and the contributions fell off by a factor of 2 to 3. This gives an overall estimate of convergence in our final expansion to 7-12 Ha accuracy. There is also an error arising from an inadequate STO basis. To obtain an estimate of this error, we did the following: One extra STO of each STO type was added, with separate calculations for each type and r-sum rule. Using only the most important CSF blocks (certainly only those in the CORE) added an additional

[4] Unless otherwise noted, the blocks are correlated.
[5] For details, see Table A1 of the Appendix.
[6] A process we refer to in Sec. IV as "via the difference tool".

error estimate of about 5 nHa, for an overall estimate of eight decimal place accuracy for the 3 ^1S (Be[2s3s]) state. Upon examining the energy convergence in Table A1 (Appendix) and comparing it with the ground state [11], one can see that the ground state converges faster than the first excited state. This can be expected, since the excited-state wave function is more difficult to describe than the ground-state wave function due to a radial hole [31].

Table 2. Overall picture of the Be 3 ^1S state (in Ha). In the table, N is the cumulative number of terms.

Term Types Added (cutoff = 0.25 nHa)	N	E(N) (Ha)	$-\Delta E$ (μHa)
$<$ 25 block CORE $>$			
$(ssss + ppss + sspp + p_0p_0p_0p_0 + p_1p_1p_{-1}p_{-1})$	15957	-14.4182 3198 5819	
+ $spps$ + $spsp$	19957	-14.4182 3648 4804	4.4989 85
+ $ddss + ssdd + sdds + sdsd$	27017	-14.4182 3931 6211	2.8314 07
+ $sppd + sdpp + pspd + dpsp + ppsd(1)$	33596	-14.4182 3984 5155	0.5289 44
+ $ffss + ssff + sffs(4) + sfsf(2)$	37868	-14.4182 3997 6977	0.1318 22
+ $ppdd + ddpp$	41618	-14.4182 4005 0580	0.0736 03
+ $s_{K_1}s_{K_1}ss(1)$	42139	-14.4182 4009 5138	0.0445 88
Adjustments			
+ all <CORE Rsum adjustments>	62566	-14.4182 4029 1767	0.1966 29
+ $pssp + psps$	66566	-14.4182 4030 5289	0.0135 22
+ $dssd(4) + dsds(3) + dpdp(3)$	70084	-14.4182 4031 0510	0.0052 21
+ $dppd(2) + pddp(2) + pdpd(1) + d_{-1}p_1p_{-1}d_1(1)$	71590	-14.4182 4031 4001	0.0034 91
+ $ppsd(2) + pdsp(3) + psdp(2) + dpps(4)$			
+ $dspp(3) + pdps(4) + spdp(0) + ppds(0)$	77092	-14.4182 4033 0658	0.0166 57
+ $dddd(1) + d_1d_1d_{-1}d_{-1}(2)$	77500	-14.4182 4033 5074	0.0044 16
+ $ddsd(3) + ddds(2)$	78445	-14.4182 4033 7852	0.0027 78
+ $ppff(1) + p_1p_1f_{-1}f_{-1}(1) + ffpp(1)$	79020	-14.4182 4034 0712	0.0028 60
+ $fssf(0) + fsfs(0) + spdf(0) + psdf(0)$			
+ $pdsf(0) + spfd(0) + dspf(0) + dpsf(0)$			
+ $pdfs(0) + sdfp(0) + sfpd(1) + sfdp(1) + dsfp(1)$	79935	-14.4182 4034 1673	0.0009 61
+ $fspd(0) + fsdp(0) + pfsd(0) + fpsd(0)$ + $fpds(0) + pfds(0) + fpds(3)$	80850	-14.4182 4034 3387	0.0017 14
+ $fdsp(0) + dfsp(0) + fdps(0) + psfd(0)$			
+ $fspd(0) + sdpf(0) + dpfs(0) + dfps(3)$	81765	-14.4182 4034 4522	0.0011 35
+ $sdff(0) + ffsd(0) + dsff(0) + ddff(0)$			
+ $pppf(0) + pffp(0) + pfpf(0) + pddf(0)$			
+ $pfpf(0) + fffp(0) + s_{K1}s_{K1}ss(2)$	82807	-14.4182 4034 6380	0.0018 58

3.1 Be 4 ^1S

The Be 3 ^1S wave function formed the basis for the Be 4 ^1S expansion, except 7s and 7p outer L orbitals were added to reflect the more diffuse nature of 4 ^1S versus 3 ^1S. Consequently, the 40 term orbital optimization is for a 23,424 term expansion, and the final optimization is for an 86 block, 37,915 CSF wave function. Table A2 (Appendix) gives the overall picture of the 4 ^1S energy convergence with a 99,874 term expansion using an s,p,d,fr_{ij} STO basis for the CSFs. The optimized exponents for 3 ^1S and 4 ^1S[7] are in line with invariant K and inner L shell s and p orbitals, except for an anomalous L_1 case for which we have no explanation other than the energy for 3 ^1S with respect to L_1 turned out to be very flat. At this point, the 203 term expansion analogous to the 3 ^1S expansion is about 0.037 μHa worse that the ECG result [19], and hence a seven digit result.

Note the increased importance of the $s_{K1}s_{K1}$ terms compared to 3 ^1S. These terms were added to introduce additional K-shell correlation and hence serve to gauge how well the K shell is represented[8]. The increased importance of these terms suggested that further testing of these term types was in order (as CSFs 204-207 show) as well as re-examination of the CORE and final adjustments, which resulted in additional blocks being added to the 4 ^1S expansion and our final 220 CSF, 99,874 term expansion. In addition to changes to the $Be^+(1s1s2s)$ core, the nature of the correlation changes as the outermost electron increases in energy (*e.g.* $3s \Rightarrow 4s$, $4s \Rightarrow 5s$, *etc.*). The implications with respect to the r_{ij} factors are

- r_{12} correlates with the K shell and will always be important;
- r_{34} correlates with open shell electrons;
- r_{13} correlates with K shell and inner L shell electrons (in the $Be^+[1s1s2s]$ core); and
- r_{14} correlates with the outermost L shell electron and will be less and less important as the outermost electron gets further and further away from the nucleus.

Note how this is reflected in the additional CSFs 204-220, where there are no r_{34} or r_{14} terms that contributed enough to be included in the expansion. Term types ($psps$+$dpps$) (1+r_{12}+r_{13}) are much more important here than in Be 3 ^1S and also are indicative of how the nature of the correlation changes as the outermost electron becomes more diffuse.

4. Results and Discussion

Table 3 shows that the current best Be 3 ^1S 82,807 expansion result is 18 nHa below the ECG results of Stanke *et al.* [19] and of Pachucki [32], and within 18 nHa of the most recent, best calculation [21]. Similarly, the current best Be 4 ^1S 99,874 expansion result is 14 nHa below the ECG result of Stanke *et al.* [19], and within 40 nHa of the most recent, best 4 ^1S calculation [21]. This table includes the results for the 5 ^1S and 6 ^1S states, which will turn out to be within 46 nHa of the most recent, best 5 ^1S result and 26 nHa better than the best previous calculation for the 6 ^1S state. The Hy-CI restriction of one r_{ij} per CSF has been previously discussed [3, 11, 12, 29], and it has been pointed out [11, 12] that the unlinked $r_{ij}r_{kl}$ (no indices in common) term types first occur in the four-electron case, with $r_{12}r_{34}$ expected to be the most important. In the most recent Be [11] and Li^- [12] work, it was pointed out that one can reason that the $r_{12}r_{34}$ double cusp leads to two convergence problems, $(ss)_K\ r_{12} \times$ [L-shell cluster] and [K-shell cluster] $\times\ (ss)_L\ r_{34}$, when the

[7] The optimized orbital exponents are tabulated further in Table 5.
[8] The CI term was moved to the end of the expansion with the other $s_{K1}s_{K1}$ terms to facilitate this.

double cusp is represented by a superposition of normal Hy-CI term types. The [K-shell cluster] and the [L-shell cluster] are both basically a linear combination of pair functions $ss + pp + dd + ff + gg + ...$

Table 3. Comparison of theoretical Be ^1S state non-relativistic energies (in Ha).

State	Technique	Author	N	$E(NR)$ (Ha)
Be 2 ^1S	ECG	Stanke *et al.* (2009) [19]		-14.6673 5648 6(6)
Be 2 ^1S	Hy-CI	Sims and Hagstrom (2014) [11]	83598	-14.6673 5649 269
Be 2 ^1S	ECG	Puchalski *et al.* (2013) [33]		-14.6673 5649 49
Be 2 ^1S	ECG	Hornyák *et al.* (2019) [21]		-14.6673 5650 7
Be 3 ^1S	ECG	Stanke *et al.* (2009) [19]		-14.4182 4032 8
Be 3 ^1S	ECG	Pachucki (2016) [32]		-14.4182 4032 845
Be 3 ^1S	Hy-CI	This work	82807	-14.4182 4034 6
Be 3 ^1S	ECG	Hornyák *et al.* (2019) [21]		-14.4182 4036 4
Be 4 ^1S	ECG	Stanke *et al.* (2009) [19]		-14.3700 8787 6
Be 4 ^1S	Hy-CI	This work	99874	-14.3700 8789 0
Be 4 ^1S	ECG	Hornyák *et al.* (2019) [21]		-14.3700 8793 0
Be 5 ^1S	ECG	Stanke *et al.* (2009) [19]		-14.3515 1165 4
Be 5 ^1S	Hy-CI	This work	99965	-14.3515 1167 6
Be 5 ^1S	ECG	Hornyák *et al.* (2019) [21]		-14.3515 1172 2
Be 6 ^1S	ECG	Stanke *et al.* (2009) [19]		-14.3424 0355 2
Be 6 ^1S	Hy-CI	This work	92930	-14.3424 0357 8
Be 7 ^1S	Hy-CI	This work	92904	-14.3372 6649 9

How well the convergence of the $r_{12}r_{34}$ term type ("double cusp problem") is treated in Hy-CI for four-electron atoms and anions was analyzed in Table 3 of the 2011 work of Sims and Hagstrom [29] for Be and in Table 3 of the 2017 work by Sims [12] for Li^-. The results suggested that (for the four-electron problem), compared to the slow, cusp-connected convergences in typical CI calculations, the convergence is fast and that this correlation type can be accurately, albeit slowly, represented within the Hy-CI model. Table 4 compiles the results from the expansions in Tables A1 and A2 of the Appendix, which explore this point for the first two excited states of Be of ^1S symmetry.

Table 4. Convergence of the $r_{12}\ r_{34}$ double cusp with a superposition of normal Hy-CI term types.

Block	Energy(E) (nHa)		Block	Energy(E) (nHa)	
	Be($2s3s$)	Be($2s4s$)		Be($2s3s$)	Be($2s4s$)
$(ss)_K\ r_{12}\ (ss)_L$	33,729,728	10,609,047	$(ss)_K\ (ss)_L\ r_{34}$	4,795,485	1,861,678
$(ss)_K\ r_{12}\ (pp)_L$	104,223	41,918	$(pp)_K\ (ss)_L\ r_{34}$	529,860	169,664
$(ss)_K\ r_{12}\ (dd)_L$	485	306	$(dd)_K\ (ss)_L\ r_{34}$	626	292
$(ss)_K\ r_{12}\ (ff)_L$	44	25	$(ff)_K\ (ss)_L\ r_{34}$	0	6
$(pp)_K\ r_{12}\ (ss)_L$	48,899	26,478	$(ss)_K\ (pp)_L\ r_{34}$	3128	2769
$(pp)_K\ r_{12}\ (pp)_L$	2344	895	$(pp)_K\ (pp)_L\ r_{34}$	2740	1082
$(pp)_K\ r_{12}\ (dd)_L$	20	9	$(dd)_K\ (pp)_L\ r_{34}$	4	10
$(pp)_K\ r_{12}\ (ff)_L$	2.6	0	$(ff)_K\ (pp)_L\ r_{34}$	0	0
$(dd)_K\ r_{12}\ (ss)_L$	35	152	$(ss)_K\ (dd)_L\ r_{34}$	9	16
$(dd)_K\ r_{12}\ (pp)_L$	2.7	3	$(pp)_K\ (dd)_L\ r_{34}$	3	3
$(dd)_K\ r_{12}\ (dd)_L$	0	0	$(dd)_K\ (dd)_L\ r_{34}$	0	1
$(dd)_K\ r_{12}\ (ff)_L$	0	0	$(ff)_K\ (dd)_L\ r_{34}$	0	0
$(ff)_K\ r_{12}\ (ss)_L$	3.6	13	$(ss)_K\ (ff)_L\ r_{34}$	3	4
$(ff)_K\ r_{12}\ (pp)_L$	0	0	$(pp)_K\ (ff)_L\ r_{34}$	0	0

These results suggest that convergence is fast and that this correlation type can be accurately, albeit slowly, represented within the Hy-CI model for the more diffuse electronic distribution of Be($2s3s$), as was the case for Li^-, and that this trend continues for Be($2s4s$) as well. Interestingly, the K-shell does not appear to be a problem, while the L-shell is not as converged in the r_{12} case. Addition of higher l STOs and blocks such as $(ss)_K\ r_{12}\ (gg)_L$, $(ss)_K\ r_{12}\ (hh)_L$, and $(ss)_K\ r_{12}\ (ii)_L$ could lead to perhaps an additional 5 nHa to 10 nHa.

Ultimately, slow convergence is built into Hy-CI for four or more electrons where one is trying to approximate the effect of the missing "double cusp" terms, as well as the $r_{ij}r_{ik}$ terms first encountered with three electrons. Previous experience with Li suggests that the linked product terms $r_{ij}r_{ik}$ should not be expected to give problems until the nanohartree level, but in going beyond the nanohartree level, the slow double cusp convergence would become even more of a problem. This suggests further study of the double cusp problem is necessary using codes explicitly designed for this (our code is not). The results do appear to support the conclusion in previous work, which stated that while 10-20 nHa accuracy can be achieved without any difficulty, doing substantially better will require greater flexibility in the atomic orbital basis, including adding $(ss)_K\ r_{12} \times [(gg)_L, (hh)_L$, and possibly $(ii)_L]$ blocks, and extensive experimentation to find the best combination of CSFs and orbitals on which to base a much larger calculation.

4.1 Be 5 ^1S

The Be 4 ^1S wave function formed the basis for the Be 5 ^1S expansion, and so the final optimization for 5 ^1S is for the same 86 block, 37,915 CSF wave function as for 4 ^1S.

Table A3 of the Appendix gives an overall picture of the 5 ^1S energy convergence with a 99,965 term expansion using an $s, p, d, f r_{ij}$ STO basis for the CSFs. The optimized exponents for Be 5 ^1S [9] continue the

[9]The optimized orbital exponents are tabulated further on in Table 5.

3 ^1S and 4 ^1S trend of invariant K and inner L shell s and p orbitals appropriate for a $Be^+(1s1s2s)$ core,[10] whereas the L_2 and L_4 exponents here are for a Be($2s5s$) excited state, so while the L_4 p orbital exponent is the same as for Be($2s4s$), the L_2 orbital exponent is more diffuse than the L_2 orbital exponent for Be($2s4s$), and the L_2 exponent for $3s \Rightarrow 5s$ is a reasonably smooth curve as it should be.

In the table, the 136 block, 62,123 term expansion is the same expansion (with different orbital exponents) as in the 99,874 term Be 4 ^1S expansion. Blocks 137-142 are based on similar terms in the 4 ^1S expansion but have been moved to immediately follow the CORE adjustments, since these terms are also "addbacks", *i.e.*, additional energy obtained by expanding orbital basis sets via the difference tool. For the *psps* blocks, we note that the r_{34} and r_{14} blocks in general are not as important as the outermost electron moves further away from the nucleus, so these blocks remain as they are in 4 ^1S but the $(1+r_{12}+r_{13})$ blocks are 7-7-7-7 instead of the 5-5-5-5 in 4 ^1S. The $s_{K1}s_{K1}$ terms, added to introduce additional K-shell correlation and hence serve to gauge how well the K shell is represented, are here comparable to their importance in Be 3 ^1S and of lesser importance than in Be 4 ^1S. This drop in importance is more than offset by an increased importance of $dpps(1+r_{12}+r_{13})$ blocks, while $\{psps, dsds\}$ $(1+r_{12}+r_{13})$ are also of increased importance compared to 3 ^1S and 4 ^1S, following the general pattern of correlation changes as the outer electron becomes more diffuse. The fact that $\{psps, dsds\}$ $(1+r_{12}+r_{13})$ is of increased importance should not be surprising considering how important the $\{psp, dsd\}$ x R blocks are in Li[11]. The result of the 99,965 term Be 5 ^1S calculation is tabulated in Table 3 and turns out to be, as noted previously, within 46 nHa of the recent, best results of Ref. [21].

4.2 Be 6 ^{1}S

The Be 5 ^{1}S wave function formed the basis for the 6 ^{1}S expansion, and so the final optimization for 6 ^1S is for the same 86 block, 37,915 CSF wave function as for 5 ^1S.

Table A4 of the Appendix gives an overall picture of the 6 ^1S energy convergence with a 92,930 term expansion using an s, p, d, fr_{ij} STO basis for the CSFs. The optimized exponents for 6 ^1S[12] continue the Be 3 ^1S, 4 ^1S, and 5 ^1S trend of invariant K and inner L shell s and p orbitals appropriate for a $Be^+(1s1s2s)$ core,[13] whereas the L_2 and L_4 exponents here are for a 6 ^1S excited state, so while the L_4 p orbital exponent is about the same as for 5 ^1S, the L_2 orbital exponent is more diffuse than the L_2 orbital exponent for 5 ^1S, and the L_2 exponent for 3s$\Rightarrow$ 6s is a reasonably smooth curve, as it should be.

The fundamental difference between this expansion and the Be 5 ^1S expansion is that, in all terms, the outer L shell electron basis in each block includes an $n = 6$ orbital since we are dealing with a 6 ^1S state. So, for example, the *spsp* $1{:}5s_K$ $2{:}5p_{L1}$ $1{:}5s_{L1}$ $2{:}5p_{L4}$ R becomes $1{:}5s_K$ $2{:}5p_{L1}$ $1{:}5s_{L1}$ $2{:}6p_{L4}$ R, where an additional 6 p_{L4} orbital has been added to the p_{L4} set. With this exception, the blocks up to the addback blocks starting at block 113 are the same as in the 5 ^1S expansion. In the addback section, for the *pppp* blocks, the r_{13} and r_{14} blocks drop out. For the final adjustments, the *dsds* blocks are too small to be included, and the outermost L shell electron has gotten far enough away from the nucleus that the r_{34} and r_{14} blocks no longer need to be included.

The 6 ^1S wave function at this point followed almost directly from the 5 ^1S wave function, with the expansion of the outer L shell electron basis in each block to include an $n = 6$ orbital where needed. Again, we see an increased importance for the $\{dpps$, *psps*, and *dsds*$\}$ $(1+r_{12}+r_{13})$ blocks compared to Be($2sns$), $n < 6$. The result of a 92,930 term calculation is tabulated in Table 4 and turns out to be, as noted previously, 26 nHa lower than the results of Stanke et al. [19].

[10] With the one anomalous Be 3 ^1S L_1 orbital exponent.
[11] See Table I of Ref. [34].
[12] The optimized orbital exponents are tabulated further on in Table 5.
[13] With the one anomalous 3 ^1S L_1 orbital exponent.

4.3 Be 7 ^1S

The Be 6 ^1S wave function formed the basis for the 7 ^1S expansion, but now in addition to making sure that the outermost orbital basis set includes an $n = 7$ orbital, the CORE blocks are expanded to include an additional L shell orbital for both the inner and outer shell electrons. Hence, the size of the 86 block, 37,915 CSF wave function used in optimizing the 6 ^1S wave function is now 52,294 CSFs, and it is this wave function that is used for the optimization of the 7 ^1S basis orbitals.

Table A5 of the Appendix gives an overall picture of the Be 7 ^1S energy convergence with a 92,904 term expansion using an s, p, d, fr_{ij} STO basis for the CSFs. The optimized exponents for Be 7^1S continue the 3 ^1S, 4 ^1S, 5 ^1S, and 6 ^1S trend of invariant K and inner L shell s and p orbitals appropriate for a $Be^+(1s1s2s)$ core,[14] whereas the L_2 and L_4 exponents here are for a 7 ^1S excited state, so while the L_4 p orbital exponent is about the same as for 6 ^1S, the L_2 orbital exponent is more diffuse than the L_2 orbital exponent for 6 ^1S, and the L_2 exponent for $3s \Rightarrow 7s$ is a reasonably smooth curve, as it should be.

The fundamental difference between this expansion and the Be 6 ^1S expansion is that, in all terms, the outer L shell electron basis in each block includes an $n = 7$ orbital, since we are dealing with a 7 ^1S state. So, for example, the $spsp$ $1{:}5s_K$ $2{:}5p_{L1}$ $1{:}5s_{L1}$ $2{:}6p_{L4}$ R becomes $1{:}5s_K$ $2{:}5p_{L1}$ $1{:}5s_{L1}$ $2{:}7p_{L4}$ R, where an additional 7 p_{L4} orbital has been added to the p_{L4} set. Since the CORE blocks now contain an outermost L $n = 8$ orbital, many of the addback blocks are superfluous and are not included in the expansion. Except for these differences, the 7 ^1S expansion looks very much like the 6 ^1S expansion, with a few less important blocks having dropped out.

5. Conclusion

Table 5 is a table of the optimum zeta values for each of the species explored here.

Table 5. Optimum zeta values for each calculated excited S state.

State	K	L_1	L_2	K_p	L_3	L_4	K_1
Be 3 ^1S	3.832	0.964	0.650	5.200	1.163	0.940	10.0
Be 4 ^1S	3.806	1.730	0.367	5.100	1.163	0.525	10.0
Be 5 ^1S	3.800	1.692	0.259	5.070	1.163	0.525	10.0
Be 6 ^1S	3.800	1.692	0.201	5.100	1.163	0.525	10.0
Be 7 ^1S	3.800	1.730	0.163	5.100	1.163	0.535	10.0

Here, K, K_p, L_1, L_3, and K_1 are basically fixed after the 3 ^1S state, because the $Be^+(1s1s2s)$ core changes very little as one approaches ionization and the outer L shell orbital gets further and further away from the nucleus. L_2 should vary smoothly as the outer electron gets further and further away from the nucleus, and indeed it does. L_4 should do the same to a lesser extent, but we find that it varies very little in fact.

The best non-relativistic energies for Be 3 ^1S, 4 ^1S, 5 ^1S, and 6 ^1S obtained are -14.4182 4034 638 Ha, -14.3700 8789 0 Ha, -14.3515 1167 6 Ha, and -14.3424 0357 8 Ha, respectively. In addition, the best non-relativistic energy for Be 7 ^1S obtained is -14.3372 6649 96 Ha. The 6 ^1S result is superior to the known reference energy for that state, while for the 7 ^1S state, there is no other comparable calculation.

We have previously shown that Hy-CI is capable of high-precision results for not only ground states, but excited states as well, for three-electron atoms, specifically the Li atom. Hy-CI has from its inception been

[14] With the one anomalous Be 3 ^1S L_1 orbital exponent.

an attempt to extend the success of the Hy method to systems with more than three electrons. A fundamental feature in the method is the restriction of one r_{ij} per CSF, which has achieved 10-20 nHa accuracy for the ground states of the Be isoelectronic series with $Z \geq 4$. For both extension of the method to $N > 4$ as well as for excited states of four-electron systems, how well the method handles the "double cusp" problem when the L shell is more diffuse than in the ground state needs to be studied. This work continues the work begun with Li^- (which turns out to have a Be($2s3s$)-like structure as calculations have shown down to the block level [12]) by examining how well Hy-CI can treat states successively more diffuse than the ground state. This is accomplished by examining successively higher states of Be of ^1S symmetry. Specifically, a study of the Be($2sns$) excited states, n = 3,7 has been carried out. Compared to Be, this is a more diffuse system, one in which a weaker "double cusp" would be expected, which should make Hy-CI more favorable, but also more CI-like, so some of the advantage of Hy-CI is lost, perhaps. Indeed, we find that r_{14}, which correlates the outermost L shell electron and to a lesser extent, r_{34}, which correlates open shell electrons, become less and less important as the outer L shell electron becomes more distant, and this compensates for blocks in which the basis has been expanded to represent the more diffuse charge distribution. Based on the calculations reported in Sec. III and Sec. IV here, one can conclude that this correlation type can be accurately represented for the more diffuse distribution of Be excited states of ^1S up through 7 ^1S. Combined with the previous Be isoelectronic series results, these calculations exemplify the level of accuracy that is now possible with Hy-CI in describing not only the ground state of Li-, Be and Be-like ions, but also excited states as well.

6. Appendix

Tables A1-A5 list the final Hy-CI expansions for the 3 ^1S, 4 ^1S, 5 ^1S, 6 ^1S , and 7 ^1S states, respectively. In the tables, ΔE for each CSF block is the amount by which that block lowers the non-relativistic energy when added to the expansion. Column 1 lists the CSF block specifications used to generate the CSF terms for the various block types, in the order electron 1 (α spin), electron 2 (β spin), electron 3 (α spin), electron 4 (β spin). For example, in the first line 1:9s_K for the first electron means the basis orbitals are 1s_K through 9s_K orbitals (where K indicates an orbital exponent appropriate for a K shell electron). All of the listed basis orbitals are used to generate all of the CSFs that are unique for this basis set selection, except that N_{max}, the sum of the powers of r in the Hartree product (HP), must be less than or equal to 16 unless an explicit r-sum is specified. The choice of terms is highly regular, there having been no attempt to cut down on the number of terms. The number of unique terms (CSFs) in a block can be computed from the listed basis orbitals and the condition that $N_{max} \leq 16$ (or $\leq$ the explicitly specified N_{max}). For example, consider 1:6s_{K1} 1:6s_{K1} 1:5s_{L1} 1:5 s_{L2} r_{34} in the last row of Table A1. There are 6 x 7 / 2 = 21 unique pairs of orbitals for electrons 1 and 2 and 5 x 5 = 25 unique pairs of orbitals for electrons 3 and 4. Since the K shell orbital exponent is different from the L shell orbital, there are (21 x 25) = 525 different CSF terms for this block. Applying the condition that the r-sum, the sum of powers of r for the four orbitals in a term, has to be $\leq$ 16, the number of terms for this CSF block is reduced to 521 (see Ref. [29] for further details).

Table A1. Hy-CI expansion of the 3 ^1S excited state of Be (in Ha), a 82,807 term s,p,d,f expansion. In the table, R_1 = $\{1,r_{12},r_{34}\}$, R_2 = $\{r_{13},r_{14}\}$, R = $\{1,r_{12},r_{34},r_{13},r_{14}\}$, N is the number of terms added and N_{tot} is the cumulative number of terms. The terms are r-sum filtered using N_{max} = 16 (see text) unless an explicit r-sum N_{max} value is given.

Block(s)	Terms Added[ab]	N	N_{tot}	E(N_{tot}) (Ha)	$-\Delta E$ (μHa)
1-25	CORE				
1-3	$1{:}9s_K\ 1{:}9s_K\ 1{:}6s_{L_1}\ 1{:}6s_{L_2}\ R_1$	3747	3747	-14.4162 5059 5738	
4	$1{:}9s_K\ 1{:}9s_K\ 1{:}6s_{L_1}\ 1{:}6s_{L_2}\ r_{13}$	1249	4996	-14.4163 3192 7799	81.3320 61
5	$1{:}6s_K\ 1{:}6s_K\ 1{:}6s_{L_1}\ 1{:}6s_{L_2}\ r_{14}$	732	5728	-14.4163 9773 6264	65.8084 65
6-10	$2{:}7p_{Kp}\ 2{:}7p_{Kp}\ 1{:}6s_{L_1}\ 1{:}6s_{L_2}\ R$	3380	9108	-14.4178 0538 7899	1407.6516 35
11	$1{:}9s_K\ 1{:}9s_K\ 2{:}6p_{L3}\ 2{:}6p_{L4}$	798	9906	-14.4180 9613 0563	290.7426 64
12	$1{:}9s_K\ 1{:}9s_K\ 2{:}6p_{L3}\ 2{:}6p_{L4}\ r_{12}$	798	10704	-14.4182 0035 3838	104.2232 75
13	$1{:}6s_K\ 1{:}6s_K\ 2{:}6p_{L3}\ 2{:}6p_{L4}\ r_{34}$	501	11205	-14.4182 0348 2155	3.1283 17
14-15	$1{:}6s_K\ 1{:}6s_K\ 2{:}6p_{L3}\ 2{:}6p_{L4}R_2$	1002	12207	-14.4182 2131 6871	17.8347 16
16-20	$2{:}6p_{Kp}\ 2{:}6p_{Kp}\ 2{:}6p_{L3}\ 2{:}6p_{L4}\ R$ [c]	1875	14082	-14.4182 2719 0961	5.8740 90
21-25	$2{:}6p_{1Kp}\ 2{:}6p_{1Kp}\ 2{:}6p_{-1L3}\ 2{:}6p_{-1L4}\ R$ [c]	1875	15957	-14.4182 3198 5819	4.7948 58
26-113	Post-CORE				
26-30	$1{:}5s_K\ 2{:}5p_{Kp}\ 2{:}5p_{L3}\ 1{:}5s_{L2}\ R$	2000	17957	-14.4182 3582 3317	3.8374 98
31-35	$1{:}5s_K\ 2{:}5p_{Kp}\ 1{:}5s_{L1}\ 2{:}5p_{L4}\ R$	2000	19957	-14.4182 3648 4804	0.6614 87
36-40	$3{:}6d_{Kp}\ 3{:}6d_{Kp}\ 1{:}5s_{L1}\ 1{:}5s_{L2}\ R$	1230	21187	-14.4182 3827 7294	1.7924 90
41-45	$1{:}5s_K\ 1{:}5s_K\ 3{:}6d_{L3}\ 3{:}6d_{L4}\ R$	1180	22367	-14.4182 3890 5873	0.6285 78
46-50	$1{:}5s_K\ 3{:}6d_{Kp}\ 3{:}6d_{L3}\ 1{:}6s_{L2}\ R$	2325	24692	-14.4182 3924 5585	0.3397 12
51-55	$1{:}5s_K\ 3{:}6d_{Kp}\ 1{:}6s_{L1}\ 3{:}6d_{L4}\ R$	2325	27017	-14.4182 3931 6211	0.0706 26
56-60	$1{:}5s_K\ 2{:}5p_{Kp}\ 2{:}5p_{L3}\ 3{:}6d_{L4}\ R$	1595	28612	-14.4182 3957 5313	0.2591 02
61-65	$1{:}5s_K\ 3{:}6d_{Kp}\ 2{:}5p_{L3}\ 2{:}5p_{L4}\ R$	1595	30207	-14.4182 3965 0678	0.0753 65
66-70	$2{:}5p_{Kp}\ 1{:}5s_K\ 2{:}5p_{L3}\ 3{:}6d_{L4}\ R$	1595	31802	-14.4182 3970 9965	0.0592 87
71-75	$3{:}6d_{Kp}\ 2{:}5p_{Kp}\ 1{:}5s_{L1}\ 2{:}5p_{L4}\ R$	1595	33397	-14.4182 3984 1050	0.1310 85
76	$2{:}5p_{Kp}\ 2{:}5p_{Kp}\ 1{:}5s_{L1}\ 3{:}6d_{L4}$	199	33596	-14.4182 3984 5155	0.0041 05
77	$4{:}7f_{Kp}\ 4{:}7f_{Kp}\ 2{:}5s_{L1}\ 2{:}5s_{L2}$	136	33732	-14.4182 3985 2156	0.0070 01
78	$4{:}7f_{Kp}\ 4{:}7f_{Kp}\ 2{:}5s_{L1}\ 2{:}5s_{L2}\ r_{12}$	136	33868	-14.4182 3985 5793	0.0036 36
79	$4{:}7f_{Kp}\ 4{:}7f_{Kp}\ 2{:}6s_{L1}\ 2{:}6s_{L2}\ r_{34}$	177	34045	-14.4182 3986 5696	0.0099 03
80	$4{:}7f_{Kp}\ 4{:}7f_{Kp}\ 2{:}5s_{L1}\ 2{:}5s_{L2}\ r_{13}$	136	34181	-14.4182 3987 0299	0.0046 03
81	$4{:}7f_{Kp}\ 4{:}7f_{Kp}\ 2{:}6s_{L1}\ 2{:}6s_{L2}\ r_{14}$	177	34358	-14.4182 3987 3145	0.0028 46
82-86	$1{:}6s_K\ 1{:}6s_K\ 4{:}7f_{L3}\ 4{:}7f_{L4}\ R$	1320	35678	-14.4182 3992 7005	0.0538 60
87-89	$1{:}6s_K\ 4{:}7f_{Kp}\ 4{:}7f_{L3}\ 2{:}6s_{L2}\ R_1$	1095	36773	-14.4182 3996 5808	0.0388 03
90	$1{:}6s_K\ 4{:}7f_{Kp}\ 4{:}7f_{L3}\ 2{:}6s_{L2}\ r_{13}$	365	37138	-14.4182 3997 3862	0.0080 56
91	$1{:}6s_K\ 4{:}7f_{Kp}\ 2{:}6s_{L1}\ 4{:}7f_{L4}$	365	37503	-14.4182 3997 6395	0.0025 33
92	$1{:}6s_K\ 4{:}7f_{Kp}\ 2{:}6s_{L1}\ 4{:}7f_{L4}\ r_{12}$	365	37868	-14.4182 3997 6977	0.0005 82
93-97	$2{:}5p_{Kp}\ 2{:}5p_{Kp}\ 3{:}6d_{L3}\ 3{:}6d_{L4}\ R$	780	38648	-14.4182 3998 9687	0.0127 10
98-102	$2{:}5p_{1Kp}\ 2{:}5p_{1Kp}\ 3{:}6d_{-1L3}\ 3{:}6d_{-1L4}\ R$	780	39428	-14.4182 4003 1439	0.0417 52
103	$3{:}6d_{Kp}\ 3{:}6d_{Kp}\ 2{:}6p_{L3}\ 2{:}6p_{L4}$	226	39654	-14.4182 4003 4023	0.0025 85
104	$3{:}6d_{Kp}\ 3{:}6d_{Kp}\ 2{:}6p_{L3}\ 2{:}6p_{L4}\ r_{12}$	226	39880	-14.4182 4003 5120	0.0010 97
105	$3{:}6d_{Kp}\ 3{:}6d_{Kp}\ 2{:}5p_{L3}\ 2{:}5p_{L4}\ r_{34}$	156	40036	-14.4182 4003 6213	0.0010 93
106-107	$3{:}6d_{Kp}\ 3{:}6d_{Kp}\ 2{:}6p_{L3}\ 2{:}6p_{L4}\ R_2$	452	40488	-14.4182 4003 9566	0.0033 53
108-112	$3{:}6d_{1Kp}\ 3{:}6d_{1Kp}\ 2{:}6p_{-1L3}\ 2{:}6p_{-1L4}\ R$	1130	41618	-14.4182 4005 0580	0.0110 14
113	$1{:}6s_{K1}\ 1{:}6s_{K1}\ 1{:}5s_{L1}\ 1{:}5s_{L2}$	521	42139	-14.4182 4009 5138	0.0445 58

Block(s)	Terms Added[ab]	N	N_{tot}	$E(N_{tot})$ (Ha)	$-\Delta E$ (μHa)
114-137	CORE Adjustments				
114	$1{:}9s_K$ $1{:}9s_K$ $1{:}9s_{L1}$ $1{:}9s_{L2}$-#1 [d]	1649	43788	-14.4182 4012 2803	0.0276 65
115	$1{:}9s_K$ $1{:}9s_K$ $1{:}9s_{L1}$ $1{:}9s_{L2}$ r_{12}-#2 [d]	1649	45437	-14.4182 4021 8158	0.0953 55
116	$1{:}9s_K$ $1{:}9s_K$ $1{:}9s_{L1}$ $1{:}9s_{L2}$ r_{34}-#3 [d]	1649	47086	-14.4182 4022 2270	0.0041 12
117	$1{:}9s_K$ $1{:}9s_K$ $1{:}9s_{L1}$ $1{:}9s_{L2}$ r_{13}-#4 [d]	1649	48735	-14.4182 4022 6962	0.0046 91
118	$1{:}9s_K$ $1{:}9s_K$ $1{:}9s_{L1}$ $1{:}9s_{L2}$ r_{14}-#5 [d]	2166	50901	-14.4182 4024 1707	0.0147 46
119	$2{:}9p_{Kp}$ $2{:}9p_{Kp}$ $1{:}9s_{L1}$ $1{:}9s_{L2}$-#6 [d]	1513	52414	-14.4182 4025 3984	0.0122 76
120	$2{:}9p_{Kp}$ $2{:}9p_{Kp}$ $1{:}9s_{L1}$ $1{:}9s_{L2}$ r12-#7	670	53084	-14.4182 4025 9573	0.0055 89
121	$2{:}9p_{Kp}$ $2{:}9p_{Kp}$ $1{:}9s_{L1}$ $1{:}9s_{L2}$ r13-#9 [d]	1513	54597	-14.4182 4026 9150	0.0095 77
122	$2{:}9p_{Kp}$ $2{:}9p_{Kp}$ $1{:}9s_{L1}$ $1{:}9s_{L2}$ r14-#10 [d]	1513	56110	-14.4182 4027 6885	0.0077 35
123	$1{:}9s_K$ $1{:}9s_K$ $2{:}8p_{L3}$ $2{:}8s_{L4}$-#11	393	56503	-14.4182 4027 7465	0.0005 80
124	$1{:}9s_K$ $1{:}9s_K$ $2{:}8p_{L3}$ $2{:}8s_{L4}$ r_{12}-#12	393	56896	-14.4182 4027 8333	0.0008 68
125	$1{:}9s_K$ $1{:}9s_K$ $2{:}8p_{L3}$ $2{:}8s_{L4}$ r_{34}-#13	690	57586	-14.4182 4027 8949	0.0006 16
126	$1{:}9s_K$ $1{:}9s_K$ $2{:}8p_{L3}$ $2{:}8s_{L4}$ r_{13}-#14	690	58276	-14.4182 4028 2071	0.0031 22
127	$1{:}9s_K$ $1{:}9s_K$ $2{:}8p_{L3}$ $2{:}8s_{L4}$ r_{14}-#15	690	58966	-14.4182 4028 9141	0.0070 70
128	$2{:}6p_{Kp}$ $2{:}6p_{Kp}$ $2{:}8p_{L3}$ $2{:}8p_{L4}$-#16 [c]	360	59326	-14.4182 4028 9440	0.0002 99
129	$2{:}6p_{Kp}$ $2{:}6p_{Kp}$ $2{:}8p_{L3}$ $2{:}8p_{L4}$ r12-#17 [c]	360	59686	-14.4182 4028 9702	0.0002 62
130	$2{:}6p_{Kp}$ $2{:}6p_{Kp}$ $2{:}8p_{L3}$ $2{:}8p_{L4}$ r34-#18 [c]	360	60046	-14.4182 4028 9933	0.0002 31
131	$2{:}6p_{Kp}$ $2{:}6p_{Kp}$ $2{:}8p_{L3}$ $2{:}8p_{L4}$ r13-#19 [c]	360	60406	-14.4182 4029 0111	0.0001 78
132	$2{:}6p_{Kp}$ $2{:}6p_{Kp}$ $2{:}8p_{L3}$ $2{:}8p_{L4}$ r14-#20 [c]	360	60766	-14.4182 4029 0313	0.0002 03
133	$2{:}6p_{1Kp}$ $2{:}6p_{1Kp}$ $2{:}8p_{-1L3}$ $2{:}8p_{-1L4}$-#21 [c]	360	61126	-14.4182 4029 0546	0.0002 33
134	$2{:}6p_{1Kp}$ $2{:}6p_{1Kp}$ $2{:}8p_{-1L3}$ $2{:}8p_{-1L4}$ r12-#22 [c]	360	61486	-14.4182 4029 0887	0.0003 41
135	$2{:}6p_{1Kp}$ $2{:}6p_{1Kp}$ $2{:}8p_{-1L3}$ $2{:}8p_{-1L4}$ r34-#23 [c]	360	61846	-14.4182 4029 0926	0.0000 39
136	$2{:}6p_{1Kp}$ $2{:}6p_{1Kp}$ $2{:}8p_{-1L3}$ $2{:}8p_{-1L4}$ r13-#24 [c]	360	62206	-14.4182 4029 1279	0.0003 53
137	$2{:}6p_{1Kp}$ $2{:}6p_{1Kp}$ $2{:}8p_{-1L3}$ $2{:}8p_{-1L4}$ r14-#25 [c]	360	62566	-14.4182 4029 1767	0.0004 88
138-203	Final Adjustments				
138-142	$2{:}5p_{Kp}$ $1{:}5s_K$ $1{:}5s_{L1}$ $2{:}5p_{L4}$ R	2000	64566	-14.4182 4030 1064	0.0092 97
143	$2{:}5p_{Kp}$ $1{:}5s_K$ $2{:}5p_{L3}$ $1{:}5s_{L2}$	400	64966	-14.4182 4030 1923	0.0008 59
144	$2{:}5p_{Kp}$ $1{:}5s_K$ $2{:}5p_{L3}$ $1{:}5s_{L2}$ r_{12}	400	65366	-14.4182 4030 2885	0.0009 61
145	$2{:}5p_{Kp}$ $1{:}5s_K$ $2{:}5p_{L3}$ $1{:}5s_{L2}$ r_{34}	400	65766	-14.4182 4030 3594	0.0007 09
146	$2{:}5p_{Kp}$ $1{:}5s_K$ $2{:}5p_{L3}$ $1{:}5s_{L2}$ r_{13}	400	66166	-14.4182 4030 3921	0.0003 27
147	$2{:}5p_{Kp}$ $1{:}5s_K$ $2{:}5p_{L3}$ $1{:}5s_{L2}$ r_{14}	400	66566	-14.4182 4030 5289	0.0013 68
148	$3{:}6d_{Kp}$ $1{:}5s_K$ $1{:}5s_{L1}$ $3{:}6d_{L4}$	395	66961	-14.4182 4030 5678	0.0003 88
149	$3{:}6d_{Kp}$ $1{:}5s_K$ $1{:}5s_{L1}$ $3{:}6d_{L4}$ r_{12}	395	67356	-14.4182 4030 6243	0.0005 66
150-151	$3{:}6d_{Kp}$ $1{:}5s_K$ $1{:}5s_{L1}$ $3{:}6d_{L4}$ R_2	790	68146	-14.4182 4030 7125	0.0008 82
152	$3{:}6d_{Kp}$ $1{:}5s_K$ $3{:}6d_{L3}$ $1{:}5s_{L2}$ r_{12}	395	68541	-14.4182 4030 7632	0.0005 06
153	$3{:}6d_{Kp}$ $1{:}5s_K$ $3{:}6d_{L3}$ $1{:}5s_{L2}$ r_{34}	395	68936	-14.4182 4030 8221	0.0005 89
154	$3{:}6d_{Kp}$ $1{:}5s_K$ $3{:}6d_{L3}$ $1{:}5s_{L2}$ r_{14}	395	69331	-14.4182 4030 8686	0.0004 65
155	$3{:}6d_{Kp}$ $2{:}5p_{Kp}$ $3{:}6d_{L3}$ $2{:}5p_{L4}$	251	69582	-14.4182 4030 9083	0.0003 98
156	$3{:}6d_{Kp}$ $2{:}5p_{Kp}$ $3{:}6d_{L3}$ $2{:}5p_{L4}$ r_{12}	251	69833	-14.4182 4030 9500	0.0004 16
157	$3{:}6d_{1Kp}$ $2{:}5p_{1Kp}$ $3{:}6d_{-1L3}$ $2{:}5p_{-1L4}$	251	70084	-14.4182 4031 0510	0.0010 10
158	$3{:}6d_{Kp}$ $2{:}5p_{Kp}$ $2{:}5p_{L3}$ $3{:}6d_{L4}$	251	70335	-14.4182 4031 1449	0.0009 40
159	$3{:}6d_{Kp}$ $2{:}5p_{Kp}$ $2{:}5p_{L3}$ $3{:}6d_{L4}$ r_{12}	251	70586	-14.4182 4031 2083	0.0006 34
160	$2{:}5p_{Kp}$ $3{:}6d_{Kp}$ $3{:}6d_{L3}$ $2{:}5p_{L4}$	251	70837	-14.4182 4031 2533	0.0004 50
161	$2{:}5p_{Kp}$ $3{:}6d_{Kp}$ $3{:}6d_{L3}$ $2{:}5p_{L4}$ r_{12}	251	71088	-14.4182 4031 3049	0.0005 16

Block(s)	Terms Added[ab]	N	N_{tot}	$E(N_{tot})$ (Ha)	$-\Delta E$ (μHa)
162	$2{:}5p_{Kp}\ 3{:}6d_{Kp}\ 2{:}5p_{L3}\ 3{:}6d_{L4}$	251	71339	-14.4182 4031 3562	0.0005 13
163	$3{:}6d_{-1Kp}\ 2{:}5p_{1Kp}\ 2{:}5p_{-1L3}\ 3{:}6d_{1L4}$	251	71590	-14.4182 4031 4001	0.0004 39
164	$2{:}5p_{Kp}\ 2{:}5p_{Kp}\ 1{:}5s_{L1}\ 3{:}6d_{L4}\ r_{12}$	199	71789	-14.4182 4031 4397	0.0003 96
165	$2{:}5p_{Kp}\ 2{:}5p_{Kp}\ 1{:}5s_{L1}\ 3{:}6d_{L4}\ r_{14}$	199	71988	-14.4182 4031 5291	0.0008 94
166	$2{:}5p_{Kp}\ 3{:}6d_{Kp}\ 1{:}5s_{L1}\ 2{:}5p_{L4}$	319	72307	-14.4182 4031 5940	0.0006 50
167	$2{:}5p_{Kp}\ 3{:}6d_{Kp}\ 1{:}5s_{L1}\ 2{:}5p_{L4}\ r_{12}$	319	72626	-14.4182 4031 8439	0.0024 98
168	$2{:}5p_{Kp}\ 3{:}6d_{Kp}\ 1{:}5s_{L1}\ 2{:}5p_{L4}\ r_{14}$	319	72945	-14.4182 4031 9254	0.0008 15
169	$2{:}5p_{Kp}\ 1{:}5s_{K}\ 3{:}6d_{L3}\ 2{:}5p_{L4}\ r_{12}$	319	73264	-14.4182 4032 0138	0.0008 84
170	$2{:}5p_{Kp}\ 1{:}5s_{K}\ 3{:}6d_{L3}\ 2{:}5p_{L4}\ r_{13}$	319	73583	-14.4182 4032 1038	0.0009 00
171	$3{:}6d_{Kp}\ 2{:}5p_{Kp}\ 2{:}5p_{L3}\ 1{:}5s_{L2}$	319	73902	-14.4182 4032 2789	0.0017 52
172	$3{:}6d_{Kp}\ 2{:}5p_{Kp}\ 2{:}5p_{L3}\ 1{:}5s_{L2}\ r_{12}$	319	74221	-14.4182 4032 5411	0.0026 22
173	$3{:}6d_{Kp}\ 2{:}5p_{Kp}\ 2{:}5p_{L3}\ 1{:}5s_{L2}\ r_{13}$	319	74540	-14.4182 4032 6584	0.0011 73
174	$3{:}6d_{Kp}\ 2{:}5p_{Kp}\ 2{:}5p_{L3}\ 1{:}5s_{L2}\ r_{14}$	319	74859	-14.4182 4032 7134	0.0005 50
175	$3{:}6d_{Kp}\ 1{:}5s_{K}\ 2{:}5p_{L3}\ 2{:}5p_{L4}$	319	75178	-14.4182 4032 7418	0.0002 84
176	$3{:}6d_{Kp}\ 1{:}5s_{K}\ 2{:}5p_{L3}\ 2{:}5p_{L4}\ r_{13}$	319	75497	-14.4182 4032 7758	0.0003 40
177	$3{:}6d_{Kp}\ 1{:}5s_{K}\ 2{:}5p_{L3}\ 2{:}5p_{L4}\ r_{14}$	319	75816	-14.4182 4032 8255	0.0004 97
178	$2{:}5p_{Kp}\ 3{:}6d_{Kp}\ 2{:}5p_{L3}\ 1{:}5s_{L2}$	319	76135	-14.4182 4032 9194	0.0009 39
179	$2{:}5p_{Kp}\ 3{:}6d_{Kp}\ 2{:}5p_{L3}\ 1{:}5s_{L2}\ r_{12}$	319	76454	-14.4182 4032 9939	0.0007 45
180	$2{:}5p_{Kp}\ 3{:}6d_{Kp}\ 2{:}5p_{L3}\ 1{:}5s_{L2}\ r_{13}$	319	76773	-14.4182 4033 0345	0.0004 06
181	$2{:}5p_{Kp}\ 3{:}6d_{Kp}\ 2{:}5p_{L3}\ 1{:}5s_{L2}\ r_{14}$	319	77092	-14.4182 4033 0658	0.0003 12
182	$3{:}6d_{Kp}\ 3{:}6d_{Kp}\ 3{:}6d_{L3}\ 3{:}6d_{L4}\ r_{34}$	136	77228	-14.4182 4033 1328	0.0006 70
183	$3{:}6d_{1Kp}\ 3{:}6d_{1Kp}\ 3{:}6d_{-1L3}\ 3{:}6d_{-1L4}$	136	77364	-14.4182 4033 1953	0.0006 25
184	$3{:}6d_{1Kp}\ 3{:}6d_{1Kp}\ 3{:}6d_{-1L3}\ 3{:}6d_{-1L4}\ r_{34}$	136	77500	-14.4182 4033 5074	0.0031 21
185	$3{:}6d_{Kp}\ 3{:}6d_{Kp}\ 1{:}5s_{L1}\ 3{:}6d_{L4}$	189	77689	-14.4182 4033 6057	0.0009 83
186	$3{:}6d_{Kp}\ 3{:}6d_{Kp}\ 1{:}5s_{L1}\ 3{:}6d_{L4}\ r_{12}$	189	77878	-14.4182 4033 6305	0.0002 48
187	$3{:}6d_{Kp}\ 3{:}6d_{Kp}\ 1{:}5s_{L1}\ 3{:}6d_{L4}\ r_{14}$	189	78067	-14.4182 4033 6812	0.0005 07
188	$3{:}6d_{Kp}\ 3{:}6d_{Kp}\ 3{:}6d_{L3}\ 1{:}5s_{L2}$	189	78256	-14.4182 4033 7268	0.0004 56
189	$3{:}6d_{Kp}\ 3{:}6d_{Kp}\ 3{:}6d_{L4}\ 1{:}5s_{L2}\ r_{13}$	189	78445	-14.4182 4033 7852	0.0005 85
190	$2{:}8p_{Kp}\ 2{:}8p_{Kp}\ 4{:}7f_{L3}\ 4{:}7f_{L4}\ \mathrm{r}_{12}$	199	78644	-14.4182 4033 8513	0.0006 61
191	$2{:}8p_{1Kp}\ 2{:}8p_{1Kp}\ 4{:}7f_{-1L3}\ 4{:}7f_{-1L4}\ \mathrm{r}_{12}$	199	78843	-14.4182 4034 0490	0.0019 76
192	$4{:}7f_{Kp}\ 4{:}7f_{Kp}\ 2{:}6p_{L3}\ 2{:}6p_{L4}\ \mathrm{r}_{14}$	177	79020	-14.4182 4034 0712	0.0002 23
193	$1{:}5s_{K}\ 4{:}7f_{Kp}\ 2{:}5p_{L3}\ 3{:}6d_{L4}$	305	79325	-14.4182 4034 0993	0.0002 81
194	$1{:}5s_{K}\ 4{:}7f_{Kp}\ 3{:}6d_{L3}\ 2{:}5p_{L4}$	305	79630	-14.4182 4034 1403	0.0004 10
195	$3{:}6d_{Kp}\ 1{:}5s_{K}\ 4{:}7f_{L3}\ 2{:}5p_{L4}$	305	79935	-14.4182 4034 1673	0.0002 70
196	$2{:}5p_{Kp}\ 4{:}7f_{Kp}\ 3{:}6d_{l3}\ 1{:}5s_{L2}$	305	80240	-14.4182 4034 2493	0.0008 21
197	$2{:}5p_{Kp}\ 4{:}7f_{Kp}\ 3{:}6d_{l3}\ 1{:}5s_{L2}\ \mathrm{r}_{12}$	305	80545	-14.4182 4034 2972	0.0004 79
198	$2{:}5p_{Kp}\ 4{:}7f_{Kp}\ 3{:}6d_{l3}\ 1{:}5s_{L2}\ \mathrm{r}_{13}$	305	80850	-14.4182 4034 3387	0.0004 15
199-201	$3{:}6d_{Kp}\ 4{:}7f_{Kp}\ 2{:}5p_{l3}\ 1{:}5s_{L2}\ \mathrm{R}_1$	915	81765	-14.4182 4034 4522	0.0011 35
202	$1{:}6s_{K1}\ 1{:}6s_{K1}\ 1{:}5s_{L1}\ 1{:}5s_{L2}\ \mathrm{r}_{12}$	521	82286	-14.4182 4034 5736	0.0012 14
203	$1{:}6s_{K1}\ 1{:}6s_{K1}\ 1{:}5s_{L1}\ 1{:}5s_{L2}\ \mathrm{r}_{34}$	521	82807	-14.4182 4034 6380	0.0006 44

[a] K shell orbital exponents are $K = 3.83157, K_p = 5.2$; [b] L shell orbital exponents are $L_1 = 0.9638, L_2 = 0.65, L_3 = 1.16274, L_4 = 0.94006$;
[c] r-sum = 24; [d] r-sum = 20.

Table A2. Hy-CI expansion of the 4 ^1S excited state of Be (in Ha), a 99,874 term s,p,d,f expansion. In the table, R_1 = $\{1,r_{12},r_{34}\}$, R_2 = $\{r_{13},r_{14}\}$, R = $\{1,r_{12},r_{34},r_{13},r_{14}\}$, N is the number of terms added, and N_{tot} is the cumulative number of terms. The terms are r-sum filtered using N_{max} = 16 (see text) unless an explicit r-sum N_{max} value is given.

Block(s)	Terms Added[ab]	N	N_{tot}	E(N_{tot}) (Ha)	$-\Delta E$ (μHa)
1-25	CORE				
1-3	$1{:}9s_K$ $1{:}9s_K$ $1{:}6s_{L_1}$ $1{:}7s_{L_2}$ R_1	4152	4152	-14.3688 8923 2777	
4	$1{:}9s_K$ $1{:}9s_K$ $1{:}6s_{L_1}$ $1{:}7s_{L_2}$ r_{13}	1334	5536	-14.3690 3454 7456	145.3146 79
5	$1{:}6s_K$ $1{:}6s_K$ $1{:}6s_{L_1}$ $1{:}7s_{L_2}$ r_{14}	836	6372	-14.3690 3682 1680	2.2742 24
6-10	$2{:}7p_{Kp}$ $2{:}7p_{Kp}$ $1{:}6s_{L_1}$ $1{:}7s_{L_2}$ R	3770	10142	-14.3698 8153 9195	844.7175 15
11	$1{:}9s_K$ $1{:}9s_K$ $2{:}6p_{L3}$ $2{:}7p_{L4}$	900	11042	-14.3700 2489 8563	143.3593 68
12	$1{:}9s_K$ $1{:}9s_K$ $2{:}6p_{L3}$ $2{:}7p_{L4}$ r_{12}	900	11942	-14.3700 6681 6954	41.9183 91
13	$1{:}6s_K$ $1{:}6s_K$ $2{:}6p_{L3}$ $2{:}7p_{L4}$ r_{34}	584	12526	-14.3700 6958 5980	2.7690 26
14-15	$1{:}6s_K$ $1{:}6s_K$ $2{:}6p_{L3}$ $2{:}7p_{L4}R_2$	1168	13694	-14.3700 7579 8398	6.2124 18
16-20	$2{:}6p_{0Kp}$ $2{:}6p_{0Kp}$ $2{:}6p_{0L3}$ $2{:}7p_{0L4}$ R [c]	2250	15944	-14.3700 7786 8173	2.0697 75
21-25	$2{:}6p_{1Kp}$ $2{:}6p_{1Kp}$ $2{:}6p_{-1L3}$ $2{:}7p_{-1L4}$ R [c]	2250	18194	-14.3700 7982 1312	1.9531 39
26-112	Post-CORE				
26-30	$1{:}5s_K$ $2{:}5p_{Kp}$ $2{:}5p_{L3}$ $1{:}5s_{L2}$ R	2000	20194	-14.3700 8313 7510	3.3161 98
31-35	$1{:}5s_K$ $2{:}5p_{Kp}$ $1{:}5s_{L1}$ $2{:}5p_{L4}$ R	2000	22194	-14.3700 8394 5046	0.8075 36
36-40	$3{:}6d_{Kp}$ $3{:}6d_{Kp}$ $1{:}5s_{L1}$ $1{:}5s_{L2}$ R	1230	23424	-14.3700 8576 5191	1.8201 45
41-45	$1{:}5s_K$ $1{:}5s_K$ $3{:}6d_{L3}$ $3{:}6d_{L4}$ R	1180	24604	-14.3700 8616 0321	0.3951 30
46-50	$1{:}5s_K$ $3{:}6d_{Kp}$ $3{:}6d_{L3}$ $1{:}6s_{L2}$ R	2325	26929	-14.3700 8651 1911	0.3515 90
51-55	$1{:}5s_K$ $3{:}6d_{Kp}$ $1{:}6s_{L1}$ $3{:}6d_{L4}$ R	2325	29254	-14.3700 8653 0577	0.0186 66
56-60	$1{:}5s_K$ $2{:}5p_{Kp}$ $2{:}5p_{L3}$ $3{:}6d_{L4}$ R	1595	30849	-14.3700 8664 4502	0.1139 25
61-65	$1{:}5s_K$ $3{:}6d_{Kp}$ $2{:}5p_{L3}$ $2{:}5p_{L4}$ R	1595	32444	-14.3700 8669 9962	0.0554 60
66-70	$2{:}5p_{Kp}$ $1{:}5s_K$ $2{:}5p_{L3}$ $3{:}6d_{L4}$ R	1595	34039	-14.3700 8680 8068	0.1081 06
71-75	$3{:}6d_{Kp}$ $2{:}5p_{Kp}$ $1{:}5s_{L1}$ $2{:}5p_{L4}$ R	1595	35634	-14.3700 8689 0055	0.0819 87
76	$2{:}5p_{Kp}$ $2{:}5p_{Kp}$ $1{:}5s_{L1}$ $3{:}6d_{L4}$	199	35833	-14.3700 8689 2303	0.0022 48
77	$4{:}7f_{Kp}$ $4{:}7f_{Kp}$ $2{:}5s_{L1}$ $2{:}5s_{L2}$	136	35969	-14.3700 8693 4379	0.0420 76
78	$4{:}7f_{Kp}$ $4{:}7f_{Kp}$ $2{:}5s_{L1}$ $2{:}5s_{L2}$ r_{12}	136	36105	-14.3700 8694 7436	0.0130 57
79	$4{:}7f_{Kp}$ $4{:}7f_{Kp}$ $2{:}6s_{L1}$ $2{:}6s_{L2}$ r_{34}	177	36282	-14.3700 8695 3786	0.0063 50
80	$4{:}7f_{Kp}$ $4{:}7f_{Kp}$ $2{:}5s_{L1}$ $2{:}5s_{L2}$ r_{13}	136	36418	-14.3700 8700 1775	0.0479 89
81	$4{:}7f_{Kp}$ $4{:}7f_{Kp}$ $2{:}6s_{L1}$ $2{:}6s_{L2}$ r_{14}	177	36595	-14.3700 8700 5380	0.0036 04
82-86	$1{:}6s_K$ $1{:}6s_K$ $4{:}7f_{L3}$ $4{:}7f_{L4}$ R	1320	37915	-14.3700 8704 3651	0.0382 71
87-89	$1{:}6s_K$ $4{:}7f_{Kp}$ $4{:}7f_{L3}$ $2{:}6s_{L2}$ R_1	1095	39010	-14.3700 8708 8108	0.0444 57
90	$1{:}6s_K$ $4{:}7f_{Kp}$ $4{:}7f_{L3}$ $2{:}6s_{L2}$ r_{13}	365	39375	-14.3700 8709 5577	0.0074 69
91	$1{:}6s_K$ $4{:}7f_{Kp}$ $2{:}6s_{L1}$ $4{:}7f_{L4}$	365	39740	-14.3700 8709 5872	0.0002 95
92	$1{:}6s_K$ $4{:}7f_{Kp}$ $2{:}6s_{L1}$ $4{:}7f_{L4}$ r_{12}	365	40105	-14.3700 8709 6056	0.0001 84
93-97	$2{:}5p_{Kp}$ $2{:}5p_{Kp}$ $3{:}6d_{L3}$ $3{:}6d_{L4}$ R	780	40885	-14.3700 8711 1337	0.0152 81
98-102	$2{:}5p_{1Kp}$ $2{:}5p_{1Kp}$ $3{:}6d_{-1L3}$ $3{:}6d_{-1L4}$ R	780	41665	-14.3700 8713 1530	0.0201 93
103	$3{:}6d_{Kp}$ $3{:}6d_{Kp}$ $2{:}6p_{L3}$ $2{:}6p_{L4}$	226	41891	-14.3700 8713 2928	0.0013 98
104	$3{:}6d_{Kp}$ $3{:}6d_{Kp}$ $2{:}6p_{L3}$ $2{:}6p_{L4}$ r_{12}	226	42117	-14.3700 8713 3729	0.0008 01
105	$3{:}6d_{Kp}$ $3{:}6d_{Kp}$ $2{:}5p_{L3}$ $2{:}5p_{L4}$ r_{34}	156	42273	-14.3700 8713 8774	0.0050 46
106-107	$3{:}6d_{Kp}$ $3{:}6d_{Kp}$ $2{:}6p_{L3}$ $2{:}6p_{L4}$ R_2	452	42725	-14.3700 8714 5136	0.0063 62
108-112	$3{:}6d_{1Kp}$ $3{:}6d_{1Kp}$ $2{:}6p_{-1L3}$ $2{:}6p_{-1L4}$ R	1130	43855	-14.3700 8716 2027	0.0168 91
113-136	CORE r-sum Adjustments				

Block(s)	Terms Added[ab]	N	N_{tot}	E(N_{tot}) (Ha)	$-\Delta E$ (μHa)
113	1:9s_K 1:9s_K 1:9s_{L1} 1:9s_{L2}-#1 [d]	1514	45369	-14.3700 8723 5369	0.0733 42
114	1:9s_K 1:9s_K 1:9s_{L1} 1:9s_{L2} r_{12}-#2 [d]	1514	46883	-14.3700 8735 2992	0.1176 23
115	1:9s_K 1:9s_K 1:9s_{L1} 1:9s_{L2} r_{34}-#3 [d]	1514	48397	-14.3700 8736 2801	0.0098 09
116	1:9s_K 1:9s_K 1:9s_{L1} 1:9s_{L2} r_{13}-#4 [d]	1514	49911	-14.3700 8739 4939	0.0321 38
117	1:9s_K 1:9s_K 1:9s_{L1} 1:9s_{L2} r_{14}-#5 [d]	2062	59173	-14.3700 8739 9722	0.0047 83
118	2:9p_{Kp} 2:9p_{Kp} 1:9s_{L1} 1:9s_{L2}-#6 [d]	1435	53408	-14.3700 8744 2258	0.0425 36
119	2:9p_{Kp} 2:9p_{Kp} 1:9s_{L1} 1:9s_{L2} r12-#7	592	54000	-14.3700 8746 7348	0.0250 90
120	2:9p_{Kp} 2:9p_{Kp} 1:9s_{L1} 1:9s_{L2} r13-#9 [d]	1435	55435	-14.3700 8750 0326	0.0329 78
121	2:9p_{Kp} 2:9p_{Kp} 1:9s_{L1} 1:9s_{L2} r14-#10 [d]	1435	56870	-14.3700 8750 6209	0.0058 83
122	1:9s_K 1:9s_K 2:8p_{L3} 2:8s_{L4}-#11	291	57161	-14.3700 8750 9080	0.0028 71
123	1:9s_K 1:9s_K 2:8p_{L3} 2:8s_{L4} r_{12}-#12	291	57452	-14.3700 8750 9989	0.0009 09
124	1:9s_K 1:9s_K 2:8p_{L3} 2:8s_{L4} r_{34}-#13	607	58059	-14.3700 8751 9068	0.0090 79
125	1:9s_K 1:9s_K 2:8p_{L3} 2:8s_{L4} r_{13}-#14	607	58666	-14.3700 8752 3990	0.0049 23
126	1:9s_K 1:9s_K 2:8p_{L3} 2:8s_{L4} r_{14}-#15	607	59273	-14.3700 8752 5902	0.0019 12
127	2:6p_{Kp} 2:6p_{Kp} 2:8p_{L3} 2:8p_{L4}-#16 [c]	285	59558	-14.3700 8752 6348	0.0004 46
128	2:6p_{Kp} 2:6p_{Kp} 2:8p_{L3} 2:8p_{L4} r12-#17 [c]	285	59843	-14.3700 8752 6933	0.0005 84
129	2:6p_{Kp} 2:6p_{Kp} 2:8p_{L3} 2:8p_{L4} r34-#18 [c]	285	60128	-14.3700 8752 7476	0.0005 44
130	2:6p_{Kp} 2:6p_{Kp} 2:8p_{L3} 2:8p_{L4} r13-#19 [c]	285	60413	-14.3700 8752 7716	0.0002 40
131	2:6p_{Kp} 2:6p_{Kp} 2:8p_{L3} 2:8p_{L4} r14-#20 [c]	285	60698	-14.3700 8752 7969	0.0002 53
132	2:6p_{1Kp} 2:6p_{1Kp} 2:8p_{-1L3} 2:8p_{-1L4}-#21 [c]	285	60983	-14.3700 8752 8440	0.0004 71
133	2:6p_{1Kp} 2:6p_{1Kp} 2:8p_{-1L3} 2:8p_{-1L4} r12-#22 [c]	285	61268	-14.3700 8752 8800	0.0003 60
134	2:6p_{1Kp} 2:6p_{1Kp} 2:8p_{-1L3} 2:8p_{-1L4} r34-#23 [c]	285	61553	-14.3700 8752 9223	0.0004 23
135	2:6p_{1Kp} 2:6p_{1Kp} 2:8p_{-1L3} 2:8p_{-1L4} r13-#24 [c]	285	61838	-14.3700 8752 9676	0.0004 53
136	2:6p_{1Kp} 2:6p_{1Kp} 2:8p_{-1L3} 2:8p_{-1L4} r14-#25 [c]	285	62123	-14.3700 8752 9980	0.0003 04
137-220	Final Adjustments				
137-141	2:5p_{Kp} 1:5s_K 1:5s_{L1} 2:5p_{L4} R	2000	64123	-14.3700 8756 4290	0.0343 10
142	2:5p_{Kp} 1:5s_K 2:5p_{L3} 1:5s_{L2}	400	64523	-14.3700 8756 8984	0.0046 94
143	2:5p_{Kp} 1:5s_K 2:5p_{L3} 1:5s_{L2} r_{12}	400	64923	-14.3700 8759 0397	0.0214 13
144	2:5p_{Kp} 1:5s_K 2:5p_{L3} 1:5s_{L2} r_{34}	400	65323	-14.3700 8759 2315	0.0019 18
145	2:5p_{Kp} 1:5s_K 2:5p_{L3} 1:5s_{L2} r_{13}	400	65723	-14.3700 8761 4636	0.0223 21
146	2:5p_{Kp} 1:5s_K 2:5p_{L3} 1:5s_{L2} r_{14}	400	66123	-14.3700 8761 5843	0.0012 07
147	3:6d_{Kp} 1:5s_K 1:5s_{L1} 3:6d_{L4}	395	66518	-14.3700 8763 1834	0.0159 91
148	3:6d_{Kp} 1:5s_K 1:5s_{L1} 3:6d_{L4} r_{12}	395	66913	-14.3700 8763 3153	0.0013 20
149-150	3:6d_{Kp} 1:5s_K 1:5s_{L1} 3:6d_{L4} R_2	790	67703	-14.3700 8763 7754	0.0046 01
151	3:6d_{Kp} 1:5s_K 3:6d_{L3} 1:5s_{L2} r_{12}	395	68098	-14.3700 8764 6577	0.0088 24
152	3:6d_{Kp} 1:5s_K 3:6d_{L3} 1:5s_{L2} r_{34}	395	68493	-14.3700 8765 1958	0.0053 81
153	3:6d_{Kp} 1:5s_K 3:6d_{L3} 1:5s_{L2} r_{14}	395	68888	-14.3700 8765 7928	0.0059 69
154	3:6d_{Kp} 2:5p_{Kp} 3:6d_{L3} 2:5p_{L4}	251	69139	-14.3700 8765 8284	0.0003 57
155	3:6d_{Kp} 2:5p_{Kp} 3:6d_{L3} 2:5p_{L4} r_{12}	251	69390	-14.3700 8766 0048	0.0017 64
156	3:6d_{1Kp} 2:5p_{1Kp} 3:6d_{-1L3} 2:5p_{-1L4}	251	69641	-14.3700 8766 0302	0.0002 54
157	3:6d_{Kp} 2:5p_{Kp} 2:5p_{L3} 3:6d_{L4}	251	69892	-14.3700 8767 4470	0.0141 68
158	3:6d_{Kp} 2:5p_{Kp} 2:5p_{L3} 3:6d_{L4} r_{12}	251	70143	-14.3700 8767 5974	0.0015 04
159	2:5p_{Kp} 3:6d_{Kp} 3:6d_{L3} 2:5p_{L4}	251	70394	-14.3700 8767 6480	0.0005 07
160	2:5p_{Kp} 3:6d_{Kp} 3:6d_{L3} 2:5p_{L4} r_{12}	251	70645	-14.3700 8767 6947	0.0004 66
161	2:5p_{Kp} 3:6d_{Kp} 2:5p_{L3} 3:6d_{L4}	251	70896	-14.3700 8768 0338	0.0033 91

Block(s)	Terms Added[ab]	N	N_{tot}	E(N_{tot}) (Ha)	$-\Delta E$ (μHa)
162	$3{:}6d_{-1Kp}$ $2{:}5p_{1Kp}$ $2{:}5p_{-1L3}$ $3{:}6d_{1L4}$	251	71147	-14.3700 8769 0164	0.0098 27
163	$2{:}5p_{Kp}$ $2{:}5p_{Kp}$ $1{:}5s_{L1}$ $3{:}6d_{L4}$ r_{12}	199	71346	-14.3700 8769 0941	0.0007 77
164	$2{:}5p_{Kp}$ $2{:}5p_{Kp}$ $1{:}5s_{L1}$ $3{:}6d_{L4}$ r_{14}	199	71545	-14.3700 8769 1324	0.0003 83
165	$2{:}5p_{Kp}$ $3{:}6d_{Kp}$ $1{:}5s_{L1}$ $2{:}5p_{L4}$	319	71864	-14.3700 8769 2432	0.0011 08
166	$2{:}5p_{Kp}$ $3{:}6d_{Kp}$ $1{:}5s_{L1}$ $2{:}5p_{L4}$ r_{12}	319	72183	-14.3700 8769 3616	0.0011 84
167	$2{:}5p_{Kp}$ $3{:}6d_{Kp}$ $1{:}5s_{L1}$ $2{:}5p_{L4}$ r_{14}	319	72502	-14.3700 8769 4475	0.0008 58
168	$2{:}5p_{Kp}$ $1{:}5s_{K}$ $3{:}6d_{L3}$ $2{:}5p_{L4}$ r_{12}	319	72821	-14.3700 8769 6866	0.0023 91
169	$2{:}5p_{Kp}$ $1{:}5s_{K}$ $3{:}6d_{L3}$ $2{:}5p_{L4}$ r_{13}	319	73140	-14.3700 8769 7693	0.0008 27
170	$3{:}6d_{Kp}$ $2{:}5p_{Kp}$ $2{:}5p_{L3}$ $1{:}5s_{L2}$	319	73459	-14.3700 8770 6143	0.0084 50
171	$3{:}6d_{Kp}$ $2{:}5p_{Kp}$ $2{:}5p_{L3}$ $1{:}5s_{L2}$ r_{12}	319	73778	-14.3700 8772 0903	0.0147 60
172	$3{:}6d_{Kp}$ $2{:}5p_{Kp}$ $2{:}5p_{L3}$ $1{:}5s_{L2}$ r_{13}	319	74097	-14.3700 8773 2086	0.0111 83
173	$3{:}6d_{Kp}$ $2{:}5p_{Kp}$ $2{:}5p_{L3}$ $1{:}5s_{L2}$ r_{14}	319	74416	-14.3700 8773 2385	0.0002 99
174	$3{:}6d_{Kp}$ $1{:}5s_{K}$ $2{:}5p_{L3}$ $2{:}5p_{L4}$	319	74735	-14.3700 8773 3471	0.0010 86
175	$3{:}6d_{Kp}$ $1{:}5s_{K}$ $2{:}5p_{L3}$ $2{:}5p_{L4}$ r_{13}	319	75054	-14.3700 8773 4661	0.0011 91
176	$3{:}6d_{Kp}$ $1{:}5s_{K}$ $2{:}5p_{L3}$ $2{:}5p_{L4}$ r_{14}	319	75373	-14.3700 8773 5377	0.0007 15
177	$2{:}5p_{Kp}$ $3{:}6d_{Kp}$ $2{:}5p_{L3}$ $1{:}5s_{L2}$	319	75692	-14.3700 8773 9396	0.0040 19
178	$2{:}5p_{Kp}$ $3{:}6d_{Kp}$ $2{:}5p_{L3}$ $1{:}5s_{L2}$ r_{12}	319	76011	-14.3700 8774 1916	0.0025 20
179	$2{:}5p_{Kp}$ $3{:}6d_{Kp}$ $2{:}5p_{L3}$ $1{:}5s_{L2}$ r_{13}	319	76330	-14.3700 8774 3867	0.0019 51
180	$2{:}5p_{Kp}$ $3{:}6d_{Kp}$ $2{:}5p_{L3}$ $1{:}5s_{L2}$ r_{14}	319	76649	-14.3700 8774 4199	0.0003 32
181	$3{:}6d_{Kp}$ $3{:}6d_{Kp}$ $3{:}6d_{L3}$ $3{:}6d_{L4}$ r_{34}	136	76785	-14.3700 8774 4356	0.0001 57
182	$3{:}6d_{1Kp}$ $3{:}6d_{1Kp}$ $3{:}6d_{-1L3}$ $3{:}6d_{-1L4}$	136	76921	-14.3700 8774 4710	0.0003 53
183	$3{:}6d_{1Kp}$ $3{:}6d_{1Kp}$ $3{:}6d_{-1L3}$ $3{:}6d_{-1L4}$ r_{34}	136	77057	-14.3700 8774 5838	0.0011 29
184	$3{:}6d_{Kp}$ $3{:}6d_{Kp}$ $1{:}5s_{L1}$ $3{:}6d_{L4}$	189	77246	-14.3700 8774 6102	0.0002 64
185	$3{:}6d_{Kp}$ $3{:}6d_{Kp}$ $1{:}5s_{L1}$ $3{:}6d_{L4}$ r_{12}	189	77435	-14.3700 8774 6228	0.0001 26
186	$3{:}6d_{Kp}$ $3{:}6d_{Kp}$ $1{:}5s_{L1}$ $3{:}6d_{L4}$ r_{14}	189	77624	-14.3700 8774 6388	0.0001 60
187	$3{:}6d_{Kp}$ $3{:}6d_{Kp}$ $3{:}6d_{L3}$ $1{:}5s_{L2}$	189	77813	-14.3700 8774 7565	0.0011 77
188	$3{:}6d_{Kp}$ $3{:}6d_{Kp}$ $3{:}6d_{L4}$ $1{:}5s_{L2}$ r_{13}	189	78002	-14.3700 8774 8561	0.0009 97
189	$2{:}8p_{Kp}$ $2{:}8p_{Kp}$ $4{:}7f_{L3}$ $4{:}7f_{L4}$ r_{12}	199	78201	-14.3700 8774 8841	0.0002 80
190	$2{:}8p_{1Kp}$ $2{:}8p_{1Kp}$ $4{:}7f_{-1L3}$ $4{:}7f_{-1L4}$ r_{12}	199	78400	-14.3700 8774 9703	0.0008 61
191	$4{:}7f_{Kp}$ $4{:}7f_{Kp}$ $2{:}6p_{L3}$ $2{:}6p_{L4}$ r_{14}	177	78577	-14.3700 8774 9805	0.0001 03
192	$1{:}5s_{K}$ $4{:}7f_{Kp}$ $2{:}5p_{L3}$ $3{:}6d_{L4}$	305	78882	-14.3700 8775 0085	0.0002 80
193	$1{:}5s_{K}$ $4{:}7f_{Kp}$ $3{:}6d_{L3}$ $2{:}5p_{L4}$	305	79187	-14.3700 8775 0566	0.0004 81
194	$3{:}6d_{Kp}$ $1{:}5s_{K}$ $4{:}7f_{L3}$ $2{:}5p_{L4}$	305	79492	-14.3700 8775 1010	0.0004 44
195	$2{:}5p_{Kp}$ $4{:}7f_{Kp}$ $3{:}6d_{l3}$ $1{:}5s_{L2}$	305	79797	-14.3700 8775 3059	0.0020 50
196	$2{:}5p_{Kp}$ $4{:}7f_{Kp}$ $3{:}6d_{l3}$ $1{:}5s_{L2}$ r_{12}	305	80102	-14.3700 8775 3996	0.0009 37
197	$2{:}5p_{Kp}$ $4{:}7f_{Kp}$ $3{:}6d_{l3}$ $1{:}5s_{L2}$ r_{13}	305	80407	-14.3700 8775 5197	0.0012 01
198-200	$3{:}6d_{Kp}$ $4{:}7f_{Kp}$ $2{:}5p_{l3}$ $1{:}5s_{L2}$ R_1	915	81322	-14.3700 8775 7991	0.0027 94
201-203	$1{:}6s_{K1}$ $1{:}6s_{K1}$ $1{:}6s_{L1}$ $1{:}6s_{L2}$ R_1	2196	83518	-14.3700 8783 1268	0.0732 77
204	$1{:}6s_{K1}$ $1{:}6s_{K1}$ $1{:}6s_{L1}$ $1{:}6s_{L2}$ r_{13}	732	84250	-14.3700 8783 3151	0.0018 83
205	$1{:}9s_{K1}$ $1{:}9s_{K1}$ $1{:}6s_{L1}$ $1{:}7s_{L2}$-#201	652	84902	-14.3700 8783 6424	0.0032 73
206	$1{:}9s_{K1}$ $1{:}9s_{K1}$ $1{:}6s_{L1}$ $1{:}7s_{L2}$ r_{12}-#202	652	85554	-14.3700 8783 8989	0.0025 65
207	$1{:}9s_{K1}$ $1{:}9s_{K1}$ $1{:}6s_{L1}$ $1{:}7s_{L2}$ r_{13}-#204	652	86206	-14.3700 8784 0036	0.0010 47
208	$4{:}7f_{Kp}$ $4{:}7f_{Kp}$ $2{:}6s_{L1}$ $1{:}7s_{L2}$-#77 [d]	273	86479	-14.3700 8784 1049	0.0010 13
209	$4{:}7f_{Kp}$ $4{:}7f_{Kp}$ $2{:}6s_{L1}$ $1{:}7s_{L2}$ r_{13}-#80	170	86649	-14.3700 8785 2992	0.0119 43
210	$1{:}7s_{K}$ $2{:}7p_{Kp}$ $2{:}7p_{L3}$ $1{:}7s_{L2}$-#26	1046	87695	-14.3700 8785 5063	0.0020 71

Block(s)	Terms Added[ab]	N	N_{tot}	E(N_{tot}) (Ha)	$-\Delta E$ (μHa)
211	1:7s_K 2:7p_{Kp} 2:7p_{L3} 1:7s_{L2} r_{12}-#27	1046	88741	-14.3700 8787 1791	0.0167 28
212	1:7s_K 2:7p_{Kp} 2:7p_{L3} 1:7s_{L2} r_{13}-#29	1046	89787	-14.3700 8787 2899	0.0011 08
213	2:7p_{Kp} 1:7s_K 2:7p_{L3} 1:7s_{L2}-#142	1046	90833	-14.3700 8787 4359	0.0014 60
214	2:7p_{Kp} 1:7s_K 2:7p_{L3} 1:7s_{L2} r_{12}-#143	1046	91879	-14.3700 8787 6448	0.0020 89
215	2:7p_{Kp} 1:7s_K 2:7p_{L3} 1:7s_{L2} r_{13}-#145	1046	92925	-14.3700 8787 7770	0.0013 22
216	3:7d_{Kp} 2:7p_{Kp} 2:7p_{L3} 1:7s_{L2}-#170	637	93562	-14.3700 8787 9517	0.0017 47
217	3:7d_{Kp} 2:7p_{Kp} 2:7p_{L3} 1:7$s_{L2}r_{12}$-#171	637	94199	-14.3700 8788 4911	0.0053 94
218	1:7s_K 1:7s_{L1} 1:7s_K 1:7s_{L2}	1800	95999	-14.3700 8788 6481	0.0015 70
219	1:7s_K 1:7s_{L1} 1:7s_K 1:7s_{L2} r_{12}	2095	98074	-14.3700 8788 7958	0.0014 77
220	1:7s_K 1:7s_{L1} 1:7s_K 1:7s_{L2} r_{13}	1800	99874	-14.3700 8789 0422	0.0024 64

[a] K shell orbital exponents are $K = 3.80618, K_p = 5.1, K_1 = 10.0$; [b] L shell orbital exponents are $L_1 = 1.73, L_2 = 0.367, L_3 = 1.163, L_4 = 0.525$; [c] r-sum = 24; [d] r-sum = 20.

Table A3. Hy-CI expansion of the 5 ^1S excited state of Be (in Ha), a 99,965 term s,p,d,f expansion. In the table, R_1 = $\{1,r_{12},r_{34}\}$, R_2 = $\{r_{13},r_{14}\}$, R = $\{1,r_{12},r_{34},r_{13},r_{14}\}$, N is the number of terms added, and N_{tot} is the cumulative number of terms. The terms are r-sum filtered using N_{max} = 16 (see text) unless an explicit r-sum N_{max} value is given.

Block(s)	Terms Added[ab]	N	N_{tot}	E(N_{tot}) (Ha)	$-\Delta E$ (μHa)
1-25	CORE				
1-3	$1{:}9s_K\ 1{:}9s_K\ 1{:}6s_{L_1}\ 1{:}7s_{L_2}\ R_1$	4152	4152	-14.3505 3008 2288	
4	$1{:}9s_K\ 1{:}9s_K\ 1{:}6s_{L_1}\ 1{:}7s_{L_2}\ r_{13}$	1334	5536	-14.3506 8541 3180	155.3308 92
5	$1{:}6s_K\ 1{:}6s_K\ 1{:}6s_{L_1}\ 1{:}7s_{L_2}\ r_{14}$	836	6372	-14.3506 9067 9336	5.2661 56
6-10	$2{:}7p_{Kp}\ 2{:}7p_{Kp}\ 1{:}6s_{L_1}\ 1{:}7s_{L_2}\ R$	3770	10142	-14.3513 6732 6585	676.6472 49
11	$1{:}9s_K\ 1{:}9s_K\ 2{:}6p_{L3}\ 2{:}7p_{L4}$	900	11042	-14.3514 6966 7949	102.3413 64
12	$1{:}9s_K\ 1{:}9s_K\ 2{:}6p_{L3}\ 2{:}7p_{L4}\ r_{12}$	900	11942	-14.3514 9298 4558	23.3166 09
13	$1{:}6s_K\ 1{:}6s_K\ 2{:}6p_{L3}\ 2{:}7p_{L4}\ r_{34}$	584	12526	-14.3514 9613 3941	3.1493 82
14-15	$1{:}6s_K\ 1{:}6s_K\ 2{:}6p_{L3}\ 2{:}7p_{L4}R_2$	1168	13694	-14.3515 0108 9176	4.9552 35
16-20	$2{:}6p_{0Kp}\ 2{:}6p_{0Kp}\ 2{:}6p_{0L3}\ 2{:}7p_{0L4}\ R$ [c]	2250	15944	-14.3515 0222 5665	1.1364 89
21-25	$2{:}6p_{1Kp}\ 2{:}6p_{1Kp}\ 2{:}6p_{-1L3}\ 2{:}7p_{-1L4}\ R$ [c]	2250	18194	-14.3515 0331 3834	1.0881 69
26-112	Post-CORE				
26-30	$1{:}5s_K\ 2{:}5p_{Kp}\ 2{:}5p_{L3}\ 1{:}5s_{L2}\ R$	2000	20194	-14.3515 0677 9198	3.4653 64
31-35	$1{:}5s_K\ 2{:}5p_{Kp}\ 1{:}5s_{L1}\ 2{:}5p_{L4}\ R$	2000	22194	-14.3515 0738 0240	0.6010 42
36-40	$3{:}6d_{Kp}\ 3{:}6d_{Kp}\ 1{:}5s_{L1}\ 1{:}5s_{L2}\ R$	1230	23424	-14.3515 0923 5708	1.8554 68
41-45	$1{:}5s_K\ 1{:}5s_K\ 3{:}6d_{L3}\ 3{:}6d_{L4}\ R$	1180	24604	-14.3515 0974 7205	0.5114 97
46-50	$1{:}5s_K\ 3{:}6d_{Kp}\ 3{:}6d_{L3}\ 1{:}6s_{L2}\ R$	2325	26929	-14.3515 1014 5365	0.3981 60
51-55	$1{:}5s_K\ 3{:}6d_{Kp}\ 1{:}6s_{L1}\ 3{:}6d_{L4}\ R$	2325	29254	-14.3515 1015 9299	0.0139 34
56-60	$1{:}5s_K\ 2{:}5p_{Kp}\ 2{:}5p_{L3}\ 3{:}6d_{L4}\ R$	1595	30849	-14.3515 1023 1314	0.0720 15
61-65	$1{:}5s_K\ 3{:}6d_{Kp}\ 2{:}5p_{L3}\ 2{:}5p_{L4}\ R$	1595	32444	-14.3515 1026 9783	0.0384 69
66-70	$2{:}5p_{Kp}\ 1{:}5s_K\ 2{:}5p_{L3}\ 3{:}6d_{L4}\ R$	1595	34039	-14.3515 1031 8475	0.0486 92
71-75	$3{:}6d_{Kp}\ 2{:}5p_{Kp}\ 1{:}5s_{L1}\ 2{:}5p_{L4}\ R$	1595	35634	-14.3515 1037 0754	0.0522 79
76	$2{:}5p_{Kp}\ 2{:}5p_{Kp}\ 1{:}5s_{L1}\ 3{:}6d_{L4}$	199	35833	-14.3515 1037 3500	0.0027 46
77	$4{:}7f_{Kp}\ 4{:}7f_{Kp}\ 2{:}5s_{L1}\ 2{:}5s_{L2}$	136	35969	-14.3515 1043 3480	0.0599 80
78	$4{:}7f_{Kp}\ 4{:}7f_{Kp}\ 2{:}5s_{L1}\ 2{:}5s_{L2}\ r_{12}$	136	36105	-14.3515 1045 0334	0.0168 54
79	$4{:}7f_{Kp}\ 4{:}7f_{Kp}\ 2{:}6s_{L1}\ 2{:}6s_{L2}\ r_{34}$	177	36282	-14.3515 1045 9537	0.0092 03
80	$4{:}7f_{Kp}\ 4{:}7f_{Kp}\ 2{:}5s_{L1}\ 2{:}5s_{L2}\ r_{13}$	136	36418	-14.3515 1050 9968	0.0504 31
81	$4{:}7f_{Kp}\ 4{:}7f_{Kp}\ 2{:}6s_{L1}\ 2{:}6s_{L2}\ r_{14}$	177	36595	-14.3515 1051 6355	0.0063 87
82-86	$1{:}6s_K\ 1{:}6s_K\ 4{:}7f_{L3}\ 4{:}7f_{L4}\ R$	1320	37915	-14.3515 1056 0598	0.0442 43
87-89	$1{:}6s_K\ 4{:}7f_{Kp}\ 4{:}7f_{L3}\ 2{:}6s_{L2}\ R_1$	1095	39010	-14.3515 1062 1506	0.0609 08
90	$1{:}6s_K\ 4{:}7f_{Kp}\ 4{:}7f_{L3}\ 2{:}6s_{L2}\ r_{13}$	365	39375	-14.3515 1063 2214	0.0107 08
91	$1{:}6s_K\ 4{:}7f_{Kp}\ 2{:}6s_{L1}\ 4{:}7f_{L4}$	365	39740	-14.3515 1063 2868	0.0006 54
92	$1{:}6s_K\ 4{:}7f_{Kp}\ 2{:}6s_{L1}\ 4{:}7f_{L4}\ r_{12}$	365	40105	-14.3515 1063 3093	0.0002 25
93-97	$2{:}5p_{Kp}\ 2{:}5p_{Kp}\ 3{:}6d_{L3}\ 3{:}6d_{L4}\ R$	780	40885	-14.3515 1063 7937	0.0048 44
98-102	$2{:}5p_{1Kp}\ 2{:}5p_{1Kp}\ 3{:}6d_{-1L3}\ 3{:}6d_{-1L4}\ R$	780	41665	-14.3515 1065 2423	0.0144 86
103	$3{:}6d_{Kp}\ 3{:}6d_{Kp}\ 2{:}6p_{L3}\ 2{:}6p_{L4}$	226	41891	-14.3515 1065 3246	0.0008 23
104	$3{:}6d_{Kp}\ 3{:}6d_{Kp}\ 2{:}6p_{L3}\ 2{:}6p_{L4}\ r_{12}$	226	42117	-14.3515 1065 3937	0.0006 91
105	$3{:}6d_{Kp}\ 3{:}6d_{Kp}\ 2{:}5p_{L3}\ 2{:}5p_{L4}\ r_{34}$	156	42273	-14.3515 1065 4612	0.0006 75
106-107	$3{:}6d_{Kp}\ 3{:}6d_{Kp}\ 2{:}6p_{L3}\ 2{:}6p_{L4}\ R_2$	452	42725	-14.3515 1065 7116	0.0025 04
108-112	$3{:}6d_{1Kp}\ 3{:}6d_{1Kp}\ 2{:}6p_{-1L3}\ 2{:}6p_{-1L4}\ R$	1130	43855	-14.3515 1066 4755	0.0076 39
113-136	CORE r-Sum Adjustments				

Block(s)	Terms Added[ab]	N	N_{tot}	E(N_{tot}) (Ha)	$-\Delta E$ (μHa)
113	1:9s_K 1:9s_K 1:9s_{L1} 1:9s_{L2}-#1 [d]	1514	45369	-14.3515 1078 7745	0.1229 90
114	1:9s_K 1:9s_K 1:9s_{L1} 1:9s_{L2} r_{12}-#2 [d]	1514	46883	-14.3515 1095 4929	0.1671 84
115	1:9s_K 1:9s_K 1:9s_{L1} 1:9s_{L2} r_{34}-#3 [d]	1514	48397	-14.3515 1096 9307	0.0143 78
116	1:9s_K 1:9s_K 1:9s_{L1} 1:9s_{L2} r_{13}-#4 [d]	1514	49911	-14.3515 1101 8927	0.0496 20
117	1:9s_K 1:9s_K 1:9s_{L1} 1:9s_{L2} r_{14}-#5 [d]	2062	51973	-14.3515 1102 5455	0.0065 28
118	2:9p_{Kp} 2:9p_{Kp} 1:9s_{L1} 1:9s_{L2}-#6 [d]	1435	53408	-14.3515 1109 6174	0.0707 19
119	2:9p_{Kp} 2:9p_{Kp} 1:9s_{L1} 1:9s_{L2} r_{12}-#7	592	54000	-14.3515 1113 0108	0.0339 34
120	2:9p_{Kp} 2:9p_{Kp} 1:9s_{L1} 1:9s_{L2} r_{13}-#9 [d]	1435	55435	-14.3515 1116 8647	0.0385 39
121	2:9p_{Kp} 2:9p_{Kp} 1:9s_{L1} 1:9s_{L2} r_{14}-#10 [d]	1435	56870	-14.3515 1117 4079	0.0054 32
122	1:9s_K 1:9s_K 2:8p_{L3} 2:8s_{L4}-#11	291	57161	-14.3515 1117 7168	0.0030 89
123	1:9s_K 1:9s_K 2:8p_{L3} 2:8s_{L4} r_{12}-#12	291	57452	-14.3515 1120 8145	0.0309 78
124	1:9s_K 1:9s_K 2:8p_{L3} 2:8s_{L4} r_{34}-#13	607	58059	-14.3515 1121 1522	0.0033 76
125	1:9s_K 1:9s_K 2:8p_{L3} 2:8s_{L4} r_{13}-#14	607	58666	-14.3515 1121 7205	0.0056 83
126	1:9s_K 1:9s_K 2:8p_{L3} 2:8s_{L4} r_{14}-#15	607	59273	-14.3515 1121 8525	0.0013 20
127	2:6p_{Kp} 2:6p_{Kp} 2:8p_{L3} 2:8p_{L4}-#16 [c]	285	59558	-14.3515 1121 9497	0.0009 72
128	2:6p_{Kp} 2:6p_{Kp} 2:8p_{L3} 2:8p_{L4} r_{12}-#17 [c]	285	59843	-14.3515 1122 0117	0.0006 21
129	2:6p_{Kp} 2:6p_{Kp} 2:8p_{L3} 2:8p_{L4} r_{34}-#18 [c]	285	60128	-14.3515 1122 0677	0.0005 59
130	2:6p_{Kp} 2:6p_{Kp} 2:8p_{L3} 2:8p_{L4} r_{13}-#19 [c]	285	60413	-14.3515 1122 0889	0.0002 12
131	2:6p_{Kp} 2:6p_{Kp} 2:8p_{L3} 2:8p_{L4} r_{14}-#20 [c]	285	60698	-14.3515 1122 1212	0.0003 24
132	2:6p_{1Kp} 2:6p_{1Kp} 2:8p_{-1L3} 2:8p_{-1L4}-#21 [c]	285	60983	-14.3515 1122 2192	0.0009 80
133	2:6p_{1Kp} 2:6p_{1Kp} 2:8p_{-1L3} 2:8p_{-1L4} r_{12}-#22 [c]	285	61268	-14.3515 1122 3157	0.0009 65
134	2:6p_{1Kp} 2:6p_{1Kp} 2:8p_{-1L3} 2:8p_{-1L4} r_{34}-#23 [c]	285	61553	-14.3515 1122 3648	0.0004 91
135	2:6p_{1Kp} 2:6p_{1Kp} 2:8p_{-1L3} 2:8p_{-1L4} r_{13}-#24 [c]	285	61838	-14.3515 1122 3889	0.0002 40
136	2:6p_{1Kp} 2:6p_{1Kp} 2:8p_{-1L3} 2:8p_{-1L4} r_{14}-#25 [c]	285	62123	-14.3515 1122 4141	0.0002 53
137-181	Final Adjustments				
137	1:7s_K 2:8p_{Kp} 2:8p_{L3} 1:7s_{L2}-#26	1346	63469	-14.3515 1124 3213	0.0190 72
138	1:7s_K 2:8p_{Kp} 2:8p_{L3} 1:7s_{L2} r_{12}-#27	1346	64815	-14.3515 1128 8578	0.0453 66
139	1:7s_K 2:8p_{Kp} 2:8p_{L3} 1:7s_{L2} r_{13}-#29	1346	66161	-14.3515 1129 8688	0.0101 10
140	4:7f_{Kp} 4:7f_{Kp} 2:7s_{L1} 2:7s_{L2}-#77 [d]	200	66361	-14.3515 1130 0410	0.0017 21
141	4:7f_{Kp} 4:7f_{Kp} 2:7s_{L1} 2:7s_{L2} r_{12}-#78	67	66428	-14.3515 1130 0841	0.0004 32
142	4:7f_{Kp} 4:7f_{Kp} 2:7s_{L1} 2:7s_{L2} r_{13}-#80	67	66495	-14.3515 1130 8758	0.0079 16
143	2:7p_{Kp} 1:7s_K 1:7s_{L1} 2:7p_{L4}	1446	67941	-14.3515 1131 2167	0.0034 09
144	2:5p_{Kp} 1:5s_K 1:5s_{L1} 2:5p_{L4} r_{12}	400	68341	-14.3515 1131 8264	0.0060 97
145	2:7p_{Kp} 1:7s_K 1:7s_{L1} 2:7p_{L4} r_{34}	1446	69787	-14.3515 1132 1998	0.0037 34
146	2:7p_{Kp} 1:7s_K 1:7s_{L1} 2:7p_{L4} r_{13}	1446	71233	-14.3515 1132 4515	0.0025 17
147	2:5p_{Kp} 1:5s_K 1:5s_{L1} 2:5p_{L4} r_{14}	400	71633	-14.3515 1132 7012	0.0024 97
148	2:7p_{Kp} 1:7s_K 2:7p_{L3} 1:7s_{L2}	1446	73079	-14.3515 1135 2397	0.0253 85
149	2:7p_{Kp} 1:7s_K 2:7p_{L3} 1:7s_{L2} r_{12}	1446	74525	-14.3515 1136 1685	0.0092 88
150	2:5p_{Kp} 1:5s_K 2:5p_{L3} 1:5s_{L2} r_{34}	400	74925	-14.3515 1136 3495	0.0018 09
151	2:7p_{Kp} 1:7s_K 2:7p_{L3} 1:7s_{L2} r_{13}	1446	76371	-14.3515 1143 2501	0.0690 07
152	2:5p_{Kp} 1:5s_K 2:5p_{L3} 1:5s_{L2} r_{14}	400	76771	-14.3515 1143 3055	0.0005 54
153	3:6d_{Kp} 1:7s_K 1:7s_{L1} 3:7d_{L4}	790	77561	-14.3515 1143 4748	0.0016 93
154	3:6d_{Kp} 1:7s_K 1:7s_{L1} 3:7d_{L4} r_{12}	790	78351	-14.3515 1143 5507	0.0007 59
155	3:6d_{Kp} 1:7s_K 1:7s_{L1} 3:7d_{L4} r_{13}	790	79141	-14.3515 1143 5758	0.0002 51
156	3:6d_{Kp} 1:5s_K 1:5s_{L1} 3:6d_{L4} r_{14}	395	79536	-14.3515 1143 6772	0.0010 14

Block(s)	Terms Added[ab]	N	N_{tot}	E(N_{tot}) (Ha)	$-\Delta E$ (μHa)
157	3:6d_{Kp} 1:7s_K 3:7d_{L3} 1:7s_{L2}	790	80326	-14.3515 1146 9306	0.0325 33
158	3:6d_{Kp} 1:7s_K 3:7d_{L3} 1:7s_{L2} r_{12}	790	81116	-14.3515 1148 3453	0.0141 48
159	3:6d_{Kp} 1:5s_K 3:6d_{L3} 1:5s_{L2} r_{34}	395	81511	-14.3515 1148 4053	0.0006 00
160	3:6d_{Kp} 1:7s_K 3:7d_{L3} 1:7s_{L2} r_{13}	790	82301	-14.3515 1149 4077	0.0100 24
161	3:6d_{Kp} 1:5s_K 3:6d_{L3} 1:5s_{L2} r_{14}	395	82696	-14.3515 1149 5261	0.0011 84
162	3:6d_{Kp} 2:5p_{Kp} 3:6d_{L3} 2:5p_{LA} r_{12}	251	82947	-14.3515 1149 6142	0.0008 81
163	3:6d_{Kp} 2:5p_{Kp} 2:5p_{L3} 3:6d_{L4}	251	83198	-14.3515 1149 7185	0.0010 43
164	3:6d_{Kp} 2:5p_{Kp} 2:5p_{L3} 3:6d_{L4} r_{12}	251	83449	-14.3515 1149 7506	0.0003 21
165	2:5p_{Kp} 3:6d_{Kp} 2:5p_{L3} 3:6d_{L4}	251	83700	-14.3515 1149 8327	0.0008 21
166	2:5p_{Kp} 3:6d_{Kp} 1:5s_{L1} 2:5p_{L4}	319	84019	-14.3515 1149 8944	0.0006 17
167	2:5p_{Kp} 1:5s_K 3:6d_{L3} 2:5p_{L4} r_{12}	319	84338	-14.3515 1150 0107	0.0011 62
168	3:6d_{Kp} 2:7p_{Kp} 2:7p_{L3} 1:7s_{L2}	815	85153	-14.3515 1155 1271	0.0511 64
169	3:6d_{Kp} 2:7p_{Kp} 2:7p_{L3} 1:7s_{L2} r_{12}	815	85968	-14.3515 1157 8597	0.0273 26
170	3:6d_{Kp} 2:7p_{Kp} 2:7p_{L3} 1:7s_{L2} r_{13}	815	86783	-14.3515 1159 8799	0.0202 02
171	2:7p_{Kp} 3:6d_{Kp} 2:7p_{L3} 1:7s_{L2}	815	87598	-14.3515 1160 0896	0.0020 97
172	2:7p_{Kp} 3:6d_{Kp} 2:7p_{L3} 1:7s_{L2} r_{12}	815	88413	-14.3515 1160 2375	0.0014 79
173	2:7p_{Kp} 3:6d_{Kp} 2:7p_{L3} 1:7s_{L2} r_{13}	815	89228	-14.3515 1160 5096	0.0027 20
174	1:6s_{K1} 1:6s_{K1} 1:7s_{L1} 1:7s_{L2}	949	90177	-14.3515 1163 9075	0.0339 79
175	1:8s_{K1} 1:8s_{K1} 1:7s_{L1} 1:7s_{L2} r$_{12}$	1371	91548	-14.3515 1166 3928	0.0248 53
176	1:6s_{K1} 1:6s_{K1} 1:7s_{L1} 1:7s_{L2} r$_{34}$	949	92497	-14.3515 1166 6025	0.0020 98
177	1:8s_{K1} 1:8s_{K1} 1:7s_{L1} 1:7s_{L2} r$_{13}$	1371	93868	-14.3515 1166 8402	0.0023 77
178	1:8s_{K1} 1:8s_{K1} 1:7s_{L1} 1:7s_{L2}-#174	422	94290	-14.3515 1166 8889	0.0004 86
179	1:7s_K 1:7s_{L1} 1:7s_K 1:7s_{L2}	1800	96090	-14.3515 1167 0654	0.0017 66
180	1:7s_K 1:7s_{L1} 1:7s_K 1:7s_{L2} r_{12}	2075	98165	-14.3515 1167 2630	0.0019 76
181	1:7s_K 1:7s_{L1} 1:7s_K 1:7s_{L2} r_{13}	1800	99965	-14.3515 1167 6045	0.0034 15

[a]K shell orbital exponents are K = 3.8, K_p = 5.07, K_1 = 10.0; [b]L shell orbital exponents are L_1 = 1.692, L_2 = 0.259, L_3 = 1.163, L_4 = 0.525;
[c]r-sum = 24; [d]r-sum = 20.

Table A4. Hy-CI expansion of the 6 ^1S excited state of Be (in Ha), a 92,930 term s,p,d,f expansion. In the table, R_1 = $\{1,r_{12},r_{34}\}$, R_2 = $\{r_{13},r_{14}\}$, R = $\{1,r_{12},r_{34},r_{13},r_{14}\}$, N is the number of terms added and N_{tot} is the cumulative number of terms. The terms are r-sum filtered using N_{max} = 16 (see text) unless an explicit r-sum N_{max} value is given.

Block(s)	Terms Added[ab]	N	N_{tot}	E(N_{tot}) (Ha)	$-\Delta$E (μHa)
1-25	CORE				
1-3	$1{:}9s_K\ 1{:}9s_K\ 1{:}6s_{L_1}\ 1{:}7s_{L_2}\ R_1$	4152	4152	-14.3414 8520 1215	
4	$1{:}9s_K\ 1{:}9s_K\ 1{:}6s_{L_1}\ 1{:}7s_{L_2}\ r_{13}$	1384	5536	-14.3416 4726 5202	162.0639 86
5	$1{:}6s_K\ 1{:}6s_K\ 1{:}6s_{L_1}\ 1{:}7s_{L_2}\ r_{14}$	836	6172	-14.3416 5196 4453	4.6992 51
6-10	$2{:}7p_{Kp}\ 2{:}7p_{Kp}\ 1{:}6s_{L_1}\ 1{:}7s_{L_2}\ R$	3770	10142	-14.3422 7779 5505	625.831 05
11	$1{:}9s_K\ 1{:}9s_K\ 2{:}6p_{L3}\ 2{:}7p_{L4}$	900	11042	-14.3423 6751 1916	89.7164 11
12	$1{:}9s_K\ 1{:}9s_K\ 2{:}6p_{L3}\ 2{:}7p_{L4}\ r_{12}$	900	11942	-14.3423 8278 7530	15.2756 14
13	$1{:}6s_K\ 1{:}6s_K\ 2{:}6p_{L3}\ 2{:}7p_{L4}\ r_{34}$	584	12526	-14.3423 8849 2445	5.7049 14
14-15	$1{:}6s_K\ 1{:}6s_K\ 2{:}6p_{L3}\ 2{:}7p_{L4}R_2$	1168	13694	-14.3423 9206 6125	3.5736 80
16-20	$2{:}6p_{0Kp}\ 2{:}6p_{0Kp}\ 2{:}6p_{0L3}\ 2{:}7p_{0L4}\ R$ [c]	2250	15944	-14.3423 9280 8996	0.7428 71
21-25	$2{:}6p_{1Kp}\ 2{:}6p_{1Kp}\ 2{:}6p_{-1L3}\ 2{:}7p_{-1L4}\ R$ [c]	2250	18194	-14.3423 9354 8636	0.7396 40
26-112	Post-CORE				
26-30	$1{:}5s_K\ 2{:}5p_{Kp}\ 2{:}5p_{L3}\ 1{:}6s_{L2}\ R$	2395	20589	-14.3423 9728 9519	3.7408 83
31-35	$1{:}5s_K\ 2{:}5p_{Kp}\ 1{:}5s_{L1}\ 2{:}6p_{L4}\ R$	2495	23084	-14.3423 9788 1241	0.5917 22
36-40	$3{:}6d_{Kp}\ 3{:}6d_{Kp}\ 1{:}5s_{L1}\ 1{:}6s_{L2}\ R$	1445	24529	-14.3423 9980 9686	1.9284 45
41-45	$1{:}5s_K\ 1{:}5s_K\ 3{:}6d_{L3}\ 3{:}6d_{L4}\ R$	1180	25709	-14.3424 0104 1058	1.2313 72
46-50	$1{:}5s_K\ 3{:}6d_{Kp}\ 3{:}6d_{L3}\ 1{:}6s_{L2}\ R$	2325	28034	-14.3424 0148 4779	0.4437 21
51-55	$1{:}5s_K\ 3{:}6d_{Kp}\ 1{:}6s_{L1}\ 3{:}6d_{L4}\ R$	2325	30359	-14.3424 0151 7899	0.0331 20
56-60	$1{:}5s_K\ 2{:}5p_{Kp}\ 2{:}5p_{L3}\ 3{:}6d_{L4}\ R$	1595	31954	-14.3424 0159 3391	0.0754 92
61-65	$1{:}5s_K\ 3{:}6d_{Kp}\ 2{:}5p_{L3}\ 2{:}6p_{L4}\ R$	1975	33929	-14.3424 0163 1968	0.0385 77
66-70	$2{:}5p_{Kp}\ 1{:}5s_K\ 2{:}5p_{L3}\ 3{:}6d_{L4}\ R$	1595	35524	-14.3424 0168 8960	0.0569 92
71-75	$3{:}6d_{Kp}\ 2{:}5p_{Kp}\ 1{:}5s_{L1}\ 2{:}6p_{L4}\ R$	1975	37499	-14.3424 0173 6432	0.0474 72
76	$2{:}5p_{Kp}\ 2{:}5p_{Kp}\ 1{:}5s_{L1}\ 3{:}6d_{L4}$	199	37698	-14.3424 0175 2822	0.0163 90
77	$4{:}7f_{Kp}\ 4{:}7f_{Kp}\ 2{:}5s_{L1}\ 2{:}6s_{L2}$	156	37854	-14.3424 0180 8892	0.0560 70
78	$4{:}7f_{Kp}\ 4{:}7f_{Kp}\ 2{:}5s_{L1}\ 2{:}6s_{L2}\ r_{12}$	156	38010	-14.3424 0182 6617	0.0177 25
79	$4{:}7f_{Kp}\ 4{:}7f_{Kp}\ 2{:}6s_{L1}\ 2{:}6s_{L2}\ r_{34}$	177	38187	-14.3424 0183 9732	0.0131 15
80	$4{:}7f_{Kp}\ 4{:}7f_{Kp}\ 2{:}5s_{L1}\ 2{:}6s_{L2}\ r_{13}$	156	38343	-14.3424 0188 9520	0.0497 88
81	$4{:}7f_{Kp}\ 4{:}7f_{Kp}\ 2{:}6s_{L1}\ 2{:}6s_{L2}\ r_{14}$	177	38520	-14.3424 0189 1756	0.0022 36
82-86	$1{:}6s_K\ 1{:}6s_K\ 4{:}7f_{L3}\ 4{:}7f_{L4}\ R$	1320	39840	-14.3424 0205 2643	0.1608 87
87-89	$1{:}6s_K\ 4{:}7f_{Kp}\ 4{:}7f_{L3}\ 2{:}6s_{L2}\ R_1$	1095	40935	-14.3424 0212 5037	0.0723 94
90	$1{:}6s_K\ 4{:}7f_{Kp}\ 4{:}7f_{L3}\ 2{:}6s_{L2}\ r_{13}$	365	41300	-14.3424 0213 7169	0.0121 32
91	$1{:}6s_K\ 4{:}7f_{Kp}\ 2{:}6s_{L1}\ 4{:}7f_{L4}$	365	41665	-14.3424 0214 1182	0.0040 13
92	$1{:}6s_K\ 4{:}7f_{Kp}\ 2{:}6s_{L1}\ 4{:}7f_{L4}\ r_{12}$	365	42030	-14.3424 0214 1516	0.0003 34
93-97	$2{:}5p_{Kp}\ 2{:}5p_{Kp}\ 3{:}6d_{L3}\ 3{:}6d_{L4}\ R$	780	42810	-14.3424 0214 5759	0.0042 43
98-102	$2{:}5p_{1Kp}\ 2{:}5p_{1Kp}\ 3{:}6d_{-1L3}\ 3{:}6d_{-1L4}\ R$	780	43590	-14.3424 0215 9395	0.0136 36
103-107	$3{:}6d_{Kp}\ 3{:}6d_{Kp}\ 2{:}6p_{L3}\ 2{:}6p_{L4}\ R$	1130	44720	-14.3424 0217 0932	0.0115 37
108-112	$3{:}6d_{1Kp}\ 3{:}6d_{1Kp}\ 2{:}6p_{-1L3}\ 2{:}6p_{-1L4}\ R$	1130	45850	-14.3424 0220 3245	0.0323 13
113-130	CORE r-Sum Adjustments				
113	$1{:}9s_K\ 1{:}9s_K\ 1{:}9s_{L1}\ 1{:}9s_{L2}$-#1 [d]	1514	47364	-14.3424 0240 1655	0.1984 10
114	$1{:}9s_K\ 1{:}9s_K\ 1{:}9s_{L1}\ 1{:}9s_{L2}\ r_{12}$-#2 [d]	1514	48878	-14.3424 0277 2629	0.3709 74
115	$1{:}9s_K\ 1{:}9s_K\ 1{:}9s_{L1}\ 1{:}9s_{L2}\ r_{34}$-#3 [d]	1514	50392	-14.3424 0280 6553	0.0339 24

Block(s)	Terms Added[ab]	N	N_{tot}	E(N_{tot}) (Ha)	$-\Delta$E (μHa)
116	$1{:}9s_K$ $1{:}9s_K$ $1{:}9s_{L1}$ $1{:}9s_{L2}$ r_{13}-#4 [d]	1514	51906	-14.3424 0287 1113	0.0645 60
117	$1{:}9s_K$ $1{:}9s_K$ $1{:}9s_{L1}$ $1{:}9s_{L2}$ r_{14}-#5 [d]	2062	53968	-14.3424 0288 1693	0.0105 80
118	$2{:}9p_{Kp}$ $2{:}9p_{Kp}$ $1{:}9s_{L1}$ $1{:}9s_{L2}$-#6 [d]	1435	55403	-14.3424 0296 5864	0.0841 71
119	$2{:}9p_{Kp}$ $2{:}9p_{Kp}$ $1{:}9s_{L1}$ $1{:}9s_{L2}$ r_{12}-#7	592	55995	-14.3424 0299 7700	0.0318 36
120	$2{:}9p_{Kp}$ $2{:}9p_{Kp}$ $1{:}9s_{L1}$ $1{:}9s_{L2}$ r_{13}-#9 [d]	1435	57430	-14.3424 0303 8382	0.0406 82
121	$2{:}9p_{Kp}$ $2{:}9p_{Kp}$ $1{:}9s_{L1}$ $1{:}9s_{L2}$ r_{14}-#10 [d]	1435	58865	-14.3424 0304 6696	0.0083 14
122	$1{:}9s_K$ $1{:}9s_K$ $2{:}8p_{L3}$ $2{:}8s_{L4}$ $-$ #11	156	59156	-14.3424 0305 1441	0.0047 45
123	$1{:}9s_K$ $1{:}9s_K$ $2{:}8p_{L3}$ $2{:}8s_{L4}$ r_{12}-#12	291	59447	-14.3424 0307 2407	0.0209 66
124	$1{:}9s_K$ $1{:}9s_K$ $2{:}8p_{L3}$ $2{:}8s_{L4}$ r_{34}-#13	607	60054	-14.3424 0307 7365	0.0049 58
125	$2{:}6p_{Kp}$ $2{:}6p_{Kp}$ $2{:}8p_{L3}$ $2{:}8p_{L4}$-#16 [c]	285	60339	-14.3424 0307 8305	0.0009 40
126	$2{:}6p_{Kp}$ $2{:}6p_{Kp}$ $2{:}8p_{L3}$ $2{:}8p_{L4}$ r_{12}-#17 [c]	285	60624	-14.3424 0307 8661	0.0003 56
127	$2{:}6p_{Kp}$ $2{:}6p_{Kp}$ $2{:}8p_{L3}$ $2{:}8p_{L4}$ r_{34}-#18 [c]	285	60909	-14.3424 0307 9251	0.0005 89
128	$2{:}6p_{1Kp}$ $2{:}6p_{1Kp}$ $2{:}8p_{-1L3}$ $2{:}8p_{-1L4}$-#21 [c]	285	61194	-14.3424 0308 1784	0.0025 33
129	$2{:}6p_{1Kp}$ $2{:}6p_{1Kp}$ $2{:}8p_{-1L3}$ $2{:}8p_{-1L4}$ r_{12}-#22 [c]	285	61479	-14.3424 0308 2588	0.0008 04
130	$2{:}6p_{1Kp}$ $2{:}6p_{1Kp}$ $2{:}8p_{-1L3}$ $2{:}8p_{-1L4}$ r_{34}-#23 [c]	285	61764	-14.3424 0308 2841	0.0002 53
131-157	Final Adjustments				
131	$1{:}7s_K$ $2{:}8p_{Kp}$ $2{:}8p_{L3}$ $1{:}7s_{L2}$-#26	1267	63031	-14.3424 0310 3753	0.0209 12
132	$1{:}7s_K$ $2{:}8p_{Kp}$ $2{:}8p_{L3}$ $1{:}7s_{L2}$ r_{12}-#27	1267	64298	-14.3424 0314 6671	0.0429 18
133	$1{:}7s_K$ $2{:}8p_{Kp}$ $2{:}8p_{L3}$ $1{:}7s_{L2}$ r_{13}-#29	1267	65565	-14.3424 0315 7117	0.0104 46
134	$4{:}7f_{Kp}$ $4{:}7f_{Kp}$ $2{:}7s_{L1}$ $2{:}7s_{L2}$-#77 [d]	259	65824	-14.3424 0315 9984	0.0028 67
135	$4{:}7f_{Kp}$ $4{:}7f_{Kp}$ $2{:}7s_{L1}$ $2{:}7s_{L2}$ r_{12}-#78 [d]	259	66083	-14.3424 0316 2248	0.0022 65
136	$4{:}7f_{Kp}$ $4{:}7f_{Kp}$ $2{:}7s_{L1}$ $2{:}7s_{L2}$ r_{13}-#80 [d]	259	66342	-14.3424 0317 8160	0.0159 12
137	$2{:}7p_{Kp}$ $1{:}7s_K$ $1{:}7s_{L1}$ $2{:}7p_{L4}$	1446	67788	-14.3424 0318 4070	0.0059 10
138	$2{:}7p_{Kp}$ $1{:}7s_K$ $1{:}7s_{L1}$ $2{:}7p_{L4}$ r_{12}	1446	69234	-14.3424 0319 3153	0.0090 83
139	$2{:}7p_{Kp}$ $1{:}7s_K$ $1{:}7s_{L1}$ $2{:}7p_{L4}$ r_{13}	1446	70680	-14.3424 0319 4737	0.0015 84
140	$2{:}7p_{Kp}$ $1{:}8s_K$ $2{:}8p_{L3}$ $1{:}7s_{L2}$	1707	72387	-14.3424 0322 6212	0.0314 75
141	$2{:}7p_{Kp}$ $1{:}8s_K$ $2{:}8p_{L3}$ $1{:}7s_{L2}$ r_{12}	1707	74094	-14.3424 0323 6529	0.0103 17
142	$2{:}7p_{Kp}$ $1{:}8s_K$ $2{:}8p_{L3}$ $1{:}7s_{L2}$ r_{13}	1707	75540	-14.3424 0331 9011	0.0824 82
143	$3{:}6d_{Kp}$ $1{:}7s_K$ $3{:}7d_{L3}$ $1{:}7s_{L2}$	790	76330	-14.3424 0335 9107	0.0400 96
144	$3{:}6d_{Kp}$ $1{:}7s_K$ $3{:}7d_{L3}$ $1{:}7s_{L2}$ r_{12}	790	77120	-14.3424 0337 2942	0.0138 34
145	$3{:}6d_{Kp}$ $1{:}7s_K$ $3{:}7d_{L3}$ $1{:}7s_{L2}$ r_{13}	790	77910	-14.3424 0338 5191	0.0122 49
146	$3{:}6d_{Kp}$ $2{:}7p_{Kp}$ $2{:}7p_{L3}$ $1{:}7s_{L2}$	815	78725	-14.3424 0344 4076	0.0588 86
147	$3{:}6d_{Kp}$ $2{:}7p_{Kp}$ $2{:}7p_{L3}$ $1{:}7s_{L2}$ r_{12}	815	79540	-14.3424 0347 2747	0.0286 71
148	$3{:}6d_{Kp}$ $2{:}7p_{Kp}$ $2{:}7p_{L3}$ $1{:}7s_{L2}$ r_{13}	815	80355	-14.3424 0349 5298	0.0225 51
149	$2{:}7p_{Kp}$ $3{:}6d_{Kp}$ $2{:}7p_{L3}$ $1{:}7s_{L2}$	815	81170	-14.3424 0349 7209	0.0019 10
150	$2{:}7p_{Kp}$ $3{:}6d_{Kp}$ $2{:}7p_{L3}$ $1{:}7s_{L2}$ r_{12}	815	81985	-14.3424 0349 8376	0.0011 67
151	$2{:}7p_{Kp}$ $3{:}6d_{Kp}$ $2{:}7p_{L3}$ $1{:}7s_{L2}$ r_{13}	815	82800	-14.3424 0350 0972	0.0025 96
152	$1{:}8s_{K1}$ $1{:}8s_{K1}$ $1{:}7s_{L1}$ $1{:}7s_{L2}$	1485	84285	-14.3424 0353 9853	0.0338 81
153	$1{:}8s_{K1}$ $1{:}8s_{K1}$ $1{:}7s_{L1}$ $1{:}7s_{L2}$ r_{12}	1485	85770	-14.3424 0356 6921	0.0270 69
154	$1{:}8s_{K1}$ $1{:}8s_{K1}$ $1{:}7s_{L1}$ $1{:}7s_{L2}$ r_{13}	1485	87255	-14.3424 0356 8927	0.0020 06
155	$1{:}7s_K$ $1{:}7s_{L1}$ $1{:}7s_K$ $1{:}7s_{L2}$	1800	89055	-14.3424 0357 1020	0.0020 93
156	$1{:}7s_K$ $1{:}7s_{L1}$ $1{:}7s_K$ $1{:}7s_{L2}$ r_{12}	2075	91130	-14.3424 0357 3919	0.0028 99
157	$1{:}7s_K$ $1{:}7s_{L1}$ $1{:}7s_K$ $1{:}7s_{L2}$ r_{13}	1800	92930	-14.3424 0357 8275	0.0043 56

[a] K shell orbital exponents are $K = 3.8, K_p = 5.1, K_1 = 10.0$; [b] L shell orbital exponents are $L_1 = 1.692, L_2 = 0.201, L_3 = 1.163, L_4 = 0.525$;
[c] r-sum = 24; [d] r-sum = 20.

Table A5. Hy-CI expansion of the 7 ^1S excited state of Be (in Ha), a 92,904 term s,p,d,f expansion. In the table, R_1 = $\{1,r_{12},r_{34}\}$, R_2 = $\{r_{13},r_{14}\}$, R = $\{1,r_{12},r_{34},r_{13},r_{14}\}$, N is the number of terms added and N_{tot} is the cumulative number of terms. The terms are r-sum filtered using N_{max} = 16 (see text) unless an explicit r-sum N_{max} value is given.

Block(s)	Terms Added[ab]	N	N_{tot}	E(N_{tot}) (Ha)	$-\Delta$E (μHa)
1-25	CORE				
1-3	$1{:}9s_K\ 1{:}9s_K\ 1{:}7s_{L_1}\ 1{:}8s_{L_2}\ R_1$	4935	4935	-14.3363 9407 4620	
4	$1{:}9s_K\ 1{:}9s_K\ 1{:}7s_{L_1}\ 1{:}8s_{L_2}\ r_{13}$	1645	6580	-14.3365 6483 7646	170.7630 26
5	$1{:}6s_K\ 1{:}6s_K\ 1{:}7s_{L_1}\ 1{:}8s_{L_2}\ r_{14}$	1047	7627	-14.3365 6873 9338	3.9016 91
6-10	$2{:}7p_{Kp}\ 2{:}7p_{Kp}\ 1{:}7s_{L_1}\ 1{:}8s_{L_2}\ R$	4505	12132	-14.3371 7236 1457	603.6221 19
11	$1{:}9s_K\ 1{:}9s_K\ 2{:}7p_{L3}\ 2{:}8p_{L4}$	1099	13231	-14.3372 3718 8188	64.8267 31
12	$1{:}9s_K\ 1{:}9s_K\ 2{:}7p_{L3}\ 2{:}8p_{L4}\ r_{12}$	1099	14330	-14.3372 4746 1370	10.2731 83
13	$1{:}6s_K\ 1{:}6s_K\ 2{:}7p_{L3}\ 2{:}8p_{L4}\ r_{34}$	754	15084	-14.3372 5343 7550	5.9761 79
14-15	$1{:}6s_K\ 1{:}6s_K\ 2{:}7p_{L3}\ 2{:}8p_{L4}R_2$	1508	16592	-14.3372 5617 9790	2.7422 40
16-20	$2{:}6p_{0Kp}\ 2{:}6p_{0Kp}\ 2{:}7p_{0L3}\ 2{:}8p_{0L4}\ R$ [c]	3150	19742	-14.3372 5672 5834	0.5460 44
21-25	$2{:}6p_{1Kp}\ 2{:}6p_{1Kp}\ 2{:}7p_{-1L3}\ 2{:}8p_{-1L4}\ R$ [c]	3150	22892	-14.3372 5727 1775	0.5459 41
26-103	Post-CORE				
26	$1{:}7s_K\ 2{:}8p_{Kp}\ 2{:}8p_{L3}\ 1{:}7s_{L2}$	1746	24638	-14.3372 5947 4732	2.2029 57
27	$1{:}7s_K\ 2{:}8p_{Kp}\ 2{:}8p_{L3}\ 1{:}7s_{L2}\ r_{12}$	1746	26384	-14.3372 6105 7663	1.5829 31
28	$1{:}5s_K\ 2{:}5p_{Kp}\ 2{:}5p_{L3}\ 1{:}7s_{L2}\ r_{34}$	555	26939	-14.3372 6124 2945	0.1852 82
29	$1{:}7s_K\ 2{:}8p_{Kp}\ 2{:}8p_{L3}\ 1{:}7s_{L2}\ r_{13}$	1746	28685	-14.3372 6142 1270	0.1783 35
30	$1{:}5s_K\ 2{:}5p_{Kp}\ 2{:}5p_{L3}\ 1{:}7s_{L2}\ r_{14}$	555	29240	-14.3372 6143 8346	0.0170 76
31-35	$1{:}5s_K\ 2{:}5p_{Kp}\ 1{:}5s_{L1}\ 2{:}7p_{L4}\ R$	2975	32215	-14.3372 6180 9006	0.3706 60
36-40	$3{:}6d_{Kp}\ 3{:}6d_{Kp}\ 1{:}5s_{L1}\ 1{:}7s_{L2}\ R$	1630	33845	-14.3372 6330 7242	1.4982 36
41-45	$1{:}5s_K\ 1{:}5s_K\ 3{:}6d_{L3}\ 3{:}7d_{L4}\ R$	1445	35290	-14.3372 6450 4666	1.1974 24
46-50	$1{:}5s_K\ 3{:}6d_{Kp}\ 3{:}6d_{L3}\ 1{:}7s_{L2}\ R$	2625	37915	-14.3372 6488 4368	0.3797 02
51-55	$1{:}5s_K\ 3{:}6d_{Kp}\ 1{:}6s_{L1}\ 3{:}7d_{L4}\ R$	2825	40740	-14.3372 6491 7287	0.0329 19
56-60	$1{:}5s_K\ 2{:}5p_{Kp}\ 2{:}5p_{L3}\ 3{:}7d_{L4}\ R$	1975	42715	-14.3372 6498 2221	0.0649 34
61-65	$1{:}5s_K\ 3{:}6d_{Kp}\ 2{:}5p_{L3}\ 2{:}7p_{L4}\ R$	2325	45040	-14.3372 6500 4798	0.0225 77
66-70	$2{:}5p_{Kp}\ 1{:}5s_K\ 2{:}5p_{L3}\ 3{:}7d_{L4}\ R$	1975	47015	-14.3372 6504 3649	0.0388 51
71-75	$3{:}6d_{Kp}\ 2{:}5p_{Kp}\ 1{:}5s_{L1}\ 2{:}7p_{L4}\ R$	2325	49340	-14.3372 6507 3121	0.0294 72
76	$2{:}5p_{Kp}\ 2{:}5p_{Kp}\ 1{:}5s_{L1}\ 3{:}7d_{L4}$	246	49586	-14.3372 6508 7073	0.0139 53
77	$4{:}7f_{Kp}\ 4{:}7f_{Kp}\ 2{:}7s_{L1}\ 2{:}7s_{L2}$ [d]	336	49922	-14.3372 6516 3497	0.0764 24
78	$4{:}7f_{Kp}\ 4{:}7f_{Kp}\ 2{:}7s_{L1}\ 2{:}7s_{L2}\ r_{12}$ [d]	336	50258	-14.3372 6520 0025	0.0365 28
79	$4{:}7f_{Kp}\ 4{:}7f_{Kp}\ 2{:}6s_{L1}\ 2{:}7s_{L2}\ r_{34}$	190	50448	-14.3372 6520 3157	0.0031 32
80	$4{:}7f_{Kp}\ 4{:}7f_{Kp}\ 2{:}7s_{L1}\ 2{:}7s_{L2}\ r_{13}$ [d]	336	50784	-14.3372 6526 4140	0.0609 82
81	$4{:}7f_{Kp}\ 4{:}7f_{Kp}\ 2{:}6s_{L1}\ 2{:}7s_{L2}\ r_{14}$	190	50974	-14.3372 6526 5085	0.0009 45
82-86	$1{:}6s_K\ 1{:}6s_K\ 4{:}7f_{L3}\ 4{:}7f_{L4}\ R$	1320	52294	-14.3372 6537 0828	0.1057 43
87	$1{:}6s_K\ 4{:}7f_{Kp}\ 4{:}7f_{L3}\ 2{:}7s_{L2}$	398	52692	-14.3372 6538 8845	0.0180 17
88	$1{:}6s_K\ 4{:}7f_{Kp}\ 4{:}7f_{L3}\ 2{:}7s_{L2}\ r_{12}$	398	53090	-14.3372 6540 7206	0.0183 61
89	$1{:}6s_K\ 4{:}7f_{Kp}\ 4{:}7f_{L3}\ 2{:}7s_{L2}\ r_{13}$	398	53488	-14.3372 6541 1028	0.0038 22
90	$1{:}6s_K\ 4{:}7f_{Kp}\ 2{:}6s_{L1}\ 4{:}7f_{L4}$	365	53853	-14.3372 6541 3827	0.0027 99
91-93	$2{:}5p_{Kp}\ 2{:}5p_{Kp}\ 3{:}6d_{L3}\ 3{:}7d_{L4}\ R_1$	567	54420	-14.3372 6541 7514	0.0036 87
94	$2{:}5p_{1Kp}\ 2{:}5p_{1Kp}\ 3{:}6d_{-1L3}\ 3{:}7d_{-1L4}$	189	54609	-14.3372 6542 1329	0.0038 14
95	$2{:}5p_{1Kp}\ 2{:}5p_{1Kp}\ 3{:}6d_{-1L3}\ 3{:}7d_{-1L4}\ r12$	189	54798	-14.3372 6542 4466	0.0031 38
96-100	$3{:}6d_{Kp}\ 3{:}6d_{Kp}\ 2{:}6p_{L3}\ 2{:}7p_{L4}\ R$	1275	56073	-14.3372 6543 8055	0.0135 89

Block(s)	Terms Added[ab]	N	N_{tot}	E(N_{tot}) (Ha)	$-\Delta$E μHa)
101-103	$3{:}6d_{1Kp}$ $3{:}6d_{1Kp}$ $2{:}7p_{-1L3}$ $2{:}7p_{-1L4}$ R_1	765	56838	-14.3372 6546 3173	0.0251 18
104-113	CORE r-sum Adjustments				
104	$1{:}9s_K$ $1{:}9s_K$ $1{:}9s_{L1}$ $1{:}9s_{L2}$-#1 [d]	1253	58091	-14.3372 6562 4771	0.1615 98
105	$1{:}9s_K$ $1{:}9s_K$ $1{:}9s_{L1}$ $1{:}9s_{L2}$ r_{12}-#2 [d]	1253	59344	-14.3372 6586 7445	0.2426 74
106	$1{:}9s_K$ $1{:}9s_K$ $1{:}9s_{L1}$ $1{:}9s_{L2}$ r_{34}-#3 [d]	1253	60597	-14.3372 6589 8010	0.0305 65
107	$1{:}9s_K$ $1{:}9s_K$ $1{:}9s_{L1}$ $1{:}9s_{L2}$ r_{13}-#4 [d]	1253	61850	-14.3372 6595 4615	0.0566 05
108	$1{:}9s_K$ $1{:}9s_K$ $1{:}9s_{L1}$ $1{:}9s_{L2}$ r_{14}-#5 [d]	1851	63701	-14.3372 6596 2860	0.0082 45
109	$2{:}9p_{Kp}$ $2{:}9p_{Kp}$ $1{:}9s_{L1}$ $1{:}9s_{L2}$-#6 [d]	1288	64989	-14.3372 6600 7422	0.0445 62
110	$2{:}9p_{Kp}$ $2{:}9p_{Kp}$ $1{:}9s_{L1}$ $1{:}9s_{L2}$ r_{12}-#7	445	65434	-14.3372 6602 4926	0.0175 05
111	$1{:}9s_K$ $1{:}9s_K$ $2{:}8p_{L3}$ $2{:}8s_{L4}$-#11	92	65526	-14.3372 6602 5902	0.0009 75
112	$1{:}9s_K$ $1{:}9s_K$ $2{:}8p_{L3}$ $2{:}8s_{L4}$ r_{12}-#12	92	65618	-14.3372 6602 9623	0.0037 21
113	$1{:}9s_K$ $1{:}9s_K$ $2{:}8p_{L3}$ $2{:}8s_{L4}$ r_{34}-#13	437	66055	-14.3372 6603 2780	0.0031 57
114-134	Final Adjustments				
114	$2{:}7p_{Kp}$ $1{:}7s_K$ $1{:}7s_{L1}$ $2{:}7p_{L4}$	1446	67501	-14.3372 6603 5873	0.0030 93
115	$2{:}7p_{Kp}$ $1{:}7s_K$ $1{:}7s_{L1}$ $2{:}7p_{L4}$ r_{12}	1446	68947	-14.3372 6604 1144	0.0052 71
116	$2{:}7p_{Kp}$ $1{:}7s_K$ $1{:}7s_{L1}$ $2{:}7p_{L4}$ r_{13}	1446	70393	-14.3372 6604 2574	0.0014 30
117	$2{:}7p_{Kp}$ $1{:}8s_K$ $2{:}8p_{L3}$ $1{:}7s_{L2}$	1707	72100	-14.3372 6606 9995	0.0274 21
118	$2{:}7p_{Kp}$ $1{:}8s_K$ $2{:}8p_{L3}$ $1{:}7s_{L2}$ r_{12}	1707	73807	-14.3372 6609 5952	0.0259 57
119	$2{:}7p_{Kp}$ $1{:}8s_K$ $2{:}8p_{L3}$ $1{:}7s_{L2}$ r_{13}	1707	75514	-14.3372 6619 1379	0.0954 27
120	$3{:}6d_{Kp}$ $1{:}7s_K$ $3{:}7d_{L3}$ $1{:}7s_{L2}$	790	76304	-14.3372 6624 4430	0.0530 51
121	$3{:}6d_{Kp}$ $1{:}7s_K$ $3{:}7d_{L3}$ $1{:}7s_{L2}$ r_{12}	790	77094	-14.3372 6625 8312	0.0138 82
122	$3{:}6d_{Kp}$ $1{:}7s_K$ $3{:}7d_{L3}$ $1{:}7s_{L2}$ r_{13}	790	77884	-14.3372 6627 2532	0.0142 20
123	$3{:}6d_{Kp}$ $2{:}7p_{Kp}$ $2{:}7p_{L3}$ $1{:}7s_{L2}$	815	78699	-14.3372 6633 5483	0.0629 51
124	$3{:}6d_{Kp}$ $2{:}7p_{Kp}$ $2{:}7p_{L3}$ $1{:}7s_{L2}$ r_{12}	815	79514	-14.3372 6636 5384	0.0299 01
125	$3{:}6d_{Kp}$ $2{:}7p_{Kp}$ $2{:}7p_{L3}$ $1{:}7s_{L2}$ r_{13}	815	80329	-14.3372 6639 3466	0.0280 81
126	$2{:}7p_{Kp}$ $3{:}6d_{Kp}$ $2{:}7p_{L3}$ $1{:}7s_{L2}$	815	81144	-14.3372 6639 6506	0.0030 40
127	$2{:}7p_{Kp}$ $3{:}6d_{Kp}$ $2{:}7p_{L3}$ $1{:}7s_{L2}$ r_{12}	815	81959	-14.3372 6639 8027	0.0015 21
128	$2{:}7p_{Kp}$ $3{:}6d_{Kp}$ $2{:}7p_{L3}$ $1{:}7s_{L2}$ r_{13}	815	82774	-14.3372 6640 0869	0.0028 42
129	$1{:}8s_{K1}$ $1{:}8s_{K1}$ $1{:}7s_{L1}$ $1{:}8s_{L2}$	1485	84259	-14.3372 6644 7675	0.0468 06
130	$1{:}8s_{K1}$ $1{:}8s_{K1}$ $1{:}7s_{L1}$ $1{:}8s_{L2}$ r_{12}	1485	85744	-14.3372 6648 3013	0.0353 38
131	$1{:}8s_{K1}$ $1{:}8s_{K1}$ $1{:}7s_{L1}$ $1{:}8s_{L2}$ r_{13}	1485	87229	-14.3372 6648 5686	0.0026 74
132	$1{:}7s_K$ $1{:}7s_{L1}$ $1{:}7s_K$ $1{:}7s_{L2}$	1800	89029	-14.3372 6648 8538	0.0028 52
133	$1{:}7s_K$ $1{:}7s_{L1}$ $1{:}7s_K$ $1{:}7s_{L2}$ r_{12}	2075	91104	-14.3372 6649 3416	0.0048 78
134	$1{:}7s_K$ $1{:}7s_{L1}$ $1{:}7s_K$ $1{:}7s_{L2}$ r_{13}	1800	92904	-14.3372 6649 9575	0.0061 59

[a] K shell orbital exponents are $K = 3.8, K_p = 5.1, K_1 = 10.0$; [b] L shell orbital exponents are $L_1 = 1.73, L_2 = 0.163, L_3 = 1.163, L_4 = 0.535$; [c] r-sum = 24; [d] r-sum = 20.

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7. References

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About the author: *James S. Sims is a computational scientist in the Scientific Applications and Visualization Group, Applied and Computational Mathematics Division of the NIST Information Technology Laboratory. The National Institute of Standards and Technology is an agency of the U.S. Department of Commerce.*