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University of Windsor

Order $\alpha^6 mc^2$ Contributions to the Fine Structure Splittings of Helium and Helium-Like Ions

by

Zong-Chao Yan

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Abstract

In this thesis, the Douglas and Kroll order $\alpha^6 mc^2$ contributions to the $1s2p\,^3P_J$ fine structure splittings of helium are evaluated using the new variational wave functions of Drake [2]. Our results improve the old calculation of Daley *et al.* [13] by several orders of magnitude. Extensions are made to two-electron ions in arbitrary angular momentum states. The other triplet states calculated are $Z = 2$, $1snp\,^3P_J$, $n = 2, \cdots, 10$; $Z = 3, \cdots, 12$, $1s2p\,^3P_J$; $Z = 3, \cdots, 12$, $1s3p\,^3P_J$; $Z = 2, \cdots, 12$, $1s3d\,^3D_J$; and $Z = 2$, $1snd\,^3D_J$, $n = 4, \cdots, 10$. The final numerical values for the reduced matrix elements and the splittings are tabulated. By including the newly calculated second-order contributions of Drake, a comparison with the present high precision experimental measurements for the $1s2p\,^3P_J$ states of helium is made.

To my wife wenying

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Chapter 1

Introduction

The study of quantum electrodynamic (QED) effects in atoms has been an active research field since the discovery of the Lamb shift in hydrogen in 1947 [1]. QED is a quantized field theory which describes the interaction of an electron with an electromagnetic field with a coupling constant, $\alpha \approx 1/137$. QED predicts new phenomena in atoms which cannot be fully explained by conventional quantum mechanics. However, from a perturbation point of view, if the non-QED part is understood sufficiently well, the QED effects can be extracted by subtraction of the non-QED part from high precision experimental results. The extracted QED contributions can further be compared with high precision QED calculations to test the validity of the theory. The hydrogen atom has thus been chosen as a major candidate for fundamental tests of QED effects since 1947, because the Schrödinger and Dirac equations for hydrogen can be solved analytically and thus the non-QED contributions can be evaluated exactly.

The second simplest atom, helium, is different from hydrogen in that it is a two electron system. Thus, the Schrödinger equation for this system cannot be solved analytically due to the existence of the Coulomb repulsive force between the two electrons. Being a prototype for studying other many electron atoms, helium has been intensively investigated since the earliest days of quantum mechanics. However, remarkable progress has been made by Drake [2] only in the past few years on the calculations of nonrelativistic energy levels of helium and helium-like ions. The new techniques involve the use of variational basis sets which include explicitly the screened hydrogenic wave function, together with double non-linear exponential parameters for each of the remaining Hylleraas-like terms. A complete optimization is performed with respect to all the non-linear parameters. Although originally designed for Rydberg states, where a direct physical picture could naturally be embedded into the construction of the wave functions, the method proved equally successful for lower lying states. The new variational method has also been applied to the ground state of lithium with parallel success [3]. As we know a major complication in the high precision calculation of helium properties is from the necessity of obtaining sufficiently accurate nonrelativistic wave functions so that the expectation values of operators of relativistic and QED corrections can be evaluated to the required precision. The difficulty has now been removed in the sense that the solutions of the Schrödinger equation for helium are essentially exact for all practical purposes, which makes it possible to take the helium atom as another high precision testing ground for both relativistic and QED effects.

Among various properties of helium, the fine structure of the $2\ ^3P_J$ states (with J the total angular momentum of the atom) has attracted much attention in the last six decades. In the theory of helium the understanding of the interaction between the two electrons becomes essential to the explanation of the fine structure. If we totally neglect the relativistic motions of the two electrons, the interaction in this static limit is just the Coulomb repulsive potential e^2/r, where $r = |\mathbf{r}_1 - \mathbf{r}_2|$. Solving the Schrödinger equation together with the Pauli exclusion principle yields only the separation between the singlet and triplet levels. There are no further splittings among the triplet states. If we wish to go beyond the static limit, that is, if we wish to include the effects produced by the motions of the two electrons, the correct interaction is no longer the instantaneous Coulomb potential. The motion of the first electron generates a magnetic field in the region of the second electron and vice versa. Therefore, we must determine not only the scalar potential but also the vector potential due to the second electron at the position of the first. The relativistic interaction Lagrangian for two electron systems, correct to the order of $(v/c)^2$, was first obtained by Darwin in 1920. However, since Breit used this Lagrangian to study the helium atom in the quantum mechanical domain, the interaction is known as the Breit interaction [4]. The Breit interaction can be reduced to a set of operators in the nonrelativistic 2×2 Pauli form which is suitable for numerical evaluation using nonrelativistic wave functions. Among these operators are the spin-orbit interaction with the nucleus H_{Zso}, the spin-orbit interaction between the electrons H_{eso}, and the spin-spin interaction between the electrons H_{ess}. These operators account largely for the fine structure splittings of the triplet states. Thus, the spin-dependent Breit interaction is (in atomic units throughout)

$$H_4 = H_{Zso} + H_{eso} + H_{ess}, \tag{1.1}$$

with

$$\begin{aligned} H_{Zso} &= \frac{1}{4}Z\alpha^2(\vec{\sigma}_1 \cdot (\frac{\vec{r}_1}{r_1^3} \times \vec{p}_1) + \vec{\sigma}_2 \cdot (\frac{\vec{r}_2}{r_2^3} \times \vec{p}_2)) \\ H_{eso} &= \frac{\alpha^2}{4r^3}(\vec{r} \times \vec{p}_2 \cdot (\vec{\sigma}_2 + 2\vec{\sigma}_1) - \vec{r} \times \vec{p}_1 \cdot (\vec{\sigma}_1 + 2\vec{\sigma}_2)) \\ H_{ess} &= \frac{1}{4}\alpha^2(\frac{1}{r^3}\vec{\sigma}_1 \cdot \vec{\sigma}_2 - \frac{3}{r^5}(\vec{\sigma}_1 \cdot \vec{r})(\vec{\sigma}_2 \cdot \vec{r})), \end{aligned}$$

where $\vec{\sigma}_1/2$ and $\vec{\sigma}_2/2$ are the spin operators for electron 1 and electron 2, and $\vec{r} = \vec{r}_1 - \vec{r}_2$. The fine structure is largest for the $1s2p\ ^3P_J$ states. Therefore, if both experiment and theory on the fine structure intervals are performed to sufficient precision, then a precise value of the fine structure constant α could be derived by the comparison of theory and experiment. Furthermore, the consistency of QED theory could be verified once this fine structure constant is compared with those derived from other sources, for example, the hydrogen fine structure and hyperfine structure, the muonium hyperfine structure, the electron $g-2$ anomaly, the Josephson effect, and the quantized Hall effect, etc. [1]. Helium is also appealing to the experimenter in that the $2\ ^3P_J$ levels are more widely spaced than those of the $2\ ^2P$ hydrogen atom, and the lifetime of the helium $2\ ^3P$ state is about 100 times longer than that of the $2\ ^2P$ hydrogen, so that the natural width of the fine structure levels in helium is much narrower. Consequently, one should be able to measure the fine structure splittings in helium to a precision over 50 times greater than in hydrogen [5].

The theoretical calculation of the fine structure of $1s2p\ ^3P_J$ states of helium to 1 ppm or better involves lengthy calculations. The steps to achieve this goal were set out by Schwartz [6] as follows. The $2\ ^3P_J$ energy levels can be expressed symbolically in the form

$$E_J = E^0 + \alpha^2 \langle B_P \rangle_J + \alpha^4 \langle B_P (E^0 - H^0)^{-1} B_P \rangle_J + \alpha^4 \langle H_D \rangle_J, \qquad (1.2)$$

where E^0 is the nonrelativistic energy, the second term is the expectation value of the spin-dependent Breit interaction [4], the third term represents the Breit interaction taken to second order (including both the spin-dependent part H_4 and spin-independent part), and the fourth term, containing H_D, is the expectation value of the sum of all order α^4 a.u. QED corrections to the Breit interaction. This series expansion in α implies four well-defined tasks. The first is the evaluation of the Breit interaction taken by first order perturbation theory, with Schrödinger wave functions, which gives the lowest $O(\alpha^2)$ contributions to the fine structure splittings. It should be noted that only the spin-dependent operators need to be calculated, because the spin-independent part contributes equally to all three levels of the triplet. This task has been completed recently with an accuracy of about 1 part in 10^9 (1 ppb level) [7]. The second task is to apply second order perturbation theory to the Breit operators. The validity of this second order approach was justified by Douglas and Kroll [8] in their systematic reduction of the Bethe-Salpeter equation. Initial calculations of limited accuracy were performed by Hambro [9] and by Lewis and Serafino [10]. The sums over all intermediate states, including the continuum, were performed by solving variationally an inhomogeneous perturbation equation according to the method of Dalgarno and Lewis [11]. There is a clear need to improve their calculations by at least 2 or 3 orders of magnitude. This has been achieved recently by Drake and the results will be published shortly. The third task is the derivation of all the spin-dependent operators of order $\alpha^6 mc^2$ (H_D term) from the covariant two electron Bethe-Salpeter equation with the nucleus considered as a fixed Coulomb field. This was accomplished by Douglas and Kroll [8], who considered all order $\alpha^6 mc^2$ corrections which arise from Feynman diagrams involving the exchange of one, two, and three photons, as well as radiative corrections to the electron magnetic moment. The final results are also presented in the nonrelativistic 2×2 Pauli form. These operators are

$$H_D = \sum_{i=1}^{15} H_D^i, \qquad (1.3)$$

where

$$
\begin{aligned}
H_D^1 &= \frac{3}{8}\alpha^3(Z\alpha)\nabla_1^2\frac{1}{r_1^3}\vec{\sigma}_1\cdot(\vec{r}_1\times\vec{p}_1)\\
H_D^2 &= -\alpha^3(Z\alpha)\frac{1}{r^3r_1^3}\vec{\sigma}_1\cdot(\vec{r}_1\times\vec{r})(\vec{r}\cdot\vec{p}_2)\\
H_D^3 &= \frac{1}{2}\alpha^3(Z\alpha)\frac{1}{r^3r_1^3}(\vec{\sigma}_1\cdot\vec{r})(\vec{\sigma}_2\cdot\vec{r}_1)\\
H_D^4 &= \frac{1}{2}\alpha^4\frac{1}{r^4}\vec{\sigma}_1\cdot(\vec{r}\times\vec{p}_2)\\
H_D^5 &= -\frac{1}{2}\alpha^4\frac{1}{r^6}(\vec{\sigma}_1\cdot\vec{r})(\vec{\sigma}_2\cdot\vec{r})\\
H_D^6 &= i\frac{1}{4}\alpha^4\nabla_1^2\frac{1}{r}\vec{\sigma}_1\cdot(\vec{p}_1\times\vec{p}_2)\\
H_D^7 &= i\frac{3}{4}\alpha^4\nabla_1^2\frac{1}{r^3}(\vec{r}\cdot\vec{p}_2)\vec{\sigma}_1\cdot(\vec{r}\times\vec{p}_1)\\
H_D^8 &= -\frac{5}{8}\alpha^4\nabla_1^2\frac{1}{r^3}\vec{\sigma}_1\cdot(\vec{r}\times\vec{p}_1)+\frac{3}{4}\alpha^4\nabla_1^2\frac{1}{r^3}\vec{\sigma}_1\cdot(\vec{r}\times\vec{p}_2)\\
H_D^9 &= i\frac{3}{8}\alpha^4\frac{1}{r^5}\vec{\sigma}_1\cdot(\vec{r}\times(\vec{r}\cdot\vec{p}_2)\vec{p}_1)\\
H_D^{10} &= -\frac{3}{2}\alpha^4\nabla_1^2\frac{1}{r^5}(\vec{\sigma}_1\cdot\vec{r})(\vec{\sigma}_2\cdot\vec{r})\\
H_D^{11} &= i\frac{1}{4}\alpha^4\nabla_1^2\frac{1}{r^3}(\vec{\sigma}_1\cdot\vec{r})(\vec{\sigma}_2\cdot\vec{p}_1)\\
H_D^{12} &= H_D^{121}+H_D^{122},\\
H_D^{121} &= -i\frac{1}{8}\alpha^4\nabla_1^2\frac{1}{r^3}[(\vec{\sigma}_1\cdot\vec{r})(\vec{\sigma}_2\cdot\vec{p}_2)+(\vec{\sigma}_2\cdot\vec{r})(\vec{\sigma}_1\cdot\vec{p}_2)]\\
H_D^{122} &= i\frac{3}{8}\alpha^4\nabla_1^2\frac{1}{r^5}(\vec{\sigma}_1\cdot\vec{r})(\vec{\sigma}_2\cdot\vec{r})(\vec{r}\cdot\vec{p}_2)\\
H_D^{13} &= -\frac{1}{16}\alpha^4\frac{1}{r^3}(\vec{\sigma}_1\cdot\vec{p}_2)(\vec{\sigma}_2\cdot\vec{p}_1)\\
H_D^{14} &= -\frac{3}{16}\alpha^4\frac{1}{r^5}\vec{\sigma}_2\cdot(\vec{r}\times(\vec{\sigma}_1\cdot(\vec{r}\times\vec{p}_1))\vec{p}_2)\\
H_D^{15} &= -0.328478965(\frac{\alpha}{\pi})^2(2H_{Zso}+\frac{4}{3}H_{eso})\\
&+ (2(-0.328478965)(\frac{\alpha}{\pi})^2+(\frac{\alpha}{2\pi})^2)H_{ess}.
\end{aligned}
$$

In addition, there are anomalous magnetic moment corrections of leading order $\alpha^5 mc^2$, nucleus relativistic recoil corrections of order $(m/M)\alpha^4 mc^2$, as well as a correction of order $(m/M)\alpha^5 mc^2$ [12]. These corrections can be taken into account by including the expectation values of operators H_5, H_{m4}, and H_{m5}, respectively, where

$$H_5=\frac{\alpha}{\pi}(H_{Zso}+\frac{2}{3}\delta_{SS'}H_{eso}+H_{ess}), \tag{1.4}$$

$$H_{m4}=\frac{m}{M}(\tilde{\Delta}_3+2H_{Zso}), \tag{1.5}$$

and

$$H_{m5} = \frac{\alpha}{2\pi}\frac{m}{M}(\tilde{\Delta}_3 + 2H_{Z so}), \quad (1.6)$$

with

$$\tilde{\Delta}_3 = \frac{Z\alpha^2}{2}(\frac{1}{r_1{}^3}\vec{\sigma}_1 \cdot (\vec{r}_1 \times \vec{p}_2) + \frac{1}{r_2{}^3}\vec{\sigma}_2 \cdot (\vec{r}_2 \times \vec{p}_1)). \quad (1.7)$$

The next higher order anomalous magnetic moment contribution is included in H_D as H_D^{15}. Thus, the total spin-dependent operator is

$$H_{fs} = H_4 + H_5 + H_{m4} + H_{m5} + H_D. \quad (1.8)$$

The last task is the evaluation of the expectation value of the H_D term. The first complete computation was due to Daley *et al.* [13] in 1972, who used variational Hylleraas wave functions with the largest wave function of 165 terms. Recalculation of the H_D term using much more accurate wave functions will definitely lead to an improvement of the old values by several orders of magnitude. This will be the objective of this thesis. It should be emphasised that the Schwartz project is originally intended for calculating the fine structure of helium up to about the 1 ppm level. Thus, we should not expect to determine, with high precision experimental results, the fine structure constant, α, better than 1 ppm as long as there is no strong cancellation among various higher order terms. In fact, order $O(\alpha^7 \ln(Z\alpha)mc^2)$ and $O(\alpha^7 mc^2)$ terms may contaminate the fine structure splittings at the 1 ppm level. Theoretical work is in progress to investigate these higher order corrections [14]. On the other hand, however, if experimental results are sufficiently higher than 1 ppm, the higher order contribution can be extracted reliably and will serve as a valuable guide in the understanding of higher order QED effects.

On the experimental side, high precision measurements of fine structures of helium and helium-like ions have been performed in recent years. Using an optical microwave atomic beam magnetic resonance technique, Hughes *et al.* measured the fine structure splittings of the $1s2p\ {}^3P_J$ states of helium to a precision of 0.7 ppm [15]. Very recently, using laser excitation of an atomic beam, Shiner *et al.* [16] have improved substantially the measurements of this fine structure. Future work is under way to reduce uncertainties below the 1 kHz level [16]. Kramer and Pipkin [5] measured the fine structure in the $1s3p\ {}^3P_J$ states of helium by using the technique of level-crossing spectroscopy, with the purpose of providing an independent test of the calculations involved in determining α from the $n = 2$ measurements. Their precision is 4.5 ppm. The experimental determinations of the fine structure intervals of $1s3d\ ^3D_J$ [17] and $1s4f\ ^3F_J$ of helium are also available [18]. High precision measurements on high-n and high-l states could also provide a unique opportunity to detect and investigate retardation effects which come from the finite exchange time of virtual photons between the outer Rydberg electron and the inner core. High precision measurements of the fine structure of other low Z atoms also exist. In Li^+, the $1s2p\ ^3P_J$ fine structure splittings were measured by Bayer *et al.* [19] and Holt *et al.* [20] and were improved recently by Riis *et al.* [21]. In Beryllium, the high precision measurements of the $1s2s\ ^3S_1 \rightarrow 1s2p\ ^3P_{0,1,2}$ transitions were reported very recently [22], from which the fine structure splittings could be extracted. Myers *et al.* [23] measured the $1s2p\ ^3P_1 -\ ^3P_2$ fine structure of $^{19}F^{7+}$ at the 31 ppm level. Very recently Hallett *et al.* [24] measured $1s2s\ ^3S_1 \rightarrow 1s2p\ ^3P_{2,0}$ wavelengths in helium-like neon.

In view of the recent advances in both theory and experiment of two electron atoms, a new possibility of re-determining the fine structure constant to a precision of about a few parts per billion (ppb level) has been raised, which could be competitive with those derived from leptonic $g-2$ studies and from condensed-matter physics. In this work we have recalculated the Douglas and Kroll $O(\alpha^6 mc^2)$ contributions to the $1s2p\ ^3P_J$ fine structure of helium and successfully extended these calculations to arbitrary states of helium and helium-like ions, using the Hylleraas-type wave functions of Drake. We have also discussed the computational method in detail, especially the method of cancelling systematically the divergences which come from the high singularity of the operators at $\vec{r}_1 = \vec{r}_2$. The precision we have achieved is consistent with that of the lowest-order spin-dependent matrix elements of the Breit interaction [7].

Chapter 2

Evaluation of the Matrix elements of the Douglas and Kroll $\alpha^6 mc^2$ Operators

2.1 Description of the Wave Function

Let us first discuss the new techniques of Drake to construct nonrelativistic wave functions of two electron atoms such as helium. The material here comes from a review article by Drake and van Wijngaarden [25] which contains the best description of this new variational approach. The Hamiltonian for a two-electron atom in the Coulomb field of a fixed nucleus of charge Z can be expressed in atomic units by

$$H = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r}, \tag{2.1}$$

where $r = |\vec{r}_1 - \vec{r}_2|$. The Schrödinger equation for this H would be separable if there were no repulsive force between the two electrons. Hylleraas was the first to take this correlation into account by including explicitly the variable r in his trial wave function for the ground state:

$$\Psi(\vec{r}_1, \vec{r}_2) = \sum_{i,j,k} a_{ijk} r_1^i r_2^j r^k e^{-\alpha r_1 - \beta r_2} \pm \text{exchange}, \tag{2.2}$$

where a_{ijk} are linear variational parameters and α and β are non-linear parameters. The usual procedure is to include all combinations of i, j, k such that $i + j + k \leq N$, where N is an interger, and then study the convergence of the calculation as N is increased. One can show that the expansion of Eq. (2.2) becomes complete as $N \to \infty$.

For any finite N, the a_{ijk} are determined by Schrödinger's variational principle

$$E(\Psi) = \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \text{Min.}, \tag{2.3}$$

which gives the system of homogeneous linear equations

$$\frac{\partial E}{\partial a_{ijk}} = 0. \tag{2.4}$$

We can consider Eq. (2.4) from a more general point of view. We can think of the functions in Eq. (2.2) as the members of a basis set

$$\begin{aligned} \chi_l &= r_1^i r_2^j r^k e^{-\alpha r_1 - \beta r_2} \\ l &= 1, 2, \cdots, P, \end{aligned}$$

where l denotes the lth distinct combination of values for i, j, k. The solutions to Eq. (2.4) correspond to finding the linear combinations

$$\Phi_m = \sum_{l=1}^{P} a_l^{(m)} \chi_l, \tag{2.5}$$

which satisfy

$$\begin{aligned} \langle\Phi_m|\Phi_n\rangle &= \delta_{m,n} \\ \langle\Phi_m|H|\Phi_n\rangle &= \varepsilon_m \delta_{m,n}. \end{aligned}$$

Thus, the solutions to Eq. (2.4) are the same as what one would obtain by diagonalizing the Hamiltonian in the orthonormal basis set constructed from the same set of functions. If there are P linearly independent functions, then one obtains P variational eigenvalues, ε_m ($m = 1, 2, \cdots, P$).

An important property of the eigenvalues obtained follows from the MATRIX INTERLEAVING THEOREM, which says that when an extra row and column are added to a matrix, the old eigenvalues fall between the new values, with the new highest higher than the old highest and the new lowest lower that the old lowest. Since, by Eq. (2.3), the lowest eigenvalue is bounded from below by the true ground state, the higher eigenvalues must similarly lie above the corresponding excited states, and move progressively downward as P is increased. The result is summarized by the Hylleraas-Undheim Theorem [26]:

When a Hamiltonian operator whose spectrum is bounded from below is diagonalized in a P-dimensional finite basis set, then the P eigenvalues are upper bounds to the first P energies of the actual spectrum.

The optimization of the nonlinear parameters in Eq. (2.2) produces a more difficult problem because the equations

$$\frac{\partial E}{\partial \alpha} = 0$$

$$\frac{\partial E}{\partial \beta} = 0 \qquad (2.6)$$

are transcendental. One must resort to a process of recalculating the variational eigenvalues for different values of α and β in order to locate the variational minimum for a given state.

The Hylleraas method has been applied with great success by many authors to the low-lying states of helium and helium-like ions, culminating in the 1960's and early 1970's with the extensive calculations of Pekeris and co-workers [27].

Despite this large body of work, there remain important problems to be solved. For low-lying states, one should overcome the problem of near linear dependence in the basis set as N increases. Another problem is to develop new techniques to deal with high-lying Rydberg states. In order to solve these problems, Drake proposed a new variational approach by doubling the basis set so that Eq. (2.2) becomes

$$\Psi(\vec{r}_1,\vec{r}_2) = a_0\Psi_0(1s,nl)+\sum_{i,j,k}[a_{ijk}\chi_{ijk}(\alpha_1,\beta_1)+b_{ijk}\chi_{ijk}(\alpha_2,\beta_2)]\mathcal{Y}^M_{l_1l_2L}(\hat{r}_1,\hat{r}_2)\pm\text{exchange} \qquad (2.7)$$

with $\Psi_0(1s,nl)$ being the screened hydrogenic wave function for the two electrons. The inclusion of Ψ_0 is to take advantage of the near screened hydrogenic nature of the excited states of two electron systems and thus, Ψ_0 is already a good approximation to the wave function. The angular function denotes a vector coupled product of solid spherical harmonics for the two electrons to form a state of total angular momentum L:

$$\mathcal{Y}^M_{l_1l_2L} = \sum_{m_1m_2}\langle l_1l_2m_1m_2|LM\rangle Y_{l_1m_1}(\hat{r}_1)Y_{l_2m_2}(\hat{r}_2), \qquad (2.8)$$

and, as before,

$$\chi_{ijk}(\alpha,\beta) = r_1^i r_2^j r^k e^{-\alpha r_1 - \beta r_2}, \tag{2.9}$$

with i, j, and k are non-negative integers. Each combination of powers i, j, k is now included twice in Eq. (2.7) with different nonlinear parameters α_1, β_1 and α_2, β_2. At first sight, one might think that this would lead to problems of linear dependence, but in fact a complete optimization of the energy with respect to all four nonlinear parameters leads to well-defined and numerically stable values for the parameters, with the two sets being well separated from each other. For the first set of terms in Eq. (2.7), the optimum values of α_1 and β_1 are close to their screened hydrogenic values $\alpha_1 \approx Z$ and $\beta_1 \approx (Z-1)/n$. These terms describe the asymptotic behavior of the wave function. For the second set of terms, the optimum values of α_2 and β_2 are much larger. These terms describe the complex inner correlation effects. The complete optimization, therefore, has the effect of dividing the basis set into two sectors with quite different distance scales, i.e., an asymptotic sector and an inner correlation sector.

The new variational method has proven to be very successful in improving the precision of calculated eigenvalues by several orders of magnitude. An important advantage in using these techniques is that they do not suffer from a loss of accuracy as one goes up the Rydberg series to moderately high values of n (i.e., $n \sim 10$).

2.2 Some Useful Expressions of Differential Operators

We adopt the Condon-Shortley convention [28] for the Clebsch-Gordan coefficient throughout this work. That is, the $3j$ symbol is related to the corresponding Clebsch-Gordan coefficient by

$$\begin{pmatrix} j_1 & j_2 & j \\ m_1 & m_2 & m \end{pmatrix} = \frac{(-1)^{j_1-j_2-m}}{\sqrt{2j+1}} \langle j_1 j_2 m_1 m_2 | j_1 j_2 j - m \rangle.$$

The Douglas and Kroll terms contain a wide variety of differential operators. It is convenient to separate the radial and angular parts of the gradient operators according to the following basic formulas written in the spherical component form:

$$\nabla_{1\mu} = \sqrt{\frac{4\pi}{3}}Y_{1\mu}(\hat{r}_1)(\frac{\partial}{\partial r_1}+\frac{r_1}{r}\frac{\partial}{\partial r}) - \sqrt{\frac{4\pi}{3}}Y_{1\mu}(\hat{r}_2)\frac{r_2}{r}\frac{\partial}{\partial r} + \nabla^y_{1\mu} \tag{2.10}$$

$$\nabla_{2\mu} = \sqrt{\frac{4\pi}{3}}Y_{1\mu}(\hat{r}_2)(\frac{\partial}{\partial r_2}+\frac{r_2}{r}\frac{\partial}{\partial r}) - \sqrt{\frac{4\pi}{3}}Y_{1\mu}(\hat{r}_1)\frac{r_1}{r}\frac{\partial}{\partial r} + \nabla^y_{2\mu}, \tag{2.11}$$

where μ =-1, 0, and 1, and $\nabla^y_{1\mu}$ and $\nabla^y_{2\mu}$ are understood to act only on the spherical harmonics. We also have the following formula (see Appendix VI of ref. [29]):

$$r\nabla_\mu Y_{lm}(\hat{r}) = \sum_{\lambda\tau} b(l;\lambda)(l,\lambda)^{1/2}\begin{pmatrix}1 & l & \lambda\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}1 & l & \lambda\\ \mu & m & \tau\end{pmatrix}Y^*_{\lambda\tau}(\hat{r}), \tag{2.12}$$

where the notation $(\alpha,\beta,\cdots) = (2\alpha+1)(2\beta+1)\cdots$ is adopted and the function $b(l;\lambda)$ is defined by

$$\begin{aligned} b(l;l-1) &= l+1 \\ b(l;l+1) &= -l. \end{aligned} \tag{2.13}$$

From the above equations it is a straightforward matter to obtain the following expressions:

$$\begin{aligned}\nabla_{1\mu}|F\mathcal{Y}^M_{l_1l_2L}\rangle &= \sum_{m_1m_2}\sum_{T\tau}(-1)^{l_1-l_2+M}(l_1,L,T)^{1/2}\begin{pmatrix}1 & l_1 & T\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}1 & l_1 & T\\ \mu & m_1 & \tau\end{pmatrix}\\ &\times \begin{pmatrix}l_1 & l_2 & L\\ m_1 & m_2 & -M\end{pmatrix}(D^{(1)}(l_1;T)F)Y^*_{T\tau}(\hat{r}_1)Y_{l_2m_2}(\hat{r}_2)\\ &+ \sum_{m_1m_2}\sum_{T\tau}(-1)^{l_1-l_2+M+1}(l_2,L,T)^{1/2}\begin{pmatrix}l_2 & 1 & T\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_2 & 1 & T\\ m_2 & \mu & \tau\end{pmatrix}\\ &\times \begin{pmatrix}l_1 & l_2 & L\\ m_1 & m_2 & -M\end{pmatrix}(D^{(1)}_0F)Y_{l_1m_1}(\hat{r}_1)Y^*_{T\tau}(\hat{r}_2)\end{aligned} \tag{2.14}$$

$$\begin{aligned}\nabla_{2\mu}|F\mathcal{Y}^M_{l_1l_2L}\rangle &= \sum_{m_1m_2}\sum_{T\tau}(-1)^{l_1-l_2+M}(l_2,L,T)^{1/2}\begin{pmatrix}1 & l_2 & T\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}1 & l_2 & T\\ \mu & m_2 & \tau\end{pmatrix}\\ &\times \begin{pmatrix}l_1 & l_2 & L\\ m_1 & m_2 & -M\end{pmatrix}(D^{(2)}(l_2;T)F)Y_{l_1m_1}(\hat{r}_1)Y^*_{T\tau}(\hat{r}_2)\\ &+ \sum_{m_1m_2}\sum_{T\tau}(-1)^{l_1-l_2+M+1}(l_1,L,T)^{1/2}\begin{pmatrix}l_1 & 1 & T\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_1 & 1 & T\\ m_1 & \mu & \tau\end{pmatrix}\\ &\times \begin{pmatrix}l_1 & l_2 & L\\ m_1 & m_2 & -M\end{pmatrix}(D^{(2)}_0F)Y^*_{T\tau}(\hat{r}_1)Y_{l_2m_2}(\hat{r}_2),\end{aligned} \tag{2.15}$$

where F is the radial part containing r_1, r_2, and r as independent variables and is written as:

$$F(r_1, r_2, r) = r_1^a r_2^b r^c e^{-\alpha r_1 - \beta r_2}, \tag{2.16}$$

and the various D operators are

$$D_0^{(1)} = \frac{r_2}{r}\frac{\partial}{\partial r} \tag{2.17}$$

$$D_0^{(2)} = \frac{r_1}{r}\frac{\partial}{\partial r} \tag{2.18}$$

$$D^{(1)}(l;T) = \frac{\partial}{\partial r_1} + \frac{r_1}{r}\frac{\partial}{\partial r} + b(l;T)\frac{1}{r_1} \tag{2.19}$$

$$D^{(2)}(l;T) = \frac{\partial}{\partial r_2} + \frac{r_2}{r}\frac{\partial}{\partial r} + b(l;T)\frac{1}{r_2}. \tag{2.20}$$

Since the Laplacian operator ∇_1^2 may be understood to act on the left-hand side wave function, we have:

$$\langle \nabla_1^2 F \mathcal{Y}_{l_1 l_2 L}^M | = B_1 + B_2 \tag{2.21}$$

with

$$B_1 = \sum_{m_1 m_2} (-1)^{l_1 - l_2 + M}(2L+1)^{1/2} \begin{pmatrix} l_1 & l_2 & L \\ m_1 & m_2 & -M \end{pmatrix} (\tilde{D}^{(1)}(l_1)F) Y_{l_1 m_1}^*(\hat{r}_1) Y_{l_2 m_2}^*(\hat{r}_2)$$

$$\begin{aligned} B_2 = {} & 2\sum_{N\nu}\sum_{H\eta}\sum_{\mu m_1 m_2} (-1)^{l_1 - l_2 + M + m_1 + 1}(l_1, l_2, L, N, H)^{1/2} \begin{pmatrix} l_1 & 1 & N \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2 & 1 & H \\ 0 & 0 & 0 \end{pmatrix} \\ & \times \begin{pmatrix} l_1 & l_2 & L \\ m_1 & m_2 & -M \end{pmatrix} \begin{pmatrix} 1 & l_1 & N \\ \mu & -m_1 & \nu \end{pmatrix} \begin{pmatrix} 1 & l_2 & H \\ \mu & m_2 & \eta \end{pmatrix} (\tilde{d}_N^{(1)}(l_1)F) Y_{N\nu}^*(\hat{r}_1) Y_{H\eta}(\hat{r}_2) \end{aligned}$$

where

$$\tilde{D}^{(1)}(l) = \frac{1}{r_1^2}\frac{\partial}{\partial r_1}(r_1^2\frac{\partial}{\partial r_1}) + \frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial}{\partial r}) - \frac{l(l+1)}{r_1^2} + \frac{2(r_1 - r_2\cos\theta)}{r}\frac{\partial^2}{\partial r_1 \partial r} \tag{2.22}$$

$$\tilde{d}_\Lambda^{(1)}(l) = b(l;\Lambda)\frac{r_2}{r_1 r}\frac{\partial}{\partial r}, \tag{2.23}$$

and $\cos\theta$ is a radial function defined by

$$\cos\theta = (r_1^2 + r_2^2 - r^2)/(2r_1 r_2). \tag{2.24}$$

Note that the formula (see p57 of ref. [29])

$$Y_{lm}(\hat{r})Y_{l'm'}(\hat{r}) = \sum_{LM}\sqrt{\frac{(l,l',L)}{4\pi}}\begin{pmatrix} l & l' & L \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l & l' & L \\ m & m' & M \end{pmatrix}Y^{*}_{LM}(\hat{r}) \qquad (2.25)$$

is useful in the reduction of products of various spherical harmonic functions. Finally we have the following expression:

$$\sum_{\mu_1\mu_2}\begin{pmatrix} 1 & 1 & K \\ \mu_1 & \mu_2 & 0 \end{pmatrix}\nabla_{1\mu_1}\nabla_{2\mu_2}[FY_{l_1m_1}(\hat{r}_1)Y_{l_2m_2}(\hat{r}_2)] = A_1^{(K)} + A_2^{(K)} + A_3^{(K)}, \qquad (2.26)$$

where

$$\begin{aligned} A_1^{(K)} &= \sum_{T\tau}\sum_{\Lambda\lambda}\sum_{\mu_1\mu_2}(l_1,l_2,T,\Lambda)^{1/2}\begin{pmatrix} 1 & l_1 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_2 & \Lambda \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_1 & T \\ \mu_1 & m_1 & \tau \end{pmatrix} \\ &\times \begin{pmatrix} 1 & l_2 & \Lambda \\ \mu_2 & m_2 & \lambda \end{pmatrix}\begin{pmatrix} 1 & 1 & K \\ \mu_1 & \mu_2 & 0 \end{pmatrix}(D_{\Lambda T}^{(K)}(l_2,l_1)F)Y^{*}_{T\tau}(\hat{r}_1)Y^{*}_{\Lambda\lambda}(\hat{r}_2) \end{aligned}$$

$$\begin{aligned} A_2^{(K)} &= \sum_{T\tau}\sum_{\Lambda\lambda}\sum_{\mu_1\mu_2}(-1)^{\tau+1}(l_1,T,T,\Lambda)^{1/2}\begin{pmatrix} 1 & l_1 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & T & \Lambda \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_1 & T \\ \mu_1 & m_1 & \tau \end{pmatrix} \\ &\times \begin{pmatrix} 1 & T & \Lambda \\ \mu_2 & -\tau & \lambda \end{pmatrix}\begin{pmatrix} 1 & 1 & K \\ \mu_1 & \mu_2 & 0 \end{pmatrix}(D_0^{(2)}D^{(1)}(l_1;T)F)Y^{*}_{\Lambda\lambda}(\hat{r}_1)Y_{l_2m_2}(\hat{r}_2) \end{aligned}$$

$$\begin{aligned} A_3^{(K)} &= \sum_{T\tau}\sum_{\Lambda\lambda}\sum_{\mu_1\mu_2}(-1)^{\tau+1}(l_2,T,T,\Lambda)^{1/2}\begin{pmatrix} 1 & l_2 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & T & \Lambda \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_2 & T \\ \mu_1 & m_2 & \tau \end{pmatrix} \\ &\times \begin{pmatrix} 1 & T & \Lambda \\ \mu_2 & -\tau & \lambda \end{pmatrix}\begin{pmatrix} 1 & 1 & K \\ \mu_1 & \mu_2 & 0 \end{pmatrix}(D^{(2)}(T;\Lambda)D_0^{(1)}F)Y_{l_1m_1}(\hat{r}_1)Y^{*}_{\Lambda\lambda}(\hat{r}_2) \end{aligned}$$

with

$$D_{\Lambda T}^{(K)}(l_2,l_1) = D^{(2)}(l_2;\Lambda)D^{(1)}(l_1;T) + (-1)^K D_0^{(2)}D_0^{(1)}. \qquad (2.27)$$

2.3 Calculation of Integrals

In the evaluation of the Douglas and Kroll operators, the matrix elements of the operators can finally be reduced to sums of integrals of the type

$$I_\Lambda(a,b,c) = \int_0^\infty r_1dr_1\int_0^\infty r_2dr_2\int_{|r_1-r_2|}^{r_1+r_2} rdr\; r_1^a r_2^b r^c e^{-\alpha r_1-\beta r_2}P_\Lambda(\cos\theta), \qquad (2.28)$$

where $\cos\theta$ is defined by Eq. (2.24) and $P_\Lambda(\cos\theta)$ is a Legendre polynomial. There are some recurrence relations which were derived by Drake [30]:

$$I_{\Lambda+1}(a,b,c) = \frac{2\Lambda+1}{c+2}I_\Lambda(a-1,b-1,c+2) + I_{\Lambda-1}(a,b,c), \quad c \neq -2, \qquad (2.29)$$

and, for the case of $c = -2$ we have

$$I_{\Lambda+1}(r_1^a, r_2^b, r^{-2}) = (2\Lambda+1)I_\Lambda(r_1^{a-1}, r_2^{b-1}, \ln r) + I_{\Lambda-1}(r_1^a, r_2^b, r^{-2}). \quad (2.30)$$

The recurrence relation involving logarithmic integrals is

$$\begin{aligned} I_{\Lambda+1}(r_1^a, r_2^b, r^c \ln r) &= \frac{(2\Lambda+1)}{c+2}[I_\Lambda(r_1^{a-1}, r_2^{b-1}, r^{c+2}\ln r) && (2.31) \\ &- \frac{1}{c+2}I_\Lambda(r_1^{a-1}, r_2^{b-1}, r^{c+2})] + I_{\Lambda-1}(r_1^a, r_2^b, r^c \ln r). && (2.32) \end{aligned}$$

In particular, from Eq. (2.24) $I_1(a,b,c)$ can be written as

$$I_1(a,b,c) = \frac{1}{2}[I_0(a+1, b-1, c) + I_0(a-1, b+1, c) - I_0(a-1, b-1, c+2)]. \quad (2.33)$$

Thus, the calculation of the integral $I_\Lambda(a,b,c)$ is reduced to evaluating $I_0(a,b,c)$ for a sufficient range of a, b, and c, which will be the main topic of this section.

It is obvious that

$$I_0(a,b,c) = A_1 + A_2 \quad (2.34)$$

with

$$\begin{aligned} A_1 &= \int_0^\infty r_1^{a+1} e^{-\alpha r_1} dr_1 \int_{r_1}^\infty r_2^{b+1} e^{-\beta r_2} dr_2 \int_{r_2-r_1}^{r_2+r_1} r^{c+1} dr \\ A_2 &= \int_0^\infty r_2^{b+1} e^{-\beta r_2} dr_2 \int_{r_2}^\infty r_1^{a+1} e^{-\alpha r_1} dr_1 \int_{r_1-r_2}^{r_1+r_2} r^{c+1} dr. \end{aligned}$$

We first treat A_1. The integration over r can be carried out:

$$\int_{r_2-r_1}^{r_2+r_1} r^{c+1} dr = \frac{1}{c+2}[(r_2+r_1)^{c+2} - (r_2-r_1)^{c+2}] = \sum_{p=\text{odd}}^{c+2} \frac{2(c+1)!}{p!(c+2-p)!} r_1^p r_2^{c+2-p}.$$

Thus,

$$\begin{aligned} A_1 &= \sum_{p=\text{odd}}^{c+2} \frac{2(c+1)!}{p!(c+2-p)!} \int_0^\infty r_1^{a+1+p} e^{-\alpha r_1} dr_1 \int_{r_1}^\infty r_2^{b+c+3-p} e^{-\beta r_2} dr_2 \\ &= \sum_{p=\text{odd}}^{c+2} \frac{2(c+1)!}{p!(c+2-p)!} \int_0^\infty r_2^{b+c+3-p} e^{-\beta r_2} dr_2 \int_0^{r_2} r_1^{a+1+p} e^{-\alpha r_1} dr_1. \quad (2.35) \end{aligned}$$

Using formula 6.5.12 of ref. [31] and formula 4, 7.621 of ref. [32],

$$\int_0^{r_2} r_1^n e^{-\alpha r_1} dr_1 = \frac{r_2^{n+1}}{n+1} e^{-\alpha r_2} {}_1F_1(1; n+2; \alpha r_2) \quad (2.36)$$

$$\int_0^\infty e^{-st} t^{b-1} {}_1F_1(a;c;kt)dt = \Gamma(b) s^{-b} F(a,b;c;ks^{-1}), \tag{2.37}$$

where ${}_1F_1(a;b;x)$ is the confluent hypergeometric function, $F(a,b;c;x)$ is the hypergeometric function, and $\Gamma(x)$ is the gamma function. A_1 can easily be integrated. A_2 can be treated in a similar way. Finally we obtain

$$\begin{aligned} I_0(a,b,c;\alpha,\beta) &= \frac{2(c+1)!(a+b+c+5)!}{(\alpha+\beta)^{a+b+c+6}} \sum_{p=\mathrm{odd}}^{c+2} \frac{1}{p!(c+2-p)!} \\ &\times [\frac{1}{a+2+p} F(1,a+b+c+6;a+3+p;\frac{\alpha}{\alpha+\beta}) \\ &+ \frac{1}{b+2+p} F(1,a+b+c+6;b+3+p;\frac{\beta}{\alpha+\beta})]. \end{aligned} \tag{2.38}$$

The above expression is convergent as long as the following conditions are satisfied:

$$a+b+c+5 \geq 0 \tag{2.39}$$

$$a \geq -2 \tag{2.40}$$

$$b \geq -2 \tag{2.41}$$

$$c \geq -1. \tag{2.42}$$

These conditions are also valid for $I_\Lambda(a,b,c)$, because $r_1^a r_2^b r^c e^{-\alpha r_1 - \beta r_2} > 0$, and $P_\Lambda(\cos\theta)$ is bounded and oscillatory, thus making $I_\Lambda(a,b,c)$ converge. It is worth mentioning here that the application of recurrence relation of Eq. (2.29) to I_Λ amounts to evaluating various I_0 with more negative powers of r_1 and r_2, which could cause individual I_0 divergence. Nevertheless, cancellation can always be performed by simply neglecting the terms in Eq. (2.38) with

$$a+2+p = 0 \tag{2.43}$$

$$a+3+p \leq 0 \tag{2.44}$$

$$b+2+p = 0 \tag{2.45}$$

$$b+3+p \leq 0. \tag{2.46}$$

Thus, only the nonsingular part of Eq. (2.38) is needed. For the integrals required in this work, the power series expansions of hypergeometric functions yield numerically accurate values with rapid convergence.

A similar method can be applied to the case of $c = -2$ by noting the expansion

$$\int_{r_2-r_1}^{r_2+r_1} r^{-1}dr = \ln\frac{r_2+r_1}{r_2-r_1} = 2\sum_{p=0}^{\infty}\frac{1}{2p+1}(\frac{r_1}{r_2})^{2p+1}.$$

This expansion gives an infinite series for the integral

$$\begin{aligned} I_0(a,b,-2;\alpha,\beta) &= \frac{2(a+b+3)!}{(\alpha+\beta)^{a+b+4}}\sum_{p=0}^{\infty}\frac{1}{2p+1} \\ &\times [\frac{1}{a+2p+3}F(1,a+b+4;a+2p+4;\frac{\alpha}{\alpha+\beta}) \\ &+ \frac{1}{b+2p+3}F(1,a+b+4;b+2p+4;\frac{\beta}{\alpha+\beta})], \end{aligned} \tag{2.47}$$

which is valid only when

$$a+b+3 \geq 0 \tag{2.48}$$

$$a \geq -2 \tag{2.49}$$

$$b \geq -2. \tag{2.50}$$

The convergence of this infinite series can be assured by the fact that each term of the expression is positive and is roughly proportional to $1/p^2$ which is a general term of a convergent series $\sum_{p=0}^{\infty} 1/p^2$. However, this series converges very slowly and should be improved before it can be used in numerical computation. If we make the following transformations in Eq. (2.47),

$$\begin{aligned} a+b+4 &\Rightarrow b \\ a+2 &\Rightarrow c \\ \frac{\alpha}{\alpha+\beta} &\Rightarrow z \\ 2p+1 &\Rightarrow n, \end{aligned}$$

then the first summation becomes

$$S = \sum_{n=\mathrm{odd}}^{\infty}\frac{1}{n(n+c)}F(1,b;n+c+1;z). \tag{2.51}$$

The hypergeometric function F can be expanded according to the definition

$$F(1,b;n+c+1;z) = \sum_{m=0}^{\infty}\frac{(1)_m(b)_m}{m!(n+c+1)_m}z^m = \sum_{m=0}^{\infty}\frac{(b)_m}{(n+c+1)_m}z^m, \tag{2.52}$$

where

$$
\begin{aligned}
(\lambda)_0 &= 1 \\
(\lambda)_n &= \lambda(\lambda+1)\cdots(\lambda+n-1).
\end{aligned}
$$

Thus Eq. (2.51) can be put into the form of

$$S = \sum_{m=0}^{\infty} (b)_m S_m(c) z^m \tag{2.53}$$

with

$$S_m(c) = \sum_{n=odd}^{\infty} \frac{1}{n(n+c)\cdots(n+c+m)}. \tag{2.54}$$

The above infinite series can be summed to a finite form by using formula 6.3.16 of ref. [31]:

$$\sum_{n=1}^{\infty}\left(\frac{1}{n} - \frac{1}{z+n}\right) = \gamma + \frac{1}{z} + \Psi(z), \tag{2.55}$$

where γ is the Euler constant

$$\gamma = 0.577215664901\cdots$$

and $\Psi(z)$ is the digamma function

$$\Psi(z) = \Gamma'(z)/\Gamma(z). \tag{2.56}$$

Eq. (2.55) is equivalent to

$$
\begin{aligned}
&\sum_{n=odd}^{\infty}\left(\frac{1}{n} - \frac{1}{z+n}\right) + \sum_{n=even}^{\infty}\left(\frac{1}{n} - \frac{1}{z+n}\right) \\
&= z\sum_{n=odd}^{\infty} \frac{1}{n(n+z)} + \frac{1}{2}\sum_{n=1}^{\infty}\left(\frac{1}{n} - \frac{1}{z/2+n}\right) \\
&= z\sum_{n=odd}^{\infty} \frac{1}{n(n+z)} + \frac{1}{2}\left(\gamma + \frac{2}{z} + \Psi\left(\frac{z}{2}\right)\right) \\
&= \gamma + \frac{1}{z} + \Psi(z),
\end{aligned}
$$

or

$$\sum_{n=odd}^{\infty} \frac{1}{n(n+z)} = \frac{1}{z}\left[\frac{\gamma}{2} + \Psi(z) - \frac{1}{2}\Psi\left(\frac{z}{2}\right)\right], \tag{2.57}$$

which is equal to $S_0(z)$. This can easily be generalized by the method of mathematical induction. The final result reads

$$S_m(c) = \sum_{k=0}^{m} \frac{(-1)^k}{k!(m-k)!} \frac{1}{c+k} [\frac{\gamma}{2} + \Psi(c+k) - \frac{1}{2}\Psi(\frac{c+k}{2})]. \tag{2.58}$$

At first sight, one might think that the existence of the oscillatory factor $(-1)^k$ in Eq. (2.58) would cause numerical cancellation for large m. However, it is necessary to extract only a few terms from the hypergeometric function F and to sum up to a finite number of terms, that is,

$$S = \sum_{m=0}^{N} (b)_m S_m(c) z^m + \sum_{n=\text{odd}}^{\infty} \frac{1}{n(n+c)} F_N(1, b; n+c+1; z), \tag{2.59}$$

where F_N is $F(1, b; n+c+1; z)$ with the first $N+1$ terms removed. With some experimentation we found that the choice of $N \sim 10$ in the present work is just adequate to greatly improve the rate of convergence without any loss of numerical stability.

Besides the general formulas, Eq. (2.38) and Eq. (2.47), there are other expressions for $I_0(a, b, c)$ which could be used under some circumstances. If we apply the expansion

$$\int r^n e^{-\alpha r} dr = -\sum_{j=0}^{n} \frac{n!}{\alpha^{n-j+1} j!} r^j e^{-\alpha r} \tag{2.60}$$

to Eq. (2.35), then we obtain

$$\begin{aligned} I_0(a,b,c) &= \frac{2}{c+2} \sum_{i=0}^{[(c+1)/2]} \binom{c+2}{2i+1} \{ \frac{q!}{\beta^{q+1}(\alpha+\beta)^{p+1}} \sum_{j=0}^{q} \frac{(p+j)!}{j!} (\frac{\beta}{\alpha+\beta})^j \\ &+ \frac{q'!}{\alpha^{q'+1}(\alpha+\beta)^{p'+1}} \sum_{j=0}^{q'} \frac{(p'+j)!}{j!} (\frac{\alpha}{\alpha+\beta})^j \}. \end{aligned} \tag{2.61}$$

In Eq. (2.61),

$$\begin{aligned} p &= a + 2i + 2 \\ q &= b + c - 2i + 2 \\ p' &= b + 2i + 2 \\ q' &= a + c - 2i + 2, \end{aligned} \tag{2.62}$$

$[x]$ is the largest integer in x, and $\binom{m}{n}$ the binomial coefficient. Eq. (2.61) applies only for $c \geq -1$ and $a,\ b \geq -2$, excluding the case of $a = -2,\ b = -2$, and $c = -1$, which would make q and q' negative.

Let us return to Eq. (2.34). Integrating over r without further expansion, the integral can be recast as

$$I_0(a,b,c) = T_1 - T_2 - T_3, \tag{2.63}$$

with

$$T_1 = \frac{1}{c+2}\int_0^\infty r_1^{a+1}e^{-\alpha r_1}dr_1\int_0^\infty r_2^{b+1}e^{-\beta r_2}(r_1+r_2)^{c+2}dr_2 \tag{2.64}$$

$$T_2 = \frac{1}{c+2}\int_0^\infty r_1^{a+1}e^{-\alpha r_1}dr_1\int_{r_1}^\infty r_2^{b+1}e^{-\beta r_2}(r_2-r_1)^{c+2}dr_2 \tag{2.65}$$

$$T_3 = \frac{1}{c+2}\int_0^\infty r_1^{a+1}e^{-\alpha r_1}dr_1\int_0^{r_1} r_2^{b+1}e^{-\beta r_2}(r_1-r_2)^{c+2}dr_2. \tag{2.66}$$

After making a transformation of $r_2 = \xi - r_1$ in Eq. (2.64) and then changing the order of integration, we have

$$T_1 = \frac{1}{c+2}\int_0^\infty \xi^{c+2}e^{-\beta\xi}d\xi\int_0^\xi r_1^{a+1}(\xi-r_1)^{b+1}e^{(\beta-\alpha)r_1}dr_1.$$

The integration over r_1 may first be carried out using formula 1, 3.383 of ref. [32]:

$$\int_0^u x^{\nu-1}(u-x)^{\mu-1}e^{\beta x}dx = B(\mu,\nu)u^{\mu+\nu-1}{}_1F_1(\nu;\mu+\nu;\beta u)$$
$$[Re\mu > 0, \quad Re\nu > 0], \tag{2.67}$$

where $B(\mu,\nu)$ is the beta function. Thus,

$$T_1 = \frac{B(b+2,a+2)}{c+2}\int_0^\infty \xi^{a+b+c+5}e^{-\beta\xi}{}_1F_1(a+2;a+b+4;(\beta-\alpha)\xi)d\xi.$$

Furthermore, using Eq. (2.37) will complete our evaluation of T_1:

$$T_1 = \frac{B(a+2,b+2)}{c+2}\frac{\Gamma(a+b+c+6)}{\beta^{a+b+c+6}}F(a+2,a+b+c+6;a+b+4;\frac{\beta-\alpha}{\beta})$$
$$\beta \geq \alpha. \tag{2.68}$$

As for the case of $\beta \leq \alpha$, the Kummer transformation (see 13.1.27 of ref. [31])

$$ {}_1F_1(a+2; a+b+4; (\beta-\alpha)\xi) = e^{(\beta-\alpha)\xi}\, {}_1F_1(b+2; a+b+4; (\alpha-\beta)\xi) \qquad (2.69) $$

can be applied, which results in Eq. (2.68) with the interchanges, $a \leftrightarrow b$ and $\alpha \leftrightarrow \beta$. The integral T_2 could be done by making a transformation of $r_2 = r_1 + \xi$:

$$ \begin{aligned} T_2 &= \frac{1}{c+2}\int_0^\infty r_1^{a+1} e^{-(\alpha+\beta)r_1} dr_1 \int_0^\infty (r_1+\xi)^{b+1} e^{-\beta\xi} \xi^{c+2} d\xi \\ &= \frac{1}{c+2}\sum_{p=0}^{b+1}\binom{b+1}{p}\int_0^\infty r_1^{a+b+2-p} e^{-(\alpha+\beta)r_1} dr_1 \int_0^\infty \xi^{p+c+2} e^{-\beta\xi} d\xi \\ &= \frac{1}{c+2}\sum_{p=0}^{b+1}\binom{b+1}{p}\frac{(a+b+2-p)!}{(\alpha+\beta)^{a+b+3-p}}\frac{(p+c+2)!}{\beta^{p+c+3}}. \end{aligned} $$

T_3 can be obtained from T_2 by the interchanging of $a \leftrightarrow b$ and $\alpha \leftrightarrow \beta$. The final expression of $I_0(a,b,c)$ is

$$ I_0(a,b,c) = T_1 - T_2 - T_3; \qquad (2.70) $$

$$ \begin{aligned} T_1 &= \frac{(a+1)!(b+1)!s!}{(a+b+3)!(c+2)}\frac{1}{\beta^{s+1}}F(a+2, s+1; a+b+4; \frac{\beta-\alpha}{\beta}), \quad \beta \geq \alpha \\ &= \frac{(a+1)!(b+1)!s!}{(a+b+3)!(c+2)}\frac{1}{\alpha^{s+1}}F(b+2, s+1; a+b+4; \frac{\alpha-\beta}{\alpha}), \quad \alpha \geq \beta \\ T_2 &= \sum_{p=0}^{b+1}\frac{(b+1)!(a+b+2-p)!}{p!(b+1-p)!(c+2)}\frac{(p+c+2)!}{(\alpha+\beta)^{a+b+3-p}\beta^{p+c+3}} \\ T_3 &= \sum_{p=0}^{a+1}\frac{(a+1)!(a+b+2-p)!}{p!(a+1-p)!(c+2)}\frac{(p+c+2)!}{(\alpha+\beta)^{a+b+3-p}\alpha^{p+c+3}}, \end{aligned} $$

where $s = a+b+c+5$. The above expression is valid for

$$ \begin{aligned} a &\geq -1 \\ b &\geq -1 \\ c &\geq -1 \end{aligned} $$

and is useful when $\alpha \sim \beta$, because, for this case, the hypergeometric function converges extremely fast. Compared with Eq. (2.61) the above expression contains only single summations.

We also need to calculate the integrals containing $\ln r$ when Eq. (2.30) is used. We first write down the following integral:

$$
\begin{aligned}
I_0(r_1^a, r_2^b, r^c \ln r) &= \int_0^\infty r_1^{a+1} e^{-\alpha r_1} dr_1 \int_{r_1}^\infty r_2^{b+1} e^{-\beta r_2} dr_2 \int_{r_2 - r_1}^{r_2 + r_1} r^{c+1} \ln r dr \\
&+ \int_0^\infty r_1^{a+1} e^{-\alpha r_1} dr_1 \int_0^{r_1} r_2^{b+1} e^{-\beta r_2} dr_2 \int_{r_1 - r_2}^{r_1 + r_2} r^{c+1} \ln r dr \quad (2.71)
\end{aligned}
$$

where the integration over r can be performed by

$$
\int r^{c+1} \ln r dr = \frac{1}{c+2} r^{c+2} \ln r - \frac{r^{c+2}}{(c+2)^2}.
$$

Thus, Eq. (2.71) becomes

$$
I_0(r_1^a, r_2^b, r^c \ln r) = H_1 - H_2 - H_3 - \frac{1}{c+2} I_0(a, b, c), \quad (2.72)
$$

with

$$
\begin{aligned}
H_1 &= \frac{1}{c+2} \int_0^\infty r_1^{a+1} e^{-\alpha r_1} dr_1 \int_0^\infty r_2^{b+1} e^{-\beta r_2} (r_1 + r_2)^{c+2} \ln(r_1 + r_2) dr_2 \\
H_2 &= \frac{1}{c+2} \int_0^\infty r_1^{a+1} e^{-\alpha r_1} dr_1 \int_{r_1}^\infty r_2^{b+1} e^{-\beta r_2} (r_2 - r_1)^{c+2} \ln(r_2 - r_1) dr_2 \\
H_3 &= \frac{1}{c+2} \int_0^\infty r_1^{a+1} e^{-\alpha r_1} dr_1 \int_0^{r_1} r_2^{b+1} e^{-\beta r_2} (r_1 - r_2)^{c+2} \ln(r_1 - r_2) dr_2.
\end{aligned}
$$

We deal with H_1 first. After making the transformation of $r_2 = \xi - r_1$ and integrating over r_1 with the use of Eq. (2.67), we have

$$
\begin{aligned}
H_1 &= \frac{1}{c+2} B(b+2, a+2) \int_0^\infty \xi^s e^{-\beta\xi} \ln \xi \, {}_1F_1(a+2; a+b+4; (\beta - \alpha)\xi) d\xi \\
&= \frac{1}{c+2} B(b+2, a+2) \sum_{q=0}^\infty \frac{(a+2)_q}{(a+b+4)_q} \frac{(\beta-\alpha)^q}{q!} \int_0^\infty \xi^{s+q} e^{-\beta\xi} \ln \xi d\xi.
\end{aligned}
$$

Here we have used the series expansion of the confluent hypergeometric function,

$$
{}_1F_1(\alpha; \gamma; z) = \sum_{n=0}^\infty \frac{(\alpha)_n}{n!(\gamma)_n} z^n, \quad (2.73)
$$

and that $s = a + b + c + 5$. Furthermore, the application of formula (see 2, 4.352 and 4, 8.365 of ref. [32])

$$
\int_0^\infty x^n e^{-\mu x} \ln x dx = \frac{n!}{\mu^{n+1}} [\Psi(n+1) - \ln \mu] \quad (2.74)
$$

yields

$$H_1 = \frac{(b+1)!}{(c+2)\beta^{s+1}}\sum_{q=0}^{\infty}\frac{(s+q)!(a+1+q)!}{(a+b+3+q)!q!}(\frac{\beta-\alpha}{\beta})^q[\Psi(s+1+q)-\ln\beta]. \qquad (2.75)$$

Although this expression is valid for both $\alpha \geq \beta$ and $\alpha \leq \beta$, it is best suited for the case of $\alpha \leq \beta$, since then an alternating series can be avoided. As for $\alpha \geq \beta$, the use of the Kummer transformation results in Eq. (2.75) with $a \leftrightarrow b$ and $\alpha \leftrightarrow \beta$ interchanged. H_2 can be treated in a similar way. Let $r_2 = r_1 + \xi$, then

$$\begin{aligned} H_2 &= \frac{1}{c+2}\int_0^{\infty} r_1^{a+1}e^{-(\alpha+\beta)r_1}dr_1\int_0^{\infty}(r_1+\xi)^{b+1}e^{-\beta\xi}\xi^{c+2}\ln\xi d\xi \\ &= \frac{1}{c+2}\sum_{p=0}^{b+1}\frac{(b+1)!}{p!(b+1-p)!}\int_0^{\infty} r_1^{a+b+2-p}e^{-(\alpha+\beta)r_1}dr_1\int_0^{\infty}\xi^{p+c+2}e^{-\beta\xi}\ln\xi d\xi \\ &= \frac{1}{c+2}\sum_{p=0}^{b+1}\frac{(b+1)!}{p!(b+1-p)!}\frac{(a+b+2-p)!}{(\alpha+\beta)^{a+b+3-p}}\frac{(p+c+2)!}{\beta^{p+c+3}}[\Psi(p+c+3)-\ln\beta], \end{aligned}$$

which also holds for H_3 when $a \leftrightarrow b$ and $\alpha \leftrightarrow \beta$ are interchanged. In summary, we have obtained the following expression:

$$I_0(r_1^a, r_2^b, r^c\ln r) = H_1 - H_2 - H_3 - \frac{1}{c+2}I_0(a,b,c), \qquad (2.76)$$

where

$$\begin{aligned} H_1 &= \frac{(b+1)!}{(c+2)\beta^{s+1}}\sum_{q=0}^{\infty}\frac{(s+q)!(a+1+q)!}{(a+b+3+q)!q!}(\frac{\beta-\alpha}{\beta})^q[\Psi(s+1+q)-\ln\beta], \quad \beta\geq\alpha \\ &= \frac{(a+1)!}{(c+2)\alpha^{s+1}}\sum_{q=0}^{\infty}\frac{(s+q)!(b+1+q)!}{(a+b+3+q)!q!}(\frac{\alpha-\beta}{\alpha})^q[\Psi(s+1+q)-\ln\alpha], \quad \beta\leq\alpha \end{aligned}$$

$$\begin{aligned} H_2 &= \frac{1}{c+2}\sum_{p=0}^{b+1}\frac{(b+1)!}{p!(b+1-p)!}\frac{(a+b+2-p)!}{(\alpha+\beta)^{a+b+3-p}}\frac{(p+c+2)!}{\beta^{p+c+3}}[\Psi(p+c+3)-\ln\beta] \\ H_3 &= \frac{1}{c+2}\sum_{p=0}^{a+1}\frac{(a+1)!}{p!(a+1-p)!}\frac{(a+b+2-p)!}{(\alpha+\beta)^{a+b+3-p}}\frac{(p+c+2)!}{\alpha^{p+c+3}}[\Psi(p+c+3)-\ln\alpha]. \end{aligned}$$

Eq. (2.76) is valid for $a, b, c \geq -1$. The above derivation may be applied to $I_0(a,b,-2)$ to obtain a similar expression:

$$I_0(a,b,-2) = K_1 - K_2 - K_3, \qquad (2.77)$$

where

$$
\begin{aligned}
K_1 &= \frac{(b+1)!}{\beta^{a+b+4}}\sum_{q=0}^{\infty}\frac{(a+1+q)!}{q!}(\frac{\beta-\alpha}{\beta})^q[\Psi(a+b+4+q)-\ln\beta], \quad \beta\geq\alpha \\
&= \frac{(a+1)!}{\alpha^{a+b+4}}\sum_{q=0}^{\infty}\frac{(b+1+q)!}{q!}(\frac{\alpha-\beta}{\alpha})^q[\Psi(a+b+4+q)-\ln\alpha], \quad \beta\leq\alpha \\
K_2 &= \sum_{p=0}^{b+1}\frac{(b+1)!}{(b+1-p)!}\frac{(a+b+2-p)!}{(\alpha+\beta)^{a+b+3-p}\beta^{p+1}}[\Psi(p+1)-\ln\beta] \\
K_3 &= \sum_{p=0}^{a+1}\frac{(a+1)!}{(a+1-p)!}\frac{(a+b+2-p)!}{(\alpha+\beta)^{a+b+3-p}\alpha^{p+1}}[\Psi(p+1)-\ln\alpha].
\end{aligned}
$$

Eq. (2.77) is valid for $a,\ b\geq -1$.

The last thing we have to do is to deal with even more singular integrals with $c<-2$. In particular, we should separate the divergent part from the whole integral that may further be combined with the corresponding exchange terms in order to obtain finite results. This can be achieved in analogy with the previous derivations that lead to Eq. (2.76) and Eq. (2.77). We list the final result without any repetition. If $c=-2-n$ with n a positive integer, then

$$
I_0(a,b,-2-n)=O_1+O_2+O_3, \tag{2.78}
$$

where

$$
\begin{aligned}
O_1 &= -\frac{1}{n}\frac{(a+1)!(b+1)!(a+b+3-n)!}{(a+b+3)!\alpha^{a+2-n}\beta^{b+2}}F(b+2,n;a+b+4;\frac{\beta-\alpha}{\beta}), \quad \beta\geq\alpha \\
&= -\frac{1}{n}\frac{(a+1)!(b+1)!(a+b+3-n)!}{(a+b+3)!\beta^{b+2-n}\alpha^{a+2}}F(a+2,n;a+b+4;\frac{\alpha-\beta}{\alpha}), \quad \beta\leq\alpha \\
O_2 &= \frac{1}{n}\sum_{j=0}^{b+1}\frac{(b+1)!}{j!(b+1-j)!}\frac{(a+b+2-j)!}{(\alpha+\beta)^{a+b+3-j}}\int_0^{\infty}\xi^{j-n}e^{-\beta\xi}d\xi \\
O_3 &= \frac{1}{n}\sum_{j=0}^{a+1}\frac{(a+1)!}{j!(a+1-j)!}\frac{(a+b+2-j)!}{(\alpha+\beta)^{a+b+3-j}}\int_0^{\infty}\xi^{j-n}e^{-\alpha\xi}d\xi.
\end{aligned}
$$

Eq. (2.78) is valid for $a,\ b\geq -1$. The divergence can easily be identified with the uncalculated integrals of $j\leq n-1$. Thus, we can obtain the following expression:

$$
I_0(a,b,-2-n)=\mathrm{Reg}I_0(a,b,-2-n)+\mathrm{Sing}I_0(a,b,-2-n), \tag{2.79}
$$

where 'Reg' stands for the regular part, and 'Sing' the singular part.

The computational methods and the formulas discussed in this section have been tested extensively for accuracy and speed and proven to be efficient in dealing with all integrals appearing in the present work.

2.4 General Procedure of Cancellation

As mentioned before, the integrals of type $I_E(a,b,c)$ with more negative powers of r generally diverge individually. However, these integrals always occur in combinations with those coming from either the direct or exchange terms of the wave function, thus, resulting in a final complete cancellation of singularity (in other words, if there still exists a residual singularity, one must have made some mistakes, because the expectation values of the Douglas and Kroll operators are proven to be convergent). It is, therefore, important to find a general scheme of eliminating the virtual singularities for arbitrary triplet states. The starting point is Eq. (2.29) by which the integral $I_E(a,b,c)$ can be written as

$$I_E(a,b,c) = \sum_{\Lambda=\omega(E)}^{E}{}' g(E;\Lambda,c+2) I_{\Lambda-1}(a-1,b-1,c+2) + I_{\omega(E)-2}(a,b,c) \quad (2.80)$$

where $c \neq -2$ and the two functions of g and ω are defined by

$$g(E;\Lambda,c+2) = (1-\delta_{E,0})(1-\delta_{E,1})\frac{2\Lambda-1}{c+2} \quad (2.81)$$

and

$$\omega(E) = \begin{cases} 2, & \text{if } E\text{=even} \\ 3, & \text{if } E\text{=odd} \end{cases} . \quad (2.82)$$

In Eq. (2.80), $\sum'$ means that the step of summation is 2. Note also that $I_E(a,b,-2)$ is convergent.

From Eq. (2.80) the following expression can be obtained immediately:

$$\sum_{E=\mu}^{M}{}' G(E) I_E(a,b,c) = \varpi_1(\mu,M;G;a,b,c) + J_1(\mu,M;G) I_{\omega(\mu)-2}(a,b,c), \quad (2.83)$$

for $c \geq -4$, where

$$J_1(\mu,M;G) = \sum_{E=\mu}^{M}{}' G(E). \quad (2.84)$$

$G(E)$ are the angular coefficients, and ϖ_1 a quantity defined by

$$\begin{aligned}
&\varpi_1(\mu, M; G; a, b, c) \qquad (2.85)\\
&= \sum_{E=\mu}^{M}{}' \sum_{\Lambda=\omega(\mu)}^{E}{}' G(E) g(E; \Lambda, c+2) I_{\Lambda-1}(a-1, b-1, c+2), \quad c \neq -2 \\
&= \sum_{E=\mu}^{M}{}' G(E) I_E(a, b, -2) - J_1(\mu, M; G) I_{\omega(\mu)-2}(a, b, -2), \quad c = -2,
\end{aligned}$$

which is convergent for $c = -3$ and $c = -4$. The second term of Eq. (2.83) may diverge and should be combined with other divergent terms to obtain finite results. By repeated applications of Eq. (2.80), the higher singular cases can be handled:

$$\begin{aligned}
\sum_{E=\mu}^{M}{}' G(E) I_E(a, b, c) &= \varpi_2(\mu, M; G; a, b, c) \\
&+ J_2(\mu, M; G; c) I_{\omega(\mu+1)-2}(a-1, b-1, c+2) \\
&+ J_1(\mu, M; G) I_{\omega(\mu)-2}(a, b, c), \qquad (2.86)
\end{aligned}$$

for $c = -5$ and -6, where

$$J_2(\mu, M; G; c) = \sum_{E=\mu}^{M}{}' \sum_{\Lambda=\omega(\mu)}^{E}{}' G(E) g(E; \Lambda, c+2), \qquad (2.87)$$

and

$$\begin{aligned}
\varpi_2(\mu, M; G; a, b, c) &= \sum_{E=\mu}^{M}{}' \sum_{\Lambda=\omega(\mu)}^{E}{}' \sum_{\Lambda_1=\omega(\mu+1)}^{\Lambda-1}{}' G(E) g(E; \Lambda, c+2) \\
&\times g(\Lambda-1; \Lambda_1, c+4) I_{\Lambda_1-1}(a-2, b-2, c+4). \qquad (2.88)
\end{aligned}$$

Note that the second and third terms of Eq. (2.86) have different degrees of divergence for $c = -5$ and -6. The most singular integrals we have met in the evaluation of the Douglas and Kroll operators are those with $c = -7$ and -8. The corresponding reduction formula is:

$$\begin{aligned}
&\sum_{E=\mu}^{M}{}' G(E) I_E(a, b, c) \qquad (2.89)\\
&= \varpi_3(\mu, M; G; a, b, c) + J_3(\mu, M; G; c) I_{\omega(\mu)-2}(a-2, b-2, c+4) \\
&+ J_2(\mu, M; G; c) I_{\omega(\mu+1)-2}(a-1, b-1, c+2) + J_1(\mu, M; G) I_{\omega(\mu)-2}(a, b, c),
\end{aligned}$$

for $c = -7$ and -8, where

$$J_3(\mu, M; G; c) = \sum_{E=\mu}^{M}{}' \sum_{\Lambda=\omega(\mu)}^{E}{}' \sum_{\Lambda_1=\omega(\mu+1)}^{\Lambda-1}{}' G(E) g(E; \Lambda, c+2) g(\Lambda-1; \Lambda_1, c+4) \quad (2.90)$$

and

$$\varpi_3(\mu, M; G; a, b, c) = \sum_{E=\mu}^{M}{}' \sum_{\Lambda=\omega(\mu)}^{E}{}' \sum_{\Lambda_1=\omega(\mu+1)}^{\Lambda-1}{}' \sum_{\Lambda_2=\omega(\mu)}^{\Lambda_1-1}{}' G(E) g(E; \Lambda, c+2)$$
$$\times g(\Lambda-1; \Lambda_1, c+4) g(\Lambda_1-1; \Lambda_2, c+6) I_{\Lambda_2-1}(a-3, b-3, c+6). \quad (2.91)$$

Also, it might be convenient to define

$$\varpi_0(\mu, M; G; a, b, c) = \sum_{E=\mu}^{M}{}' G(E) I_E(a, b, c), \quad c \geq -2, \quad (2.92)$$

which has no divergent part.

From the above discussion it can be seen that we only need to deal with the singular integrals of type $I_E(a, b, c)$ with $E = 0$ and 1, rather than ones of a higher E value. This strategy is the key point that allows our calculation to be applicable, in principle, to arbitrary triplet states of two electron atoms.

Let us develop some special formulas for integrals of the form $I_E(a, b, c)$, with $E = 0$ and 1. By Eq. (2.24) and

$$(r_1^2 + r_2^2) P_1(\cos\theta) - 2r_1 r_2 = r^2 P_1(\cos\theta) + \frac{4}{3} r_1 r_2 (P_2(\cos\theta) - 1), \quad (2.93)$$

we can derive the following reduction formula straightforwardly:

$$I_{\omega(\mu)-2}(a+2, b, c) + I_{\omega(\mu)-2}(a, b+2, c) - 2I_{\omega(\mu+1)-2}(a+1, b+1, c)$$
$$= \eta(\mu, c+5) I_{\omega(\mu)-2}(a, b, c+2), \quad c \neq -2, \quad (2.94)$$

where

$$\eta(\mu, c) = \begin{cases} 1, & \text{if } \mu = \text{even} \\ (c+1)/(c-3), & \text{if } \mu = \text{odd}, \end{cases} \quad (2.95)$$

and $c \neq 3$. In the right hand side, the degree of singularity at $r = 0$ is reduced by 2 compared with that of the left hand side. The following are the reduction formulas of another type [33]:

$$I_0(a, b, c-2; \alpha, \beta) - I_1(a-1, b+1, c-2; \alpha, \beta)$$
$$= \frac{1}{c}[-(a+1) I_0(a-2, b, c; \alpha, \beta) + \alpha I_0(a-1, b, c; \alpha, \beta)], \quad (2.96)$$

for $a+1 \neq 0$ and $c \neq 0$, and

$$\begin{aligned} &I_0(a,b,c-2;\alpha,\beta) - I_1(a+1,b-1,c-2;\alpha,\beta) \\ &= \frac{1}{c}[-(b+1)I_0(a,b-2,c;\alpha,\beta) + \beta I_0(a,b-1,c;\alpha,\beta)], \end{aligned} \tag{2.97}$$

for $b+1 \neq 0$ and $c \neq 0$. Thus, the quantity defined by

$$\mathrm{Dif}(a,b;a',b';c,\alpha,\beta;i,j) = I_i(a,b,c;\alpha,\beta) - I_j(a',b',c;\alpha,\beta), \tag{2.98}$$

where $(i,j) = (0,1)$ or $(1,0)$, $a = a' \pm 1$, and $b = b' \mp 1$, is convergent as long as $c \geq -4$.

Eqs. (2.94), (2.96), and (2.97) are mainly applied to the cancellation between the direct-direct (or exchange-exchange) terms. For more singular operators, however, the direct-direct type cancellation is not enough to eliminate the singularity completely. Under this circumstance, one has to resort to the exchange part of the wave function that can provide the partners (that is, the divergent terms having similar singularity) for cancellation. This is due to the fact that the wave functions for the triplet states are antisymmetric in space so that the wavefunctions are zero at $r = 0$.

Let us go on to consider this problem. As expressed in Eq. (2.79), the singular part of $I_0(a,b,c)$ can be separated from the convergent part uniquely. In particular, from Eq. (2.78) we have:

$$\mathrm{Sing}I_0(a,b,-3;\alpha,\beta) = \frac{(a+b+2)!}{(\alpha+\beta)^{a+b+3}}\left(\int_0^\infty \xi^{-1}e^{-\alpha\xi}d\xi + \int_0^\infty \xi^{-1}e^{-\beta\xi}d\xi\right) \tag{2.99}$$

$$\begin{aligned} \mathrm{Sing}I_0(a,b,-4;\alpha,\beta) &= \frac{1}{2}\frac{(a+b+2)!}{(\alpha+\beta)^{a+b+3}}\left(\int_0^\infty \xi^{-2}e^{-\alpha\xi}d\xi + \int_0^\infty \xi^{-2}e^{-\beta\xi}d\xi\right) \\ &+ \frac{1}{2}\frac{(a+b+1)!}{(\alpha+\beta)^{a+b+2}}\left((a+1)\int_0^\infty \xi^{-1}e^{-\alpha\xi}d\xi + (b+1)\int_0^\infty \xi^{-1}e^{-\beta\xi}d\xi\right). \end{aligned} \tag{2.100}$$

The typical combination of singular integrals appearing in the present work is

$$\Pi_0(a,b,\alpha,\beta;a',b',\alpha',\beta';c) = I_0(a,b,c;\alpha,\beta) - I_0(a',b',c;\alpha',\beta'), \tag{2.101}$$

where $a+b = a'+b'$ and $\alpha+\beta = \alpha'+\beta'$. With the help of the following two expressions (see 2, 3.434 and 1, 3.421 of ref. [32]):

$$\int_0^\infty (e^{-\mu x} - e^{-\nu x})\frac{1}{x}dx = \ln\frac{\nu}{\mu} \tag{2.102}$$

$$\int_0^\infty (e^{-\alpha' x} - e^{-\beta' x})(e^{-\beta x} - e^{-\alpha x})\frac{1}{x^2}dx$$
$$= (\alpha + \beta')\ln(\alpha + \beta') + (\alpha' + \beta)\ln(\alpha' + \beta)$$
$$-(\alpha + \alpha')\ln(\alpha + \alpha') - (\beta + \beta')\ln(\beta + \beta'), \qquad (2.103)$$

as well as with eqs. (2.79), (2.99), and (2.100), Π_0 can be worked out without any residual singularity:

$$\Pi_0(a, b, \alpha, \beta; a', b', \alpha', \beta'; -3)$$
$$= \mathrm{Reg}I_0(a, b, -3; \alpha, \beta) - \mathrm{Reg}I_0(a', b', -3; \alpha', \beta') + \frac{(z+2)!}{\tau^{z+3}}\ln\frac{\alpha'\beta'}{\alpha\beta} \quad (2.104)$$

$$\Pi_0(a, b, \alpha, \beta; a', b', \alpha', \beta'; -4)$$
$$= \mathrm{Reg}I_0(a, b, -4; \alpha, \beta) - \mathrm{Reg}I_0(a', b', -4; \alpha', \beta')$$
$$+\frac{1}{2}\frac{(z+2)!}{\tau^{z+3}}(\alpha\ln\alpha + \beta\ln\beta - \alpha'\ln\alpha' - \beta'\ln\beta')$$
$$+\frac{1}{2}\frac{(z+1)!}{\tau^{z+2}}[\ln\frac{\alpha'\beta'}{\alpha\beta} + a\ln\frac{\alpha'}{\alpha} + b\ln\frac{\beta'}{\beta} + (a - a')\ln\frac{\beta'}{\alpha'}] \qquad (2.105)$$

with

$$\begin{aligned} z &= a + b = a' + b' \\ \tau &= \alpha + \beta = \alpha' + \beta'. \end{aligned} \qquad (2.106)$$

Finally, by Eq. (2.33) and Eq. (2.101), one introduces a useful quantity

$$\mathrm{Can}(a, b, \alpha, \beta; a', b', \alpha', \beta'; c; i, j) = I_i(a, b, c; \alpha, \beta) - I_j(a', b', c; \alpha', \beta'), \qquad (2.107)$$

where $a + b = a' + b'$ and $\alpha + \beta = \alpha' + \beta'$, and $i, j = 0, 1$. Eq. (2.107) is regular at $r = 0$ for $c \geq -4$.

2.5 Evaluation of the Matrix Elements

After the previous preparation we are in a position to evaluate the matrix elements of the Douglas and Kroll operators. However since the procedure of calculation is lengthy and similar for all operators, we present the analysis for a typical case in detail. We thus choose the operator H_D^{13} for this purpose. We adopt the LS coupling scheme in our calculation. The quantity we are going to evaluate is:

$$\Delta E_D^{13} = \frac{1}{16}\alpha^4 \langle \gamma' L' S' J' M_{J'} | (\vec{\sigma}_1 \cdot \frac{1}{r^3}\vec{\nabla}_2)(\vec{\sigma}_2 \cdot \vec{\nabla}_1) | \gamma LSJM_J \rangle. \qquad (2.108)$$

The above integrand can be decoupled (see 5.52 of [34]) into the products of the spin and orbital parts:

$$(\vec{\sigma}_1 \cdot \vec{\nabla}_2)(\vec{\sigma}_2 \cdot \vec{\nabla}_1) = \sum_K (-1)^K [\vec{\sigma}_1 \otimes \vec{\sigma}_2]^{(K)} \cdot [\vec{\nabla}_2 \otimes \vec{\nabla}_1]^{(K)}, \qquad (2.109)$$

where K means the rank of an irreducible tensor operator. Thus, Eq. (2.108) becomes

$$\Delta E_D^{13} = \frac{1}{16}\alpha^4 \sum_K \delta_{JJ'}\delta_{M_J M_{J'}} (-1)^{K+L+S'+J} \begin{Bmatrix} L' & S' & J \\ S & L & K \end{Bmatrix} \times \langle \gamma' L' \| \frac{1}{r^3}[\vec{\nabla}_2 \otimes \vec{\nabla}_1]^{(K)} \| \gamma L \rangle \langle S' \| [\vec{\sigma}_1 \otimes \vec{\sigma}_2]^{(K)} \| S \rangle, \qquad (2.110)$$

where a standard formula has been used (see 5.71 of ref. [34]):

$$\langle \gamma' L' S' J' M_{J'} | A^{(K)} \cdot \Sigma^{(K)} | \gamma LSJM_J \rangle = \delta_{JJ'}\delta_{M_J M_{J'}} (-1)^{L+S'+J} \begin{Bmatrix} L' & S' & J \\ S & L & K \end{Bmatrix} \langle \gamma' L' \| A^{(K)} \| \gamma L \rangle \langle S' \| \Sigma^{(K)} \| S \rangle \qquad (2.111)$$

with $A^{(K)}$ being an irreducible tensor operator of rank K with respect to $\vec{L}$ and $\Sigma^{(K)}$ an irreducible tensor operator of rank K with respect to $\vec{S}$, and the matrix elements with $\|$ represent the reduced matrix elements of the corresponding operators. The reduced matrix element for the spin part can be easily calculated [34]:

$$\langle S' \| [\vec{\sigma}_1 \otimes \vec{\sigma}_2]^{(K)} \| S \rangle = 6(S, S', K)^{1/2} \begin{Bmatrix} 1/2 & 1/2 & 1 \\ 1/2 & 1/2 & 1 \\ S' & S & K \end{Bmatrix}, \qquad (2.112)$$

which implies that the above $9j$ symbol is zero unless K is an even integer; this is because the $9j$ symbol is multiplied by $(-1)^X$ with X being the sum of all the nine parameters if we interchange the first two rows, and also because $S = S'$ in our work. Also we even don't need to consider the case of $K = 0$ which corresponds to a scalar $\vec{\sigma}_1 \cdot \vec{\sigma}_2$ in Eq. (2.109) and, thus, contributes equally to the triplet states. Using the Wigner-Eckart theorem (see 5.14 of ref. [34]), the reduced matrix element for the orbital part can be evaluated through

$$\langle \gamma' L' M' | R_0^{(K)} | \gamma LM \rangle = (-1)^{L'-M'} \begin{pmatrix} L' & K & L \\ -M' & 0 & M \end{pmatrix} \langle \gamma' L' \| R^{(K)} \| \gamma L \rangle, \qquad (2.113)$$

where

$$R^{(K)} = \frac{1}{r^3}[\vec{\nabla}_2 \otimes \vec{\nabla}_1]^{(K)}. \tag{2.114}$$

The operator $R_0^{(K)}$ may further be expanded as (see 5.36 of [34])

$$\begin{aligned} R_0^{(K)} &= \frac{1}{r^3}\sqrt{2K+1}\sum_{\mu_1\mu_2}\begin{pmatrix} 1 & 1 & K \\ \mu_1 & \mu_2 & 0 \end{pmatrix}\nabla_{2\mu_1}\nabla_{1\mu_2} \\ &= \frac{1}{r^3}(-1)^K\sqrt{2K+1}\sum_{\mu_1\mu_2}\begin{pmatrix} 1 & 1 & K \\ \mu_1 & \mu_2 & 0 \end{pmatrix}\nabla_{1\mu_1}\nabla_{2\mu_2}. \end{aligned} \tag{2.115}$$

According to the construction of our wave function (see Eq. (2.7)), the state vector $|\gamma LM\rangle$ is a linear superposition of the following basis set:

$$\{|F\mathcal{Y}^{M}_{l_1l_2L}\rangle\}$$

$$F(a,b,c;\alpha,\beta) = r_1^a r_2^b r^c e^{-\alpha r_1-\beta r_2}.$$

Therefore, the main task is to calculate the following matrix element:

$$\begin{aligned} T &\equiv \langle F'\mathcal{Y}^{M'}_{l_1'l_2'L'}|R_0^{(K)}|F\mathcal{Y}^{M}_{l_1l_2L}\rangle \\ &= \sqrt{2K+1}(-1)^K\sum_{\mu_1\mu_2}\begin{pmatrix} 1 & 1 & K \\ \mu_1 & \mu_2 & 0 \end{pmatrix}\langle F'\mathcal{Y}^{M'}_{l_1'l_2'L'}|\frac{1}{r^3}\nabla_{1\mu_1}\nabla_{2\mu_2}|F\mathcal{Y}^{M}_{l_1l_2L}\rangle. \end{aligned} \tag{2.116}$$

Using Eq. (2.26) and letting

$$\begin{aligned} B &= \sqrt{2K+1}(-1)^K\langle F'\mathcal{Y}^{M'}_{l_1'l_2'L'}|\frac{1}{r^3} \\ T_i &= B\sum_{m_1m_2}(-1)^{l_1-l_2+M}(2L+1)^{1/2}\begin{pmatrix} l_1 & l_2 & L \\ m_1 & m_2 & -M \end{pmatrix}A_i^{(K)}, \end{aligned} \tag{2.117}$$

we obtain:

$$T = \int d\vec{r}_1 d\vec{r}_2 \sum_{r=1}^{3} T_i = \int d\tau d\Omega \sum_{r=1}^{3} T_i, \tag{2.118}$$

where the volume element is

$$d\vec{r}_1 d\vec{r}_2 = \underbrace{r_1 dr_1 r_2 dr_2 r dr}_{d\tau}\underbrace{\sin\theta_1 d\theta_1 d\phi_1 d\chi}_{d\Omega}, \tag{2.119}$$

with θ_1 and ϕ_1 being the polar angles of the vector $\vec{r}_1$, and χ the angle of rotation of the rigid triangle formed by $\vec{r}_1$, $\vec{r}_2$, and $\vec{r}$ about the $\vec{r}_1$ direction. With the help of Eq. (2.25) and the angular integral [30]:

$$\int Y_{E\epsilon}(\hat{r}_1)Y_{P\rho}(\hat{r}_2)d\Omega = 2\pi(-1)^{\epsilon}P_E(\cos\theta)\delta_{PE}\delta_{\rho-\epsilon}, \tag{2.120}$$

one obtains:

$$\begin{aligned}\int T_1 d\Omega &= \frac{1}{2}\sqrt{2K+1}(-1)^K(l_1,l_2,L,l_1',l_2',L')^{1/2} \\ &\times \sum_{T\Lambda E}(T,\Lambda,E)G(T_1,0)G(T_1)\frac{F'}{r^3}(D^{(K)}_{\Lambda T}(l_2,l_1)F)P_E(\cos\theta),\end{aligned} \tag{2.121}$$

where

$$G(T_1,0)=\begin{pmatrix}1 & l_1 & T\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}1 & l_2 & \Lambda\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_1' & T & E\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_2' & \Lambda & E\\ 0 & 0 & 0\end{pmatrix} \tag{2.122}$$

$$\begin{aligned}G(T_1) &= \sum_{m_1m_2}\sum_{m_1'm_2'}\sum_{\mu_1\mu_2}\sum_{\tau\lambda\epsilon}(-1)^{\epsilon}\begin{pmatrix}l_1 & l_2 & L\\ m_1 & m_2 & -M\end{pmatrix}\begin{pmatrix}l_1' & l_2' & L'\\ m_1' & m_2' & -M'\end{pmatrix} \\ &\times \begin{pmatrix}1 & 1 & K\\ \mu_1 & \mu_2 & 0\end{pmatrix}\begin{pmatrix}1 & l_1 & T\\ \mu_1 & m_1 & \tau\end{pmatrix}\begin{pmatrix}1 & l_2 & \Lambda\\ \mu_2 & m_2 & \lambda\end{pmatrix} \\ &\times \begin{pmatrix}l_1' & T & E\\ m_1' & \tau & \varepsilon\end{pmatrix}\begin{pmatrix}l_2' & \Lambda & E\\ m_2' & \lambda & -\varepsilon\end{pmatrix}.\end{aligned} \tag{2.123}$$

In Eq. (2.121) we have neglected a phase factor which is

$$(-1)^{l_1-l_2+M+l_1'-l_2'+M'} = 1,$$

because $l_1-l_2+l_1'-l_2'$ =even, due to the existence of Eq. (2.122), and $M=M'$ (see Eq. (2.124) below). Using the standard graphical methods of dealing with angular momentum [29], Eq. (2.123) can be recast into

$$\begin{aligned}G(T_1) &= (-1)^{L'-M'}\begin{pmatrix}L' & K & L\\ -M' & 0 & M\end{pmatrix} \\ &\times (-1)^{L'+1+l_1+l_2'}\begin{Bmatrix}L' & l_1' & l_2'\\ E & \Lambda & T\end{Bmatrix}\begin{Bmatrix}L & l_1 & l_2\\ K & 1 & 1\\ L' & T & \Lambda\end{Bmatrix}.\end{aligned} \tag{2.124}$$

Similarly,

$$\begin{aligned}\int T_2 d\Omega &= \frac{1}{2}\sqrt{2K+1}(-1)^K(l_1,l_2,L,l_1',l_2',L')^{1/2} \\ &\times \sum_{T\Lambda E}(T,\Lambda,E)G(T_2,0)G(T_2)\frac{F'}{r^3}(D^{(2)}_0D^{(1)}(l_1;T)F)P_E(\cos\theta)\end{aligned} \tag{2.125}$$

$$G(T_2,0)=\begin{pmatrix}1 & l_1 & T\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}1 & T & \Lambda\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_1' & \Lambda & E\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_2' & l_2 & E\\ 0 & 0 & 0\end{pmatrix} \quad (2.126)$$

$$\begin{aligned} G(T_2) &= (-1)^{L'-M'}\begin{pmatrix}L' & K & L\\ -M' & 0 & M\end{pmatrix} \\ &\times (-1)^{L'+L+l_1+l_2'+K}\begin{Bmatrix}L & l_1 & l_2\\ \Lambda & L' & K\end{Bmatrix}\begin{Bmatrix}L' & l_1' & l_2'\\ E & l_2 & \Lambda\end{Bmatrix}\begin{Bmatrix}1 & 1 & K\\ l_1 & \Lambda & T\end{Bmatrix} \quad (2.127)\end{aligned}$$

$$\begin{aligned} \int T_3 d\Omega &= \frac{1}{2}\sqrt{2K+1}(-1)^K(l_1,l_2,L,l_1',l_2',L')^{1/2} \\ &\times \sum_{T\Lambda E}(T,\Lambda,E)G(T_3,0)G(T_3)\frac{F'}{r^3}(D^{(2)}(T;\Lambda)D_0^{(1)}F)P_E(\cos\theta) \quad (2.128)\end{aligned}$$

$$G(T_3,0)=\begin{pmatrix}1 & l_2 & T\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}1 & T & \Lambda\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_1' & l_1 & E\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_2' & \Lambda & E\\ 0 & 0 & 0\end{pmatrix} \quad (2.129)$$

$$\begin{aligned} G(T_3) &= (-1)^{L'-M'}\begin{pmatrix}L' & K & L\\ -M' & 0 & M\end{pmatrix} \\ &\times (-1)^{l_1+l_2'+K}\begin{Bmatrix}L & l_1 & l_2\\ \Lambda & K & L'\end{Bmatrix}\begin{Bmatrix}L' & l_1' & l_2'\\ E & \Lambda & l_1\end{Bmatrix}\begin{Bmatrix}1 & 1 & K\\ l_2 & \Lambda & T\end{Bmatrix}. \quad (2.130)\end{aligned}$$

We consider Eq. (2.121) first. According to Eq. (2.27), one has

$$\frac{F'}{r^3}D^{(K)}_{\Lambda T}(l_2,l_1)F = F_{11}+F_{12}b(l_1;T)+F_{13}b(l_2;\Lambda)+F_{14}b(l_1;T)b(l_2;\Lambda), \quad (2.131)$$

where

$$\begin{aligned} F_{11} &= \sum_{i=1}^{9}S_i \quad (2.132)\\ S_1 &= abF(\tilde{a}-1,\tilde{b}-1,\tilde{c}-3;\tilde{\alpha},\tilde{\beta})\\ S_2 &= -a\beta F(\tilde{a}-1,\tilde{b},\tilde{c}-3;\tilde{\alpha},\tilde{\beta})\\ S_3 &= -b\alpha F(\tilde{a},\tilde{b}-1,\tilde{c}-3;\tilde{\alpha},\tilde{\beta})\\ S_4 &= \alpha\beta F(\tilde{a},\tilde{b},\tilde{c}-3;\tilde{\alpha},\tilde{\beta})\\ S_5 &= cbF(\tilde{a}+1,\tilde{b}-1,\tilde{c}-5;\tilde{\alpha},\tilde{\beta})\\ S_6 &= caF(\tilde{a}-1,\tilde{b}+1,\tilde{c}-5;\tilde{\alpha},\tilde{\beta})\\ S_7 &= -c\alpha F(\tilde{a},\tilde{b}+1,\tilde{c}-5;\tilde{\alpha},\tilde{\beta})\\ S_8 &= -c\beta F(\tilde{a}+1,\tilde{b},\tilde{c}-5;\tilde{\alpha},\tilde{\beta})\\ S_9 &= (1+(-1)^K)c(c-2)F(\tilde{a}+1,\tilde{b}+1,\tilde{c}-7;\tilde{\alpha},\tilde{\beta}),\end{aligned}$$

or for brevity,

$$S_i = \mathrm{coe}(S_i)F(\tilde{a}+a'(i),\tilde{b}+b'(i),\tilde{c}+c'(i)), \quad i=1,2,\cdots,9, \tag{2.133}$$

and

$$\begin{aligned} F_{12} &= bF(\tilde{a}-1,\tilde{b}-1,\tilde{c}-3)-\beta F(\tilde{a}-1,\tilde{b},\tilde{c}-3) \\ &+ cF(\tilde{a}-1,\tilde{b}+1,\tilde{c}-5) \end{aligned} \tag{2.134}$$

$$\begin{aligned} F_{13} &= aF(\tilde{a}-1,\tilde{b}-1,\tilde{c}-3)-\alpha F(\tilde{a},\tilde{b}-1,\tilde{c}-3) \\ &+ cF(\tilde{a}+1,\tilde{b}-1,\tilde{c}-5) \end{aligned} \tag{2.135}$$

$$F_{14} = F(\tilde{a}-1,\tilde{b}-1,\tilde{c}-3) \tag{2.136}$$

with the notations of

$$\begin{aligned} \tilde{a} &= a+a' \\ \tilde{b} &= b+b' \\ \tilde{c} &= c+c' \\ \tilde{\alpha} &= \alpha+\alpha' \\ \tilde{\beta} &= \beta+\beta'. \end{aligned}$$

In the following, we do not write out $\tilde{\alpha}$ and $\tilde{\beta}$ explicitly to save space. Introducing

$$G_{11}(E) = \sum_{T\Lambda}(T,\Lambda,E)G(T_1,0)\tilde{G}(T_1) \tag{2.137}$$
$$G_{12}(E) = \sum_{T\Lambda}(T,\Lambda,E)G(T_1,0)\tilde{G}(T_1)b(l_1;T) \tag{2.138}$$
$$G_{13}(E) = \sum_{T\Lambda}(T,\Lambda,E)G(T_1,0)\tilde{G}(T_1)b(l_2;\Lambda) \tag{2.139}$$
$$G_{14}(E) = \sum_{T\Lambda}(T,\Lambda,E)G(T_1,0)\tilde{G}(T_1)b(l_1;T)b(l_2;\Lambda), \tag{2.140}$$

where $\tilde{G}(T_i)$ are $G(T_i)$ with

$$(-1)^{L'-M'}\begin{pmatrix} L' & K & L \\ -M' & 0 & M \end{pmatrix}$$

removed, then one obtains the contribution from T_1 which is denoted by D_1:

$$\begin{aligned} D_1 &= \{(-1)^{L'-M'}\begin{pmatrix} L' & K & L \\ -M' & 0 & M \end{pmatrix}\}^{-1} \int T_1 d\tau d\Omega \\ &= U(13)\sum_{i=1}^{4}\sum_{E} G_{1i}(E) \int F_{1i} P_E(\cos\theta) d\tau \end{aligned} \tag{2.141}$$

with

$$U(13) = \frac{1}{2}\sqrt{2K+1}(-1)^K (l_1, l_2, L, l_1', l_2', L')^{1/2}. \tag{2.142}$$

Similarly,

$$\begin{aligned} D_2 &= \{(-1)^{L'-M'}\begin{pmatrix} L' & K & L \\ -M' & 0 & M \end{pmatrix}\}^{-1} \int T_2 d\tau d\Omega \\ &= U(13)\sum_{i=1}^{2}\sum_{E} G_{2i}(E) \int F_{2i} P_E(\cos\theta) d\tau \end{aligned} \tag{2.143}$$

with

$$\begin{aligned} F_{21} &= acF(\tilde{a},\tilde{b},\tilde{c}-5) - \alpha cF(\tilde{a}+1,\tilde{b},\tilde{c}-5) \\ &+ c(c-2)F(\tilde{a}+2,\tilde{b},\tilde{c}-7) \end{aligned} \tag{2.144}$$

$$F_{22} = cF(\tilde{a},\tilde{b},\tilde{c}-5) \tag{2.145}$$

$$G_{21}(E) = \sum_{T\Lambda}(T,\Lambda,E)G(T_2,0)\tilde{G}(T_2) \tag{2.146}$$

$$G_{22}(E) = \sum_{T\Lambda}(T,\Lambda,E)G(T_2,0)\tilde{G}(T_2)b(l_1;T), \tag{2.147}$$

and

$$\begin{aligned} D_3 &= \{(-1)^{L'-M'}\begin{pmatrix} L' & K & L \\ -M' & 0 & M \end{pmatrix}\}^{-1} \int T_3 d\tau d\Omega \\ &= U(13)\sum_{i=1}^{2}\sum_{E} G_{3i}(E) \int F_{3i} P_E(\cos\theta) d\tau \end{aligned} \tag{2.148}$$

with

$$\begin{aligned} F_{31} &= (b+1)cF(\tilde{a},\tilde{b},\tilde{c}-5) - \beta cF(\tilde{a},\tilde{b}+1,\tilde{c}-5) \\ &+ c(c-2)F(\tilde{a},\tilde{b}+2,\tilde{c}-7) \end{aligned} \tag{2.149}$$

$$F_{32} = cF(\tilde{a},\tilde{b},\tilde{c}-5) \tag{2.150}$$

$$G_{31}(E) = \sum_{T\Lambda}(T,\Lambda,E)G(T_3,0)\tilde{G}(T_3) \tag{2.151}$$

$$G_{32}(E) = \sum_{T\Lambda}(T,\Lambda,E)G(T_3,0)\tilde{G}(T_3)b(T;\Lambda). \tag{2.152}$$

Note that the ranges of summations over E are determined by the triangular rule of $3j$ symbols contained in $G(T_i,0)$, (see Eqs.(2.122), (2.126), and (2.129)), namely, if we define

$$M_1 = \min(l_1 + l_1' + 1, l_2 + l_2' + 1) \tag{2.153}$$

$$M_2 = \min(l_1 + l_1' + 2, l_2 + l_2') \tag{2.154}$$

$$M_3 = \min(l_1 + l_1', l_2 + l_2' + 2) \tag{2.155}$$

$$\mu_i = \omega(M_i) - 2, \quad i = 1,2,3, \tag{2.156}$$

then

$$\mu_i \leq E \leq M_i \quad \text{for} \quad G(T_i,0). \tag{2.157}$$

Finally, Eq. (2.116) become

$$T = (-1)^{L'-M'}\begin{pmatrix} L' & K & L \\ -M' & 0 & M \end{pmatrix}U(13)D \tag{2.158}$$

$$D = (D_1 + D_2 + D_3)/U(13) \tag{2.159}$$

It is obvious that the individual integrals contained in D_i are divergent for low $\tilde{c}$ by remembering the fact that $I_E(a,b,c)$ diverges unless $c \geq -2$. Thus one has to perform the cancellation procedure among them. After substituting the expressions of F_{ij} into D_i, one can group the following terms with similar singularity:

$$\Delta = \sum_E G_{12}(E)cI_E(\tilde{a}-1,\tilde{b}+1,\tilde{c}-5) + \sum_E G_{13}(E)cI_E(\tilde{a}+1,\tilde{b}-1,\tilde{c}-5)$$
$$+\sum_E G_{22}(E)cI_E(\tilde{a},\tilde{b},\tilde{c}-5) + \sum_E G_{31}(E)cI_E(\tilde{a},\tilde{b},\tilde{c}-5) + \sum_E G_{32}(E)cI_E(\tilde{a},\tilde{b},\tilde{c}-5).$$

Of course there are other groups of terms with similar singularity. However, we demonstrate the cancellation procedure only for Δ in order to avoid unnecessary repetition. Applying Eq. (2.83) and then Eq. (2.98), one has:

$$\Delta = c\varpi_1(\mu_1, M_1; G_{12}; \tilde{a}-1, \tilde{b}+1, \tilde{c}-5)$$

$$
\begin{aligned}
&+ \quad cJ_1(\mu_1, M_1; G_{12}) I_{\omega(\mu_1)-2}(\tilde{a}-1, \tilde{b}+1, \tilde{c}-5) \\
&+ \quad c\varpi_1(\mu_1, M_1; G_{13}; \tilde{a}+1, \tilde{b}-1, \tilde{c}-5) \\
&+ \quad cJ_1(\mu_1, M_1; G_{13}) I_{\omega(\mu_1)-2}(\tilde{a}+1, \tilde{b}-1, \tilde{c}-5) \\
&+ \quad c\varpi_1(\mu_2, M_2; G_{22}; \tilde{a}, \tilde{b}, \tilde{c}-5) \\
&+ \quad cJ_1(\mu_2, M_2; G_{22}) I_{\omega(\mu_1+1)-2}(\tilde{a}, \tilde{b}, \tilde{c}-5) \\
&+ \quad c\varpi_1(\mu_3, M_3; G_{31}; \tilde{a}, \tilde{b}, \tilde{c}-5) \\
&+ \quad cJ_1(\mu_3, M_3; G_{31}) I_{\omega(\mu_1+1)-2}(\tilde{a}, \tilde{b}, \tilde{c}-5) \\
&+ \quad c\varpi_1(\mu_3, M_3; G_{32}; \tilde{a}, \tilde{b}, \tilde{c}-5) \\
&+ \quad cJ_1(\mu_3, M_3; G_{32}) I_{\omega(\mu_1+1)-2}(\tilde{a}, \tilde{b}, \tilde{c}-5) \\
&= \quad c\varpi_1(\mu_1, M_1; G_{12}; \tilde{a}-1, \tilde{b}+1, \tilde{c}-5) \\
&+ \quad c\varpi_1(\mu_1, M_1; G_{13}; \tilde{a}+1, \tilde{b}-1, \tilde{c}-5) \\
&+ \quad c\varpi_1(\mu_2, \max(M_2, M_3); G_{22}+G_{31}+G_{32}; \tilde{a}, \tilde{b}, \tilde{c}-5) \\
&+ \quad cJ_1(\mu_1, M_1; G_{12}) \mathrm{Dif}(\tilde{a}-1, \tilde{b}+1; \tilde{a}, \tilde{b}; \tilde{c}-5, \tilde{\alpha}, \tilde{\beta}; \omega(\mu_1)-2, \omega(\mu_1+1)-2) \\
&+ \quad cJ_1(\mu_1, M_1; G_{13}) \mathrm{Dif}(\tilde{a}+1, \tilde{b}-1; \tilde{a}, \tilde{b}; \tilde{c}-5, \tilde{\alpha}, \tilde{\beta}; \omega(\mu_1)-2, \omega(\mu_1+1)-2) \\
&+ \quad c\xi(l_1', l_2', l_1, l_2) I_{\omega(\mu_1+1)-2}(\tilde{a}, \tilde{b}, \tilde{c}-5), \qquad (2.160)
\end{aligned}
$$

where we have defined

$$
\begin{aligned}
\xi(l_1', l_2', l_1, l_2) \quad &= \quad J_1(\mu_1, M_1; G_{12}) + J_1(\mu_1, M_1; G_{13}) \\
&+ \quad J_1(\mu_2, M_2; G_{22}) + J_1(\mu_3, M_3; G_{31}) + J_1(\mu_3, M_3; G_{32}). \qquad (2.161)
\end{aligned}
$$

In Eq. (2.160), every term, except the last term, is convergent due to the existence of the coefficient c, thus, there is no singularity for $c = 0$. The further cancellation is necessary by resorting to the exchange terms. By including the exchange counterparts of the above divergent term, the last term of Eq. (2.160) will be replaced by

$$
\begin{aligned}
\Delta_c \quad &= \quad c\xi(l_1', l_2', l_1, l_2) I_{\omega(\mu_1+1)-2}(\tilde{a}, \tilde{b}, \tilde{c}-5; \tilde{\alpha}, \tilde{\beta}) \\
&+ \quad c\xi(l_2', l_1', l_2, l_1) I_{\omega(\mu_1+1)-2}(\tilde{b}, \tilde{a}, \tilde{c}-5; \tilde{\beta}, \tilde{\alpha}) \\
&- \quad c\xi(l_2', l_1', l_1, l_2) I_{\omega(\mu_1+1+L)-2}(\tilde{a}', \tilde{b}', \tilde{c}-5; \tilde{\alpha}', \tilde{\beta}') \\
&- \quad c\xi(l_1', l_2', l_2, l_1) I_{\omega(\mu_1+1+L)-2}(\tilde{b}', \tilde{a}', \tilde{c}-5; \tilde{\beta}', \tilde{\alpha}') \qquad (2.162)
\end{aligned}
$$

with the notations of

$$\begin{aligned}\tilde{a}' &= a + b' \\ \tilde{b}' &= b + a' \\ \tilde{\alpha}' &= \alpha + \beta' \\ \tilde{\beta}' &= \beta + \alpha'.\end{aligned}$$

Since we have the following symmetric property:

$$I_E(a, b, c; \alpha, \beta) = I_E(b, a, c; \beta, \alpha), \tag{2.163}$$

Eq. (2.162) becomes

$$\begin{aligned}\Delta_c &= c\tilde{\xi}(l_1', l_2', l_1, l_2) I_{\omega(\mu_1+1)-2}(\tilde{a}, \tilde{b}, \tilde{c} - 5; \tilde{\alpha}, \tilde{\beta}) \\ &- c\tilde{\xi}(l_2', l_1', l_1, l_2) I_{\omega(\mu_1+1+L)-2}(\tilde{a}', \tilde{b}', \tilde{c} - 5; \tilde{\alpha}', \tilde{\beta}')\end{aligned} \tag{2.164}$$

with

$$\tilde{\xi}(l_1', l_2', l_1, l_2) = \xi(l_1', l_2', l_1, l_2) + \xi(l_2', l_1', l_2, l_1). \tag{2.165}$$

Further cancellation can be made using Eq. (2.107) to get

$$\begin{aligned}\Delta_c &= c\tilde{\xi}(l_1', l_2', l_1, l_2) \\ &\times \mathrm{Can}(\tilde{a}, \tilde{b}, \tilde{\alpha}, \tilde{\beta}; \tilde{a}', \tilde{b}', \tilde{\alpha}', \tilde{\beta}'; \tilde{c} - 5; \omega(\mu_1 + 1) - 2, \omega(\mu_1 + 1 + L) - 2) \\ &+ c(\tilde{\xi}(l_1', l_2', l_1, l_2) - \tilde{\xi}(l_2', l_1', l_1, l_2)) I_{\omega(\mu_1+1+L)-2}(\tilde{a}', \tilde{b}', \tilde{c} - 5; \tilde{\alpha}', \tilde{\beta}').\end{aligned} \tag{2.166}$$

The last term in Eq. (2.166) would diverge for low c unless the coefficient were identical to zero. The coefficient does equal to zero which may be verified either analytically or numerically, that is,

$$\tilde{\xi}(l_1', l_2', l_1, l_2) \equiv \tilde{\xi}(l_2', l_1', l_1, l_2), \tag{2.167}$$

and, thus, the singularity in Δ is completely eliminated.

2.6 Final Numerical Values

2.6.1 Convergence Study and Comparison

All the numerical calculations in this study are performed on an IBM RISC/6000 350 workstation using quadruple precision. It is important to avoid recalculating the basic integrals of type $I_0(a, b, c; \alpha, \beta)$ in order to save computing time. To ensure that the algorithms for evaluating $I_0(a, b, c; \alpha, \beta)$ are correct, a number of different analytical expressions of this integral are used for comparisons. The cpu time for a complete computation of one triplet, including the different sizes of the basis sets, is about four days. Before making comparison with the old results of Daley *et al.*, we should note here that our notations for the Douglas and Kroll operators differ from the notations used in ref. [13]. Table 2.1 is a one-to-one correspondence:

Table 2.1: Notations used in this work and in Daley *et al.* work

This work	H_D^1	H_D^2	H_D^3	H_D^4	H_D^5	H_D^6	H_D^7	H_D^8
Ref. [13]	H_1^6	H_2^6	H_3^6	H_4^6	H_5^6	H_8^6	H_9^6	$H_6^6 + H_7^6$
This work	H_D^9	H_D^{10}	H_D^{11}	$H_D^{121} + H_D^{122}$	H_D^{13}	H_D^{14}	H_D^{15}	$m/M\,\Delta_3$
Ref. [13]	H_{10}^6	H_{13}^6	H_{14}^6	H_{15}^6	H_{12}^6	H_{11}^6	H_{16}^6	H'_N

Table 2.2: Coefficients $f(H)$ and $d(H)$ for obtaining the fine structure intervals.

H	H_D^1	H_D^2	H_D^3	H_D^4	H_D^5	H_D^6	H_D^7	H_D^8	H_D^9	H_D^{10}
f	$-\frac{3}{8}Z$	Z	$\frac{1}{2}Z$	$-\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{4}$	$-\frac{3}{4}$	-1	$-\frac{3}{8}$	$-\frac{3}{2}$
$-d$	5	4	4	4	4	5	5	5	5	5
H	H_D^{11}	H_D^{121}	H_D^{122}	H_D^{13}	H_D^{14}	Δ_3	H_{cso}	H_{Zso}	H_{css}	
f	$\frac{1}{4}$	$-\frac{1}{4}$	$\frac{3}{8}$	$\frac{1}{16}$	$-\frac{3}{16}$	$-Z$	$\frac{3}{2}$	$-\frac{1}{2}Z$	$-\frac{3}{4}$	
$-d$	5	5	5	5	5	3	3	3	3	

The fine structure intervals are determined from the reduced matrix elements according to the formula

$$\nu_{ij}(H) = \alpha^p Z^{-d(H)}(\mu/m)^{-d(H)} f(H) C_{ij}^{(K)}(L)\langle\|H\|\rangle \quad \text{in } 2R_\infty, \tag{2.168}$$

where the last factor in the above expression represents the reduced matrix element of operator H; $p = 4$ is for the Douglas-Kroll operators, and $p = 2$ is for the Breit operators and $\tilde{\Delta}_3$; $d(H)$ is the degree of homogeneity of operator H; $\mu = mM/(m+M)$ is the reduced mass; $K = 1$ is for spin-orbit type operators, and $K = 2$ is for spin-spin type operators; and (i,j) can be either $(L-1, L)$ or $(L, L+1)$ or $(L-1, L+1)$. The coefficients $C_{ij}^{(K)}$ are given by

$$C_{L-1,L}^{(1)} = \sqrt{6}\begin{Bmatrix} L & 1 & L-1 \\ 1 & L & 1 \end{Bmatrix} + \sqrt{6}\begin{Bmatrix} L & 1 & L \\ 1 & L & 1 \end{Bmatrix} \quad (2.169)$$

$$C_{L,L+1}^{(1)} = -\sqrt{6}\begin{Bmatrix} L & 1 & L \\ 1 & L & 1 \end{Bmatrix} - \sqrt{6}\begin{Bmatrix} L & 1 & L+1 \\ 1 & L & 1 \end{Bmatrix} \quad (2.170)$$

$$C_{L-1,L}^{(2)} = 2\sqrt{5}\begin{Bmatrix} L & 1 & L-1 \\ 1 & L & 2 \end{Bmatrix} + 2\sqrt{5}\begin{Bmatrix} L & 1 & L \\ 1 & L & 2 \end{Bmatrix} \quad (2.171)$$

$$C_{L,L+1}^{(2)} = -2\sqrt{5}\begin{Bmatrix} L & 1 & L \\ 1 & L & 2 \end{Bmatrix} - 2\sqrt{5}\begin{Bmatrix} L & 1 & L+1 \\ 1 & L & 2 \end{Bmatrix}. \quad (2.172)$$

The coefficients $f(H)$ and $d(H)$ are listed in Table 2.2. It is easy to show that

$$C_{L-1,L+1}^{(1)} - \frac{2L+1}{L+1} C_{L,L+1}^{(1)} = 0 \quad (2.173)$$

$$C_{L-1,L+1}^{(2)} + \frac{2L+1}{(2L-1)(L+1)} C_{L,L+1}^{(2)} = 0. \quad (2.174)$$

Thus, if we define the following two quantities,

$$\nu_{ss} = \nu_{L-1,L+1} - \frac{2L+1}{L+1}\nu_{L,L+1} \quad (2.175)$$

$$\nu_{so} = \nu_{L-1,L+1} + \frac{2L+1}{(2L-1)(L+1)}\nu_{L,L+1}, \quad (2.176)$$

then within first order perturbation theory, ν_{ss} only contains the contributions of spin-spin type interactions, and ν_{so} only contains the contributions of spin-orbital type interactions.

In Eq. (2.168), the two factors $Z^{-d(H)}$ and $(\mu/m)^{-d(H)}$ come from some scaling transformations as follows. Assume that A is an operator which is homogeneous of degree n in two electron coordinate space such that

$$A(\beta\vec{r_1}, \beta\vec{r_2}) = \beta^n A(\vec{r_1}, \vec{r_2}), \quad (2.177)$$

and A and Ψ satisfy the original Schrödinger's equation

$$[-\frac{\hbar^2}{2\mu}(\nabla_1^2 + \nabla_2^2) - \frac{\hbar^2}{M}\nabla_1 \cdot \nabla_2 - Ze^2(\frac{1}{r_1} + \frac{1}{r_2}) + \frac{e^2}{r_{12}} + A(\vec{r_1}, \vec{r_2})]\Psi = E\Psi, \quad (2.178)$$

and also assume that A_a and A_s are A expressed in atomic and in scaled atomic energy units respectively, with the corresponding wavefunctions Ψ_a and Ψ_s:

$$[-\frac{1}{2\frac{\mu}{m}}(\nabla_1^2+\nabla_2^2)-\frac{1}{\frac{M}{m}}\nabla_1\cdot\nabla_2-Z(\frac{1}{r_1}+\frac{1}{r_2})+\frac{1}{r_{12}}+A_a(\vec{r_1},\vec{r_2})]\Psi_a=E_a\Psi_a, \quad (2.179)$$

$$[-\frac{1}{2}(\nabla_1^2+\nabla_2^2)-\frac{\mu}{M}\nabla_1\cdot\nabla_2-\frac{1}{r_1}-\frac{1}{r_2}+\frac{Z^{-1}}{r_{12}}+A_s(\vec{r_1},\vec{r_2})]\Psi_s=E_s\Psi_s; \quad (2.180)$$

then, if all the wavefunctions above are normalized to 1, we can obtain the following scaling law:

$$\langle\Psi|A|\Psi\rangle=\langle\Psi_s|A_a|\Psi_s\rangle Z^{-n}(\frac{\mu}{m})^{-n}(2R_\infty), \quad (2.181)$$

In this work, all operators are expressed in atomic units and wavefunctions are in scaled atomic units.

The results for the $1s2p\ ^3P_J$ states of helium are presented in Table 2.5, together with a detailed account of the convergence process as the size of the basis set is enlarged, and a comparison with the previous calculations for this triplet by Daley *et al.* [13]. In the table, we have converted the results of Daley *et al.* to the corresponding reduced matrix elements defined by Eq. (2.168), using their fundamental constants. The extrapolated values are obtained by taking differences between successive calculations, and by assuming that these differences obey either $b\exp(-a\Omega)$ or $b\Omega^{-a}$ for large Ω, where Ω labels the size of basis set in the variational calculations of wavefunctions. The exponential law reflects a faster convergence rate, and the power law a slower convergence rate. The least square method is used to obtain the best fit parameters. The final extrapolated result is a weighted average of these two single extrapolations, being closer to the one which has the smaller uncertainty. The convergence study presented in Table 2.5 shows that the present work improves by at least 2 or 3 orders of magnitude in accuracy over the previous results.

We have also evaluated all expectation values for the $1s2p\ ^3P_J$ states of helium by including the mass polarization operator $-\mu/M\nabla_1\cdot\nabla_2$ in the unperturbed Hamiltonian. This procedure in effect sums to infinity the perturbation series in μ/M. However, since μ/M is small, it is accurate enough to keep only the first order contribution in μ/M:

$$\langle\Psi_M|H|\Psi_M\rangle=\langle\Psi_\infty|H|\Psi_\infty\rangle(1+c\frac{\mu}{M}), \quad (2.182)$$

where Ψ_M is the wavefunction with the mass polarization term included, and Ψ_∞ is the wavefunction without the mass polarization; the parameter ϵ can be extracted by differencing, as listed in Table 2.3.

Thus, the result from the first order perturbation calculation can be expressed as follows:

$$\Delta E^1 = \langle \Psi_\infty | H_4 + H_5 + H_{m4} + H_{m5} + H_D | \Psi_\infty \rangle + \delta H_\mu^1, \tag{2.183}$$

where the last term δH_μ^1 is the correction due to the inclusion of the mass polarization $\epsilon\mu/M$ term from Table 2.3.

Table 2.3: First order coefficients ϵ for mass polarization corrections to the Douglas and Kroll operators H_D^i and $\tilde{\Delta}_3$, and the Breit operators H_{eso}, H_{Zso}, and H_{ess}.

He Z=2 $1s2p\ ^3P_J$					
H_D^1	7.629(18)	H_D^8	3.758(35)	H_D^{14}	-0.961(95)
H_D^2	-1.6954(21)	H_D^9	4.085(87)	$\tilde{\Delta}_3$	2.856485(13)
H_D^3	-28.0784(11)	H_D^{10}	2.815(10)	H_{eso}	3.106409(27)
H_D^4	3.6757(11)	H_D^{11}	3.280(26)	H_{Zso}	3.359873(13)
H_D^5	3.21655(76)	H_D^{121}	2.968(17)	H_{ess}	2.400909(16)
H_D^6	250.206(19)	H_D^{122}	-5.2(1.5)		
H_D^7	-20.02(78)	H_D^{13}	5.013(39)		

Very recently, Drake has greatly improved the second-order energy calculations of Lewis and Serafino [10], with uncertainties less than 1 kHz. By including his results, full comparisons with the present high precision experimental measurements for the $1s2p\ ^3P_J$ states of helium are possible. Table 2.4 lists all the theoretical contributions through order $O(\alpha^6 mc^2)$ and the best experimental data of Hughes *et al.* [15] and Shiner *et al.* [16]. The mass polarization term is included directly in the unperturbed Hamiltonian. The two experimental measurements are not in particularly good agreement with each other. Their values differ by 118 kHz and 23 kHz for ν_{01} and ν_{12} respectively which are greater than their error bars. With no explanation for this, another independent measurement may resolve the discrepancy. The theoretical values agree with the values of Hughes *et al.*, and differ from the values of Shiner *et* *al.* by 108 kHz and 31 kHz. However, a recent study [14] shows that the phenomenological treatment of the $\alpha^6 mc^2$ radiative part of Douglas and Kroll is not sufficiently accurate. A new correction [14] has been found which contributes 10.888207(11) kHz to ν_{01} and 21.776414(22) kHz to ν_{12}. Furthermore, order $O(\alpha^7 \ln(Z\alpha) mc^2)$ and $O(\alpha^7 mc^2)$ contributions are important at 50 to 100 kHz level [35]. A meaningful comparison with experiment at 10 kHz level must include these effects. Work on this problem [35] is in progress. On the other hand, comparisons with high precision experimental measurements on helium and helium-like ions in other states, for example, He $1s3p\ ^3P_J$ and Li^+ $1s2p\ ^3P_J$, may help clarify the situation.

Table 2.4: Comparison of theoretical and experimental fine structure intervals for the $1s2p\ ^3P_J$ states of helium[a].

Term	ν_{01}	ν_{12}
H_4	29552.444002(61)	2316.279442(99)
H_5	54.68537423(11)	-22.53894618(16)
H_{m4}	1.45177443195(71)	2.90354486639(14)
H_{m5}	0.00168610449(0)	0.003372209(0)
H_D	-3.332735(13)	1.532968(21)
δH_μ^1	9.890379(88)	1.05179(14)
Second order	1.713458(90)	-8.02868(38)
$\nu_{\rm theo}$	29616.85394(11)	2291.20350(39)
$\nu_{\rm L.\&S.}$[b]	29616.904(43)	2291.283(81)
$\nu_{\rm exp}$ I[c]	29616.844(21)	2291.196(5)
$\nu_{\rm exp}$ II[d]	29616.962(3)	2291.173(3)
$\nu_{\rm theo} - \nu_{\rm exp}$ I	0.010	0.008
$\nu_{\rm theo} - \nu_{\rm exp}$ II	-0.108	0.031
	ν_{ss}	ν_{so}
Theory	28471.25219(72)	35344.86269(72)
Experiment I	28471.246(23)	35344.834(23)
Experiment II	28471.375(5)	35344.894(5)

[a] In MHz. Here $m/M = 1.370933543 \times 10^{-4}$, $\alpha^{-1} = 137.0359895(61)$, $R_\infty = 109737.315709(18)\ \mathrm{cm}^{-1}$, and $c = 2.99792458 \times 10^{10}\ \mathrm{cm \cdot sec^{-1}}$.
[b] Lewis and Serafino Ref. [10]. [c] Hughes *et al.* Ref. [15]. [d] Shiner *et al.* Ref. [16].

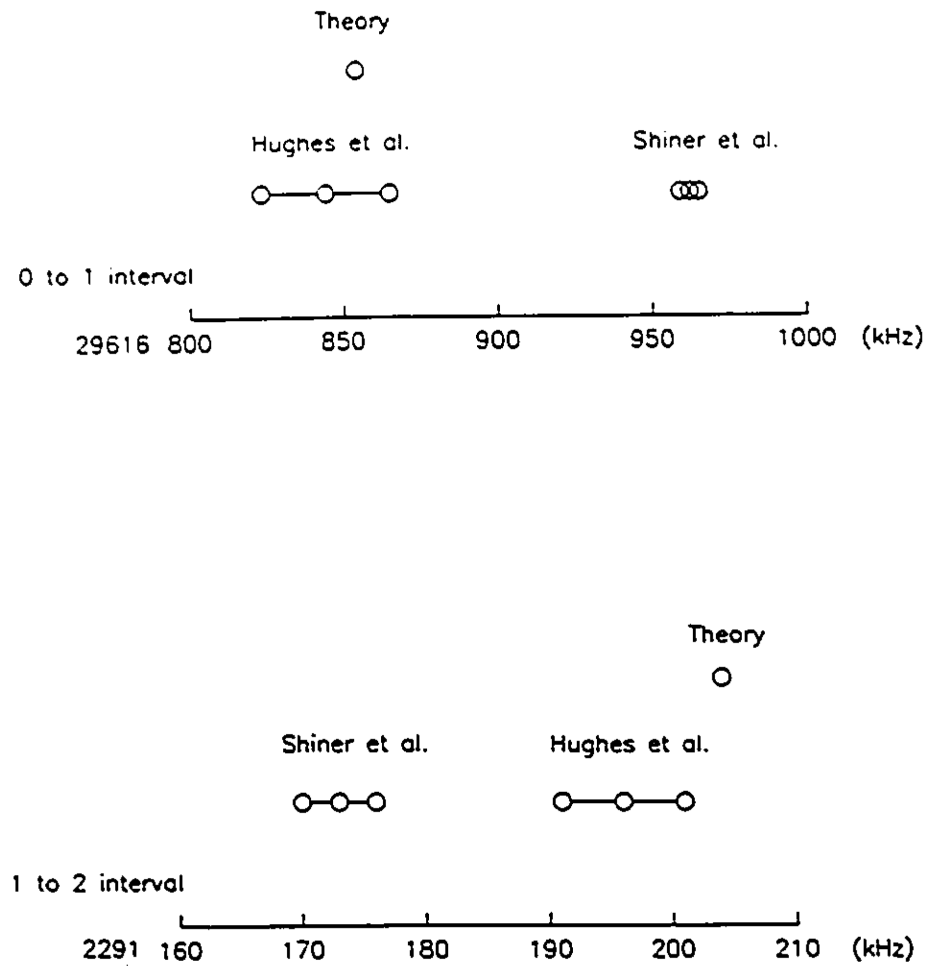

Figure 2.1: Schematic of the comparison between theory and experimental measurements for the helium $1s2p\,^3P_J$ intervals.

Table 2.5: Convergence study of the reduced matrix elements[a] of the Douglas and Kroll operators H^i_D and $\dot{\Delta}_3$, and the Breit operators H_{sso}, H_{soo} and H_{sss} for $Z=2$ $1s2p\,^3P_J$ states of He .

N^b	H^1_D	H^2_D	H^3_D	H^4_D
104	114.57881	-6.2839668	1.42499986	52.9087312
145	114.47321	-6.2839877	1.42578001	52.9049458
197	114.43786	-6.2838386	1.42588942	52.9051216
264	114.42609	-6.2837216	1.42591358	52.9057895
342	114.42081	-6.2836781	1.42592570	52.9052894
436	114.41930	-6.2836491	1.42593489	52.9050915
539	114.41820	-6.2836393	1.42593704	52.9050257
658	114.41722	-6.2836340	1.42593824	52.9049976
724	114.41686	-6.2836333	1.42593873	52.9049953
804	114.41719	-6.2836316	1.42593864	52.9049875
∞	114.41657(19)	-6.2836298(13)	1.42593890(15)	52.9049785(55)
Old[c]	114.128	-6.3094	1.439	52.886
	H^5_D	H^6_D	H^7_D	H^8_D
104	-22.6877402	0.33344252	3.25962	-101.21919
145	-22.6848844	0.33618661	3.28797	-101.17313
197	-22.6843416	0.33733827	3.29038	-101.16768
264	-22.6843819	0.33798037	3.28662	-101.17177
342	-22.6841707	0.33806028	3.29075	-101.16599
436	-22.6840899	0.33810488	3.29289	-101.16295
539	-22.6840614	0.33811641	3.29374	-101.16175
658	-22.6840500	0.33812115	3.29419	-101.16113
724	-22.6840488	0.33812220	3.29422	-101.16108
804	-22.6840457	0.33812394	3.29438	-101.16086
∞	-22.6840435(17)	0.33812395(62)	3.29490(25)	-101.16020(34)
Old[c]	-22.686	0.275	3.297	-101.209
	H^9_D	H^{10}_D	H^{11}_D	H^{12i}_D
104	-8.864306	36.650751	37.994320	-59.242153
145	-8.853349	36.634470	37.951660	-59.200504
197	-8.852008	36.630634	37.941345	-59.190550
264	-8.852967	36.630623	37.940899	-59.190274
342	-8.851538	36.628932	37.936449	-59.185842
436	-8.850787	36.628061	37.934157	-59.183558
539	-8.850493	36.627707	37.933238	-59.182642
658	-8.850338	36.627530	37.932771	-59.182175
724	-8.850326	36.627513	37.932726	-59.182131
804	-8.850272	36.627452	37.932569	-59.181974
∞	-8.850129(75)	36.627397(36)	37.932428(97)	-59.181829(98)
Old[c]	-8.871	36.6649	38.0480	

Table 2.5 (continued).

	H_D^{122}	H_D^{13}	H_D^{14}	Δ_3
104	0.232483	-11.568482	1.653849	152.415940046
145	0.248027	-11.551884	1.658763	152.41007724
197	0.251730	-11.547916	1.659933	152.41101717
264	0.251638	-11.547755	1.659923	152.41116777
342	0.253348	-11.545908	1.660522	152.41112555
436	0.254217	-11.544948	1.660832	152.41107764
539	0.254572	-11.544571	1.660955	152.41107460
658	0.254749	-11.544373	1.661020	152.41108043
724	0.254765	-11.544353	1.661026	152.41107881
804	0.254826	-11.544289	1.661047	152.41107871
∞	0.254884(37)	-11.544224(44)	1.661070(15)	152.41107920(19)
Old[c]		-11.58	1.653	152.417

$-\frac{1}{4}H_D^{121} + \frac{3}{8}H_D^{122}$	14.891038(28)
Old[c]	14.9036

	H_{eso}	H_{Zso}	H_{ess}
104	-105.07878702	-106.12349681	-50.356995938
145	-105.07889601	-106.12197360	-50.356672100
197	-105.07911229	-106.12176382	-50.356628169
264	-105.07926594	-106.12173632	-50.356654646
342	-105.07920506	-106.12172293	-50.356630547
436	-105.07918871	-106.12171965	-50.356624637
539	-105.07918400	-106.12171781	-50.356622565
658	-105.07918244	-106.12171645	-50.356622033
724	-105.07918235	-106.12171627	-50.356621979
804	-105.07918200	-106.12171656	-50.356621833
∞	-105.07918174(27)	-106.12171634(12)	-50.356621703(76)

[a]In 10^{-4} a.u..
[b]N is the number of terms in the doubled basis sets.
[c]Daley *et al.*, Ref. [13].

2.6.2 Final Numerical Values

Tables 2.6 and 2.7 contain our final results of the numerical calculations for the reduced matrix elements of the spin-dependent Breit operators and the Douglas-Kroll operators, as well as the total contributions to the triplet splittings, for the various triplets of the helium and helium-like ions, without the mass polarization term $\mu/M\nabla_1 \cdot \nabla_2$. The fundamental constants used in conversion are:

$$\begin{aligned} \alpha^{-1} &= 137.0359895(61) \\ R_\infty &= 109737.315709(18)\ \text{cm}^{-1} \\ c &= 2.99792458 \times 10^{10}\ \text{cm sec}^{-1}, \end{aligned}$$

where α^{-1} and c are from Cohen and Taylor [36], while R_∞ is from the more recent measurement of Biraben *et al.* [37]. As for the mass ratios, the binding energy corrections have been taken into account.

Table 2.6: Reduced matrix elements[a] of the Douglas and Kroll operators H_D^i and $\tilde{\Delta}_3$, and the Breit operators H_{eso}, H_{Zso}, and H_{ess}.

He Z=2 $1s2p\ ^3P_J$

H_D^1	114.41657(19)	H_D^8	-101.16020(34)	H_D^{14}	1.661070(15)
H_D^2	-6.2836298(13)	H_D^9	-8.850429(75)	$\tilde{\Delta}_3$	152.41107920(19)
H_D^3	1.42593890(15)	H_D^{10}	36.627397(36)	H_{eso}	-105.07918174(27)
H_D^4	52.90497785(55)	H_D^{11}	37.932428(97)	H_{Zso}	-106.12171634(12)
H_D^5	-22.68404435(17)	H_D^{121}	-59.181829(98)	H_{ess}	-50.356621703(76)
H_D^6	0.33812395(62)	H_D^{122}	0.254884(37)		
H_D^7	3.29490(25)	H_D^{13}	-11.544224(44)		

Li^+ Z=3 $1s2p\ ^3P_J$

H_D^1	289.5815444(14)	H_D^8	-244.27395(33)	H_D^{14}	1.675722(36)
H_D^2	-6.6843158(29)	H_D^9	-25.558933(81)	$\tilde{\Delta}_3$	313.47333016(96)
H_D^3	-5.04701413(10)	H_D^{10}	82.91636(11)	H_{eso}	-217.56508837(32)
H_D^4	128.1501669(97)	H_D^{11}	97.23008(27)	H_{Zso}	-217.600168470(53)
H_D^5	-53.0164859(36)	H_D^{121}	-138.89394(28)	H_{ess}	-97.926999616(91)
H_D^6	10.5276448(33)	H_D^{122}	-3.01440(11)		
H_D^7	-8.81570(22)	H_D^{13}	-35.56543(11)		

Be^{2+} Z=4 $1s2p\ ^3P_J$

H_D^1	409.082583(34)	H_D^8	-345.45628(37)	H_D^{14}	0.827009(32)
H_D^2	-6.0269206(27)	H_D^9	-38.476828(89)	$\tilde{\Delta}_3$	406.608299520(60)
H_D^3	-10.40731552(10)	H_D^{10}	114.391656(94)	H_{eso}	-285.27415316(30)
H_D^4	178.9033185(91)	H_D^{11}	140.61398(24)	H_{Zso}	-283.461822645(19)
H_D^5	-73.0701901(30)	H_D^{121}	-194.70066(24)	H_{ess}	-125.532042490(76)
H_D^6	19.5700484(29)	H_D^{122}	-6.729139(94)		
H_D^7	-22.44181(27)	H_D^{13}	-54.343368(96)		

B^{3+} Z=5 $1s2p\ ^3P_J$

H_D^1	490.815627(69)	H_D^8	-416.72582(32)	H_D^{14}	-0.060820(27)
H_D^2	-5.3954423(24)	H_D^9	-47.926323(77)	$\tilde{\Delta}_3$	465.36896876(44)
H_D^3	-14.267390064(94)	H_D^{10}	136.202413(81)	H_{eso}	-329.08393334(23)
H_D^4	213.5953491(75)	H_D^{11}	171.64204(20)	H_{Zso}	-325.56626123874(53)
H_D^5	-86.6659125(22)	H_D^{121}	-233.89923(20)	H_{ess}	-143.136794612(54)
H_D^6	26.3789258(25)	H_D^{122}	-9.833578(80)		
H_D^7	-33.66816(23)	H_D^{13}	-68.089920(83)		

[a] In 10^{-4} a.u..

C^{4+} Z=6 $1s2p\,^3P_J$

H_D^1	549.468552(12)	H_D^8	-468.93692(28)	H_D^{14}	-0.834504(25)
H_D^2	-4.8847695(22)	H_D^9	-54.994877(69)	$\tilde{\Delta}_3$	505.56663016(44)
H_D^3	-17.100325790(87)	H_D^{10}	152.039035(71)	H_{eso}	-359.55103628(20)
H_D^4	238.5180962(66)	H_D^{11}	194.57037(18)	H_{Zso}	-354.611188225(11)
H_D^5	-96.3899745(19)	H_D^{121}	-262.58191(18)	H_{ess}	-155.286336665(35)
H_D^6	31.5180559(22)	H_D^{122}	-12.318012(70)		
H_D^7	-42.56982(20)	H_D^{13}	-78.366552(74)		

N^{5+} Z=7 $1s2p\,^3P_J$

H_D^1	593.4044623(37)	H_D^8	-508.63466(25)	H_D^{14}	-1.483878(22)
H_D^2	-4.4787091(19)	H_D^9	-60.440990(61)	$\tilde{\Delta}_3$	534.73812075(37)
H_D^3	-19.248536082(80)	H_D^{10}	164.012967(63)	H_{eso}	-381.91639360(19)
H_D^4	257.2114958(59)	H_D^{11}	212.10117(16)	H_{Zso}	-375.809810441(37)
H_D^5	-103.6634070(18)	H_D^{121}	-284.37710(16)	H_{ess}	-164.162940385(27)
H_D^6	35.4899399(19)	H_D^{122}	-14.311985(62)		
H_D^7	-49.66961(18)	H_D^{13}	-86.278347(67)		

O^{6+} Z=8 $1s2p\,^3P_J$

H_D^1	627.4746252(56)	H_D^8	-539.76443(23)	H_D^{14}	-2.026813(20)
H_D^2	-4.1525177(17)	H_D^9	-64.750982(55)	$\tilde{\Delta}_3$	556.85404595(32)
H_D^3	-20.927043706(74)	H_D^{10}	173.366612(57)	H_{eso}	-399.01617276(18)
H_D^4	271.7246414(54)	H_D^{11}	225.90213(15)	H_{Zso}	-391.947821006(50)
H_D^5	-109.2996698(17)	H_D^{121}	-301.46220(15)	H_{ess}	-170.927898637(22)
H_D^6	38.6363096(17)	H_D^{122}	-15.933785(57)		
H_D^7	-55.41841(16)	H_D^{13}	-92.535276(61)		

F^{7+} Z=9 $1s2p\,^3P_J$

H_D^1	654.637629(15)	H_D^8	-564.79942(21)	H_D^{14}	-2.483565(19)
H_D^2	-3.8863739(15)	H_D^9	-68.240508(51)	$\tilde{\Delta}_3$	574.19069302(25)
H_D^3	-22.272125770(66)	H_D^{10}	180.867940(54)	H_{eso}	-412.50763664(17)
H_D^4	283.3075560(51)	H_D^{11}	237.03317(14)	H_{Zso}	-404.638034426(46)
H_D^5	-113.7917774(16)	H_D^{121}	-315.19917(14)	H_{ess}	-176.252957578(19)
H_D^6	41.1839672(14)	H_D^{122}	-17.272895(54)		
H_D^7	-60.14923(15)	H_D^{13}	-97.598068(58)		

Table 2.6 (continued)

Ne^{8+} Z=10 $1s2p\ ^3P_J$

H_D^1	676.787253(26)	H_D^8	-585.35535(19)	H_D^{14}	-2.871336(18)
H_D^2	-3.66580016(13)	H_D^9	-71.120478(47)	$\tilde{\Delta}_3$	588.14298388(21)
H_D^3	-23.3729736645(61)	H_D^{10}	187.014103(50)	H_{cso}	-423.42098174(16)
H_D^4	292.7610861(47)	H_D^{11}	246.19308(13)	H_{Zso}	-414.875980670(42)
H_D^5	-117.4542326(15)	H_D^{121}	-326.47671(13)	H_{css}	-180.552872427(16)
H_D^6	43.2860111(13)	H_D^{122}	-18.394534(49)		
H_D^7	-64.10143(14)	H_D^{13}	-101.774355(53)		

Na^{9+} Z=11 $1s2p\ ^3P_J$

H_D^1	695.187430(23)	H_D^8	-602.52803(18)	H_D^{14}	-3.203747(16)
H_D^2	-3.48036619(12)	H_D^9	-73.536230(44)	$\tilde{\Delta}_3$	599.61222973(16)
H_D^3	-24.289977976(56)	H_D^{10}	192.140104(46)	H_{cso}	-432.42929244(15)
H_D^4	300.6203342(44)	H_D^{11}	253.85892(12)	H_{Zso}	-423.308490884(39)
H_D^5	-120.4965365(14)	H_D^{121}	-335.89709(12)	H_{css}	-184.097313940(14)
H_D^6	45.0484513(12)	H_D^{122}	-19.346282(46)		
H_D^7	-67.44802(13)	H_D^{13}	-105.275955(50)		

Mg^{10+} Z=12 $1s2p\ ^3P_J$

H_D^1	710.712139(20)	H_D^8	-617.08501(17)	H_D^{14}	-3.491363(16)
H_D^2	-3.3224601(11)	H_D^9	-75.590764(41)	$\tilde{\Delta}_3$	609.20628742(12)
H_D^3	-25.065322372(51)	H_D^{10}	196.479461(44)	H_{cso}	-439.99055929(14)
H_D^4	307.2557786(41)	H_D^{11}	260.36644(11)	H_{Zso}	-430.373717292(37)
H_D^5	-123.0634068(14)	H_D^{121}	-343.88193(11)	H_{css}	-187.069107643(12)
H_D^6	46.5466144(11)	H_D^{122}	-20.162227(43)		
H_D^7	-70.31573(12)	H_D^{13}	-108.252870(47)		

He Z=2 $1s3p\ ^3P_J$

H_D^1	38.0245582(18)	H_D^8	-30.547703(33)	H_D^{14}	0.4055521(40)
H_D^2	-1.251994866(33)	H_D^9	-2.8665114(73)	$\tilde{\Delta}_3$	44.88683329(43)
H_D^3	-0.409229803(14)	H_D^{10}	10.6913608(96)	H_{cso}	-30.001479195(13)
H_D^4	16.24184718(31)	H_D^{11}	11.584554(26)	H_{Zso}	-30.77960476(12)
H_D^5	-6.78381661(47)	H_D^{121}	-17.506914(26)	H_{css}	-13.7685988633(12)
H_D^6	1.05527902(45)	H_D^{122}	0.0132774(94)		
H_D^7	0.102087(28)	H_D^{13}	-3.977775(12)		

Table 2.6 (continued)

He Z=2 $1s4p\,^3P_J$

H_D^1	16.469155(19)	H_D^8	-12.862017(51)	H_D^{14}	0.1585156(52)
H_D^2	-0.45208927(23)	H_D^9	-1.231124(12)	$\tilde{\Delta}_3$	18.698191117(76)
H_D^3	-0.279696651(13)	H_D^{10}	4.453488(13)	H_{eso}	-12.395386803(28)
H_D^4	6.86825446(12)	H_D^{11}	4.891274(33)	H_{Zso}	-12.792325462(70)
H_D^5	-2.84799205(75)	H_D^{121}	-7.324861(34)	H_{ess}	-5.6108981368(42)
H_D^6	0.57139113(52)	H_D^{122}	-0.003336(13)		
H_D^7	-0.075914(52)	H_D^{13}	-1.733770(15)		

He Z=2 $1s5p\,^3P_J$

H_D^1	8.5035360(83)	H_D^8	-6.560103(10)	H_D^{14}	0.0781059(17)
H_D^2	-0.21440587(44)	H_D^9	-0.6332798(30)	$\tilde{\Delta}_3$	9.487450539(69)
H_D^3	-0.166660592(64)	H_D^{10}	2.2606308(41)	H_{eso}	-6.267982014(35)
H_D^4	3.509353800(94)	H_D^{11}	2.497546(11)	H_{Zso}	-6.486716797(64)
H_D^5	-1.45074976(15)	H_D^{121}	-3.725617(11)	H_{ess}	-2.8199322924(69)
H_D^6	0.3202182(11)	H_D^{122}	-0.00037687(41)		
H_D^7	-0.0657144(45)	H_D^{13}	-0.8971626(49)		

He Z=2 $1s6p\,^3P_J$

H_D^1	4.93511(24)	H_D^8	-3.7830494(19)	H_D^{14}	0.04420140(57)
H_D^2	-0.11880196(16)	H_D^9	-0.36682859(52)	$\tilde{\Delta}_3$	5.455493884(98)
H_D^3	-0.103420753(40)	H_D^{10}	1.3003471(13)	H_{eso}	-3.597900200(27)
H_D^4	2.02561110(11)	H_D^{11}	1.4411119(44)	H_{Zso}	-3.729111270(50)
H_D^5	-0.836053050(32)	H_D^{121}	-2.1453377(40)	H_{ess}	-1.6134046355(41)
H_D^6	0.19348337(72)	H_D^{122}	-0.0028240(12)		
H_D^7	-0.04619435(72)	H_D^{13}	-0.5212570(19)		

He Z=2 $1s7p\,^3P_J$

H_D^1	3.110793(12)	H_D^8	-2.3752901(27)	H_D^{14}	0.02744312(46)
H_D^2	-0.07280987(30)	H_D^9	-0.230922755(69)	$\tilde{\Delta}_3$	3.419476341(65)
H_D^3	-0.067659032(16)	H_D^{10}	0.8152331(15)	H_{eso}	-2.252831607(46)
H_D^4	1.27253759(31)	H_D^{11}	0.9051426(35)	H_{Zso}	-2.337129534(51)
H_D^5	-0.524741165(42)	H_D^{121}	-1.3458466(38)	H_{ess}	-1.008275348(15)
H_D^6	0.12478144(51)	H_D^{122}	-0.0020089(13)		
H_D^7	-0.0320840(80)	H_D^{13}	-0.3287216(16)		

He $Z=2$ $1s8p\ ^3P_J$

H_D^1	2.08382(23)	H_D^8	-1.58737336(66)	H_D^{14}	0.018208408(93)
H_D^2	-0.04789821(11)	H_D^9	-0.15457850(22)	$\tilde{\Delta}_3$	2.28262679(22)
H_D^3	-0.046384529(63)	H_D^{10}	0.5442812900(56)	H_{eso}	-1.502870209(75)
H_D^4	0.850721022(77)	H_D^{11}	0.60501354(55)	H_{Zso}	-1.560032711(25)
H_D^5	-0.350594071(46)	H_D^{121}	-0.89890596(42)	H_{ess}	-0.67178263S(49)
H_D^6	0.08480790(42)	H_D^{122}	-0.001439935(19)		
H_D^7	-0.02274897(11)	H_D^{13}	-0.22028991(41)		

He $Z=2$ $1s9p\ ^3P_J$

H_D^1	1.46344(15)	H_D^8	-1.112655(12)	H_D^{14}	0.012697390(93)
H_D^2	-0.03321101(34)	H_D^9	-0.1084761(14)	$\tilde{\Delta}_3$	1.5987064(79)
H_D^3	-0.03306890(15)	H_D^{10}	0.3812458S7(65)	H_{eso}	-1.05210269(22)
H_D^4	0.596477(32)	H_D^{11}	0.42413330(73)	H_{Zso}	-1.09256519(32)
H_D^5	-0.24569767(97)	H_D^{121}	-0.62982828(74)	H_{ess}	-0.469888918(98)
H_D^6	0.06012092(98)	H_D^{122}	-0.001061488(46)		
H_D^7	-0.016666(31)	H_D^{13}	-0.15470074(26)		

He $Z=2$ $1s10p\ ^3P_J$

H_D^1	1.0660916(33)	H_D^8	-0.809730-40(17)	H_D^{14}	0.009207824(37)
H_D^2	-0.023982S2(35)	H_D^9	-0.079006195(21)	$\tilde{\Delta}_3$	1.16282942(12)
H_D^3	-0.024354811(51)	H_D^{10}	0.277327907(60)	H_{eso}	-0.765020545(45)
H_D^4	0.434112846(58)	H_D^{11}	0.30870033(31)	H_{Zso}	-0.794673459(34)
H_D^5	-0.1787880259(73)	H_D^{121}	-0.45824410(26)	H_{ess}	-0.3414652239(82)
H_D^6	0.04410452(41)	H_D^{122}	-0.000798450(52)		
H_D^7	-0.01239795(20)	H_D^{13}	-0.11273669(15)		

Li^+ $Z=3$ $1s3p\ ^3P_J$

H_D^1	96.145140(12)	H_D^8	-73.891621(18)	H_D^{14}	0.1762155(50)
H_D^2	-1.20882835(45)	H_D^9	-8.1099214(48)	$\tilde{\Delta}_3$	87.73303938(42)
H_D^3	-3.143813667(21)	H_D^{10}	24.185687(11)	H_{eso}	-60.277365304(10)
H_D^4	38.206136440(21)	H_D^{11}	29.349390(28)	H_{Zso}	-62.108902773(95)
H_D^5	-15.37465475(21)	H_D^{121}	-41.226605(29)	H_{ess}	-26.0641920043(31)
H_D^6	5.8667301(11)	H_D^{122}	-1.1416240(95)		
H_D^7	-5.240306(12)	H_D^{13}	-11.824495(14)		

Be^{2+} Z=4 $1s3p\ {}^3P_J$

H_D^1	137.283596(85)	H_D^8	-105.422756(83)	H_D^{14}	-0.2463325(72)
H_D^2	-1.16968864(42)	H_D^9	-12.201720(16)	$\tilde{\Delta}_3$	111.76204939(16)
H_D^3	-5.212990605(31)	H_D^{10}	33.658163(18)	H_{cso}	-78.5397103148(46)
H_D^4	53.0894528(12)	H_D^{11}	42.545125(35)	H_{Zso}	-81.06678182(10)
H_D^5	-21.08849444(75)	H_D^{121}	-58.370225(39)	H_{css}	-33.3001817620(14)
H_D^6	9.99705377(89)	H_D^{122}	-2.392091(15)		
H_D^7	-10.661139(54)	H_D^{13}	-17.931973(18)		

B^{3+} Z=5 $1s3p\ {}^3P_J$

H_D^1	166.263255(54)	H_D^8	-128.112421(62)	H_D^{14}	-0.6314892(50)
H_D^2	-1.17165413(41)	H_D^9	-15.232164(18)	$\tilde{\Delta}_3$	126.81931258(25)
H_D^3	-5.6818409410(15)	H_D^{10}	40.379049(12)	H_{cso}	-90.4811258391(81)
H_D^4	63.37886115(98)	H_D^{11}	52.125055(26)	H_{Zso}	-93.47571675(11)
H_D^5	-25.01161768(45)	H_D^{121}	-70.691602(28)	H_{css}	-37.9973451547(62)
H_D^6	13.12541301(90)	H_D^{122}	-3.4288875(95)		
H_D^7	-15.039546(32)	H_D^{13}	-22.427585(14)		

C^{4+} Z=6 $1s3p\ {}^3P_J$

H_D^1	187.496927(64)	H_D^8	-144.979364(46)	H_D^{14}	-0.9514448(39)
H_D^2	-1.18951327(40)	H_D^9	-17.520750(14)	$\tilde{\Delta}_3$	137.10415545(30)
H_D^3	-7.7578085010(64)	H_D^{10}	45.3379445(92)	H_{cso}	-98.8599144234(94)
H_D^4	70.83960189(78)	H_D^{11}	59.282254(22)	H_{Zso}	-102.18582983(14)
H_D^5	-27.84631001(31)	H_D^{121}	-79.848325(23)	H_{css}	-41.2826041899(72)
H_D^6	15.50679088(81)	H_D^{122}	-4.2578411(86)		
H_D^7	-18.490829(22)	H_D^{13}	-25.806938(11)		

N^{5+} Z=7 $1s3p\ {}^3P_J$

H_D^1	203.643684(68)	H_D^8	-157.937721(45)	H_D^{14}	-1.2137441(36)
H_D^2	-1.21204163(40)	H_D^9	-19.296668(13)	$\tilde{\Delta}_3$	144.56781203(29)
H_D^3	-8.574608987(44)	H_D^{10}	49.130110(11)	H_{cso}	-105.0531626065(18)
H_D^4	76.47539171(87)	H_D^{11}	64.798793(21)	H_{Zso}	-108.62487680(16)
H_D^5	-29.98312558(31)	H_D^{121}	-86.882827(23)	H_{css}	-43.7067113382(65)
H_D^6	17.36100927(73)	H_D^{122}	-4.923647(11)		
H_D^7	-21.238140(23)	H_D^{13}	-28.4203935(98)		

O^{6+} Z=8 $1s3p\ ^3P_J$

H_D^1	216.306835(72)	H_D^8	-168.177876(41)	H_D^{14}	-1.4300611(34)
H_D^2	-1.234874195(39)	H_D^9	-20.709803(12)	$\tilde{\Delta}_3$	150.22891972(21)
H_D^3	-9.2139855408(49)	H_D^{10}	52.117393(15)	H_{cso}	-109.8137366399(25)
H_D^4	80.87494143(79)	H_D^{11}	69.168129(20)	H_{Zso}	-113.57458939(16)
H_D^5	-31.64889191(29)	H_D^{121}	-92.441905(23)	H_{css}	-45.5680590451(63)
H_D^6	18.83880522(65)	H_D^{122}	-5.465809(14)		
H_D^7	-23.461493(22)	H_D^{13}	-30.4946784(90)		

F^{7+} Z=9 $1s3p\ ^3P_J$

H_D^1	226.491502(74)	H_D^8	-176.462064(37)	H_D^{14}	-1.6104318(32)
H_D^2	-1.25640029(38)	H_D^9	-21.858830(11)	$\tilde{\Delta}_3$	154.66933427(17)
H_D^3	-9.727331352(48)	H_D^{10}	54.528573(11)	H_{cso}	-113.5857252378(28)
H_D^4	84.40143246(78)	H_D^{11}	72.708892(19)	H_{Zso}	-117.49642509(16)
H_D^5	-32.98277233(26)	H_D^{121}	-96.939390(22)	H_{css}	-47.0418188168(61)
H_D^6	20.04134198(58)	H_D^{122}	-5.913997(10)		
H_D^7	-25.291180(21)	H_D^{13}	-32.1779717(83)		

Ne^{8+} Z=10 $1s3p\ ^3P_J$

H_D^1	234.854506(75)	H_D^8	-183.296093(34)	H_D^{14}	-1.7626231(30)
H_D^2	-1.27610944(36)	H_D^9	-22.8104061(99)	$\tilde{\Delta}_3$	158.24512054(14)
H_D^3	-10.148217229(44)	H_D^{10}	56.5142420(89)	H_{cso}	-116.6473926626(34)
H_D^4	87.28966981(84)	H_D^{11}	75.633679(18)	H_{Zso}	-120.67964506(15)
H_D^5	-34.07442446(23)	H_D^{121}	-100.649806(21)	H_{css}	-48.2374362951(57)
H_D^6	21.03759747(54)	H_D^{122}	-6.2898137(85)		
H_D^7	-26.820134(19)	H_D^{13}	-33.5698267(75)		

Na^{9+} Z=11 $1s3p\ ^3P_J$

H_D^1	241.841367(73)	H_D^8	-189.027070(31)	H_D^{14}	-1.8925008(28)
H_D^2	-1.29394019(35)	H_D^9	-23.6108447(91)	$\tilde{\Delta}_3$	161.18625316(11)
H_D^3	-10.499380590(41)	H_D^{10}	58.1771613(76)	H_{cso}	-119.1817548826(25)
H_D^4	89.69770835(88)	H_D^{11}	78.088960(17)	H_{Zso}	-123.31453873(15)
H_D^5	-34.98405406(21)	H_D^{121}	-103.761521(20)	H_{css}	-49.2267578951(55)
H_D^6	21.87574433(49)	H_D^{122}	-6.6090220(74)		
H_D^7	-28.115249(18)	H_D^{13}	-34.7391303(68)		

Mg^{10+} Z=12 $1s3p\,^3P_J$

H_D^1	247.764204(69)	H_D^8	-193.900408(30)	H_D^{14}	-2.0044934(27)
H_D^2	-1.31000405(33)	H_D^9	-24.2931926(87)	$\tilde{\Delta}_3$	163.64784232(10)
H_D^3	-10.796723432(39)	H_D^{10}	59.5896860(73)	H_{eso}	-121.3140356993(13)
H_D^4	91.73564567(74)	H_D^{11}	80.178591(16)	H_{Zso}	-125.53132162(14)
H_D^5	-35.75352528(20)	H_D^{121}	-106.407713(19)	H_{ess}	-50.0588772055(54)
H_D^6	22.59025927(45)	H_D^{122}	-6.8832598(70)		
H_D^7	-29.225456(17)	H_D^{13}	-35.7348767(64)		

He Z=2 $1s3d\,^3D_J$

H_D^1	0.77555047(63)	H_D^8	-6.81319119(30)	H_D^{14}	0.080986821(61)
H_D^2	-2.8251270339(26)	H_D^9	-0.023569209(78)	$\tilde{\Delta}_3$	4.11731840(11)
H_D^3	1.2689423634(30)	H_D^{10}	1.63100181(12)	H_{eso}	-8.57010183972(60)
H_D^4	1.051588166(14)	H_D^{11}	0.99193358(45)	H_{Zso}	-8.5851192833(11)
H_D^5	-0.361030647(17)	H_D^{121}	-2.45161433(42)	H_{ess}	-2.999940535700(69)
H_D^6	-0.985056902(14)	H_D^{122}	0.01323870(12)		
H_D^7	1.09808287(18)	H_D^{13}	0.16682564(23)		

Li^+ Z=3 $1s3d\,^3D_J$

H_D^1	3.18646509(99)	H_D^8	-16.91456262(81)	H_D^{14}	0.326069409(77)
H_D^2	-6.668649513(29)	H_D^9	-0.152865278(28)	$\tilde{\Delta}_3$	6.229493299(14)
H_D^3	2.884280428(75)	H_D^{10}	4.05985902(34)	H_{eso}	-20.414342160(18)
H_D^4	3.52562628(35)	H_D^{11}	2.75307703(33)	H_{Zso}	-20.3425343010(62)
H_D^5	-1.17668022(82)	H_D^{121}	-6.1499918(16)	H_{ess}	-7.041735223(74)
H_D^6	-1.53084419(23)	H_D^{122}	0.02294783(20)		
H_D^7	1.98082973(12)	H_D^{13}	0.5968232(12)		

Be^{2+} Z=4 $1s3d\,^3D_J$

H_D^1	5.6541067(11)	H_D^8	-24.77429239(30)	H_D^{14}	0.56696996(32)
H_D^2	-9.464827340(22)	H_D^9	-0.324818439(23)	$\tilde{\Delta}_3$	6.46552937(20)
H_D^3	4.0300622347(43)	H_D^{10}	5.948107424(17)	H_{eso}	-29.145865927(12)
H_D^4	5.81820943(27)	H_D^{11}	4.2700039(11)	H_{Zso}	-28.9058115012(27)
H_D^5	-1.913127105(34)	H_D^{121}	-9.0659744(15)	H_{ess}	-9.9685390333(25)
H_D^6	-1.51329519(17)	H_D^{122}	0.00921175(13)		
H_D^7	2.26825188(62)	H_D^{13}	0.97478668(95)		

Table 2.6 (continued)

B^{3+} Z=5 $1s3d\ {}^3D_J$

H_D^1	7.72944031(57)	H_D^8	-30.63831920(23)	H_D^{14}	0.76354681(20)
H_D^2	-11.460683170(20)	H_D^9	-0.489347779(38)	$\tilde{\Delta}_3$	6.15939166(47)
H_D^3	4.8389018239(23)	H_D^{10}	7.35392484(18)	H_{cso}	-35.4343352015(88)
H_D^4	7.6663106659(51)	H_D^{11}	5.46479948(23)	H_{Zso}	-35.0180273076(21)
H_D^5	-2.498341288(24)	H_D^{121}	-11.25840391(80)	H_{css}	-12.0542693420(38)
H_D^6	-1.32201154(55)	H_D^{122}	-0.01428196(19)		
H_D^7	2.30718558395(54)	H_D^{13}	1.26201302(64)		

C^{4+} Z=6 $1s3d\ {}^3D_J$

H_D^1	9.41353379(31)	H_D^8	-35.0957721710(45)	H_D^{14}	0.91966303(40)
H_D^2	-12.932137869(15)	H_D^9	-0.6333805436(42)	$\tilde{\Delta}_3$	5.72444646(47)
H_D^3	5.4316421039(36)	H_D^{10}	8.420417055(21)	H_{cso}	-40.09962328(11)
H_D^4	9.132011834(14)	H_D^{11}	6.40349328(80)	H_{Zso}	-39.52340940473(77)
H_D^5	-2.958369432(24)	H_D^{121}	-12.93304898(79)	H_{css}	-13.591097959(27)
H_D^6	-1.09449957(38)	H_D^{122}	-0.039638215(57)		
H_D^7	2.251107(14)	H_D^{13}	1.47915105(60)		

N^{5+} Z=7 $1s3d\ {}^3D_J$

H_D^1	10.78178606(23)	H_D^8	-38.57264574(14)	H_D^{14}	1.0445018(18)
H_D^2	-14.054692367(20)	H_D^9	-0.756386976(25)	$\tilde{\Delta}_3$	5.28683014(56)
H_D^3	5.882145395(21)	H_D^{10}	9.250914035(74)	H_{cso}	-43.67500726(13)
H_D^4	10.3059679(13)	H_D^{11}	7.15205926(80)	H_{Zso}	-42.95979198712(64)
H_D^5	-3.3246274(15)	H_D^{121}	-14.2435900532(63)	H_{css}	-14.763309658(14)
H_D^6	-0.8745096(10)	H_D^{122}	-0.06380416(14)		
H_D^7	2.161177(20)	H_D^{13}	1.64660368(56)		

O^{6+} Z=8 $1s3d\ {}^3D_J$

H_D^1	11.90570482(20)	H_D^8	-41.350623474(15)	H_D^{14}	1.14580727(15)
H_D^2	-14.936648989(15)	H_D^9	-0.861061294(12)	$\tilde{\Delta}_3$	4.88394579(57)
H_D^3	6.2351955460(41)	H_D^{10}	9.91356625(16)	H_{cso}	-46.49384501160(40)
H_D^4	11.2609892230(76)	H_D^{11}	7.75967231(76)	H_{Zso}	-45.65915025767(51)
H_D^5	-3.621303872(22)	H_D^{121}	-15.29316690(71)	H_{css}	-15.6842629650(19)
H_D^6	-0.674634416(94)	H_D^{122}	-0.08581979(16)		
H_D^7	2.062406608(46)	H_D^{13}	1.77876142(54)		

Table 2.6 (continued)

F^{7+} Z=9 $1s3d\ ^3D_J$

H_D^1	12.84110480(16)	H_D^8	-43.616871133(24)	H_D^{14}	1.22932229(14)
H_D^2	-15.646744359(16)	H_D^9	-0.950502467(15)	$\tilde{\Delta}_3$	4.52406190(55)
H_D^3	6.5189292963(56)	H_D^{10}	10.453541555(13)	H_{eso}	-48.769575358816(44)
H_D^4	12.05027465509(49)	H_D^{11}	8.26126214(67)	H_{Zso}	-47.832148443677(41)
H_D^5	-3.865697993(21)	H_D^{121}	-16.15092226(62)	H_{ess}	-16.42579267144(13)
H_D^6	-0.496948390(80)	H_D^{122}	-0.10551977(14)		
H_D^7	1.965062477(31)	H_D^{13}	1.88532614(49)		

Ne^{8+} Z=10 $1s3d\ ^3D_J$

H_D^1	13.62966535(14)	H_D^8	-45.498754592(32)	H_D^{14}	1.29918790(12)
H_D^2	-16.230212707(19)	H_D^9	-1.027456492(19)	$\tilde{\Delta}_3$	4.20574469(45)
H_D^3	6.7517457239(53)	H_D^{10}	10.90152345(11)	H_{eso}	-50.64358490776(58)
H_D^4	12.7121475377(34)	H_D^{11}	8.68162996(54)	H_{Zso}	-49.61740133312(94)
H_D^5	-4.070121672(20)	H_D^{121}	-16.86418135(50)	H_{ess}	-17.03513869280(83)
H_D^6	-0.34001512(18)	H_D^{122}	-0.12304736(11)		
H_D^7	1.873295844(22)	H_D^{13}	1.97288533(43)		

Na^{9+} Z=11 $1s3d\ ^3D_J$

H_D^1	14.30234285(16)	H_D^8	-47.0853007882(96)	H_D^{14}	1.35841149(51)
H_D^2	-16.717871638(34)	H_D^9	-1.094178102(34)	$\tilde{\Delta}_3$	3.92462591(42)
H_D^3	6.946123477(15)	H_D^{10}	11.27889985(17)	H_{eso}	-52.21268665(11)
H_D^4	13.274427335(10)	H_D^{11}	9.03863864(84)	H_{Zso}	-51.1093256862(59)
H_D^5	-4.24343359(24)	H_D^{121}	-17.46616502(29)	H_{ess}	-17.544472359(34)
H_D^6	-0.20142300(26)	H_D^{122}	-0.1386395(19)		
H_D^7	1.7885347(60)	H_D^{13}	2.04600659(43)		

Mg^{10+} Z=12 $1s3d\ ^3D_J$

H_D^1	14.88231988(36)	H_D^8	-48.440344292(25)	H_D^{14}	1.40920327(66)
H_D^2	-17.131373330(16)	H_D^9	-1.152473382(22)	$\tilde{\Delta}_3$	3.67582692(37)
H_D^3	7.1108012063(61)	H_D^{10}	11.60099508(15)	H_{eso}	-53.54517934153(61)
H_D^4	13.7576121121(16)	H_D^{11}	9.34539540(38)	H_{Zso}	-52.37424647595(64)
H_D^5	-4.392117560(30)	H_D^{121}	-17.98077598(57)	H_{ess}	-17.976392906(18)
H_D^6	-0.07868469(15)	H_D^{122}	-0.1525283(14)		
H_D^7	1.710842762(40)	H_D^{13}	2.10793329(38)		

He Z=2 $1s4d\ ^3D_J$

H_D^1	0.430591318(32)	H_D^8	-2.9297433(25)	H_D^{14}	0.04333314(15)
H_D^2	-1.190827933(23)	H_D^9	-0.01398163(61)	$\tilde{\Delta}_3$	1.71297924(98)
H_D^3	0.5226270532(19)	H_D^{10}	0.70261356(46)	H_{eso}	-3.6242490881(14)
H_D^4	0.509191197(15)	H_D^{11}	0.4411934(12)	H_{Zso}	-3.63137325730(25)
H_D^5	-0.173147146(42)	H_D^{121}	-1.0574449(12)	H_{ess}	-1.2610234059(41)
H_D^6	-0.35658047872(74)	H_D^{122}	0.00700368(46)		
H_D^7	0.4209919(18)	H_D^{13}	0.08590763(49)		

He Z=2 $1s5d\ ^3D_J$

H_D^1	0.244991592(96)	H_D^8	-1.51286657(85)	H_D^{14}	0.024336448(75)
H_D^2	-0.6093773684(91)	H_D^9	-0.00816149(29)	$\tilde{\Delta}_3$	0.87098992(10)
H_D^3	0.26452470638(81)	H_D^{10}	0.36309007(25)	H_{eso}	-1.8573775772(19)
H_D^4	0.276252002(28)	H_D^{11}	0.23116243(63)	H_{Zso}	-1.86118345081(30)
H_D^5	-0.093560915(24)	H_D^{121}	-0.54680223(63)	H_{ess}	-0.6444372271(18)
H_D^6	-0.1684873818(49)	H_D^{122}	0.00390397(25)		
H_D^7	0.20550901(49)	H_D^{13}	0.04751692(25)		

He Z=2 $1s6d\ ^3D_J$

H_D^1	0.14948206(10)	H_D^8	-0.8794632(11)	H_D^{14}	0.014755103(88)
H_D^2	-0.352521409(47)	H_D^9	-0.00504557(28)	$\tilde{\Delta}_3$	0.50207284(79)
H_D^3	0.1521073490(17)	H_D^{10}	0.21115405(23)	H_{eso}	-1.0753413729(54)
H_D^4	0.164748647(88)	H_D^{11}	0.13540994(65)	H_{Zso}	-1.07759004788(87)
H_D^5	-0.055680586(28)	H_D^{121}	-0.31810505(64)	H_{ess}	-0.3725278542(24)
H_D^6	-0.0930613323(37)	H_D^{122}	0.00235610(24)		
H_D^7	0.11576605(83)	H_D^{13}	0.02858472(27)		

He Z=2 $1s7d\ ^3D_J$

H_D^1	0.09705874(16)	H_D^8	-0.55530851(83)	H_D^{14}	0.009545761(51)
H_D^2	-0.2219387828(44)	H_D^9	-0.00330070(20)	$\tilde{\Delta}_3$	0.315423(10)
H_D^3	0.09541383678(22)	H_D^{10}	0.13335666(16)	H_{eso}	-0.6773326248(77)
H_D^4	0.105598077(62)	H_D^{11}	0.08588693(41)	H_{Zso}	-0.6787655887(14)
H_D^5	-0.035645433(17)	H_D^{121}	-0.20094676(41)	H_{ess}	-0.2344286548(21)
H_D^6	-0.0569132090(85)	H_D^{122}	0.00152013(16)		
H_D^7	0.07170041(60)	H_D^{13}	0.01840818(16)		

Table 2.6 (continued)

He Z=2 $1s8d\ ^3D_J$

H_D^1	0.06628985(35)	H_D^8	-0.37264703(50)	H_D^{14}	0.006504889(39)
H_D^2	-0.1486531005(47)	H_D^9	-0.00226551(12)	$\tilde{\Delta}_3$	0.2109512(27)
H_D^3	0.06375564679(15)	H_D^{10}	0.08950351(11)	H_{eso}	-0.4538133672(34)
H_D^4	0.071545119(35)	H_D^{11}	0.05780279(29)	H_{Zso}	-0.45478048855(66)
H_D^5	-0.024131589(11)	H_D^{121}	-0.13488674(28)	H_{ess}	-0.1569725171(12)
H_D^6	-0.0373908600(49)	H_D^{122}	0.00103379(11)		
H_D^7	0.04750909(37)	H_D^{13}	0.01250746(12)		

He Z=2 $1s9d\ ^3D_J$

H_D^1	0.04716869(11)	H_D^8	-0.26202150(33)	H_D^{14}	0.004621450(24)
H_D^2	-0.10438836675(92)	H_D^9	-0.001617141(79)	$\tilde{\Delta}_3$	0.1479876(41)
H_D^3	0.04469784093(18)	H_D^{10}	0.062939301(67)	H_{eso}	-0.3187479920(20)
H_D^4	0.0506340412(23)	H_D^{11}	0.04072320(18)	H_{Zso}	-0.31943062427(45)
H_D^5	-0.0170693302(69)	H_D^{121}	-0.09486239(17)	H_{ess}	-0.11020816563(56)
H_D^6	-0.0259056306(51)	H_D^{122}	0.000733631(68)		
H_D^7	0.03311492(24)	H_D^{13}	0.008868388(71)		

He Z=2 $1s10d\ ^3D_J$

H_D^1	0.034703635(26)	H_D^8	-0.19116780(38)	H_D^{14}	0.003396522(25)
H_D^2	-0.0760901973(13)	H_D^9	-0.001192535(88)	$\tilde{\Delta}_3$	0.10779875(35)
H_D^3	0.03254275127(20)	H_D^{10}	0.045922919(82)	H_{eso}	-0.2323751995(24)
H_D^4	0.037112880(27)	H_D^{11}	0.02975271(20)	H_{Zso}	-0.23287458112(71)
H_D^5	-0.0125064329(86)	H_D^{121}	-0.06922013(20)	H_{ess}	-0.08032065624(73)
H_D^6	-0.0186997636(68)	H_D^{122}	0.000538706(80)		
H_D^7	0.02400881(28)	H_D^{13}	0.006508667(74)		

Table 2.7: Theoretical contributions to the fine structures of helium-like ions[a].

Term	$\nu_{L-1,L}$	$\nu_{L,L+1}$	$\nu_{L-1,L+1}$
He Z=2 $1s2p\ ^3P_J$, $m/M=1.370933543\times 10^{-4}$			
H_4	29552.444002(61)	2316.279442(99)	31868.72344(15)
H_5	54.68537423(11)	-22.53894618(16)	32.14642805(24)
H_{m4}	1.45177413195(71)	2.903548639(14)	4.355322958(21)
H_{m5}	0.0016861049(0)	0.003372209(0)	0.005058314(0)
H_D	-3.332735(13)	1.532968(21)	-1.799766(31)
Sum	29605.250102(62)	2298.18039(10)	31903.43049(15)
ν_{ss}	28456.159909(44)	ν_{so}	35350.70107(30)
Li^+ Z=3 $1s2p\ ^3P_J$, $m/M=7.820814724\times 10^{-5}$			
H_4	155306.46158(24)	-62171.34705(38)	93135.11452(57)
H_5	263.18330243(45)	-339.54401508(61)	-76.36071265(92)
H_{m4}	8.685449509(87)	17.37089902(17)	26.05634853(26)
H_{m5}	0.01008736(0)	0.02017473(0)	0.03026209(0)
H_D	-45.97156(21)	61.36922(16)	15.39766(24)
Sum	155532.36886(32)	-62432.13078(42)	93100.23808(62)
ν_{ss}	186748.43425(29)	ν_{so}	-547.9581(12)
Be^{2+} Z=4 $1s2p\ ^3P_J$, $m/M=6.088575076\times 10^{-5}$			
H_4	344757.57459(50)	-443272.49395(83)	-98514.9194(13)
H_5	497.55415737(92)	-1626.1530573(13)	-1138.5988999(20)
H_{m4}	27.451016048(14)	54.902032097(28)	82.353048145(42)
H_{m5}	0.03188187 9(0)	0.063763758(0)	0.095645638(0)
H_D	-173.40758(79)	577.19621(72)	403.7886(11)
Sum	345109.20406(94)	-444276.4850(11)	-99167.2809(17)
ν_{ss}	567247.44656(93)	ν_{so}	-765582.0084(32)
B^{3+} Z=5 $1s2p\ ^3P_J$, $m/M=4.984116218\times 10^{-5}$			
H_4	478587.20932(73)	-1565665.0881(12)	-1087077.8788(19)
H_5	428.3938631(13)	-5003.3133990(19)	-4574.9195360(29)
H_{m4}	62.28435201(20)	124.56870402(40)	186.85305603(59)
H_{m5}	0.07233765(0)	0.14467531(0)	0.21701297(0)
H_D	-249.2854(21)	2926.7060(20)	2677.4206(30)
Sum	478828.6744(22)	-1567616.9821(23)	-1088788.3077(35)
ν_{ss}	1262637.1655(23)	ν_{so}	-3440213.7808(66)

[a]In MHz. The fundamental constants used here are $\alpha^{-1} = 137.0359895(61)$, $R_\infty = 109737.315709(18)\ \mathrm{cm}^{-1}$, and $c = 2.99792458 \times 10^{10}\ \mathrm{cm\cdot sec}^{-1}$.

Table 2.7 (continued)

Term	$\nu_{L-1,L}$	$\nu_{L,L+1}$	$\nu_{L-1,L+1}$
C^{4+} Z=6 $1s2p\,^3P_J$, m/M=4.572753026 × 10^{-5}			
H_4	350311.7932(10)	-4028935.7451(19)	-3678623.9519(28)
H_5	-476.3204565(18)	-11938.5541613(29)	-12414.8746177(44)
H_{m4}	127.94757851(37)	255.89515701(75)	383.8427355(11)
H_{m5}	0.14859957(0)	0.29719914(0)	0.4457987(0)
H_D	419.1257(46)	10473.8372(42)	10892.9629(63)
Sum	350382.6946(47)	-4030144.2697(46)	-3679761.5751(69)
ν_{ss}	2365454.8295(50)	ν_{so}	-9724977.980(13)
N^{5+} Z=7 $1s2p\,^3P_J$, m/M=3.918641850 × 10^{-5}			
H_4	-334038.9258(16)	-8607912.2869(31)	-8941951.2127(46)
H_5	-2951.9026180(29)	-24346.6085073(52)	-27298.5111253(79)
H_{m4}	213.86418946(50)	427.7283789(10)	641.5925684(15)
H_{m5}	0.24838396(0)	0.4967679(0)	0.7451519(0)
H_D	3639.1790(88)	29943.0539(80)	33582.233(12)
Sum	-333137.5368(89)	-8601887.6164(85)	-8935025.153(13)
ν_{ss}	3967806.2714(96)	ν_{so}	-21837856.578(24)
O^{6+} Z=8 $1s2p\,^3P_J$, m/M=3.430655299 × 10^{-5}			
H_4	-1956023.0256(25)	-16252509.6761(49)	-18208532.7017(73)
H_5	-7937.0943762(48)	-44538.8598819(91)	-52475.954258(14)
H_{m4}	331.42824024(64)	662.8564805(13)	994.2847207(19)
H_{m5}	0.38492401(0)	0.7698480(0)	1.1547720(0)
H_D	13074.810(15)	73159.784(14)	86234.594(21)
Sum	-1950553.497(16)	-16223225.126(15)	-18173778.623(22)
ν_{ss}	6161059.066(17)	ν_{so}	-42508616.312(41)
F^{7+} Z=9 $1s2p\,^3P_J$, m/M=2.888255457 × 10^{-5}			
H_4	-4984799.4269(35)	-28087987.4498(68)	-33072786.877(10)
H_5	-16574.1581963(67)	-75234.065055(13)	-91808.223251(19)
H_{m4}	459.54996801(68)	919.0999360(14)	1378.6499040(20)
H_{m5}	0.53372584(0)	1.0674516(0)	1.6011775(0)
H_D	35172.371(26)	159160.442(24)	194332.814(36)
Sum	-4965741.130(27)	-28003140.905(25)	-32968882.035(37)
ν_{ss}	9035829.322(29)	ν_{so}	-74973593.393(69)

Table 2.7 (continued)

Term	$\nu_{L-1,L}$	$\nu_{L,L+1}$	$\nu_{L-1,L+1}$
Ne^{8+} Z=10 $1s2p\ ^3P_J$, m/M=2.744689933 × 10^{-5}			
H_4	-9977020.0341(46)	-45414245.3413(90)	-55391265.375(14)
H_5	-30208.4919198(90)	-119556.448387(17)	-149764.940306(26)
H_{m4}	680.19513240(83)	1360.3902648(17)	2040.5853972(25)
H_{m5}	0.78998530(0)	1.5799706(0)	2.3699559(0)
H_D	80268.506(42)	316661.725(40)	396930.231(60)
Sum	-9926279.035(42)	-45215778.095(41)	-55142057.129(61)
ν_{ss}	12681610.013(45)	ν_{so}	-122965724.27(11)
Na^{9+} Z=11 $1s2p\ ^3P_J$, m/M=2.386818081 × 10^{-5}			
H_4	-17577130.5824(60)	-69707413.020(12)	-87284543.602(18)
H_5	-50389.599972(12)	-181039.939290(23)	-231429.539263(35)
H_{m4}	881.21242286(83)	1762.4248457(17)	2643.6372686(25)
H_{m5}	1.02344875(0)	2.0468975(0)	3.0703462(0)
H_D	163886.803(62)	586919.670(60)	750806.474(90)
Sum	-17462751.143(63)	-69299768.817(61)	-86762519.960(91)
ν_{ss}	17187133.265(67)	ν_{so}	-190712173.19(17)
Mg^{10+} Z=12 $1s2p\ ^3P_J$, m/M=2.287802960 × 10^{-5}			
H_4	-28516844.2376(76)	-102617355.978(15)	-131134200.216(23)
H_5	-78869.472622(15)	-263621.582847(30)	-342491.055470(45)
H_{m4}	1213.44623560(88)	2426.8924712(18)	3640.3387068(26)
H_{m5}	1.40930083(0)	2.8186167(0)	4.2279251(0)
H_D	308207.537(92)	1026911.261(87)	1335118.30(13)
Sum	-28286291.818(92)	-101851636.589(89)	-130137928.41(13)
ν_{ss}	22639526.477(99)	ν_{so}	-282915383.29(25)
He Z=2 $1s3p\ ^3P_J$, m/M=1.370933543 × 10^{-4}			
H_4	8096.547975(14)	665.851571(27)	8762.399545(41)
H_5	14.821165882(31)	-6.424656252(63)	8.396509630(94)
H_{m4}	0.442445323(14)	0.884890646(28)	1.327335969(42)
H_{m5}	0.000513860(0)	0.001027720(0)	0.001541581(0)
H_D	-0.9647178(26)	0.5356784(22)	-0.4290393(33)
Sum	8110.847382(14)	660.848511(27)	8771.695893(41)
ν_{ss}	7780.4231265(29)	ν_{so}	9762.968660(82)

Table 2.7 (continued)

Term	$\nu_{L-1,L}$	$\nu_{L,L+1}$	$\nu_{L-1,L+1}$
He Z=2 $1s4p\ ^3P_J$, $m/M=1.370933543 \times 10^{-4}$			
H_4	3300.0109539(96)	272.450931(19)	3572.461885(28)
H_5	6.018620365(21)	-2.660565333(40)	3.358055032(60)
H_{m4}	0.1852257962(32)	0.3704515925(65)	0.5556773887(97)
H_{m5}	0.0002151230(0)	0.0004302461(0)	0.000645369(0)
H_D	-0.4003971(35)	0.2355801(35)	-0.1648170(52)
Sum	3305.814618(10)	270.396828(19)	3576.211446(29)
ν_{ss}	3170.6162041(44)	ν_{so}	3981.806688(57)
He Z=2 $1s5p\ ^3P_J$, $m/M=1.370933543 \times 10^{-4}$			
H_4	1658.512882(10)	136.907128(19)	1795.420011(28)
H_5	3.019733606(21)	-1.347374775(39)	1.672358832(58)
H_{m4}	0.0941120793(29)	0.1882241585(59)	0.2823362378(88)
H_{m5}	0.0001093026(0)	0.0002186053(0)	0.000327908(0)
H_D	-0.2028882(10)	0.12244941(72)	-0.0804388(11)
Sum	1661.423949(10)	135.870646(19)	1797.294595(28)
ν_{ss}	1593.4886261(41)	ν_{so}	2001.100564(57)
He Z=2 $1s6p\ ^3P_J$, $m/M=1.370933543 \times 10^{-4}$			
H_4	948.8832078(76)	78.283670(15)	1027.166878(22)
H_5	1.726108516(16)	-0.774113203(30)	0.951995313(45)
H_{m4}	0.0541445764(34)	0.1082891529(69)	0.162433729(10)
H_{m5}	0.0000628840(0)	0.0001257680(0)	0.000188652(0)
H_D	-0.1165983(45)	0.0713048(89)	-0.045293(13)
Sum	950.5469255(88)	77.689277(17)	1028.236202(26)
ν_{ss}	911.7022871(24)	ν_{so}	1144.770118(52)
He Z=2 $1s7p\ ^3P_J$, $m/M=1.370933543 \times 10^{-4}$			
H_4	592.978766(12)	48.896464(20)	641.875229(30)
H_5	1.078097178(25)	-0.484993410(37)	0.593103769(56)
H_{m4}	0.0339456670(26)	0.0678913340(52)	0.1018370011(78)
H_{m5}	0.0000394248(0)	0.0000788496(0)	0.0001182744(0)
H_D	-0.07305046(44)	0.04504758(55)	-0.02800288(83)
Sum	594.017797(12)	48.524488(20)	642.542285(30)
ν_{ss}	569.7555534(88)	ν_{so}	715.329017(59)

Table 2.7 (continued)

Term	$\nu_{L-1,L}$	$\nu_{L,L+1}$	$\nu_{L-1,L+1}$
He $Z=2$ $1s8p\ ^3P_J$, $m/M=1.370933543 \times 10^{-4}$			
H_4	395.076723(26)	32.564870(28)	427.641593(42)
H_5	0.718037754(57)	-0.323666104(47)	0.394371651(71)
H_{m4}	0.0226627342(70)	0.045325468(14)	0.067988203(21)
H_{m5}	0.0000263207(6)	0.000052641(0)	0.000078962(0)
H_D	-0.048751541(33)	0.030221018(45)	-0.018530524(67)
Sum	395.768698(26)	32.316803(28)	428.085501(42)
ν_{ss}	379.610296(27)	ν_{so}	476.560705(79)
He $Z=2$ $1s9p\ ^3P_J$, $m/M=1.370933543 \times 10^{-4}$			
H_4	276.339069(70)	22.77091(11)	299.10998(16)
H_5	0.50211544(15)	-0.22664803(21)	0.27546741(32)
H_{m4}	0.01587412(25)	0.03174824(50)	0.04762235(74)
H_{m5}	0.00001843(0)	0.00003687(0)	0.00005530(0)
H_D	-0.0341362(28)	0.0212427(56)	-0.0128934(84)
Sum	276.822941(70)	22.59729(11)	299.42023(16)
ν_{ss}	265.524296(55)	ν_{so}	333.31616(32)
He $Z=2$ $1s10p\ ^3P_J$, $m/M=1.370933543 \times 10^{-4}$			
H_4	200.8118732(95)	16.543606(17)	217.355480(26)
H_5	0.364817848(18)	-0.164836011(30)	0.199981837(46)
H_{m4}	0.0115464835(40)	0.0230929671(79)	0.034639451(12)
H_{m5}	0.0000134101(0)	0.0000268203(0)	0.000040230(0)
H_D	-0.024829292(65)	0.01548334(12)	-0.00934595(19)
Sum	201.1634217(95)	16.417374(17)	217.580795(26)
ν_{ss}	192.9547349(46)	ν_{so}	242.206855(52)
Li^+ $Z=3$ $1s3p\ ^3P_J$, $m/M=7.820814724 \times 10^{-5}$			
H_4	40280.894092(56)	-18658.25157(11)	21622.64252(17)
H_5	66.53427395(13)	-97.40170795(26)	-30.86743400(39)
H_{m4}	2.321370661(39)	4.642741321(78)	6.96411198(12)
H_{m5}	0.002696062(0)	0.005392125(0)	0.00808818(0)
H_D	-12.418185(21)	21.214099(12)	8.795914(18)
Sum	40337.334248(59)	-18729.79105(11)	21607.54320(17)
ν_{ss}	49702.229771(25)	ν_{so}	-6487.14337(34)

Table 2.7 (continued)

Term	$\nu_{L-1,L}$	$\nu_{L,L+1}$	$\nu_{L-1,L+1}$
Be^{2+} Z=4 $1s3p\ ^3P_J$, m/M=6.088575076 × 10^{-5}			
H_4	84637.68584(19)	-131221.88516(37)	-46584.19933(56)
H_5	113.10786631(43)	-471.785193380(86)	-358.6773275(13)
H_{m4}	6.842390494(43)	13.684780989(86)	20.52717148(13)
H_{m5}	0.007946819(0)	0.01589363(0)	0.02384045(0)
H_D	-39.57332(18)	200.32184(25)	160.74852(38)
Sum	84718.07072(26)	-131479.64784(45)	-46761.57713(67)
ν_{ss}	150457.89464(16)	ν_{so}	-243981.0489(13)
B^{3+} Z=5 $1s3p\ ^3P_J$, m/M=4.984116218 × 10^{-5}			
H_4	103907.97730(52)	-461901.4564(10)	-357993.4791(15)
H_5	53.4932720(12)	-1448.6462037(24)	-1395.1529317(36)
H_{m4}	14.85510758(12)	29.71021515(25)	44.56532273(37)
H_{m5}	0.01725286(0)	0.03450573(0)	0.05175860(0)
H_D	-11.16372(39)	1020.02438(59)	1008.86066(88)
Sum	103965.17921(65)	-462300.3335(12)	-358335.1543(18)
ν_{ss}	335115.34597(32)	ν_{so}	-1051785.6546(35)
C^{4+} Z=6 $1s3p\ ^3P_J$, m/M=4.572753026 × 10^{-5}			
H_4	34964.1816(13)	-1187416.8101(27)	-1152452.6285(40)
H_5	-273.4835605(31)	-3467.5531689(62)	-3741.0367294(94)
H_{m4}	29.59625139(28)	59.19250278(57)	88.78875417(85)
H_{m5}	0.03437337(0)	0.06874675(0)	0.10312013(0)
H_D	358.2310(10)	3662.7749(18)	4021.0059(27)
Sum	35078.5597(17)	-1187162.3271(32)	-1152083.7674(49)
ν_{ss}	628659.72323(64)	ν_{so}	-2932827.2581(97)
N^{5+} Z=7 $1s3p\ ^3P_J$, m/M=3.918641850 × 10^{-5}			
H_4	-211258.6023(27)	-2536417.2781(54)	-2747675.8804(81)
H_5	-1089.2620163(63)	-7088.732615(13)	-8177.994632(19)
H_{m4}	48.36713292(44)	96.73426584(88)	145.1013988(13)
H_{m5}	0.05617406(0)	0.1123481(0)	0.1685221(0)
H_D	1771.5295(27)	10499.2480(48)	12270.7775(72)
Sum	-210527.9115(38)	-2532909.9161(72)	-2743437.828(11)
ν_{ss}	1055927.0465(16)	ν_{so}	-6542802.702(22)

Table 2.7 (continued)

Term	$\nu_{L-1,L}$	$\nu_{L,L+1}$	$\nu_{L-1,L+1}$
O^{6+} Z=8 $1s3p\,^3P_J$, m/M=3.430655299 × 10^{-5}			
H_4	-749779.9259(46)	-4789432.2459(93)	-5539212.172(14)
H_5	-2675.561969(11)	-12992.904110(22)	-15668.466080(32)
H_{m4}	73.66780848(54)	147.3356170(11)	221.0034254(16)
H_{m5}	0.08555851(0)	0.1711170(0)	0.2566755(0)
H_D	5618.1386(65)	25707.185(11)	31325.323(17)
Sum	-746763.5960(80)	-4776570.459(15)	-5523334.055(22)
ν_{ss}	1641521.6333(40)	ν_{so}	-12688189.742(43)
F^{7+} Z=9 $1s3p\,^3P_J$, m/M=2.888255457 × 10^{-5}			
H_4	-1721578.8304(73)	-8278945.754(15)	-10000524.584(22)
H_5	-5374.412907(17)	-21981.489313(34)	-27355.902220(51)
H_{m4}	100.75223452(63)	201.5044690(13)	302.2567036(19)
H_{m5}	0.11701463(0)	0.2340292(0)	0.3510439(0)
H_D	14308.708(12)	56022.319(23)	70331.028(34)
Sum	-1712543.666(14)	-8244703.185(27)	-9957246.851(41)
ν_{ss}	2409807.9265(53)	ν_{so}	-22324301.629(81)
Ne^{8+} Z=10 $1s3p\,^3P_J$, m/M=2.744689933 × 10^{-5}			
H_4	-3293554.335(11)	-13389188.380(22)	-16682742.715(32)
H_5	-9588.025315(25)	-34976.054890(50)	-44564.080204(75)
H_{m4}	147.47097309(81)	294.9419462(16)	442.4129193(24)
H_{m5}	0.17127423(0)	0.3425484(0)	0.5138227(0)
H_D	31674.833(22)	111617.743(43)	143292.576(65)
Sum	-3271319.885(25)	-13312251.407(48)	-16583571.292(72)
ν_{ss}	3384805.8181(77)	ν_{so}	-36551948.40(14)
Na^{9+} Z=11 $1s3p\,^3P_J$, m/M=2.386818081 × 10^{-5}			
H_4	-5658627.484(15)	-20556605.638(30)	-26215233.122(46)
H_5	-15779.102848(35)	-53019.550784(71)	-68798.65363(11)
H_{m4}	189.29278214(92)	378.5855643(18)	567.8783464(28)
H_{m5}	0.21998464(0)	0.4396929(0)	0.6595394(0)
H_D	63436.500(38)	207122.481(74)	270558.98(11)
Sum	-5610780.574(41)	-20402123.682(80)	-26012904.26(12)
ν_{ss}	4590281.267(11)	ν_{so}	-56616089.78(24)

Table 2.7 (continued)

Term	$\nu_{L-1,L}$	$\nu_{L,L+1}$	$\nu_{L-1,L+1}$
Mg^{10+} Z=12 $1s3p\ ^3P_J$, m/M=2.287802960 × 10^{-5}			
H_4	-9035565.990(20)	-30269122.567(41)	-39304688.557(61)
H_5	-24470.325444(47)	-77274.382849(95)	-101744.70829(14)
H_{m4}	258.6349261(12)	517.2698522(23)	775.9047783(35)
H_{m5}	0.3003811(0)	0.6007622(0)	0.9011434(0)
H_D	117730.776(61)	362755.62(12)	480486.40(18)
Sum	-8942046.604(64)	-29983123.46(13)	-38925170.06(19)
ν_{ss}	6049515.126(16)	ν_{so}	-83899855.25(38)
He Z=2 $1s3d\ ^3D_J$, m/M=1.370933543 × 10^{-4}			
H_4	1298.16549791(15)	101.60546480(22)	1399.77096270(36)
H_5	1.99707561684(30)	-1.29148185560(44)	0.70559376124(74)
H_{m4}	-0.1253304819(30)	-0.1879957229(45)	-0.3133262048(74)
H_{m5}	-0.0001455600(0)	-0.0002183400(0)	-0.0003639001(0)
H_D	-0.1281304480(23)	-0.0378160444(23)	-0.165946524(32)
Sum	1299.90896700(15)	100.08795283(22)	1399.99691984(36)
ν_{ss}	1233.183665111(40)	ν_{so}	1455.60133808(48)
Li^{+} Z=3 $1s3d\ ^3D_J$, m/M=7.820814724 × 10^{-5}			
H_4	6861.716601(72)	-4331.391577(48)	2530.325024(36)
H_5	7.75034074(17)	-22.34332527(11)	-14.592984537(72)
H_{m4}	-1.1435649794(12)	-1.7153474691(18)	-2.8589124485(31)
H_{m5}	-0.0013281475(0)	-0.0019922213(0)	-0.0033203689(0)
H_D	-2.22216821(47)	-0.32778987(43)	-2.54995808(59)
Sum	6866.099880(72)	-4355.780032(48)	2510.319848(36)
ν_{ss}	9769.95323(10)	ν_{so}	90.442053(34)
Be^{2+} Z=4 $1s3d\ ^3D_J$, m/M=6.088575076 × 10^{-5}			
H_4	11364.138258(16)	-32028.281244(23)	-20664.142985(38)
H_5	-1.315179110(28)	-115.963954103(38)	-117.279133213(62)
H_{m4}	-4.474141742(39)	-6.711212613(59)	-11.185354354(98)
H_{m5}	-0.005196312(0)	-0.007794468(0)	-0.01299078(0)
H_D	-12.1934006(17)	0.6947715(20)	-11.4986291(30)
Sum	11346.150341(16)	-32150.269433(23)	-20804.119093(38)
ν_{ss}	32779.6632964(84)	ν_{so}	-38665.379889(51)

Table 2.7 (continued)

Term	$\nu_{L-1,L}$	$\nu_{L,L+1}$	$\nu_{L-1,L+1}$
B^{3+} Z=5 $1s3d\ ^3D_J$, m/M=4.984116218 × 10^{-5}			
H_4	-905.606894(28)	-117265.389812(36)	-118170.996706(57)
H_5	-67.908725742(55)	-371.094095578(63)	-439.002821320(97)
H_{m4}	-11.49963767(19)	-17.24945650(28)	-28.74909416(47)
H_{m5}	-0.01335579(0)	-0.02003368(0)	-0.03338948(0)
H_D	-39.4235162(37)	13.6555963(39)	-25.7679199(59)
Sum	-1024.452129(29)	-117640.097802(36)	-118664.549931(58)
ν_{ss}	77402.279739(25)	ν_{so}	-184020.159821(76)
C^{4+} Z=6 $1s3d\ ^3D_J$, m/M=4.572753026 × 10^{-5}			
H_4	-56038.41707(50)	-309882.79116(70)	-365921.2082(11)
H_5	-258.85129112(86)	-912.8280638(11)	-1171.6793549(18)
H_{m4}	-25.62309965(36)	-38.4346494S(54)	-64.0577491З(90)
H_{m5}	-0.02975891(0)	-0.04463837(0)	-0.0743972(0)
H_D	-92.080707(54)	71.687813(81)	-20.39289(13)
Sum	-56415.00192(51)	-310762.41070(71)	-367177.4126(12)
ν_{ss}	150759.93854(30)	ν_{so}	-539823.1963(15)
N^{5+} Z=7 $1s3d\ ^3D_J$, m/M=3.918641850 × 10^{-5}			
H_4	-190507.14057(89)	-675299.2350(13)	-865806.3756(22)
H_5	-665.0837443(14)	-1902.4533463(21)	-2567.5370906(34)
H_{m4}	-45.3431370(67)	-68.0147056(10)	-113.3578426(17)
H_{m5}	-0.05266196(0)	-0.0789929(0)	-0.1316549(0)
H_D	-168.30074(17)	250.09911(26)	81.79837(43)
Sum	-191385.92086(91)	-677019.6830(13)	-868405.6038(22)
ν_{ss}	259960.53445(25)	ν_{so}	-1244527.6499(30)
O^{6+} Z=8 $1s3d\ ^3D_J$, m/M=3.430655299 × 10^{-5}			
H_4	-451165.626778(38)	-1294498.788795(31)	-1745664.415573(37)
H_5	-1401.657055078(89)	-3537.408217754(71)	-4939.065272832(84)
H_{m4}	-73.2982493(10)	-109.9473740(15)	-183.2456233(26)
H_{m5}	-0.0851293(0)	-0.1276939(0)	-0.2128232(0)
H_D	-243.204818(33)	692.254757(28)	449.049939(35)
Sum	-452883.872030(51)	-1297454.017324(42)	-1750337.889354(51)
ν_{ss}	412085.472853(67)	ν_{so}	-2471145.676757(64)

Table 2.7 (continued)

Term	$\nu_{L-1,L}$	$\nu_{L,L+1}$	$\nu_{L-1,L+1}$
F^{7+} Z=9 $1s3d\,^3D_J$, m/M=2.888255457 × 10^{-5}			
H_4	-895253.581697(38)	-2264050.519008(35)	-3159304.100705(47)
H_5	-2607.750401441(87)	-6051.337699299(79)	-8659.088100741(11)
H_{m4}	-104.9885954(13)	-157.4828932(20)	-262.4714886(33)
H_{m5}	-0.1219347(0)	-0.1829021(0)	-0.3048369(0)
H_D	-251.792179(52)	1641.691573(44)	1389.899394(56)
Sum	-898218.234808(64)	-2268617.830930(56)	-3166836.065737(74)
ν_{ss}	614193.652479(82)	ν_{so}	-4427179.305143(95)
Ne^{8+} Z=10 $1s3d\,^3D_J$, m/M=2.744689933 × 10^{-5}			
H_4	-1590374.83986(61)	-3696051.72433(91)	-5286426.5642(15)
H_5	-4446.6067450(14)	-9713.9407683(21)	-14160.5475134(35)
H_{m4}	-159.4520087(16)	-239.1780131(24)	-398.6300218(40)
H_{m5}	-0.1851891(0)	-0.2777836(0)	-0.4629728(0)
H_D	-67.652303(74)	3480.382965(69)	3412.730662(95)
Sum	-1595048.73610(61)	-3702524.73793(91)	-5297573.4740(15)
ν_{ss}	873301.08918(10)	ν_{so}	-7354531.6618(20)
Na^{9+} Z=11 $1s3d\,^3D_J$, m/M=2.386818081 × 10^{-5}			
H_4	-2614549.2665(33)	-5718256.3428(44)	-8332805.6093(71)
H_5	-7105.6823447(58)	-14831.3120563(71)	-21936.994401(11)
H_{m4}	-210.9430777(19)	-316.4146165(28)	-527.3576942(47)
H_{m5}	-0.2449913(0)	-0.3674870(0)	-0.6124784(0)
H_D	522.40486(59)	6773.43883(78)	7295.8437(13)
Sum	-2621343.7321(33)	-5726630.9981(44)	-8347974.7302(72)
ν_{ss}	1196410.2667(23)	ν_{so}	-11529436.3958(96)
Mg^{10+} Z=12 $1s3d\,^3D_J$, m/M=2.287802960 × 10^{-5}			
H_4	-4056126.8396(11)	-8473872.20590(74)	-12529999.04546(46)
H_5	-10796.4048084(26)	-21745.4073433(17)	-32541.8121517(11)
H_{m4}	-295.5519173(23)	-443.3278760(34)	-738.8797933(57)
H_{m5}	-0.3432568(0)	-0.5148853(0)	-0.8581422(0)
H_D	1847.94675(47)	12319.55485(48)	14167.50160(70)
Sum	-4065371.1928(12)	-8483741.90115(88)	-12549113.09394(84)
ν_{ss}	1590456.7413(17)	ν_{so}	-17262303.03903(97)

Table 2.7 (continued)

Term	$\nu_{L-1,L}$	$\nu_{L,L+1}$	$\nu_{L-1,L+1}$
He $Z=2$ $1s4d\ ^3D_J$, $m/M=1.370933543 \times 10^{-4}$			
H_4	546.7158957(24)	44.2588833(32)	590.9747790(53)
H_5	0.8392767969(42)	-0.5431630219(52)	0.2961137750(82)
H_{m4}	-0.053814674(28)	-0.080722011(41)	-0.134536684(69)
H_{m5}	-0.000062500(0)	-0.000093751(0)	-0.000156252(0)
H_D	-0.054590222(91)	-0.01472052(10)	-0.06931075(16)
Sum	547.4467051(24)	43.6201840(32)	591.0668891(53)
ν_{ss}	518.3665824(17)	ν_{so}	615.3003247(70)
He $Z=2$ $1s5d\ ^3D_J$, $m/M=1.370933543 \times 10^{-4}$			
H_4	279.64601397(60)	22.99419004(55)	302.64020400(74)
H_5	0.4288673220(13)	-0.2776385364(10)	0.1512287856(12)
H_{m4}	-0.0277768495(29)	-0.0416652742(43)	-0.0694421237(72)
H_{m5}	-0.0000322603(0)	-0.0000483904(0)	-0.0000806507(0)
H_D	-0.028068637(42)	-0.007239622(39)	-0.035308259(53)
Sum	280.01900354(60)	22.66759822(55)	302.68660176(75)
ν_{ss}	264.90727140(76)	ν_{so}	315.27971188(96)
He $Z=2$ $1s6d\ ^3D_J$, $m/M=1.370933543 \times 10^{-4}$			
H_4	161.7336890(11)	13.4115422(13)	175.1452311(21)
H_5	0.2479024637(21)	-0.1605109919(22)	0.0873914718(33)
H_{m4}	-0.016144374(22)	-0.024216561(33)	-0.040360935(56)
H_{m5}	-0.000018750(0)	-0.000028125(0)	-0.000046875(0)
H_D	-0.016278951(45)	-0.004095426(48)	-0.020374377(72)
Sum	161.9491494(11)	13.2226911(13)	175.1718404(21)
ν_{ss}	153.13402197(99)	ν_{so}	182.5177799(28)
He $Z=2$ $1s7d\ ^3D_J$, $m/M=1.370933543 \times 10^{-4}$			
H_4	101.8080163(13)	8.4853141(18)	110.2933304(30)
H_5	0.1559986898(24)	-0.1010145991(29)	0.0549840907(47)
H_{m4}	-0.01019245(29)	-0.01528868(43)	-0.02548113(72)
H_{m5}	-0.00001183(0)	-0.00001775(0)	-0.00002959(0)
H_D	-0.010264298(32)	-0.002542951(35)	-0.012807249(53)
Sum	101.9435464(14)	8.3664501(19)	110.3099966(31)
ν_{ss}	96.36591299(88)	ν_{so}	114.9580244(41)

Table 2.7 (continued)

Term	$\nu_{L-1,L}$	$\nu_{L,L+1}$	$\nu_{L-1,L+1}$
He Z=2 $1s8d\ ^3D_J$, $m/M=1.370933543 \times 10^{-4}$			
H_4	68.1834927(14)	5.7015936(19)	73.8850863(32)
H_5	0.1044543060(23)	-0.0676417000(31)	0.0368126060(50)
H_{m4}	-0.006839859(54)	-0.010259788(82)	-0.01709965(14)
H_{m5}	-0.0000007943(0)	-0.000011915(0)	-0.000001985(0)
H_D	-0.006881717(23)	-0.001687895(25)	-0.008569612(39)
Sum	68.2742175(14)	5.6219923(19)	73.8962098(32)
ν_{ss}	64.52622257(73)	ν_{so}	77.0195388(43)
He Z=2 $1s9d\ ^3D_J$, $m/M=1.370933543 \times 10^{-4}$			
H_4	47.87704450(35)	4.01258765(48)	51.88963215(79)
H_5	0.07333501693(62)	-0.04749156529(78)	0.02584345516(12)
H_{m4}	-0.00480931(12)	-0.00721396(17)	-0.01202327(29)
H_{m5}	-0.00000558(0)	-0.00000837(0)	-0.00001396(0)
H_D	-0.004835738(13)	-0.001177844(14)	-0.006013581(21)
Sum	47.94072888(37)	3.95669590(51)	51.89742478(84)
ν_{ss}	45.30293161(23)	ν_{so}	54.0955892(11)
He Z=2 $1s10d\ ^3D_J$, $m/M=1.370933543 \times 10^{-4}$			
H_4	34.89653503(42)	2.92940991(57)	37.82594494(93)
H_5	0.05344674406(76)	-0.03461292785(93)	0.01883381162(15)
H_{m4}	-0.0035086198(98)	-0.005262930(15)	-0.008771550(25)
H_{m5}	-0.000004074(0)	-0.000006112(0)	-0.000010187(0)
H_D	-0.003526517(15)	-0.000854676(16)	-0.004381193(24)
Sum	34.94294256(42)	2.88867327(57)	37.83161583(93)
ν_{ss}	33.01716038(30)	ν_{so}	39.4364343(12)

Chapter 3

Summary and Conclusions

Advances in both theory and experiment raise the possibility that a value for the fine structure constant α competitive with that derived from the quantum Hall effect can be obtained from the $1s2p\ ^3P_J$ fine structure splittings of helium. The fine structure problem cannot be fully explained unless QED effects are taken into account. The Douglas-Kroll operators, together with the spin-dependent Breit operators and the Breit interaction taken to second order, account for the QED effects up to $\alpha^6 mc^2$.

In this thesis, the expectation values of the Douglas-Kroll fine structure operators and the spin-dependent Breit operators have been evaluated numerically, with high precision, using the wave functions of Drake, for the different triplets of helium and helium-like ions. The triplet splittings we have calculated are $Z = 2$, $1snp\ ^3P_J$, $n = 2, \cdots, 10$; $Z = 3, \cdots, 12$, $1s2p\ ^3P_J$; $Z = 3, \cdots, 12$, $1s3p\ ^3P_J$; $Z = 2, \cdots, 12$, $1s3d\ ^3D_J$; and $Z = 2$, $1snd\ ^3D_J$, $n = 4, \cdots, 10$; but our computer codes apply, in principle, for arbitrary Z, n, and L. We have improved the old calculation of Daley *et al.* for the deepest triplet states of helium, $1s2p\ ^3P_J$, by several orders of magnitude.

As for the computational methods, the results of this work provide a general scheme for analysing and cancelling the divergent parts of integrals which commonly arise in the calculation of higher-order QED corrections with nonrelativistic correlated wave functions. Also, general formulas are obtained for evaluating the remaining finite parts of matrix elements. Although simpler results can be obtained for various special cases, the general formulas are more broadly applicable, and they provide a valuable check that the cancellations are done correctly.

Therefore, the understanding of the fine structures of helium and helium-like ions up to order $\alpha^6 mc^2$ will be completed once the second-order perturbation calculations of the Breit interaction are finished. However, order $O(\alpha^7 \ln(Z\alpha) mc^2)$ and $O(\alpha^7 mc^2)$ contributions must be included in order to match the present experimental precision. One immediate application of the isoelectronic sequence for a triplet splitting is to extract the coefficients of the terms $\alpha^6 mc^2 Z^6$, $\alpha^6 mc^2 Z^5$, $\alpha^6 mc^2 Z^4$, etc., which come from the theory of Z^{-1} expansion [38]. The leading two coefficients can also be calculated from the single-particle Dirac wave functions with the inclusion of the relativistic Breit operators. If these are subtracted from the calculated energies, estimates of the higher order (in Z^{-1}) coefficients can be obtained. This will allow detailed comparisons with the recent relativistic multiconfiguration calculations of Chen, Cheng and Johnson [39].

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Appendix A

Final Analytical Expressions

In this appendix, we list our final expressions of the matrix elements of the Douglas and Kroll operators, as well as those of the spin-dependent Breit operators. All the intermediate steps leading to the final expressions can, in principle, be filled without major difficulties by the procedures demonstrated in section 2. Besides, some notations used below have local meanings only. As we know, the Douglas and Kroll operators are spin-dependent. The spin part of an operator can be easily calculated, which equals to either

$$\langle S'\|\vec{\sigma}_1\|S\rangle = \sqrt{6}(-1)^S(S,S')^{1/2}\begin{Bmatrix} 1/2 & S' & 1/2 \\ S & 1/2 & 1 \end{Bmatrix}$$

or

$$\langle S'\|[\vec{\sigma}_1 \otimes \vec{\sigma}_2]^{(K)}\|S\rangle = 6(S,S',K)^{1/2}\begin{Bmatrix} 1/2 & 1/2 & 1 \\ 1/2 & 1/2 & 1 \\ S' & S & K \end{Bmatrix},$$

depending on how many spin operators the operator contains. As for the orbital part, it will be calculated through the Wigner-Eckart theorem:

$$\langle \gamma' L' M' | R_Q^{(K)} | \gamma L M\rangle = (-1)^{L'-M'}\begin{pmatrix} L' & K & L \\ -M' & Q & M \end{pmatrix}\langle \gamma' L' \| R^{(K)} \| \gamma L\rangle.$$

(1) H_D^1:

$$\begin{aligned} \Delta E_D^1 &= -\frac{3i}{8} Z\alpha^4 \delta_{JJ'}\delta_{M_J M_{J'}}(-1)^{L+S'+J}\begin{Bmatrix} L' & S' & J \\ S & L & 1 \end{Bmatrix} \\ &\times \langle \gamma' L' \| R^{(1)} \| \gamma L\rangle \langle S' \| \vec{\sigma}_1^{(1)} \| S\rangle \end{aligned}$$

with

$$\mathbf{R} = \nabla_1^2 \frac{1}{r_1^3}\vec{r}_1 \times \vec{\nabla}_1.$$

The orbital part is

$$\langle F'\mathcal{Y}^{M'}_{l_1'l_2'L'}|R_0^{(1)}|F\mathcal{Y}^{M}_{l_1l_2L}\rangle = (-1)^{L'-M'}\begin{pmatrix} L' & 1 & L \\ -M' & 0 & M \end{pmatrix} U(1)D,$$

where

$$U(1) = -i\frac{\sqrt{6}}{2}(l_1, l_2, L, l_1', l_2', L')^{1/2},$$

$$\begin{aligned}
D &= \sum_{\Omega}\sum_{i=1}^{5} G_{112}(\Omega)\mathrm{coe}(H_i)I_\Omega(\tilde{a}+a'(i)-1, \tilde{b}, \tilde{c}+c'(i); \tilde{\alpha}, \tilde{\beta}) \\
&+ \sum_{\Omega}\sum_{i=1}^{2} G_{112}(\Omega)\mathrm{coe}(J_i)[\frac{\Omega+1}{2\Omega+1}I_{\Omega+1}(\tilde{a}+a(i)-1, \tilde{b}+1, \tilde{c}-2; \tilde{\alpha}, \tilde{\beta}) \\
&+ \frac{\Omega}{2\Omega+1}I_{\Omega-1}(\tilde{a}+a(i)-1, \tilde{b}+1, \tilde{c}-2; \tilde{\alpha}, \tilde{\beta})] \\
&+ \sum_{\Omega}\sum_{i=1}^{5} G_{12}(\Omega)\mathrm{coe}(H_i)cI_\Omega(\tilde{a}+a'(i), \tilde{b}+1, \tilde{c}+c'(i)-2; \tilde{\alpha}, \tilde{\beta}) \\
&+ \sum_{\Omega}\sum_{i=1}^{2} G_{12}(\Omega)\mathrm{coe}(J_i)c[\frac{\Omega+1}{2\Omega+1}I_{\Omega+1}(\tilde{a}+a(i), \tilde{b}+2, \tilde{c}-4; \tilde{\alpha}, \tilde{\beta}) \\
&+ \frac{\Omega}{2\Omega+1}I_{\Omega-1}(\tilde{a}+a(i), \tilde{b}+2, \tilde{c}-4; \tilde{\alpha}, \tilde{\beta})] \\
&+ \sum_{\Omega} G_{212}(\Omega)c'I_\Omega(\tilde{a}-4, \tilde{b}+1, \tilde{c}-2; \tilde{\alpha}, \tilde{\beta}) \\
&+ \sum_{\Omega} G_{221}(\Omega)cc'I_\Omega(\tilde{a}-3, \tilde{b}+2, \tilde{c}-4; \tilde{\alpha}, \tilde{\beta}).
\end{aligned}$$

Also,

$\mathrm{coe}(H_i)$	$a'(i)$	$c'(i)$
$(a'-l_1')(a'+1+l_1')$	-4	0
$-2\alpha'(a'+1)$	-3	0
α'^2	-2	0
$c'(2a'+c'+1)$	-2	-2
$-2\alpha'c'$	-1	-2

$\mathrm{coe}(J_i)$	$a(i)$
$-2a'c'$	-3
$2\alpha'c'$	-2

The angular coefficients are:

$$G_{112}(\Omega) = \sum_{T\Gamma}(T, \Gamma, \Omega)G(T_{11}, 0)\tilde{G}(T_{11})b(l_1; T)$$

$$
\begin{aligned}
G_{12}(\Omega) &= \sum_{T\Gamma}(T,\Gamma,\Omega)G(T_{12},0)\tilde{G}(T_{12}) \\
G_{212}(\Omega) &= \sum_{N'H'T\Gamma}(N',H',T,\Gamma,\Omega)G(T_{21},0)\tilde{G}(T_{21})2b(l_1';N')b(l_1;T) \\
G_{221}(\Omega) &= \sum_{N'H'T\Gamma}(N',H',T,\Gamma,\Omega)G(T_{22},0)\tilde{G}(T_{22})2b(l_1';N')
\end{aligned}
$$

with

$$
\begin{aligned}
G(T_{11},0) &= \begin{pmatrix} 1 & l_1 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & T & \Gamma \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_1' & \Gamma & \Omega \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & l_2 & \Omega \\ 0 & 0 & 0 \end{pmatrix} \\
\tilde{G}(T_{11}) &= (-1)^{1+l_1+l_2'+L+L'}\begin{Bmatrix} L & l_1 & l_2 \\ \Gamma & L' & 1 \end{Bmatrix}\begin{Bmatrix} L' & l_1' & l_2' \\ \Omega & l_2 & \Gamma \end{Bmatrix}\begin{Bmatrix} 1 & 1 & 1 \\ l_1 & \Gamma & T \end{Bmatrix} \\
G(T_{12},0) &= \begin{pmatrix} 1 & l_1 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2 & 1 & \Gamma \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_1' & T & \Omega \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & \Gamma & \Omega \\ 0 & 0 & 0 \end{pmatrix} \\
\tilde{G}(T_{12}) &= (-1)^{l_1+l_2'+L'}\begin{Bmatrix} L' & l_1' & l_2' \\ \Omega & \Gamma & T \end{Bmatrix}\begin{Bmatrix} L & l_1 & l_2 \\ 1 & 1 & 1 \\ L' & T & \Gamma \end{Bmatrix} \\
G(T_{21},0) &= \begin{pmatrix} l_1' & 1 & N' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & 1 & H' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_1 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & T & \Gamma \\ 0 & 0 & 0 \end{pmatrix} \\
&\times \begin{pmatrix} N' & \Gamma & \Omega \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} H' & l_2 & \Omega \\ 0 & 0 & 0 \end{pmatrix} \\
\tilde{G}(T_{21}) &= (-1)^{L+l_1+l_2'}\begin{Bmatrix} L & l_1 & l_2 \\ \Gamma & L' & 1 \end{Bmatrix}\begin{Bmatrix} L' & l_1' & l_2' \\ 1 & H' & N' \end{Bmatrix} \\
&\times \begin{Bmatrix} 1 & 1 & 1 \\ l_1 & \Gamma & T \end{Bmatrix}\begin{Bmatrix} L' & \Gamma & l_2 \\ \Omega & H' & N' \end{Bmatrix} \\
G(T_{22},0) &= \begin{pmatrix} l_1' & 1 & N' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & 1 & H' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_1 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2 & 1 & \Gamma \\ 0 & 0 & 0 \end{pmatrix} \\
&\times \begin{pmatrix} N' & T & \Omega \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} H' & \Gamma & \Omega \\ 0 & 0 & 0 \end{pmatrix} \\
\tilde{G}(T_{22}) &= (-1)^{1+l_1+l_2'}\begin{Bmatrix} L & l_1 & l_2 \\ 1 & 1 & 1 \\ L' & T & \Gamma \end{Bmatrix}\begin{Bmatrix} L' & l_1' & l_2' \\ 1 & H' & N' \end{Bmatrix}\begin{Bmatrix} \Gamma & T & L' \\ N' & H' & \Omega \end{Bmatrix}.
\end{aligned}
$$

H_D^1 is the only operator which has no singularity.

(2) H_D^2:

$$
\begin{aligned}
\Delta E_D^2 &= iZ\alpha^4\delta_{JJ'}\delta_{M_JM_{J'}}(-1)^{L+S'+J}\begin{Bmatrix} L' & S' & J \\ S & L & 1 \end{Bmatrix} \\
&\times \langle\gamma'L'\|R^{(1)}\|\gamma L\rangle\langle S'\|\vec{\sigma}_i^{(1)}\|S\rangle
\end{aligned}
$$

with

$$
\mathbf{R} = -\frac{1}{r^3r_1^3}(\vec{r}_1\times\vec{r}_2)(\vec{r}\cdot\vec{\nabla}_2).
$$

The orbital part is

$$\langle F'\mathcal{Y}^{M'}_{l_1'l_2'L'}|R_0^{(1)}|F\mathcal{Y}^{M}_{l_1l_2L}\rangle = (-1)^{L'-M'}\begin{pmatrix} L' & 1 & L \\ -M' & 0 & M \end{pmatrix} U(2)D,$$

where

$$U(2) = i\frac{\sqrt{6}}{2}(l_1, l_2, L, l_1', l_2', L')^{1/2}$$

$$\begin{aligned}
D &= \varpi_1(\mu_{11}, M_{11}; bG_{111} + G_{112}; \tilde{a}-1, \tilde{b}, \tilde{c}-3; \tilde{\alpha}, \tilde{\beta}) \\
&- \beta\varpi_1(\mu_{11}, M_{11}; G_{111}; \tilde{a}-1, \tilde{b}+1, \tilde{c}-3; \tilde{\alpha}, \tilde{\beta}) \\
&+ c\varpi_1(\mu_{11}, M_{11}; G_{111}; \tilde{a}-1, \tilde{b}+2, \tilde{c}-5; \tilde{\alpha}, \tilde{\beta}) \\
&+ c\varpi_1(\mu_{12}, M_{12}; G_{12}; \tilde{a}, \tilde{b}+1, \tilde{c}-5; \tilde{\alpha}, \tilde{\beta}) \\
&+ \varpi_1(\mu_{21}, M_{21}; bG_{211} + G_{212}; \tilde{a}-2, \tilde{b}+1, \tilde{c}-3; \tilde{\alpha}, \tilde{\beta}) \\
&- \beta\varpi_1(\mu_{21}, M_{21}; G_{211}; \tilde{a}-2, \tilde{b}+2, \tilde{c}-3; \tilde{\alpha}, \tilde{\beta}) \\
&+ c\varpi_1(\mu_{21}, M_{21}; G_{211}; \tilde{a}-2, \tilde{b}+3, \tilde{c}-5; \tilde{\alpha}, \tilde{\beta}) \\
&+ c\varpi_1(\mu_{22}, M_{22}; G_{22}; \tilde{a}-1, \tilde{b}+2, \tilde{c}-5; \tilde{\alpha}, \tilde{\beta}).
\end{aligned}$$

Also,

$$\begin{aligned}
M_{11} &= \min(l_1 + l_1' + 2, l_2 + l_2' + 2) \\
M_{12} &= \min(l_1 + l_1' + 3, l_2 + l_2' + 1) \\
M_{21} &= \min(l_1 + l_1' + 1, l_2 + l_2' + 3) \\
M_{22} &= \min(l_1 + l_1' + 2, l_2 + l_2' + 2) \\
\mu_{ij} &= \omega(M_{ij}) - 2, \quad i, j = 1, 2.
\end{aligned}$$

The angular coefficients are:

$$\begin{aligned}
G_{111}(\Omega) &= \sum_{\Lambda NT\Gamma} (\Lambda, N, T, \Gamma, \Omega) G(T_{11}, 0)\tilde{G}(T_{11}) \\
G_{112}(\Omega) &= \sum_{\Lambda NT\Gamma} (\Lambda, N, T, \Gamma, \Omega) G(T_{11}, 0)\tilde{G}(T_{11}) b(l_2; T) \\
G_{12}(\Omega) &= \sum_{\Lambda NT\Gamma} (\Lambda, N, T, \Gamma, \Omega) G(T_{12}, 0)\tilde{G}(T_{12}) \\
G_{211}(\Omega) &= \sum_{\Lambda NT\Gamma} (\Lambda, N, T, \Gamma, \Omega) G(T_{21}, 0)\tilde{G}(T_{21}) \\
G_{212}(\Omega) &= \sum_{\Lambda NT\Gamma} (\Lambda, N, T, \Gamma, \Omega) G(T_{21}, 0)\tilde{G}(T_{21}) b(l_2; T) \\
G_{22}(\Omega) &= \sum_{\Lambda NT\Gamma} (\Lambda, N, T, \Gamma, \Omega) G(T_{22}, 0)\tilde{G}(T_{22})
\end{aligned}$$

with

$$
\begin{aligned}
G(T_{11},0) &= \begin{pmatrix} 1 & 1 & \Gamma \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} \Gamma & l_1' & \Lambda \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_2' & N \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_2 & T \\ 0 & 0 & 0 \end{pmatrix} \\
&\times \begin{pmatrix} \Lambda & l_1 & \Omega \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} N & T & \Omega \\ 0 & 0 & 0 \end{pmatrix} \\
\tilde{G}(T_{11}) &= (-1)^{1+L'} \sum_{\lambda_1\lambda_2\lambda_3} (-1)^{\lambda_1+\lambda_2+\lambda_3}(\lambda_1,\lambda_2,\lambda_3)\begin{Bmatrix} \lambda_1 & l_1 & \Gamma \\ \Lambda & l_1' & \Omega \end{Bmatrix}\begin{Bmatrix} L & l_1 & l_2 \\ 1 & T & \lambda_2 \end{Bmatrix} \\
&\times \begin{Bmatrix} l_1 & \lambda_1 & \Gamma \\ 1 & 1 & \lambda_2 \end{Bmatrix}\begin{Bmatrix} N & T & \Omega \\ \lambda_2 & \lambda_3 & L \end{Bmatrix}\begin{Bmatrix} \lambda_2 & \lambda_1 & 1 \\ l_1' & \lambda_3 & \Omega \end{Bmatrix}\begin{Bmatrix} L & \lambda_3 & N \\ 1 & 1 & 1 \\ L' & l_1' & l_2' \end{Bmatrix} \\
G(T_{12},0) &= \begin{pmatrix} 1 & 1 & \Gamma \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} \Gamma & l_1' & \Lambda \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_2' & N \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_1 & T \\ 0 & 0 & 0 \end{pmatrix} \\
&\times \begin{pmatrix} \Lambda & T & \Omega \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} N & l_2 & \Omega \\ 0 & 0 & 0 \end{pmatrix} \\
\dot{G}(T_{12}) &= (-1)^{1+l_1'} \sum_{\lambda_1}(2\lambda_1+1)\begin{Bmatrix} l_2 & l_1 & L \\ \lambda_1 & N & \Omega \end{Bmatrix}\begin{Bmatrix} l_1 & T & 1 \\ \Lambda & \lambda_1 & \Omega \end{Bmatrix} \\
&\times \begin{Bmatrix} \lambda_1 & 1 & \Lambda \\ \Gamma & l_1' & 1 \end{Bmatrix}\begin{Bmatrix} L & \lambda_1 & N \\ 1 & 1 & 1 \\ L' & l_1' & l_2' \end{Bmatrix} \\
G(T_{21},0) &= \begin{pmatrix} 1 & 1 & \Gamma \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_1' & 1 & \Lambda \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & \Gamma & N \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_2 & T \\ 0 & 0 & 0 \end{pmatrix} \\
&\times \begin{pmatrix} \Lambda & l_1 & \Omega \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} N & T & \Omega \\ 0 & 0 & 0 \end{pmatrix} \\
\tilde{G}(T_{21}) &= (-1)^{1+L+l_1'} \sum_{\lambda_1\lambda_2}(-1)^{\lambda_1+\lambda_2}(\lambda_1,\lambda_2)\begin{Bmatrix} L & l_1 & l_2 \\ \lambda_1 & \Lambda & 1 \\ N & \Omega & T \end{Bmatrix}\begin{Bmatrix} \lambda_2 & \Gamma & \lambda_1 \\ 1 & \Lambda & 1 \end{Bmatrix} \\
&\times \begin{Bmatrix} 1 & \lambda_2 & l_1' \\ \Lambda & 1 & 1 \end{Bmatrix}\begin{Bmatrix} N & \Gamma & l_2' \\ \lambda_2 & L & \lambda_1 \end{Bmatrix}\begin{Bmatrix} L & \lambda_2 & l_2' \\ l_1' & L' & 1 \end{Bmatrix} \\
G(T_{22},0) &= \begin{pmatrix} 1 & 1 & \Gamma \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_1' & 1 & \Lambda \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & \Gamma & N \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_1 & T \\ 0 & 0 & 0 \end{pmatrix} \\
&\times \begin{pmatrix} \Lambda & T & \Omega \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} N & l_2 & \Omega \\ 0 & 0 & 0 \end{pmatrix} \\
\tilde{G}(T_{22}) &= (-1)^{1+L+l_2'} \sum_{\lambda_1\lambda_2}(-1)^{\lambda_1+\lambda_2}(\lambda_1,\lambda_2)\begin{Bmatrix} l_2 & l_1 & L \\ \lambda_1 & N & \Omega \end{Bmatrix}\begin{Bmatrix} l_1 & T & 1 \\ \Lambda & \lambda_1 & \Omega \end{Bmatrix} \\
&\times \begin{Bmatrix} \Gamma & \lambda_2 & \lambda_1 \\ L & N & l_2' \end{Bmatrix}\begin{Bmatrix} L & \lambda_2 & l_2' \\ l_1' & L' & 1 \end{Bmatrix}\begin{Bmatrix} \lambda_2 & \Gamma & \lambda_1 \\ 1 & \Lambda & 1 \end{Bmatrix}\begin{Bmatrix} 1 & \lambda_2 & l_1' \\ \Lambda & 1 & 1 \end{Bmatrix}.
\end{aligned}
$$

(3) H_D^3:

$$
\Delta E_D^3 = \frac{1}{2} Z\alpha^4 \delta_{JJ'}\delta_{M_J M_{J'}} \sum_K (-1)^{K+L+S'+J}\begin{Bmatrix} L' & S' & J \\ S & L & K \end{Bmatrix}
$$

$$\times \quad \langle \gamma' L' \| R^{(K)} \| \gamma L \rangle \langle S' \| [\vec{\sigma}_1 \otimes \vec{\sigma}_2]^{(K)} \| S \rangle$$

with

$$R^{(K)} = \frac{1}{r^3 r_1^3} [\vec{r} \otimes \vec{r}_1]^{(K)}.$$

The orbital part is

$$\langle F' \mathcal{Y}^{M'}_{l_1' l_2' L'} | R_Q^{(K)} | F \mathcal{Y}^{M}_{l_1 l_2 L} \rangle \;=\; (-1)^{L'-M'} \begin{pmatrix} L' & K & L \\ -M' & Q & M \end{pmatrix} U(3) D,$$

where

$$U(3) = \frac{1}{2} \sqrt{2K+1} (l_1, l_2, L, l_1', l_2', L')^{1/2}$$

$$\begin{aligned} D &= \varpi_1(\mu_1, M_1; G_1; \tilde{a}-1, \tilde{b}, \tilde{c}-3; \tilde{\alpha}, \tilde{\beta}) \\ &+ \varpi_1(\mu_2, M_2; G_2; \tilde{a}-2, \tilde{b}+1, \tilde{c}-3; \tilde{\alpha}, \tilde{\beta}) \\ &+ J_1(\mu_1, M_1; G_1) \mathrm{Dif}(\tilde{a}-1, \tilde{b}; \tilde{a}-2, \tilde{b}+1; \tilde{c}-3, \tilde{\alpha}, \tilde{\beta}; \omega(\mu_1)-2, \omega(\mu_1+1)-2) \end{aligned}$$

Also,

$$\begin{aligned} M_1 &= \min(l_1 + l_1' + 2, l_2 + l_2') \\ M_2 &= \min(l_1 + l_1' + 1, l_2 + l_2' + 1) \\ \mu_i &= \omega(M_i) - 2, \quad i = 1, 2 \end{aligned}$$

The angular coefficients are:

$$\begin{aligned} G_1(E) &= \sum_N (N, E) G(T_1, 0) \tilde{G}(T_1) \\ G_2(E) &= \sum_{HN} (H, N, E) G(T_2, 0) \tilde{G}(T_2) \end{aligned}$$

with

$$\begin{aligned} G(T_1, 0) &= \begin{pmatrix} 1 & 1 & K \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} K & l_1 & N \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1' & N & E \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2' & l_2 & E \\ 0 & 0 & 0 \end{pmatrix} \\ \tilde{G}(T_1) &= (-1)^{L+L'+l_2'} \begin{Bmatrix} L & l_1 & l_2 \\ N & L' & K \end{Bmatrix} \begin{Bmatrix} L' & l_1' & l_2' \\ E & l_2 & N \end{Bmatrix} \\ G(T_2, 0) &= \begin{pmatrix} 1 & l_1 & H \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & l_2 & N \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1' & H & E \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2' & N & E \\ 0 & 0 & 0 \end{pmatrix} \\ \tilde{G}(T_2) &= (-1)^{L'+l_1+l_2'} \begin{Bmatrix} L' & l_1' & l_2' \\ E & N & H \end{Bmatrix} \begin{Bmatrix} L & l_1 & l_2 \\ K & 1 & 1 \\ L' & H & N \end{Bmatrix}. \end{aligned}$$

(4) H_D^4:

$$\begin{aligned}\Delta E_D^4 &= -\frac{1}{2} i\alpha^4 \delta_{JJ'}\delta_{M_J M_{J'}}(-1)^{L+S'+J}\begin{Bmatrix} L' & S' & J \\ S & L & 1 \end{Bmatrix} \\ &\times \langle\gamma' L'\|R^{(1)}\|\gamma L\rangle\langle S'\|\vec{\sigma}_1\|S\rangle\end{aligned}$$

with

$$\mathbf{R} = \frac{1}{r^4}(\vec{r}\times\vec{\nabla}_2).$$

The orbital part is

$$\langle F'\mathcal{Y}^{M'}_{l_1'l_2'L'}|R_0^{(1)}|F\mathcal{Y}^{M}_{l_1 l_2 L}\rangle = (-1)^{L'-M'}\begin{pmatrix} L' & 1 & L \\ -M' & 0 & M \end{pmatrix} U(4)D,$$

where

$$U(4) = i\frac{\sqrt{6}}{2}(l_1, l_2, L, l_1', l_2', L')^{1/2}$$

$$\begin{aligned}D &= \varpi_1(\mu_1, M_1; bG_{11} + G_{12}; \tilde{a}+1, \tilde{b}-1, \tilde{c}-4; \tilde{\alpha}, \tilde{\beta}) \\ &- \beta\varpi_1(\mu_1, M_1; G_{11}; \tilde{a}+1, \tilde{b}, \tilde{c}-4; \tilde{\alpha}, \tilde{\beta}) \\ &+ \varpi_1(\mu_3, M_3; G_{32}; \tilde{a}, \tilde{b}, \tilde{c}-4; \tilde{\alpha}, \tilde{\beta}) \\ &+ J_1(\mu_1, M_1; G_{12})\mathrm{Dif}(\tilde{a}+1, \tilde{b}-1; \tilde{a}, \tilde{b}; \tilde{c}-4, \tilde{\alpha}, \tilde{\beta}; \omega(\mu_1)-2, \omega(\mu_1+1)-2).\end{aligned}$$

Also,

$$\begin{aligned}M_1 &= \min(l_1 + l_1' + 1, l_2 + l_2' + 1) \\ M_3 &= \min(l_1 + l_1', l_2 + l_2' + 2) \\ \mu_i &= \omega(M_i) - 2, \quad i = 1, 3.\end{aligned}$$

The angular coefficients are:

$$\begin{aligned}G_{11}(\Omega) &= \sum_{TH}(T, H, \Omega)G(T_1, 0)\tilde{G}(T_1) \\ G_{12}(\Omega) &= \sum_{TH}(T, H, \Omega)G(T_1, 0)\tilde{G}(T_1)b(l_2; T) \\ G_{32}(\Omega) &= \sum_{TH}(T, H, \Omega)G(T_3, 0)\tilde{G}(T_3)b(l_2; T)\end{aligned}$$

with

$$\begin{aligned}
G(T_1,0) &= \begin{pmatrix} 1 & l_1 & H \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_2 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_1' & H & \Omega \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & T & \Omega \\ 0 & 0 & 0 \end{pmatrix} \\
\tilde{G}(T_1) &= (-1)^{l_1+l_2'+L'}\begin{Bmatrix} L & l_1 & l_2 \\ 1 & 1 & 1 \\ L' & H & T \end{Bmatrix}\begin{Bmatrix} L' & H & T \\ \Omega & l_2' & l_1' \end{Bmatrix} \\
G(T_3,0) &= \begin{pmatrix} 1 & l_2 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & T & H \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_1' & l_1 & \Omega \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & H & \Omega \\ 0 & 0 & 0 \end{pmatrix} \\
\tilde{G}(T_3) &= (-1)^{1+l_1'+l_2}\begin{Bmatrix} L & l_2 & l_1 \\ H & L' & 1 \end{Bmatrix}\begin{Bmatrix} l_2 & 1 & T \\ 1 & H & 1 \end{Bmatrix}\begin{Bmatrix} L' & l_1 & H \\ \Omega & l_2' & l_1' \end{Bmatrix}.
\end{aligned}$$

(5) H_D^5:

$$\begin{aligned}
\Delta E_D^5 &= -\frac{1}{2}\alpha^4\delta_{JJ'}\delta_{M_JM_{J'}}\sum_K(-1)^{K+L+S'+J}\begin{Bmatrix} L' & S' & J \\ S & L & K \end{Bmatrix} \\
&\times \langle\gamma'L'\|R^{(K)}\|\gamma L\rangle\langle S'\|[\vec{\sigma}_1\otimes\vec{\sigma}_2]^{(K)}\|S\rangle
\end{aligned}$$

with

$$R^{(K)} = \frac{1}{r^6}[\vec{r}\otimes\vec{r}]^{(K)}.$$

The orbital part is

$$\langle F'\mathcal{Y}^{M'}_{l_1'l_2'L'}|R_Q^{(K)}|F\mathcal{Y}^{M}_{l_1l_2L}\rangle = (-1)^{L'-M'}\begin{pmatrix} L' & K & L \\ -M' & Q & M \end{pmatrix}U(5)D,$$

where

$$U(5) = \frac{1}{2}\sqrt{2K+1}(l_1,l_2,L,l_1',l_2',L')^{1/2}$$

$$\begin{aligned}
D &= \varpi_0(\mu_1,M_1;G_1;\tilde{a}+2,\tilde{b},-2;\tilde{\alpha},\tilde{\beta}) \\
&+ \varpi_0(\mu_2,M_2;G_2;\tilde{a},\tilde{b}+2,-2;\tilde{\alpha},\tilde{\beta}) \\
&+ \varpi_0(\mu_3,M_3;G_3;\tilde{a}+1,\tilde{b}+1,-2;\tilde{\alpha},\tilde{\beta}), \quad \tilde{c}=4
\end{aligned}$$

$$\begin{aligned}
D &= \varpi_1(\mu_1,M_1;G_1;\tilde{a}+2,\tilde{b},-4;\tilde{\alpha},\tilde{\beta}) \\
&+ \varpi_1(\mu_2,M_2;G_2;\tilde{a},\tilde{b}+2,-4;\tilde{\alpha},\tilde{\beta}) \\
&+ \varpi_1(\mu_3,M_3;G_3;\tilde{a}+1,\tilde{b}+1,-4;\tilde{\alpha},\tilde{\beta}) \\
&+ J_1(\mu_1,M_1;G_1)\eta(\mu_1,1)I_{\omega(\mu_1)-2}(\tilde{a},\tilde{b},-2;\tilde{\alpha},\tilde{\beta}), \quad \tilde{c}=2
\end{aligned}$$

$$
\begin{aligned}
D &= \varpi_2(\mu_1, M_1; G_1; \tilde{a}+2, \tilde{b}, \tilde{c}-6; \tilde{\alpha}, \tilde{\beta}) \\
&+ \varpi_2(\mu_2, M_2; G_2; \tilde{a}, \tilde{b}+2, \tilde{c}-6; \tilde{\alpha}, \tilde{\beta}) \\
&+ \varpi_2(\mu_3, M_3; G_3; \tilde{a}+1, \tilde{b}+1, \tilde{c}-6; \tilde{\alpha}, \tilde{\beta}) \\
&+ \gamma_1 \mathrm{Dif}(\tilde{a}+1, \tilde{b}-1; \tilde{a}, \tilde{b}; \tilde{c}-4, \tilde{\alpha}, \tilde{\beta}; \omega(\mu_1+1)-2, \omega(\mu_1)-2) \\
&+ \gamma_2 \mathrm{Dif}(\tilde{a}-1, \tilde{b}+1; \tilde{a}, \tilde{b}; \tilde{c}-4, \tilde{\alpha}, \tilde{\beta}; \omega(\mu_1+1)-2, \omega(\mu_1)-2) \\
&+ [\tilde{\gamma}(l_1', l_2', l_1, l_2)\mathrm{Can}(\tilde{a}, \tilde{b}, \tilde{\alpha}, \tilde{\beta}; \tilde{a}', \tilde{b}', \tilde{\alpha}', \tilde{\beta}'; \tilde{c}-4; \omega(\mu_1)-2, \omega(\mu_1+L)-2) \\
&+ (\tilde{\gamma}(l_1', l_2', l_1, l_2) - \tilde{\gamma}(l_2', l_1', l_1, l_2)) I_{\omega(\mu_1+L)-2}(\tilde{a}', \tilde{b}', \tilde{c}-1; \tilde{\alpha}', \tilde{\beta}')] \\
&\times \delta(X_R, 1)\delta(X_L, 1), \quad \tilde{c} \neq 2, 4,
\end{aligned}
$$

where '$X_R = 1$' means the direct part of the wave function on the right hand side of the matrix element, '$X_L = 1$' the direct part of the wave function on the left hand side. We can prove that the coefficient (which will be defined below) of the last term equals to zero at least when $\tilde{c} = 0, 1$:

$$
\tilde{\gamma}(l_1', l_2', l_1, l_2) - \tilde{\gamma}(l_2', l_1', l_1, l_2) = 0, \quad \tilde{c} = 0, 1.
$$

Hence, there is no residual divergence. Also,

$$
\begin{aligned}
M_1 &= \min(l_1 + l_1' + 2, l_2 + l_2') \\
M_2 &= \min(l_1 + l_1', l_2 + l_2' + 2) \\
M_3 &= \min(l_1 + l_1' + i, l_2 + l_2' + 1) \\
\mu_i &= \omega(M_i) - 2, \quad i = 1, 2, 3
\end{aligned}
$$

The angular coefficients are:

$$
\begin{aligned}
G_1(E) &= \sum_N (N, E) G(T_1, 0)\tilde{G}(T_1) \\
G_2(E) &= \sum_N (N, E) G(T_2, 0)\tilde{G}(T_2) \\
G_3(E) &= 2\sum_{HN} (H, N, E) G(T_3, 0)\tilde{G}(T_3)
\end{aligned}
$$

with

$$
G(T_1, 0) = \begin{pmatrix} 1 & 1 & K \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} K & l_1 & N \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_1' & N & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & l_2 & E \\ 0 & 0 & 0 \end{pmatrix}
$$

$$\tilde{G}(T_1) = (-1)^{L+L'+l_2'}\begin{Bmatrix} L & l_1 & l_2 \\ N & L' & K \end{Bmatrix}\begin{Bmatrix} L' & l_1' & l_2' \\ E & l_2 & N \end{Bmatrix}$$

$$G(T_2,0) = \begin{pmatrix} 1 & 1 & K \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} K & l_2 & N \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_1' & l_1 & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & N & E \\ 0 & 0 & 0 \end{pmatrix}$$

$$\tilde{G}(T_2) = (-1)^{l_1'}\begin{Bmatrix} L & l_1 & l_2 \\ N & K & L' \end{Bmatrix}\begin{Bmatrix} L' & l_1' & l_2' \\ E & N & l_1 \end{Bmatrix}$$

$$G(T_3,0) = \begin{pmatrix} 1 & l_1 & H \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_2 & N \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_1' & H & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & N & E \\ 0 & 0 & 0 \end{pmatrix}$$

$$\tilde{G}(T_3) = (-1)^{L'+l_1+l_2'}\begin{Bmatrix} L' & l_1' & l_2' \\ E & N & H \end{Bmatrix}\begin{Bmatrix} L & l_1 & l_2 \\ K & 1 & 1 \\ L' & H & N \end{Bmatrix}.$$

We have also defined:

$$\begin{aligned} \gamma_1(l_1', l_2', l_1, l_2; \tilde{c}-4) &= J_2(\mu_1, M_1; G_1; \tilde{c}-6) \\ \gamma_2(l_1', l_2', l_1, l_2; \tilde{c}-4) &= J_2(\mu_2, M_2; G_2; \tilde{c}-6) \\ \gamma_3(l_1', l_2', l_1, l_2; \tilde{c}-4) &= J_2(\mu_3, M_3; G_3; \tilde{c}-6) \\ &+ J_2(\mu_1, M_1; G_1)\eta(\mu_1, \tilde{c}-1) \end{aligned}$$

$$\begin{aligned} \gamma(l_1', l_2', l_1, l_2; \tilde{c}-4) &= \gamma_1(l_1', l_2', l_1, l_2; \tilde{c}-4) \\ &+ \gamma_2(l_1', l_2', l_1, l_2; \tilde{c}-4) \\ &+ \gamma_3(l_1', l_2', l_1, l_2; \tilde{c}-4) \end{aligned}$$

$$\begin{aligned} \tilde{\gamma}(l_1', l_2', l_1, l_2; \tilde{c}-4) &= \gamma(l_1', l_2', l_1, l_2; \tilde{c}-4) \\ &+ \gamma(l_2', l_1', l_2, l_1; \tilde{c}-4) \end{aligned}$$

(6) H_D^6:

$$\begin{aligned} \Delta E_D^6 &= -\frac{1}{4} i\alpha^4 \delta_{JJ'}\delta_{M_J M_{J'}}(-1)^{L+S'+J}\begin{Bmatrix} L' & S' & J \\ S & L & 1 \end{Bmatrix} \\ &\times \langle \gamma' L' \| R^{(1)} \| \gamma L\rangle\langle S' \| \vec{\sigma}_1 \| S\rangle \end{aligned}$$

with

$$\mathbf{R} = \nabla_1^2 \frac{1}{r}(\vec{\nabla}_1 \times \vec{\nabla}_2).$$

The orbital part is

$$\langle F'\mathcal{Y}^{M'}_{l_1' l_2' L'} | R_0^{(1)} | F\mathcal{Y}^{M}_{l_1 l_2 L}\rangle = (-1)^{L'-M'}\begin{pmatrix} L' & 1 & L \\ -M' & 0 & M \end{pmatrix} U(6)D,$$

where

$$U(6) = -i\frac{\sqrt{6}}{2}(l_1, l_2, L, l_1', l_2', L')^{1/2}$$

$$\begin{aligned}
D &= \sum_{i=1}^{7}\sum_{j=1}^{8} O_{ij}^{(1)} \varpi_1(\mu_{11}, M_{11}; G_{111}; \tilde{a} + a_{ij}^{(1)}, \tilde{b} + b_{ij}^{(1)}, \tilde{c} + c_{ij}^{(1)}; \tilde{\alpha}, \tilde{\beta}) \\
&+ \sum_{i=1}^{7} \mathrm{coe}(S_i) \varpi_0(\mu_{11}, M_{11}; bG_{112} + aG_{113} + G_{114}; \\
&\quad \tilde{a} + a'(i) - 1, \tilde{b} + b'(i) - 1, \tilde{c} + c'(i); \tilde{\alpha}, \tilde{\beta}) \\
&- \beta \sum_{i=1}^{7} \mathrm{coe}(S_i) \varpi_0(\mu_{11}, M_{11}; G_{112}; \tilde{a} + a'(i) - 1, \tilde{b} + b'(i), \tilde{c} + c'(i); \tilde{\alpha}, \tilde{\beta}) \\
&- \alpha \sum_{i=1}^{7} \mathrm{coe}(S_i) \varpi_0(\mu_{11}, M_{11}; G_{113}; \tilde{a} + a'(i), \tilde{b} + b'(i) - 1, \tilde{c} + c'(i); \tilde{\alpha}, \tilde{\beta}) \\
&+ 2c' \sum_{i=1}^{8} \mathrm{coe}(Q_i) \varpi_1(\mu_{21}, M_{21}, G_{211}; \tilde{a} + a(i) - 1, \tilde{b} + b(i) + 1, \tilde{c} + c(i) - 3; \tilde{\alpha}, \tilde{\beta}) \\
&+ \varpi_0(\mu_{21}, M_{21}; 2bc'G_{212} + 2ac'G_{213} + 2c'G_{214}; \tilde{a} - 2, \tilde{b}, \tilde{c} - 3; \tilde{\alpha}, \tilde{\beta}) \\
&- 2\beta c' \varpi_0(\mu_{21}, M_{21}; G_{212}; \tilde{a} - 2, \tilde{b} + 1, \tilde{c} - 3; \tilde{\alpha}, \tilde{\beta}) \\
&- 2\alpha c' \varpi_0(\mu_{21}, M_{21}; G_{213}; \tilde{a} - 1, \tilde{b}, \tilde{c} - 3; \tilde{\alpha}, \tilde{\beta}) \\
&+ \Delta_1 + \Delta_2
\end{aligned}$$

$$\begin{aligned}
\Delta_1 &= \sum_{i=1}^{7} \mathrm{coe}(S_i) c \\
&\times [\varpi_1(\mu_{11}, M_{11}; G_{112}; \tilde{a} + a'(i) - 1, \tilde{b} + b'(i) + 1, \tilde{c} + c'(i) - 2; \tilde{\alpha}, \tilde{\beta}) \\
&+ \varpi_1(\mu_{11}, M_{11}; G_{113}; \tilde{a} + a'(i) + 1, \tilde{b} + b'(i) - 1, \tilde{c} + c'(i) - 2; \tilde{\alpha}, \tilde{\beta}) \\
&+ \varpi_1(\min(\mu_{12}, \mu_{13}), \max(M_{12}, M_{13}); G_{12} + G_{13}; \\
&\quad \tilde{a} + a'(i), \tilde{b} + b'(i), \tilde{c} + c'(i) - 2; \tilde{\alpha}, \tilde{\beta}) \\
&+ J_1(\mu_{11}, M_{11}; G_{112}) \mathrm{Dif}(\tilde{a} + a'(i) - 1, \tilde{b} + b'(i) + 1; \tilde{a} + a'(i), \tilde{b} + b'(i); \\
&\quad \tilde{c} + c'(i) - 2, \tilde{\alpha}, \tilde{\beta}; \omega(\mu_{11}) - 2, \omega(\mu_{11} + 1) - 2) \\
&+ J_1(\mu_{11}, M_{11}; G_{113}) \mathrm{Dif}(\tilde{a} + a'(i) + 1, \tilde{b} + b'(i) - 1; \tilde{a} + a'(i), \tilde{b} + b'(i); \\
&\quad \tilde{c} + c'(i) - 2, \tilde{\alpha}, \tilde{\beta}; \omega(\mu_{11}) - 2, \omega(\mu_{11} + 1) - 2)]
\end{aligned}$$

$$\Delta_2 = 2cc'[\varpi_1(\mu_{21}, M_{21}; G_{212}; \tilde{a} - 2, \tilde{b} + 2, \tilde{c} - 5; \tilde{\alpha}, \tilde{\beta})$$

$$
\begin{aligned}
&+ \quad \varpi_1(\mu_{21}, M_{21}; G_{213}; \tilde{a}, \tilde{b}, \tilde{c} - 5; \tilde{\alpha}, \tilde{\beta}) \\
&+ \quad \varpi_1(\min(\mu_{22}, \mu_{23}), \max(M_{22}, M_{23}); G_{22} + G_{23}; \tilde{a} - 1, \tilde{b} + 1, \tilde{c} - 5; \tilde{\alpha}, \tilde{\beta}) \\
&+ \quad J_1(\mu_{21}, M_{21}; G_{212})\mathrm{Dif}(\tilde{a} - 2, \tilde{b} + 2; \tilde{a} - 1, \tilde{b} + 1; \\
&\qquad \tilde{c} - 5, \tilde{\alpha}, \tilde{\beta}; \omega(\mu_{11} + 1) - 2, \omega(\mu_{11}) - 2) \\
&+ \quad J_1(\mu_{21}, M_{21}; G_{213})\mathrm{Dif}(\tilde{a}, \tilde{b}; \tilde{a} - 1, \tilde{b} + 1; \\
&\qquad \tilde{c} - 5, \tilde{\alpha}, \tilde{\beta}; \omega(\mu_{11} + 1) - 2, \omega(\mu_{11}) - 2)].
\end{aligned}
$$

Also,

$\mathrm{coe}(Q_i)$	$a(i)$	$b(i)$	$c(i)$
ab	-1	-1	0
$-a\beta$	-1	0	0
$-b\alpha$	0	-1	0
$\alpha\beta$	0	0	0
ca	-1	1	-2
$-c\alpha$	0	1	-2
$-c\beta$	1	0	-2
cb	1	-1	-2

$\mathrm{coe}(S_i)$	$a'(i)$	$b'(i)$	$c'(i)$
$a'(a'+1+c') - l_1{}'(l_1{}'+1)$	-2	0	-1
$-\alpha'[2(a'+1)+c']$	-1	0	-1
α'^2	0	0	-1
$c'(c'+1+a')$	0	0	-3
$-a'c'$	-2	2	-3
$-\alpha'c'$	1	0	-3
$\alpha'c'$	-1	2	-3

$$
\begin{aligned}
O_{ij}^{(1)} &= \mathrm{coe}(S_i) \cdot \mathrm{coe}(Q_j) \\
a_{ij}^{(1)} &= a'(i) + a(j) \\
b_{ij}^{(1)} &= b'(i) + b(j) \\
c_{ij}^{(1)} &= c'(i) + c(j)
\end{aligned}
$$

$$
\begin{aligned}
M_{11} &= \min(l_1 + l_1{}' + 1, l_2 + l_2{}' + 1) \\
M_{12} &= \min(l_1 + l_1{}' + 2, l_2 + l_2{}') \\
M_{13} &= \min(l_1 + l_1{}', l_2 + l_2{}' + 2)
\end{aligned}
$$

$$
\begin{aligned}
M_{21} &= \min(l_1 + l_1{}' + 2, l_2 + l_2{}' + 2) \\
M_{22} &= \min(l_1 + l_1{}' + 3, l_2 + l_2{}' + 1) \\
M_{23} &= \min(l_1 + l_1{}' + 1, l_2 + l_2{}' + 3) \\
\mu_{ij} &= \omega(M_{ij}) - 2, \quad i = 1,2, \quad j = 1,2,3.
\end{aligned}
$$

The angular coefficients are:

$$
\begin{aligned}
G_{111}(\Omega) &= \sum_{T\Lambda}(T,\Lambda,\Omega)G(T_{11},0)\tilde{G}(T_{11}) \\
G_{112}(\Omega) &= \sum_{T\Lambda}(T,\Lambda,\Omega)G(T_{11},0)\tilde{G}(T_{11})b(l_1;T) \\
G_{113}(\Omega) &= \sum_{T\Lambda}(T,\Lambda,\Omega)G(T_{11},0)\tilde{G}(T_{11})b(l_2;\Lambda) \\
G_{114}(\Omega) &= \sum_{T\Lambda}(T,\Lambda,\Omega)G(T_{11},0)\tilde{G}(T_{11})b(l_1;T)b(l_2;\Lambda) \\
G_{12}(\Omega) &= \sum_{T\Lambda}(T,\Lambda,\Omega)G(T_{12},0)\tilde{G}(T_{12})b(l_1;T) \\
G_{13}(\Omega) &= \sum_{T\Lambda}(T,\Lambda,\Omega)G(T_{13},0)\tilde{G}(T_{13})b(T;\Lambda) \\
G_{211}(\Omega) &= \sum_{N'H'T\Lambda}(N',H',T,\Lambda,\Omega)G(T_{21},0)\tilde{G}(T_{21})b(l_1{}';N') \\
G_{212}(\Omega) &= \sum_{N'H'T\Lambda}(N',H',T,\Lambda,\Omega)G(T_{21},0)\tilde{G}(T_{21})b(l_1{}';N')b(l_1;T) \\
G_{213}(\Omega) &= \sum_{N'H'T\Lambda}(N',H',T,\Lambda,\Omega)G(T_{21},0)\tilde{G}(T_{21})b(l_1{}';N')b(l_2;\Lambda) \\
G_{214}(\Omega) &= \sum_{N'H'T\Lambda}(N',H',T,\Lambda,\Omega)G(T_{21},0)\tilde{G}(T_{21})b(l_1{}';N')b(l_1;T)b(l_2;\Lambda) \\
G_{22}(\Omega) &= \sum_{N'H'T\Lambda}(N',H',T,\Lambda,\Omega)G(T_{22},0)\tilde{G}(T_{22})b(l_1{}';N')b(l_1;T) \\
G_{23}(\Omega) &= \sum_{N'H'T\Lambda}(N',H',T,\Lambda,\Omega)G(T_{23},0)\tilde{G}(T_{23})b(l_1{}';N')b(T;\Lambda)
\end{aligned}
$$

with

$$
\begin{aligned}
G(T_{11},0) &= \begin{pmatrix} 1 & l_1 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_2 & \Lambda \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_1' & T & \Omega \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & \Lambda & \Omega \\ 0 & 0 & 0 \end{pmatrix} \\
\tilde{G}(T_{11}) &= (-1)^{1+l_1+l_2'+L'}\begin{Bmatrix} L' & T & \Lambda \\ \Omega & l_2' & l_1' \end{Bmatrix}\begin{Bmatrix} L & l_1 & l_2 \\ 1 & 1 & 1 \\ L' & T & \Lambda \end{Bmatrix} \\
G(T_{12},0) &= \begin{pmatrix} 1 & l_1 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & T & \Lambda \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_1' & \Lambda & \Omega \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & l_2 & \Omega \\ 0 & 0 & 0 \end{pmatrix} \\
\tilde{G}(T_{12}) &= (-1)^{1+l_1+l_2'+L+L'}\begin{Bmatrix} 1 & 1 & 1 \\ l_1 & \Lambda & T \end{Bmatrix}\begin{Bmatrix} L & l_1 & l_2 \\ \Lambda & L' & 1 \end{Bmatrix}\begin{Bmatrix} L' & l_1' & l_2' \\ \Omega & l_2 & \Lambda \end{Bmatrix}
\end{aligned}
$$

$$G(T_{13},0) = \begin{pmatrix} 1 & l_2 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & T & \Lambda \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_1' & l_1 & \Omega \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & \Lambda & \Omega \\ 0 & 0 & 0 \end{pmatrix}$$

$$\bar{G}(T_{13}) = (-1)^{1+l_1'+l_2}\begin{Bmatrix} L' & 1 & L \\ l_2 & l_1 & \Lambda \end{Bmatrix}\begin{Bmatrix} 1 & 1 & 1 \\ T & l_2 & \Lambda \end{Bmatrix}\begin{Bmatrix} L' & l_1 & \Lambda \\ \Omega & l_2' & l_1' \end{Bmatrix}$$

$$G(T_{21},0) = \begin{pmatrix} l_1' & 1 & N' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & 1 & H' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_1 & T \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times \begin{pmatrix} 1 & l_2 & \Lambda \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} N' & T & \Omega \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} H' & \Lambda & \Omega \\ 0 & 0 & 0 \end{pmatrix}$$

$$\bar{G}(T_{21}) = (-1)^{l_1+l_2'}\begin{Bmatrix} L' & T & \Lambda \\ \Omega & H' & N' \end{Bmatrix}\begin{Bmatrix} L' & l_1' & l_2' \\ 1 & H' & N' \end{Bmatrix}\begin{Bmatrix} L & l_1 & l_2 \\ 1 & 1 & 1 \\ L' & T & \Lambda \end{Bmatrix}$$

$$G(T_{22},0) = \begin{pmatrix} l_1' & 1 & N' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & 1 & H' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_1 & T \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times \begin{pmatrix} 1 & T & \Lambda \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} N' & \Lambda & \Omega \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} H' & l_2 & \Omega \\ 0 & 0 & 0 \end{pmatrix}$$

$$\bar{G}(T_{22}) = (-1)^{L+l_1'+l_2}\begin{Bmatrix} 1 & 1 & 1 \\ l_1 & \Lambda & T \end{Bmatrix}\begin{Bmatrix} L & l_1 & l_2 \\ \Lambda & L' & 1 \end{Bmatrix}$$

$$\times \begin{Bmatrix} L' & \Lambda & l_2 \\ \Omega & H' & N' \end{Bmatrix}\begin{Bmatrix} L' & l_1' & l_2' \\ 1 & H' & N' \end{Bmatrix}$$

$$G(T_{23},0) = \begin{pmatrix} l_1' & 1 & N' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & 1 & H' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_2 & T \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times \begin{pmatrix} 1 & T & \Lambda \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} N' & l_1 & \Omega \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} H' & \Lambda & \Omega \\ 0 & 0 & 0 \end{pmatrix}$$

$$\bar{G}(T_{23}) = (-1)^{l_1+l_2'+L'}\begin{Bmatrix} L' & 1 & L \\ l_2 & l_1 & \Lambda \end{Bmatrix}\begin{Bmatrix} 1 & 1 & 1 \\ T & l_2 & \Lambda \end{Bmatrix}$$

$$\times \begin{Bmatrix} L' & l_1 & \Lambda \\ \Omega & H' & N' \end{Bmatrix}\begin{Bmatrix} L' & l_1' & l_2' \\ 1 & H' & N' \end{Bmatrix}.$$

(7) $H_D^{\bar{7}}$:

$$\Delta E_D^{\bar{7}} = -\frac{3}{4}i\alpha^4\delta_{JJ'}\delta_{M_JM_{J'}}(-1)^{L+S'+J}\begin{Bmatrix} L' & S' & J \\ S & L & 1 \end{Bmatrix}$$
$$\times \langle\gamma' L'\|R^{(1)}\|\gamma L\rangle\langle S'\|\vec{\sigma}_1\|S\rangle$$

with

$$\mathbf{R} = \nabla_1^2(\frac{\vec{r}}{r^3}\cdot\vec{\nabla}_2)(\vec{r}\times\vec{\nabla}_1)$$

The orbital part is

$$\langle F'\mathcal{Y}^{M'}_{l_1'l_2'L'}|R_0^{(1)}|F\mathcal{Y}^{M}_{l_1l_2L}\rangle = (-1)^{L'-M'}\begin{pmatrix} L' & 1 & L \\ -M' & 0 & M \end{pmatrix}U(7)D,$$

where

$$U(7) = -i\sqrt{\frac{3}{2}}(l_1, l_2, L, l_1', l_2', L')^{1/2}$$

and

$$D = \sum_{i=1}^{14} \text{Term}(i).$$

For Term(1),

$$\begin{aligned}
T_1(k) &\equiv \varpi_k(\mu_{11}, M_{11}; G_{112}; A+1, B+b^{(2)}(j), C-3; \tilde{\alpha}, \tilde{\beta}) \\
&+ \varpi_k(\mu_{31}, M_{31}; G_{312}; A, B+b^{(2)}(j)+1, C-3; \tilde{\alpha}, \tilde{\beta}) \\
\text{Term}(1) &= \sum_{i=1}^{7}\sum_{j=1}^{2} \text{coe}(S_i)\text{coe}(A_j^{(2)})\Delta_1(ij) \\
\Delta_1(ij) &= T_1(0), \quad C \geq 1 \\
\Delta_1(ij) &= T_1(1) + J_1(\mu_{11}, M_{11}; G_{112})\text{Dif}(A+1, B+b^{(2)}(j); A, B+b^{(2)}(j)+1; \\
&\quad C-3, \tilde{\alpha}, \tilde{\beta}; \omega(\mu_{11})-2, \omega(\mu_{11}+1)-2), \quad C \leq 0.
\end{aligned}$$

For Term(2),

$$\begin{aligned}
T_2(k) &\equiv \varpi_k(\mu_{11}, M_{11}; G_{112} - G_{142} + G_{322}; A+1, B+1, C-5; \tilde{\alpha}, \tilde{\beta}) \\
&+ \varpi_k(\mu_{12}, M_{12}; G_{122}; A+2, B, C-5; \tilde{\alpha}, \tilde{\beta}) \\
&- \varpi_k(\mu_{33}, M_{33}; G_{332}; A-1, B+3, C-5; \tilde{\alpha}, \tilde{\beta}) \\
&+ \varpi_k(\mu_{13}, M_{13}; -G_{132} + G_{312} - G_{342}; A, B+2, C-5; \tilde{\alpha}, \tilde{\beta}) \\
\text{Term}(2) &= \sum_{i=1}^{7} \text{coe}(S_i)c\Delta_2(i) \\
\Delta_2(i) &= T_2(0), \quad C \geq 3 \\
\Delta_2(i) &= T_2(1) + J_1(\mu_{11}, M_{11}; G_{112})[-\eta(\mu_{11}+1, C)I_{\omega(\mu_{11}+1)-2}(A, B, C-3) \\
&+ \eta(\mu_{11}, C)I_{\omega(\mu_{11})-2}(A-1, B+1, C-3)], \quad 1 \leq C \leq 2 \\
\Delta_2(i) &= T_2(2) + \gamma_1\text{Dif}(A+1, B-1; A, B; C-3, \tilde{\alpha}, \tilde{\beta}; \\
&\quad \omega(\mu_{11})-2, \omega(\mu_{11}+1)-2) \\
&+ (\gamma_1+\gamma_2)\text{Dif}(A, B; A-1, B+1; C-3, \tilde{\alpha}, \tilde{\beta}; \\
&\quad \omega(\mu_{11}+1)-2, \omega(\mu_{11})-2) \\
&- \gamma_4\text{Dif}(A-1, B+1; A-2, B+2; C-3, \tilde{\alpha}, \tilde{\beta}; \\
&\quad \omega(\mu_{11})-2, \omega(\mu_{11}+1)-2), \quad C \leq 0.
\end{aligned}$$

For Term(3),

$$\begin{aligned}
T_3(k) &\equiv \varpi_k(\mu_{11}, M_{11}; G_{114}; A+1, B-1, C-3; \tilde{\alpha}, \tilde{\beta}) \\
&- \varpi_k(\mu_{13}, M_{13}; G_{134}; A, B, C-3; \tilde{\alpha}, \tilde{\beta}) \\
\text{Term}(3) &= \sum_{i=1}^{7} \text{coe}(S_i)\Delta_3(i) \\
\Delta_3(i) &= T_3(0), \quad C \geq 1 \\
\Delta_3(i) &= T_3(1), \quad C \leq 0.
\end{aligned}$$

For Term(4),

$$\begin{aligned}
T_4(k) &\equiv \varpi_k(\mu_{13}, M_{13}; G_{131}; A_1+1, B_1, C_1-3; \tilde{\alpha}, \tilde{\beta}) \\
&+ \varpi_k(\mu_{33}, M_{33}; G_{331}; A_1, B_1+1, C_1-3; \tilde{\alpha}, \tilde{\beta}) \\
\text{Term}(4) &= \sum_{i=1}^{7}\sum_{j=1}^{6} \text{coe}(S_i)\text{coe}(C_j^{(1)})\Delta_4(ij) \\
\Delta_4(ij) &= T_4(0), \quad C_1 \geq 1 \\
\Delta_4(ij) &= T_4(1), \quad -1 \leq C_1 \leq 0 \\
\Delta_4(ij) &= T_4(2) + \gamma_5 \text{Dif}(A_1, B_1-1; A_1-1, B_1; C_1-1, \tilde{\alpha}, \tilde{\beta}; \\
&\quad \omega(\mu_{11})-2, \omega(\mu_{11}+1)-2), \quad C_1 \leq -2.
\end{aligned}$$

For Term(5),

$$\begin{aligned}
T_5(k) &\equiv \varpi_k(\mu_{13}, M_{13}; G_{132}; A, B+\bar{b}^{(2)}(j), C-3; \tilde{\alpha}, \tilde{\beta}) \\
&+ \varpi_k(\mu_{33}, M_{33}; G_{332}; A-1, B+\bar{b}^{(2)}(j)+1, C-3; \tilde{\alpha}, \tilde{\beta}) \\
\text{Term}(5) &= \sum_{i=1}^{7}\sum_{j=1}^{2} \text{coe}(S_i)\text{coe}(C_j^{(2)})\Delta_5(ij) \\
\Delta_5(ij) &= T_5(0), \quad C \geq 1 \\
\Delta_5(ij) &= T_5(1) + J_1(\mu_{11}, M_{11}; G_{112})\text{Dif}(A, B+\bar{b}^{(2)}(j); A-1, B+\bar{b}^{(2)}(j)+1; \\
&\quad C-3, \tilde{\alpha}, \tilde{\beta}; \omega(\mu_{11}+1)-2, \omega(\mu_{11})-2), \quad C \leq 0.
\end{aligned}$$

For Term(6),

$$\begin{aligned}
T_6(k) &\equiv \varpi_k(\mu_{13}, M_{13}; G_{133}; A+\bar{a}^{(3)}(j)+1, B, C-3; \tilde{\alpha}, \tilde{\beta}) \\
\text{Term}(6) &= \sum_{i=1}^{7}\sum_{j=1}^{2} \text{coe}(S_i)\text{coe}(C_j^{(3)})\Delta_6(ij)
\end{aligned}$$

$$\Delta_6(ij) = T_6(0), \quad C \geq 1$$

$$\Delta_6(ij) = T_6(1), \quad C \leq 0.$$

For Term(7),

$$\begin{aligned}
T_7(k) &\equiv \varpi_k(\mu_{14}, M_{14}; G_{141}; A + \bar{a}(j) + 1, B + 1, C - 5; \tilde{\alpha}, \tilde{\beta}) \\
&+ \varpi_k(\mu_{34}, M_{34}; G_{341}; A + \bar{a}(j), B + 2, C - 5; \tilde{\alpha}, \tilde{\beta}) \\
\text{Term}(7) &= \sum_{i=1}^{7}\sum_{j=1}^{2} \text{coe}(S_i)\text{coe}(D_j)\Delta_7(ij) \\
\Delta_7(ij) &= T_7(0), \quad C \geq 3 \\
\Delta_7(ij) &= T_7(1), \quad 1 \leq C \leq 2 \\
\Delta_7(ij) &= T_7(2) + \gamma_7 \text{Dif}(A + \bar{a}(j), B; A + \bar{a}(j) - 1, B + 1; \\
&\quad C - 3, \tilde{\alpha}, \tilde{\beta}; \omega(u_{11} + 1) - 2, \omega(\mu_{11}) - 2), \quad C \leq 0.
\end{aligned}$$

For Term(8),

$$\begin{aligned}
T_8(k) &\equiv \varpi_k(\mu_{21}, M_{21}; G_{212}; \tilde{a}, \tilde{b} + b^{(2)}(i) + 1, \tilde{c} - 5; \tilde{\alpha}, \tilde{\beta}) \\
&+ \varpi_k(\mu_{41}, M_{41}; G_{412}; \tilde{a} - 1, \tilde{b} + b^{(2)}(i) + 2, \tilde{c} - 5; \tilde{\alpha}, \tilde{\beta}) \\
\text{Term}(8) &= \sum_{i=1}^{2} \text{coe}(A_i^{(2)}) c' \Delta_8(i) \\
\Delta_8(i) &= T_8(0), \quad \tilde{c} \geq 3 \\
\Delta_8(i) &= T_8(1), \quad \tilde{c} \leq 2.
\end{aligned}$$

For Term(9),

$$\begin{aligned}
T_9(k) &\equiv \varpi_k(\mu_{22}, M_{22}; G_{222}; \tilde{a} + 1, \tilde{b} + 1, \tilde{c} - 7; \tilde{\alpha}, \tilde{\beta}) \\
&+ \varpi_k(\mu_{21}, M_{21}; G_{212} - G_{242} + G_{422}; \tilde{a}, \tilde{b} + 2, \tilde{c} - 7; \tilde{\alpha}, \tilde{\beta}) \\
&+ \varpi_k(\mu_{23}, M_{23}; -G_{232} + G_{412} - G_{442}; \tilde{a} - 1, \tilde{b} + 3, \tilde{c} - 7; \tilde{\alpha}, \tilde{\beta}) \\
&- \varpi_k(\mu_{43}, M_{43}; G_{432}; \tilde{a} - 2, \tilde{b} + 4, \tilde{c} - 7; \tilde{\alpha}, \tilde{\beta}) \\
\text{Term}(9) &= cc'\Delta_9 \\
\Delta_9 &= T_9(0), \quad \tilde{c} \geq 5 \\
\Delta_9 &= T_9(1), \quad 3 \leq \tilde{c} \leq 4 \\
\Delta_9 &= T_9(2) + \gamma_9 \text{Dif}(\tilde{a}, \tilde{b}; \tilde{a} - 1, \tilde{b} + 1; \tilde{c} - 5, \tilde{\alpha}, \tilde{\beta};
\end{aligned}$$

$$\omega(\mu_{11}+1)-2,\omega(\mu_{11})-2)$$

$$+ \quad (\gamma_9+\gamma_{10})\mathrm{Dif}(\tilde{a}-1,\tilde{b}+1;\tilde{a}-2,\tilde{b}+2;\tilde{c}-5,\tilde{\alpha},\tilde{\beta};$$

$$\omega(\mu_{11})-2,\omega(\mu_{11}+1)-2)$$

$$- \quad \gamma_{12}\mathrm{Dif}(\tilde{a}-2,\tilde{b}+2;\tilde{a}-3,\tilde{b}+3;\tilde{c}-5,\tilde{\alpha},\tilde{\beta};$$

$$\omega(\mu_{11}+1)-2,\omega(\mu_{11})-2), \quad \tilde{c}\le 2.$$

For Term(10),

$$\begin{aligned}
T_{10}(k) &\equiv \varpi_k(\mu_{21},M_{21};G_{214};\tilde{a},\tilde{b},\tilde{c}-5;\tilde{\alpha},\tilde{\beta})\\
&\quad - \varpi_k(\mu_{23},M_{23};G_{234};\tilde{a}-1,\tilde{b}+1,\tilde{c}-5;\tilde{\alpha},\tilde{\beta})\\
\mathrm{Term}(10) &= c'\Delta_{10}\\
\Delta_{10} &= T_{10}(0), \quad \tilde{c}\ge 3\\
\Delta_{10} &= T_{10}(1), \quad \tilde{c}\le 2.
\end{aligned}$$

For Term(11),

$$\begin{aligned}
T_{11}(k) &\equiv \varpi_k(\mu_{23},M_{23};G_{231};A_2,B_2+1,C_2-5;\tilde{\alpha},\tilde{\beta})\\
&\quad + \varpi_k(\mu_{43},M_{43};G_{431};A_2-1,B_2+2,C_2-5;\tilde{\alpha},\tilde{\beta})\\
\mathrm{Term}(11) &= \sum_{i=1}^{6}\mathrm{coe}(C_i^{(1)})c'\Delta_{11}(i)\\
\Delta_{11}(i) &= T_{11}(0), \quad C_2\ge 3\\
\Delta_{11}(i) &= T_{11}(1), \quad 1\le C_2\le 2\\
\Delta_{11}(i) &= T_{11}(2)+\gamma_{13}\mathrm{Dif}(A_2-1,B_2;A_2-2,B_2+1;\\
&\quad C_2-3,\tilde{\alpha},\tilde{\beta};\omega(\mu_{11}+1)-2,\omega(\mu_{11})-2), \quad C_2\le 0.
\end{aligned}$$

For Term(12),

$$\begin{aligned}
T_{12}(k) &\equiv \varpi_k(\mu_{23},M_{23};G_{232};\tilde{a}-1,\tilde{b}+\bar{b}^{(2)}(i)+1,\tilde{c}-5;\tilde{\alpha},\tilde{\beta})\\
&\quad + \varpi_k(\mu_{43},M_{43};G_{432};\tilde{a}-2,\tilde{b}+\bar{b}^{(2)}(i)+2,\tilde{c}-5;\tilde{\alpha},\tilde{\beta})\\
\mathrm{Term}(12) &= \sum_{i=1}^{2}\mathrm{coe}(C_i^{(2)})c'\Delta_{12}(i)\\
\Delta_{12}(i) &= T_{12}(0), \quad \tilde{c}\ge 3\\
\Delta_{12}(i) &= T_{12}(1), \quad \tilde{c}\le 2.
\end{aligned}$$

For Term(13),

$$
\begin{aligned}
T_{13}(k) &\equiv \varpi_k(\mu_{23}, M_{23}; G_{233}; \tilde{a} + \bar{a}^{(3)}(i), \tilde{b} + 1, \tilde{c} - 5; \tilde{\alpha}, \tilde{\beta}) \\
\text{Term}(13) &= \sum_{i=1}^{2} \text{coc}(C_i^{(3)}) c' \Delta_{13}(i) \\
\Delta_{13}(i) &= T_{13}(0), \quad \tilde{c} \geq 3 \\
\Delta_{13}(i) &= T_{13}(1), \quad \tilde{c} \leq 2.
\end{aligned}
$$

For Term(14),

$$
\begin{aligned}
T_{14}(k) &\equiv \varpi_k(\mu_{24}, M_{24}; G_{241}; \tilde{a} + \bar{\bar{a}}(i), \tilde{b} + 2, \tilde{c} - 7; \tilde{\alpha}, \tilde{\beta}) \\
&+ \varpi_k(\mu_{44}, M_{44}; G_{441}; \tilde{a} + \bar{\bar{a}}(i) - 1, \tilde{b} + 3, \tilde{c} - 7; \tilde{\alpha}, \tilde{\beta}) \\
\text{Term}(14) &= \sum_{i=1}^{2} \text{coc}(D_i) c' \Delta_{14}(i) \\
\Delta_{14}(i) &= T_{14}(0), \quad \tilde{c} \geq 5 \\
\Delta_{14}(i) &= T_{14}(1), \quad 3 \leq \tilde{c} \leq 4 \\
\Delta_{14}(i) &= T_{14}(2) + \gamma_5 \text{Dif}(\tilde{a} + \bar{\bar{a}}(i) - 1, \tilde{b} + 1; \tilde{a} + \bar{\bar{a}}(i) - 2, \tilde{b} + 2; \tilde{c} - 5, \tilde{\alpha}, \tilde{\beta}; \\
&\quad \omega(\mu_{11}) - 2, \omega(\mu_{11} + 1) - 2), \quad \tilde{c} \leq 2.
\end{aligned}
$$

Also,

$$
\begin{aligned}
M_{11} &= \min(l_1 + l_1' + 3, l_2 + l_2' + 1) \\
M_{12} &= \min(l_1 + l_1' + 4, l_2 + l_2') \\
M_{13} &= \min(l_1 + l_1' + 2, l_2 + l_2' + 2) \\
M_{14} &= \min(l_1 + l_1' + 3, l_2 + l_2' + 1) \\
M_{15} &= \min(l_1 + l_1' + 1, l_2 + l_2' + 3) \\
M_{16} &= \min(l_1 + l_1' + 2, l_2 + l_2' + 2) \\
M_{21} &= \min(l_1 + l_1' + 4, l_2 + l_2' + 2) \\
M_{22} &= \min(l_1 + l_1' + 5, l_2 + l_2' + 1) \\
M_{23} &= \min(l_1 + l_1' + 3, l_2 + l_2' + 3) \\
M_{24} &= \min(l_1 + l_1' + 4, l_2 + l_2' + 2) \\
M_{25} &= \min(l_1 + l_1' + 2, l_2 + l_2' + 4)
\end{aligned}
$$

$$
\begin{aligned}
M_{26} &= \min(l_1 + l_1' + 3, l_2 + l_2' + 3) \\
M_{31} &= \min(l_1 + l_1' + 2, l_2 + l_2' + 2) \\
M_{32} &= \min(l_1 + l_1' + 3, l_2 + l_2' + 1) \\
M_{33} &= \min(l_1 + l_1' + 1, l_2 + l_2' + 3) \\
M_{34} &= \min(l_1 + l_1' + 2, l_2 + l_2' + 2) \\
M_{35} &= \min(l_1 + l_1', l_2 + l_2' + 4) \\
M_{36} &= \min(l_1 + l_1' + 1, l_2 + l_2' + 3) \\
M_{41} &= \min(l_1 + l_1' + 3, l_2 + l_2' + 3) \\
M_{42} &= \min(l_1 + l_1' + 4, l_2 + l_2' + 2) \\
M_{43} &= \min(l_1 + l_1' + 2, l_2 + l_2' + 4) \\
M_{44} &= \min(l_1 + l_1' + 3, l_2 + l_2' + 3) \\
M_{45} &= \min(l_1 + l_1' + 1, l_2 + l_2' + 5) \\
M_{46} &= \min(l_1 + l_1' + 2, l_2 + l_2' + 4) \\
\mu_{ij} &= \omega(M_{ij}) - 2, \quad i = 1, \cdots, 4, \quad j = 1, \cdots, 6
\end{aligned}
$$

$$
\begin{aligned}
A &\equiv \tilde{a} + a'(i) \\
B &\equiv \tilde{b} + b'(i) \\
C &\equiv \tilde{c} + a'(i) \\
A_1 &\equiv \tilde{a} + a'(i) + \bar{a}^{(1)}(j) \\
B_1 &\equiv \tilde{b} + b'(i) + \bar{b}^{(1)}(j) \\
C_1 &\equiv \tilde{c} + c'(i) + \bar{c}^{(1)}(j) \\
A_2 &\equiv \tilde{a} + \bar{a}^{(1)}(i) \\
B_2 &\equiv \tilde{b} + \bar{b}^{(1)}(i) \\
C_2 &\equiv \tilde{c} + \bar{c}^{(1)}(i)
\end{aligned}
$$

$\mathrm{coe}(S_i)$	$a'(i)$	$b'(i)$	$c'(i)$
$a'(a'+1+c')-l_1{}'(l_1{}'+1)$	-2	0	0
$-\alpha'[2(a'+1)+c']$	-1	0	0
α'^2	0	0	0
$c'(c'+1+a')$	0	0	-2
$-a'c'$	-2	2	-2
$-\alpha'c'$	1	0	-2
$\alpha'c'$	-1	2	-2

$\mathrm{coe}(A_i^{(1)})$	$a^{(1)}(i)$	$b^{(1)}(i)$	$c^{(1)}(i)$
ab	0	-1	0
$-a\beta$	0	0	0
$-b\alpha$	1	-1	0
$\alpha\beta$	1	0	0
ca	0	1	-2
cb	2	-1	-2
$-c\alpha$	1	1	-2
$-c\beta$	2	0	-2
$c(c-2)$	2	1	-4

$\mathrm{coe}(A_i^{(2)})$	$a^{(2)}(i)$	$b^{(2)}(i)$	$c^{(2)}(i)$
b	0	-1	0
$-\beta$	0	0	0
c	0	1	-2

$\mathrm{coe}(A_i^{(3)})$	$a^{(3)}(i)$	$b^{(3)}(i)$	$c^{(3)}(i)$
a	0	-1	0
$-\alpha$	1	-1	0
c	2	-1	-2

$\mathrm{coe}(C_i^{(1)})$	$\bar{a}^{(1)}(i)$	$\bar{b}^{(1)}(i)$	$\bar{c}^{(1)}(i)$
$-a(b+1)$	-1	0	0
$a\beta$	-1	1	0
$-\alpha\beta$	0	1	0
$\alpha(b+1)$	0	0	0
$-ac$	-1	2	-2
αc	0	2	-2

$\mathrm{coe}(C_i^{(2)})$	$\bar{a}^{(2)}(i)$	$\bar{b}^{(2)}(i)$	$\bar{c}^{(2)}(i)$
$-(b+1)$	-1	0	0
β	-1	1	0
$-c$	-1	2	-2

$coe(C_i^{(3)})$	$\bar{a}^{(3)}(i)$	$\bar{b}^{(3)}(i)$	$\bar{c}^{(3)}(i)$
α	0	0	0
$-a$	-1	0	0

$coe(D_i)$	$\bar{a}(i)$	$\bar{b}(i)$	$c(i)$
$-ac$	0	1	-2
αc	1	1	-2

The angular coefficients are:

$$G_{112}(\Omega) = \sum_{T\Gamma NE}(T,\Gamma,N,E,\Omega)G(T_{11},0)\tilde{G}(T_{11})b(l_1;T)$$
$$G_{114}(\Omega) = \sum_{T\Gamma NE}(T,\Gamma,N,E,\Omega)G(T_{11},0)\tilde{G}(T_{11})b(l_1;T)b(l_2;N)$$

$$G_{122}(\Omega) = \sum_{T\Gamma NE}(T,\Gamma,N,E,\Omega)G(T_{12},0)\tilde{G}(T_{12})b(l_1;T)$$

$$G_{131}(\Omega) = \sum_{T\Gamma NE}(T,\Gamma,N,E,\Omega)G(T_{13},0)\tilde{G}(T_{13})$$
$$G_{132}(\Omega) = \sum_{T\Gamma NE}(T,\Gamma,N,E,\Omega)G(T_{13},0)\tilde{G}(T_{13})b(l_1;\Gamma)$$
$$G_{133}(\Omega) = \sum_{T\Gamma NE}(T,\Gamma,N,E,\Omega)G(T_{13},0)\tilde{G}(T_{13})b(T;N)$$
$$G_{134}(\Omega) = \sum_{T\Gamma NE}(T,\Gamma,N,E,\Omega)G(T_{13},0)\tilde{G}(T_{13})b(l_1;\Gamma)b(T;N)$$

$$G_{141}(\Omega) = \sum_{T\Gamma NE}(T,\Gamma,N,E,\Omega)G(T_{14},0)\tilde{G}(T_{14})$$
$$G_{142}(\Omega) = \sum_{T\Gamma NE}(T,\Gamma,N,E,\Omega)G(T_{14},0)\tilde{G}(T_{14})b(l_1;\Gamma)$$

$$G_{212}(\Omega) = 2\sum_{N'H'T\Gamma NE}(N',H',T,\Gamma,N,E,\Omega)G(T_{21},0)\tilde{G}(T_{21})b(l_1';N')b(l_1;T)$$
$$G_{214}(\Omega) = 2\sum_{N'H'T\Gamma NE}(N',H',T,\Gamma,N,E,\Omega)G(T_{21},0)\tilde{G}(T_{21})b(l_1';N')b(l_1;T)b(l_2;N)$$

$$G_{222}(\Omega) = 2\sum_{N'H'T\Gamma NE}(N',H',T,\Gamma,N,E,\Omega)G(T_{22},0)\tilde{G}(T_{22})b(l_1';N')b(l_1;T)$$

$$G_{231}(\Omega) = 2\sum_{N'H'T\Gamma NE}(N',H',T,\Gamma,N,E,\Omega)G(T_{23},0)\tilde{G}(T_{23})b(l_1';N')$$
$$G_{232}(\Omega) = 2\sum_{N'H'T\Gamma NE}(N',H',T,\Gamma,N,E,\Omega)G(T_{23},0)\tilde{G}(T_{23})b(l_1';N')b(l_1;\Gamma)$$

$$G_{233}(\Omega) = 2 \sum_{N'H'T\Gamma NE} (N', H', T, \Gamma, N, E, \Omega) G(T_{23}, 0) \tilde{G}(T_{23}) b(l_1'; N') b(T; N)$$

$$G_{234}(\Omega) = 2 \sum_{N'H'T\Gamma NE} (N', H', T, \Gamma, N, E, \Omega) G(T_{23}, 0) \tilde{G}(T_{23}) b(l_1'; N') b(l_1; \Gamma) b(T; N)$$

$$G_{241}(\Omega) = 2 \sum_{N'H'T\Gamma NE} (N', H', T, \Gamma, N, E, \Omega) G(T_{24}, 0) \tilde{G}(T_{24}) b(l_1'; N')$$

$$G_{242}(\Omega) = 2 \sum_{N'H'T\Gamma NE} (N', H', T, \Gamma, N, E, \Omega) G(T_{24}, 0) \tilde{G}(T_{24}) b(l_1'; N') b(l_1; \Gamma)$$

$$G_{312}(\Omega) = \sum_{T\Gamma NE} (T, \Gamma, N, E, \Omega) G(T_{31}, 0) \tilde{G}(T_{31}) b(l_1; T)$$

$$G_{322}(\Omega) = \sum_{T\Gamma NE} (T, \Gamma, N, E, \Omega) G(T_{32}, 0) \tilde{G}(T_{32}) b(l_1; T)$$

$$G_{331}(\Omega) = \sum_{T\Gamma NE} (T, \Gamma, N, E, \Omega) G(T_{33}, 0) \tilde{G}(T_{33})$$

$$G_{332}(\Omega) = \sum_{T\Gamma NE} (T, \Gamma, N, E, \Omega) G(T_{33}, 0) \tilde{G}(T_{33}) b(l_1; \Gamma)$$

$$G_{341}(\Omega) = \sum_{T\Gamma NE} (T, \Gamma, N, E, \Omega) G(T_{34}, 0) \tilde{G}(T_{34})$$

$$G_{342}(\Omega) = \sum_{T\Gamma NE} (T, \Gamma, N, E, \Omega) G(T_{34}, 0) \tilde{G}(T_{34}) b(l_1; \Gamma)$$

$$G_{412}(\Omega) = 2 \sum_{N'H'T\Gamma NE} (N', H', T, \Gamma, N, E, \Omega) G(T_{41}, 0) \tilde{G}(T_{41}) b(l_1'; N') b(l_1; T)$$

$$G_{422}(\Omega) = 2 \sum_{N'H'T\Gamma NE} (N', H', T, \Gamma, N, E, \Omega) G(T_{42}, 0) \tilde{G}(T_{42}) b(l_1'; N') b(l_1; T)$$

$$G_{431}(\Omega) = 2 \sum_{N'H'T\Gamma NE} (N', H', T, \Gamma, N, E, \Omega) G(T_{43}, 0) \tilde{G}(T_{43}) b(l_1'; N')$$

$$G_{432}(\Omega) = 2 \sum_{N'H'T\Gamma NE} (N', H', T, \Gamma, N, E, \Omega) G(T_{43}, 0) \tilde{G}(T_{43}) b(l_1'; N') b(l_1; \Gamma)$$

$$G_{441}(\Omega) = 2 \sum_{N'H'T\Gamma NE} (N', H', T, \Gamma, N, E, \Omega) G(T_{44}, 0) \tilde{G}(T_{44}) b(l_1'; N')$$

$$G_{442}(\Omega) = 2 \sum_{N'H'T\Gamma NE} (N', H', T, \Gamma, N, E, \Omega) G(T_{44}, 0) \tilde{G}(T_{44}) b(l_1'; N') b(l_1; \Gamma)$$

with

$$
\begin{aligned}
G(T_{11},0) &= \begin{pmatrix} 1 & l_1 & T \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & l_2 & N \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & T & \Gamma \\ 0 & 0 & 0 \end{pmatrix} \\
&\times \begin{pmatrix} 1 & l_1' & E \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} E & \Gamma & \Omega \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2' & N & \Omega \\ 0 & 0 & 0 \end{pmatrix} \\
\tilde{G}(T_{11}) &= (-1) \begin{Bmatrix} L & l_1 & l_2 \\ \Gamma & L' & 1 \end{Bmatrix} \begin{Bmatrix} 1 & 1 & 1 \\ l_1 & \Gamma & T \end{Bmatrix} \begin{Bmatrix} L' & l_1' & l_2' \\ \Gamma & E & \Omega \\ l_2 & 1 & N \end{Bmatrix} \\
G(T_{12},0) &= \begin{pmatrix} 1 & l_1 & T \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & T & \Gamma \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \Gamma & 1 & N \\ 0 & 0 & 0 \end{pmatrix} \\
&\times \begin{pmatrix} 1 & l_1' & E \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} E & N & \Omega \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2' & l_2 & \Omega \\ 0 & 0 & 0 \end{pmatrix} \\
\tilde{G}(T_{12}) &= (-1)^{L'+1} \begin{Bmatrix} L & l_1 & l_2 \\ \Gamma & L' & 1 \end{Bmatrix} \begin{Bmatrix} L' & l_1' & l_2' \\ \Omega & l_2 & \Gamma \end{Bmatrix} \begin{Bmatrix} 1 & 1 & 1 \\ l_1 & \Gamma & T \end{Bmatrix} \begin{Bmatrix} \Gamma & N & 1 \\ E & l_1' & \Omega \end{Bmatrix}
\end{aligned}
$$

$$
\begin{aligned}
G(T_{13},0) &= \begin{pmatrix} 1 & l_1 & \Gamma \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2 & 1 & T \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & T & N \\ 0 & 0 & 0 \end{pmatrix} \\
&\times \begin{pmatrix} 1 & l_1' & E \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} E & \Gamma & \Omega \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2' & N & \Omega \\ 0 & 0 & 0 \end{pmatrix} \\
\tilde{G}(T_{13}) &= (-1)^{L'+1} \begin{Bmatrix} L & l_1 & l_2 \\ 1 & 1 & 1 \\ L' & \Gamma & T \end{Bmatrix} \begin{Bmatrix} L' & l_1' & l_2' \\ T & 1 & N \\ \Gamma & E & \Omega \end{Bmatrix} \\
G(T_{14},0) &= \begin{pmatrix} 1 & l_1 & \Gamma \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2 & 1 & T \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \Gamma & 1 & N \\ 0 & 0 & 0 \end{pmatrix} \\
&\times \begin{pmatrix} 1 & l_1' & E \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} E & N & \Omega \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2' & T & \Omega \\ 0 & 0 & 0 \end{pmatrix} \\
\tilde{G}(T_{14}) &= (-1)^{L+L'+1} \begin{Bmatrix} L & l_1 & l_2 \\ 1 & 1 & 1 \\ L' & \Gamma & T \end{Bmatrix} \begin{Bmatrix} L' & l_1' & l_2' \\ \Omega & T & \Gamma \end{Bmatrix} \begin{Bmatrix} \Gamma & N & 1 \\ E & l_1' & \Omega \end{Bmatrix}
\end{aligned}
$$

$$
\begin{aligned}
G(T_{15},0) &= \begin{pmatrix} l_2 & 1 & T \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & T & \Gamma \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & \Gamma & N \\ 0 & 0 & 0 \end{pmatrix} \\
&\times \begin{pmatrix} 1 & l_1' & E \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} E & l_1 & \Omega \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2' & N & \Omega \\ 0 & 0 & 0 \end{pmatrix} \\
\tilde{G}(T_{15}) &= (-1)^{L+L'+1} \begin{Bmatrix} L & l_1 & l_2 \\ \Gamma & 1 & L' \end{Bmatrix} \begin{Bmatrix} 1 & 1 & 1 \\ l_2 & \Gamma & T \end{Bmatrix} \begin{Bmatrix} L' & l_1' & l_2' \\ l_1 & E & \Omega \\ \Gamma & 1 & N \end{Bmatrix}
\end{aligned}
$$

$$
G(T_{16},0) = \begin{pmatrix} l_1 & 1 & N \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2 & 1 & T \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & T & \Gamma \\ 0 & 0 & 0 \end{pmatrix}
$$

$$\times \begin{pmatrix} 1 & l_1' & E \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} E & N & \Omega \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2' & \Gamma & \Omega \\ 0 & 0 & 0 \end{pmatrix}$$

$$\tilde{G}(T_{16}) = (-1)^{L+1} \begin{Bmatrix} L & l_1 & l_2 \\ \Gamma & 1 & L' \end{Bmatrix} \begin{Bmatrix} L' & l_1' & l_2' \\ \Omega & \Gamma & l_1 \end{Bmatrix} \begin{Bmatrix} 1 & 1 & 1 \\ l_2 & \Gamma & T \end{Bmatrix} \begin{Bmatrix} l_1 & N & 1 \\ E & l_1' & \Omega \end{Bmatrix}$$

$$G(T_{21},0) = \begin{pmatrix} l_1' & 1 & N' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2' & 1 & H' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & l_1 & T \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & l_2 & N \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times \begin{pmatrix} 1 & T & \Gamma \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & N' & E \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} E & \Gamma & \Omega \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} H' & N & \Omega \\ 0 & 0 & 0 \end{pmatrix}$$

$$\tilde{G}(T_{21}) = (-1)^{L'+1} \begin{Bmatrix} L & l_1 & l_2 \\ \Gamma & L' & 1 \end{Bmatrix} \begin{Bmatrix} L' & l_1' & l_2' \\ 1 & H' & N' \end{Bmatrix} \begin{Bmatrix} 1 & 1 & 1 \\ l_1 & \Gamma & T \end{Bmatrix} \begin{Bmatrix} L' & \Gamma & l_2 \\ N' & E & 1 \\ H' & \Omega & N \end{Bmatrix}$$

$$G(T_{22},0) = \begin{pmatrix} l_1' & 1 & N' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2' & 1 & H' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & l_1 & T \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & T & \Gamma \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times \begin{pmatrix} \Gamma & 1 & N \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & N' & E \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} E & N & \Omega \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} H' & l_2 & \Omega \\ 0 & 0 & 0 \end{pmatrix}$$

$$\tilde{G}(T_{22}) = (-1) \begin{Bmatrix} L & l_1 & l_2 \\ \Gamma & L' & 1 \end{Bmatrix} \begin{Bmatrix} 1 & 1 & 1 \\ l_1 & \Gamma & T \end{Bmatrix} \begin{Bmatrix} l_2 & \Gamma & L' \\ N' & H' & \Omega \end{Bmatrix}$$

$$\times \begin{Bmatrix} \Gamma & N & 1 \\ E & N' & \Omega \end{Bmatrix} \begin{Bmatrix} L' & l_1' & l_2' \\ 1 & H' & N' \end{Bmatrix}$$

$$G(T_{23},0) = \begin{pmatrix} l_1' & 1 & N' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2' & 1 & H' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & l_1 & \Gamma \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2 & 1 & T \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times \begin{pmatrix} 1 & T & N \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & N' & E \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} E & \Gamma & \Omega \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} H' & N & \Omega \\ 0 & 0 & 0 \end{pmatrix}$$

$$\tilde{G}(T_{23}) = (-1) \begin{Bmatrix} L' & l_1' & l_2' \\ 1 & H' & N' \end{Bmatrix} \begin{Bmatrix} L & l_1 & l_2 \\ 1 & 1 & 1 \\ L' & \Gamma & T \end{Bmatrix} \begin{Bmatrix} L' & \Gamma & T \\ H' & \Omega & N \\ N' & E & 1 \end{Bmatrix}$$

$$G(T_{24},0) = \begin{pmatrix} l_1' & 1 & N' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2' & 1 & H' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & l_1 & \Gamma \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2 & 1 & T \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times \begin{pmatrix} \Gamma & 1 & N \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & N' & E \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} E & N & \Omega \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} H' & T & \Omega \\ 0 & 0 & 0 \end{pmatrix}$$

$$\tilde{G}(T_{24}) = (-1)^{1+L} \begin{Bmatrix} L' & l_1' & l_2' \\ 1 & H' & N' \end{Bmatrix} \begin{Bmatrix} T & \Gamma & L' \\ N' & H' & \Omega \end{Bmatrix} \begin{Bmatrix} \Gamma & N & 1 \\ E & N' & \Omega \end{Bmatrix} \begin{Bmatrix} L & l_1 & l_2 \\ 1 & 1 & 1 \\ L' & \Gamma & T \end{Bmatrix}$$

$$G(T_{25},0) = \begin{pmatrix} l_1' & 1 & N' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2' & 1 & H' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2 & 1 & T \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & T & \Gamma \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times \begin{pmatrix} \Gamma & 1 & N \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & N' & E \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} E & l_1 & \Omega \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} H' & N & \Omega \\ 0 & 0 & 0 \end{pmatrix}$$

$$\tilde{G}(T_{25}) = (-1)^{1+L} \begin{Bmatrix} L & l_1 & l_2 \\ \Gamma & 1 & L' \end{Bmatrix} \begin{Bmatrix} L' & l_1' & l_2' \\ 1 & H' & N' \end{Bmatrix} \begin{Bmatrix} 1 & 1 & 1 \\ l_2 & \Gamma & T \end{Bmatrix} \begin{Bmatrix} L' & N' & H' \\ l_1 & E & \Omega \\ \Gamma & 1 & N \end{Bmatrix}$$

$$G(T_{26}, 0) = \begin{pmatrix} l_1' & 1 & N' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2' & 1 & H' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & 1 & N \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2 & 1 & T \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times \begin{pmatrix} 1 & T & \Gamma \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & N' & E \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} E & N & \Omega \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} H' & \Gamma & \Omega \\ 0 & 0 & 0 \end{pmatrix}$$

$$\tilde{G}(T_{26}) = (-1)^{1+L+L'} \begin{Bmatrix} L & l_1 & l_2 \\ \Gamma & 1 & L' \end{Bmatrix} \begin{Bmatrix} L' & l_1' & l_2' \\ 1 & H' & N' \end{Bmatrix}$$

$$\times \begin{Bmatrix} 1 & 1 & 1 \\ l_2 & \Gamma & T \end{Bmatrix} \begin{Bmatrix} \Gamma & l_1 & L' \\ N' & H' & \Omega \end{Bmatrix} \begin{Bmatrix} l_1 & N & 1 \\ E & N' & \Omega \end{Bmatrix}$$

$$G(T_{31}, 0) = \begin{pmatrix} 1 & l_1 & T \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & l_2 & N \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & T & \Gamma \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times \begin{pmatrix} l_1' & \Gamma & \Omega \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & l_2' & E \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} E & N & \Omega \\ 0 & 0 & 0 \end{pmatrix}$$

$$\tilde{G}(T_{31}) = (-1)^{1+L'} \begin{Bmatrix} L & l_1 & l_2 \\ \Gamma & L' & 1 \end{Bmatrix} \begin{Bmatrix} L' & l_1' & l_2' \\ \Omega & l_2 & \Gamma \end{Bmatrix} \begin{Bmatrix} 1 & 1 & 1 \\ l_1 & \Gamma & T \end{Bmatrix} \begin{Bmatrix} l_2 & N & 1 \\ E & l_2' & \Omega \end{Bmatrix}$$

$$G(T_{32}, 0) = \begin{pmatrix} 1 & l_1 & T \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & T & \Gamma \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \Gamma & 1 & N \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times \begin{pmatrix} l_1' & N & \Omega \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & l_2' & E \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} E & l_2 & \Omega \\ 0 & 0 & 0 \end{pmatrix}$$

$$\tilde{G}(T_{32}) = (-1) \begin{Bmatrix} 1 & 1 & 1 \\ l_1 & \Gamma & T \end{Bmatrix} \begin{Bmatrix} L & l_1 & l_2 \\ \Gamma & L' & 1 \end{Bmatrix} \begin{Bmatrix} L' & l_1' & l_2' \\ \Gamma & N & 1 \\ l_2 & \Omega & E \end{Bmatrix}$$

$$G(T_{33}, 0) = \begin{pmatrix} 1 & l_1 & \Gamma \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2 & 1 & T \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & T & N \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times \begin{pmatrix} l_1' & \Gamma & \Omega \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & l_2' & E \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} E & N & \Omega \\ 0 & 0 & 0 \end{pmatrix}$$

$$\tilde{G}(T_{33}) = \begin{Bmatrix} L' & l_1' & l_2' \\ \Omega & T & \Gamma \end{Bmatrix} \begin{Bmatrix} T & N & 1 \\ E & l_2' & \Omega \end{Bmatrix} \begin{Bmatrix} L & l_1 & l_2 \\ L' & \Gamma & T \\ 1 & 1 & 1 \end{Bmatrix}$$

$$G(T_{34}, 0) = \begin{pmatrix} 1 & l_1 & \Gamma \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2 & 1 & T \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \Gamma & 1 & N \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times \begin{pmatrix} l_1' & N & \Omega \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & l_2' & E \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} E & T & \Omega \\ 0 & 0 & 0 \end{pmatrix}$$

$$\tilde{G}(T_{34}) = (-1)^{L'} \begin{Bmatrix} L & l_1 & l_2 \\ L' & \Gamma & T \\ 1 & 1 & 1 \end{Bmatrix} \begin{Bmatrix} L' & l_1' & l_2' \\ \Gamma & N & 1 \\ T & \Omega & E \end{Bmatrix}$$

$$G(T_{35}, 0) = \begin{pmatrix} l_2 & 1 & T \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & T & \Gamma \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & \Gamma & N \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times \begin{pmatrix} l_1' & l_1 & \Omega \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & l_2' & E \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} E & N & \Omega \\ 0 & 0 & 0 \end{pmatrix}$$

$$\tilde{G}(T_{35}) = (-1)^{1+L} \begin{Bmatrix} L & l_1 & l_2 \\ \Gamma & 1 & L' \end{Bmatrix} \begin{Bmatrix} L' & l_1' & l_2' \\ \Omega & \Gamma & l_1 \end{Bmatrix} \begin{Bmatrix} 1 & 1 & 1 \\ l_2 & \Gamma & T \end{Bmatrix} \begin{Bmatrix} \Gamma & N & 1 \\ E & l_2' & \Omega \end{Bmatrix}$$

$$G(T_{36}, 0) = \begin{pmatrix} l_1 & 1 & N \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2 & 1 & T \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & T & \Gamma \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times \begin{pmatrix} l_1' & N & \Omega \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & l_2' & E \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} E & \Gamma & \Omega \\ 0 & 0 & 0 \end{pmatrix}$$

$$\tilde{G}(T_{36}) = (-1)^{L+L'+1} \begin{Bmatrix} L & l_1 & l_2 \\ \Gamma & 1 & L' \end{Bmatrix} \begin{Bmatrix} 1 & 1 & 1 \\ l_2 & \Gamma & T \end{Bmatrix} \begin{Bmatrix} L' & l_1' & l_2' \\ l_1 & N & 1 \\ \Gamma & \Omega & E \end{Bmatrix}$$

$$G(T_{41}, 0) = \begin{pmatrix} l_1' & 1 & N' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2' & 1 & H' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & l_1 & T \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & l_2 & N \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times \begin{pmatrix} 1 & T & \Gamma \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} N' & \Gamma & \Omega \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & H' & E \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} E & N & \Omega \\ 0 & 0 & 0 \end{pmatrix}$$

$$\tilde{G}(T_{41}) = (-1) \begin{Bmatrix} L & l_1 & l_2 \\ \Gamma & L' & 1 \end{Bmatrix} \begin{Bmatrix} L' & l_1' & l_2' \\ 1 & H' & N' \end{Bmatrix}$$

$$\times \begin{Bmatrix} 1 & 1 & 1 \\ l_1 & \Gamma & T \end{Bmatrix} \begin{Bmatrix} l_2 & N & 1 \\ E & H' & \Omega \end{Bmatrix} \begin{Bmatrix} \Gamma & l_2 & L' \\ H' & N' & \Omega \end{Bmatrix}$$

$$G(T_{42}, 0) = \begin{pmatrix} l_1' & 1 & N' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2' & 1 & H' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & l_1 & T \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & T & \Gamma \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times \begin{pmatrix} \Gamma & 1 & N \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} N' & N & \Omega \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & H' & E \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} E & l_2 & \Omega \\ 0 & 0 & 0 \end{pmatrix}$$

$$\tilde{G}(T_{42}) = (-1)^{L'+1} \begin{Bmatrix} 1 & 1 & 1 \\ l_1 & \Gamma & T \end{Bmatrix} \begin{Bmatrix} L & l_1 & l_2 \\ \Gamma & L' & 1 \end{Bmatrix} \begin{Bmatrix} L' & l_1' & l_2' \\ 1 & H' & N' \end{Bmatrix} \begin{Bmatrix} L' & \Gamma & l_2 \\ N' & N & \Omega \\ H' & 1 & E \end{Bmatrix}$$

$$G(T_{43}, 0) = \begin{pmatrix} l_1' & 1 & N' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2' & 1 & H' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & l_1 & \Gamma \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2 & 1 & T \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times \begin{pmatrix} 1 & T & N \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} N' & \Gamma & \Omega \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & H' & E \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} E & N & \Omega \\ 0 & 0 & 0 \end{pmatrix}$$

$$\tilde{G}(T_{43}) = (-1)^{L'} \begin{Bmatrix} L' & l_1' & l_2' \\ 1 & H' & N' \end{Bmatrix} \begin{Bmatrix} \Gamma & T & L' \\ H' & N' & \Omega \end{Bmatrix} \begin{Bmatrix} T & N & 1 \\ E & H' & \Omega \end{Bmatrix} \begin{Bmatrix} L & l_1 & l_2 \\ L' & \Gamma & T \\ 1 & 1 & 1 \end{Bmatrix}$$

$$G(T_{44}, 0) = \begin{pmatrix} l_1' & 1 & N' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2' & 1 & H' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & l_1 & \Gamma \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2 & 1 & T \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times \begin{pmatrix} \Gamma & 1 & N \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} N' & N & \Omega \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & H' & E \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} E & T & \Omega \\ 0 & 0 & 0 \end{pmatrix}$$

$$\tilde{G}(T_{44}) = \begin{Bmatrix} L' & l_1' & l_2' \\ 1 & H' & N' \end{Bmatrix} \begin{Bmatrix} L & l_1 & l_2 \\ L' & \Gamma & T \\ 1 & 1 & 1 \end{Bmatrix} \begin{Bmatrix} L' & \Gamma & T \\ N' & N & \Omega \\ H' & 1 & E \end{Bmatrix}$$

$$G(T_{45}, 0) = \begin{pmatrix} l_1' & 1 & N' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2' & 1 & H' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2 & 1 & T \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & T & \Gamma \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times \begin{pmatrix} 1 & \Gamma & N \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} N' & l_1 & \Omega \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & H' & E \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} E & N & \Omega \\ 0 & 0 & 0 \end{pmatrix}$$

$$\tilde{G}(T_{45}) = (-1)^{1+L+L'} \begin{Bmatrix} L & l_1 & l_2 \\ \Gamma & 1 & L' \end{Bmatrix} \begin{Bmatrix} L' & l_1' & l_2' \\ 1 & H' & N' \end{Bmatrix} \begin{Bmatrix} 1 & 1 & 1 \\ l_2 & \Gamma & T \end{Bmatrix}$$

$$\times \begin{Bmatrix} \Gamma & N & 1 \\ E & H' & \Omega \end{Bmatrix} \begin{Bmatrix} l_1 & \Gamma & L' \\ H' & N' & \Omega \end{Bmatrix}$$

$$G(T_{46}, 0) = \begin{pmatrix} l_1' & 1 & N' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2' & 1 & H' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & 1 & N \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2 & 1 & T \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times \begin{pmatrix} 1 & T & \Gamma \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} N' & N & \Omega \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & H' & E \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} E & \Gamma & \Omega \\ 0 & 0 & 0 \end{pmatrix}$$

$$\tilde{G}(T_{46}) = (-1)^{1+L} \begin{Bmatrix} L & l_1 & l_2 \\ \Gamma & 1 & L' \end{Bmatrix} \begin{Bmatrix} L' & l_1' & l_2' \\ 1 & H' & N' \end{Bmatrix} \begin{Bmatrix} 1 & 1 & 1 \\ l_2 & \Gamma & T \end{Bmatrix} \begin{Bmatrix} L' & N' & H' \\ l_1 & N & 1 \\ \Gamma & \Omega & E \end{Bmatrix}.$$

We have also defined:

$$\gamma_1(C) = J_2(\mu_{12}, M_{12}; G_{122}; C-5)$$

$$\gamma_2(C) = J_2(\mu_{11}, M_{11}; G_{112}; C-5) - J_2(\mu_{14}, M_{14}; G_{142}; C-5)$$

$$+ J_2(\mu_{32}, M_{32}; G_{322}; C-5) - (\sum_E G_{112}(E))\eta(\mu_{11}+1, C)$$

$$\gamma_3(C) = -J_2(\mu_{13}, M_{13}; G_{132}; C-5) + J_2(\mu_{31}, M_{31}; G_{312}; C-5)$$

$$- J_2(\mu_{34}, M_{34}; G_{342}; C-5) + (\sum_E G_{112}(E))\eta(\mu_{11}, C)$$

$$\gamma_4(C) = -J_2(\mu_{33}, M_{33}; G_{332}; C-5)$$

$$
\begin{aligned}
\gamma_5(C_1) &= J_2(\mu_{13}, M_{13}; G_{131}; C_1 - 3) \\
\gamma_6(C_1) &= J_2(\mu_{33}, M_{33}; G_{331}; C_1 - 3) \\
\gamma_7(C) &= J_2(\mu_{14}, M_{14}; G_{141}; C - 5) \\
\gamma_8(C) &= J_2(\mu_{34}, M_{34}; G_{341}; C - 5)
\end{aligned}
$$

$$
\begin{aligned}
\gamma_9(\tilde{c}) &= J_2(\mu_{22}, M_{22}; G_{222}; \tilde{c} - 7) \\
\gamma_{10}(\tilde{c}) &= J_2(\mu_{21}, M_{21}; G_{212}; \tilde{c} - 7) - J_2(\mu_{24}, M_{24}; G_{242}; \tilde{c} - 7) \\
&+ J_2(\mu_{42}, M_{42}; G_{422}; \tilde{c} - 7) \\
\gamma_{11}(\tilde{c}) &= -J_2(\mu_{23}, M_{23}; G_{232}; \tilde{c} - 7) + J_2(\mu_{41}, M_{41}; G_{412}; \tilde{c} - 7) \\
&- J_2(\mu_{44}, M_{44}; G_{442}; \tilde{c} - 7) \\
\gamma_{12}(\tilde{c}) &= -J_2(\mu_{43}, M_{43}; G_{432}; \tilde{c} - 7)
\end{aligned}
$$

$$
\begin{aligned}
\gamma_{13}(C_2) &= J_2(\mu_{23}, M_{23}; G_{231}; C_2 - 5) \\
\gamma_{14}(C_2) &= J_2(\mu_{43}, M_{43}; G_{431}; C_2 - 5) \\
\gamma_{15}(\tilde{c}) &= J_2(\mu_{24}, M_{24}; G_{241}; \tilde{c} - 7) \\
\gamma_{16}(\tilde{c}) &= J_2(\mu_{44}, M_{44}; G_{441}; \tilde{c} - 7).
\end{aligned}
$$

(8) H_D^8:

$$
\begin{aligned}
\Delta E_D^8 &= -i\alpha^4 \delta_{JJ'} \delta_{M_J M_{J'}} (-1)^{L+S'+J} \begin{Bmatrix} L' & S' & J \\ S & L & 1 \end{Bmatrix} \\
&\times \langle \gamma' L' \| R^{(1)} \| \gamma L \rangle \langle S' \| \vec{\sigma}_1 \| S \rangle
\end{aligned}
$$

with

$$
\mathbf{R} = \nabla_1^2 \frac{\vec{r}}{r^3} \times (\frac{3}{4} \vec{\nabla}_2 - \frac{5}{8} \vec{\nabla}_1).
$$

The orbital part is

$$
\langle F' \mathcal{Y}^{M'}_{l_1' l_2' L'} | R_0^{(1)} | F \mathcal{Y}^{M}_{l_1 l_2 L} \rangle = (-1)^{L'-M'} \begin{pmatrix} L' & 1 & L \\ -M' & 0 & M \end{pmatrix} U(8) D,
$$

where

$$
U(8) = i\frac{\sqrt{6}}{16}(l_1, l_2, L, l_1', l_2', L')^{1/2}
$$

$$
\begin{aligned}
D &= 6\sum_{i=1}^{7}\text{coe}(S_i)\varpi_1(\mu_{13}, M_{13}; bG_{131} + G_{132}; A+1, B-1, C; \tilde\alpha, \tilde\beta) \\
&- 5\sum_{i=1}^{7}\text{coe}(S_i)\varpi_1(\mu_{13}, M_{13}; aG_{131} + G_{133}; A-1, B+1, C; \tilde\alpha, \tilde\beta) \\
&- 6\beta\sum_{i=1}^{7}\text{coe}(S_i)\varpi_1(\mu_{13}, M_{13}; G_{131}; A+1, B, C; \tilde\alpha, \tilde\beta) \\
&+ 5\alpha\sum_{i=1}^{7}\text{coe}(S_i)\varpi_1(\mu_{13}, M_{13}; G_{131}; A, B+1, C; \tilde\alpha, \tilde\beta) \\
&+ \sum_{i=1}^{7}\text{coe}(S_i)\varpi_1(\min(\mu_{11}, \mu_{12}), \max(M_{11}, M_{12}); 5G_{112} + 6G_{122}; A, B, C; \tilde\alpha, \tilde\beta) \\
&+ 6J_1(\mu_{12}, M_{12}; G_{122})\sum_{i=1}^{7}\text{coe}(S_i)\text{Dif}(A, B; A+1, B-1; \\
&\quad C, \tilde\alpha, \tilde\beta; \omega(\mu_{11}) - 2, \omega(\mu_{11}+1) - 2) \\
&+ 5J_1(\mu_{11}, M_{11}; G_{112})\sum_{i=1}^{7}\text{coe}(S_i)\text{Dif}(A, B; A-1, B+1; \\
&\quad C, \tilde\alpha, \tilde\beta; \omega(\mu_{11}) - 2, \omega(\mu_{11}+1) - 2) \\
&+ 6c'\varpi_1(\mu_{23}, M_{23}; bG_{231} + G_{232}; \tilde a, \tilde b, \tilde c - 5; \tilde\alpha, \tilde\beta) \\
&- 5c'\varpi_1(\mu_{23}, M_{23}; aG_{231} + G_{233}; \tilde a - 2, \tilde b + 2, \tilde c - 5; \tilde\alpha, \tilde\beta) \\
&- 6\beta c'\varpi_1(\mu_{23}, M_{23}; G_{231}; \tilde a, \tilde b + 1, \tilde c - 5; \tilde\alpha, \tilde\beta) \\
&+ 5\alpha c'\varpi_1(\mu_{23}, M_{23}; G_{231}; \tilde a - 1, \tilde b + 2, \tilde c - 5; \tilde\alpha, \tilde\beta) \\
&+ c'\varpi_1(\min(\mu_{21}, \mu_{22}), \max(M_{21}, M_{22}); 5G_{212} + 6G_{222}; \tilde a - 1, \tilde b + 1, \tilde c - 5; \tilde\alpha, \tilde\beta) \\
&+ 5c'J_1(\mu_{21}, M_{21}; G_{212})\text{Dif}(\tilde a - 1, \tilde b + 1; \tilde a - 2, \tilde b + 2; \\
&\quad \tilde c - 5, \tilde\alpha, \tilde\beta; \omega(\mu_{11}+1) - 2, \omega(\mu_{11}) - 2) \\
&+ 6c'J_1(\mu_{22}, M_{22}; G_{222})\text{Dif}(\tilde a - 1, \tilde b + 1; \tilde a, \tilde b; \\
&\quad \tilde c - 5, \tilde\alpha, \tilde\beta; \omega(\mu_{11}+1) - 2, \omega(\mu_{11}) - 2).
\end{aligned}
$$

Also,

$$
\begin{aligned}
M_{11} &= \min(l_1 + l_1' + 2, l_2 + l_2') \\
M_{12} &= \min(l_1 + l_1', l_2 + l_2' + 2) \\
M_{13} &= \min(l_1 + l_1' + 1, l_2 + l_2' + 1) \\
M_{21} &= \min(l_1 + l_1' + 3, l_2 + l_2' + 1)
\end{aligned}
$$

$$
\begin{aligned}
M_{22} &= \min(l_1 + l_1' + 1, l_2 + l_2' + 3) \\
M_{23} &= \min(l_1 + l_1' + 2, l_2 + l_2' + 2) \\
\mu_{ij} &= \omega(M_{ij}) - 2, \quad i = 1,2, \quad j = 1,2,3
\end{aligned}
$$

$$
\begin{aligned}
A &\equiv \tilde{a} + a'(i) \\
B &\equiv \tilde{b} + b'(i) \\
C &\equiv \tilde{c} + c'(i)
\end{aligned}
$$

$\mathrm{coe}(S_i)$	$a'(i)$	$b'(i)$	$c'(i)$
$a'(a'+1+c') - l_1'(l_1'+1)$	-2	0	-3
$-\alpha'[2(a'+1)+c']$	-1	0	-3
α'^2	0	0	-3
$c'(c'+1+a')$	0	0	-5
$-a'c'$	-2	2	-5
$-\alpha'c'$	1	0	-5
$\alpha'c'$	-1	2	-5

The angular coefficients are:

$$
\begin{aligned}
G_{112}(E) &= \sum_{TH}(T,H,E)G(T_{11},0)\tilde{G}(T_{11})b(l_1;T) \\
G_{122}(E) &= \sum_{TH}(T,H,E)G(T_{12},0)\tilde{G}(T_{12})b(l_2;T) \\
G_{131}(E) &= \sum_{TH}(T,H,E)G(T_{13},0)\tilde{G}(T_{13}) \\
G_{132}(E) &= \sum_{TH}(T,H,E)G(T_{13},0)\tilde{G}(T_{13})b(l_2;T) \\
G_{133}(E) &= \sum_{TH}(T,H,E)G(T_{13},0)\tilde{G}(T_{13})b(l_1;H) \\
G_{212}(E) &= \sum_{N'H'TH}(N',H',T,H,E)G(T_{21},0)\tilde{G}(T_{21})2b(l_1';N')b(l_1;T) \\
G_{222}(E) &= \sum_{N'H'TH}(N',H',T,H,E)G(T_{22},0)\tilde{G}(T_{22})2b(l_1';N')b(l_2;T) \\
G_{231}(E) &= \sum_{N'H'TH}(N',H',T,H,E)G(T_{23},0)\tilde{G}(T_{23})2b(l_1';N') \\
G_{232}(E) &= \sum_{N'H'TH}(N',H',T,H,E)G(T_{23},0)\tilde{G}(T_{23})2b(l_1';N')b(l_2;T) \\
G_{233}(E) &= \sum_{N'H'TH}(N',H',T,H,E)G(T_{23},0)\tilde{G}(T_{23})2b(l_1';N')b(l_1;H)
\end{aligned}
$$

with

$$
G(T_{11},0) = \begin{pmatrix} 1 & l_1 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & T & H \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_1' & H & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & l_2 & E \\ 0 & 0 & 0 \end{pmatrix}
$$

$$\tilde{G}(T_{11}) = (-1)^{1+L+L'+l_1+l_2'}\left\{\begin{array}{ccc} L & l_1 & l_2 \\ H & L' & 1 \end{array}\right\}\left\{\begin{array}{ccc} L' & l_1' & l_2' \\ E & l_2 & H \end{array}\right\}\left\{\begin{array}{ccc} 1 & 1 & 1 \\ l_1 & H & T \end{array}\right\}$$

$$G(T_{12},0) = \begin{pmatrix} 1 & l_2 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & T & H \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_1' & l_1 & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & H & E \\ 0 & 0 & 0 \end{pmatrix}$$

$$\tilde{G}(T_{12}) = (-1)^{1+l_1+l_2'}\left\{\begin{array}{ccc} L & l_1 & l_2 \\ H & 1 & L' \end{array}\right\}\left\{\begin{array}{ccc} L' & l_1' & l_2' \\ E & H & l_1 \end{array}\right\}\left\{\begin{array}{ccc} 1 & 1 & 1 \\ l_2 & H & T \end{array}\right\}$$

$$G(T_{13},0) = \begin{pmatrix} 1 & l_1 & H \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2 & 1 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_1' & H & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & T & E \\ 0 & 0 & 0 \end{pmatrix}$$

$$\tilde{G}(T_{13}) = (-1)^{L'+l_1+l_2'}\left\{\begin{array}{ccc} L' & l_1' & l_2' \\ E & T & H \end{array}\right\}\left\{\begin{array}{ccc} L & l_1 & l_2 \\ 1 & 1 & 1 \\ L' & H & T \end{array}\right\}$$

$$\begin{aligned} G(T_{21},0) &= \begin{pmatrix} l_1' & 1 & N' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & 1 & H' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_1 & T \\ 0 & 0 & 0 \end{pmatrix} \\ &\times \begin{pmatrix} 1 & T & H \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} N' & H & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} H' & l_2 & E \\ 0 & 0 & 0 \end{pmatrix} \end{aligned}$$

$$\begin{aligned} \tilde{G}(T_{21}) &= (-1)^{L+l_1+l_2'}\left\{\begin{array}{ccc} L & l_1 & l_2 \\ H & L' & 1 \end{array}\right\}\left\{\begin{array}{ccc} L' & l_1' & l_2' \\ 1 & H' & N' \end{array}\right\} \\ &\times \left\{\begin{array}{ccc} L' & H & l_2 \\ E & H' & N' \end{array}\right\}\left\{\begin{array}{ccc} 1 & 1 & 1 \\ l_1 & H & T \end{array}\right\} \end{aligned}$$

$$\begin{aligned} G(T_{22},0) &= \begin{pmatrix} l_1' & 1 & N' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & 1 & H' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_2 & T \\ 0 & 0 & 0 \end{pmatrix} \\ &\times \begin{pmatrix} 1 & T & H \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} N' & l_1 & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} H' & H & E \\ 0 & 0 & 0 \end{pmatrix} \end{aligned}$$

$$\begin{aligned} \tilde{G}(T_{22}) &= (-1)^{L'+l_1+l_2'}\left\{\begin{array}{ccc} L & l_1 & l_2 \\ H & 1 & L' \end{array}\right\}\left\{\begin{array}{ccc} L' & l_1' & l_2' \\ 1 & H' & N' \end{array}\right\} \\ &\times \left\{\begin{array}{ccc} 1 & 1 & 1 \\ l_2 & H & T \end{array}\right\}\left\{\begin{array}{ccc} L' & l_1 & H \\ E & H' & N' \end{array}\right\} \end{aligned}$$

$$\begin{aligned} G(T_{23},0) &= \begin{pmatrix} l_1' & 1 & N' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & 1 & H' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_1 & H \\ 0 & 0 & 0 \end{pmatrix} \\ &\times \begin{pmatrix} l_2 & 1 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} N' & H & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} H' & T & E \\ 0 & 0 & 0 \end{pmatrix} \end{aligned}$$

$$\tilde{G}(T_{23}) = (-1)^{1+l_1+l_2'}\left\{\begin{array}{ccc} L' & l_1' & l_2' \\ 1 & H' & N' \end{array}\right\}\left\{\begin{array}{ccc} L' & H & T \\ E & H' & N' \end{array}\right\}\left\{\begin{array}{ccc} L & l_1 & l_2 \\ 1 & 1 & 1 \\ L' & H & T \end{array}\right\}.$$

(9) H_D^9:

$$\begin{aligned} \Delta E_D^9 &= -\frac{3}{8} i\alpha^4 \delta_{JJ'}\delta_{M_J M_{J'}}(-1)^{L+S'+J}\left\{\begin{array}{ccc} L' & S' & J \\ S & L & 1 \end{array}\right\} \\ &\times \langle\gamma' L'\|R^{(1)}\|\gamma L\rangle\langle S'\|\vec{\sigma}_1\|S\rangle \end{aligned}$$

with

$$\mathbf{R} = \frac{1}{r^5}\vec{r} \times (\vec{r} \cdot \vec{\nabla}_2)\vec{\nabla}_1.$$

The orbital part is

$$\langle F'\mathcal{Y}^{M'}_{l_1'l_2'L'}|R^{(1)}_0|F\mathcal{Y}^{M}_{l_1l_2L}\rangle = (-1)^{L'-M'}\begin{pmatrix} L' & 1 & L \\ -M' & 0 & M \end{pmatrix}U(9)D,$$

where

$$U(9) = i\frac{\sqrt{6}}{2}(l_1, l_2, L, l_1', l_2', L')^{1/2}$$

and

$$D = \sum_{i=1}^{8}\text{Term}(i).$$

For Term(1),

$$\begin{aligned} T_1(k) &\equiv \varpi_k(\mu_{11}, M_{11}; G_{114}; \tilde{a}+1, \tilde{b}-1, \tilde{c}-5; \tilde{\alpha}, \tilde{\beta}) \\ &+ \varpi_k(\mu_{41}, M_{41}; G_{414}; \tilde{a}, \tilde{b}, \tilde{c}-5; \tilde{\alpha}, \tilde{\beta}) \\ \text{Term}(1) &= T_1(0), \quad \tilde{c} \geq 3 \\ \text{Term}(1) &= T_1(1), \quad 1 \leq \tilde{c} < 3 \\ \text{Term}(1) &= T_1(2) + \gamma_1\text{Dif}(\tilde{a}, \tilde{b}-2; \tilde{a}-1, \tilde{b}-1; \\ &\quad \tilde{c}-3, \tilde{\alpha}, \tilde{\beta}; \omega(\mu_{11}+1)-2, \omega(\mu_{11})-2), \quad \tilde{c} = 0. \end{aligned}$$

For Term(2),

$$\begin{aligned} T_2(k) &\equiv \varpi_k(\mu_{11}, M_{11}; G_{112}+G_{342}+G_{442}; \tilde{a}+1, \tilde{b}+1, \tilde{c}-7; \tilde{\alpha}, \tilde{\beta}) \\ &+ \varpi_k(\min(\mu_{13}, \mu_{14}, \mu_{41}), \max(M_{13}, M_{14}, M_{41}); \\ &\quad G_{132}+G_{142}+G_{413}; \tilde{a}+2, \tilde{b}, \tilde{c}-7; \tilde{\alpha}, \tilde{\beta}) \\ &+ \varpi_k(\mu_{24}, M_{24}; G_{242}+G_{312}+G_{412}; \tilde{a}, \tilde{b}+2, \tilde{c}-7; \tilde{\alpha}, \tilde{\beta}) \\ &+ \varpi_k(\mu_{21}, M_{21}; G_{212}; \tilde{a}-1, \tilde{b}+3, \tilde{c}-7; \tilde{\alpha}, \tilde{\beta}) \\ \text{Term}(2) &= c\Delta_2 \\ \Delta_2 &= T_2(0), \quad \tilde{c} \geq 5 \\ \Delta_2 &= T_2(1) + J_1(\mu_{11}, M_{11}; G_{112})[\eta(\mu_{11}, \tilde{c}-2)I_{\omega(\mu_{11})-2}(\tilde{a}-1, \tilde{b}+1, \tilde{c}-5) \end{aligned}$$

$$
\begin{aligned}
& - \quad \eta(\mu_{11}+1,\tilde{c}-2) I_{\omega(\mu_{11}+1)-2}(\tilde{a},\tilde{b},\tilde{c}-5)], \quad 3 \le \tilde{c} < 5 \\
\Delta_2 &= T_2(2) + \gamma_4 \mathrm{Dif}(\tilde{a}+1,\tilde{b}-1;\tilde{a},\tilde{b}; \\
& \quad \tilde{c}-5,\tilde{\alpha},\tilde{\beta};\omega(\mu_{11})-2,\omega(\mu_{11}+1)-2) \\
&+ (\gamma_3+\gamma_4)\mathrm{Dif}(\tilde{a},\tilde{b};\tilde{a}-1,\tilde{b}+1; \\
& \quad \tilde{c}-5,\tilde{\alpha},\tilde{\beta};\omega(\mu_{11}+1)-2,\omega(\mu_{11})-2) \\
&+ (\gamma_3+\gamma_4+\gamma_5)\mathrm{Dif}(\tilde{a}-1,\tilde{b}+1;\tilde{a}-2,\tilde{b}+2; \\
& \quad \tilde{c}-5,\tilde{\alpha},\tilde{\beta};\omega(\mu_{11})-2,\omega(\mu_{11}+1)-2), \quad 0 \le \tilde{c} < 3.
\end{aligned}
$$

For Term(3),

$$\mathrm{Term}(3) = 0.$$

For Term(4),

$$
\begin{aligned}
T_4(k) &\equiv \varpi_k(\mu_{21}, M_{21}; G_{211}; A, B+2, C-5; \tilde{\alpha}, \tilde{\beta}) \\
&+ \varpi_k(\mu_{41}, M_{41}; G_{411}; A+1, B+1, C-5; \tilde{\alpha}, \tilde{\beta}) \\
\mathrm{Term}(4) &= \sum_{i=1}^{8} \mathrm{coe}(A_i^{(1)}) \Delta_4(i) \\
\Delta_4(i) &= T_4(0), \quad C \ge 3 \\
\Delta_4(i) &= T_4(1), \quad 1 \le C < 3 \\
\Delta_4(i) &= T_4(2) + \gamma_7 \mathrm{Dif}(A-1, B+1; A, B; \\
& \quad C-3, \tilde{\alpha}, \tilde{\beta}; \omega(\mu_{11}+1)-2, \omega(\mu_{11})-2), \quad C = 0.
\end{aligned}
$$

For Term(5),

$$
\begin{aligned}
T_5(k) &\equiv \varpi_k(\mu_{11}, M_{11}; G_{112}; \tilde{a}+1, \tilde{b}+b^{(2)}(i), \tilde{c}-5; \tilde{\alpha}, \tilde{\beta}) \\
&+ \varpi_k(\mu_{31}, M_{31}; G_{312}+G_{412}; \tilde{a}, \tilde{b}+b^{(2)}(i)+1, \tilde{c}-5; \tilde{\alpha}, \tilde{\beta}) \\
&+ \varpi_k(\mu_{21}, M_{21}; G_{212}; \tilde{a}-1, \tilde{b}+b^{(2)}(i)+2, \tilde{c}-5; \tilde{\alpha}, \tilde{\beta}) \\
\mathrm{Term}(5) &= \sum_{i=1}^{2} \mathrm{coe}(A_i^{(2)}) \Delta_5(i) + \mathrm{Term}(5)' \\
\Delta_5(i) &= T_5(0), \quad \tilde{c} \ge 3 \\
\Delta_5(i) &= T_5(1) + J_1(\mu_{11}, M_{11}; G_{112}) \eta(\mu_{11}, \tilde{c}) I_{\omega(\mu_{11})-2}(\tilde{a}-1, \tilde{b}+b^{(2)}(i), \tilde{c}-3), \\
& \quad 1 \le \tilde{c} < 3
\end{aligned}
$$

$$
\begin{aligned}
\Delta_5(i) &= T_5(2) + \gamma_9 \mathrm{Dif}(\tilde{a}, \tilde{b} + b^{(2)}(i) - 1; \tilde{a} - 1, \tilde{b} + b^{(2)}(i); \\
&\quad \tilde{c} - 3, \tilde{\alpha}, \tilde{\beta}; \omega(\mu_{11} + 1) - 2, \omega(\mu_{11}) - 2) \\
&+ (\gamma_9 + \gamma_{11}) \mathrm{Dif}(\tilde{a} - 1, \tilde{b} + b^{(2)}(i); \tilde{a} - 2, \tilde{b} + b^{(2)}(i) + 1; \\
&\quad \tilde{c} - 3, \tilde{\alpha}, \tilde{\beta}; \omega(\mu_{11}) - 2, \omega(\mu_{11} + 1) - 2), \quad \tilde{c} = 0 \\
\mathrm{Term}(5)' &= [b S_5(l_1{}' l_2{}' l_1 l_2) \mathrm{Can}(\tilde{a} - 2, \tilde{b}, \tilde{\alpha}, \tilde{\beta}; \tilde{a}' - 2, \tilde{b}', \tilde{\alpha}', \tilde{\beta}'; \\
&\quad \tilde{c} - 3; \omega(\mu_{11} + 1) - 2, \omega(\mu_{11} + 1 + L) - 2) \\
&- \beta S_5(l_1{}' l_2{}' l_1 l_2) \mathrm{Can}(\tilde{a} - 2, \tilde{b} + 1, \tilde{\alpha}, \tilde{\beta}; \tilde{a}' - 2, \tilde{b}' + 1, \tilde{\alpha}', \tilde{\beta}'; \\
&\quad \tilde{c} - 3; \omega(\mu_{11} + 1) - 2, \omega(\mu_{11} + 1 + L) - 2) \\
&+ a S_5(l_2{}' l_1{}' l_2 l_1) \mathrm{Can}(\tilde{a}, \tilde{b} - 2, \tilde{c}, \tilde{\beta}; \tilde{a}', \tilde{b}' - 2, \tilde{\alpha}', \tilde{\beta}'; \\
&\quad \tilde{c} - 3; \omega(\mu_{11} + 1) - 2, \omega(\mu_{11} + 1 + L) - 2) \\
&- \alpha S_5(l_2{}' l_1{}' l_2 l_1) \mathrm{Can}(\tilde{a} + 1, \tilde{b} - 2, \tilde{\alpha}, \tilde{\beta}; \tilde{a}' + 1, \tilde{b}' - 2, \tilde{\alpha}', \tilde{\beta}'; \\
&\quad \tilde{c} - 3; \omega(\mu_{11} + 1) - 2, \omega(\mu_{11} + 1 + L) - 2)] \delta(X_R, 1) \delta(X_L, 1) \delta(\tilde{c}, 0).
\end{aligned}
$$

For Term(6),

$$
\begin{aligned}
T_6(k) &\equiv \varpi_k(\mu_{41}, M_{41}; G_{413}; \tilde{a} + a^{(3)}(i) + 1, \tilde{b}, \tilde{c} - 5; \tilde{\alpha}, \tilde{\beta}) \\
\mathrm{Term}(6) &= \sum_{i=1}^{2} \mathrm{coe}(A_i^{(3)}) \Delta_6(i) + \mathrm{Term}(6)' \\
\Delta_6(i) &= T_6(0), \quad \tilde{c} \geq 3 \\
\Delta_6(i) &= T_6(1), \quad 1 \leq \tilde{c} < 3 \\
\Delta_6(i) &= T_6(2), \quad \tilde{c} = 0 \\
\mathrm{Term}(6)' &= [(a\gamma_{12}(l_1{}' l_2{}' l_1 l_2) + b\gamma_{12}(l_2{}' l_1{}' l_2 l_1)) \mathrm{Can}(\tilde{a} - 1, \tilde{b} - 1, \tilde{\alpha}, \tilde{\beta}; \tilde{a}' - 1, \tilde{b}' - 1, \\
&\quad \tilde{\alpha}', \tilde{\beta}'; \tilde{c} - 3; \omega(\mu_{11}) - 2, \omega(\mu_{11} + L) - 2) \\
&- \alpha\gamma_{12}(l_1{}' l_2{}' l_1 l_2) \mathrm{Can}(\tilde{a}, \tilde{b} - 1, \tilde{\alpha}, \tilde{\beta}; \tilde{a}', \tilde{b}' - 1, \tilde{\alpha}', \tilde{\beta}'; \\
&\quad \tilde{c} - 3; \omega(\mu_{11}) - 2, \omega(\mu_{11} + L) - 2) \\
&- \beta\gamma_{12}(l_2{}' l_1{}' l_2 l_1) \mathrm{Can}(\tilde{a} - 1, \tilde{b}, \tilde{\alpha}, \tilde{\beta}; \tilde{a}' - 1, \tilde{b}', \tilde{\alpha}', \tilde{\beta}'; \\
&\quad \tilde{c} - 3; \omega(\mu_{11}) - 2, \omega(\mu_{11} + L) - 2)] \delta(X_R, 1) \delta(X_L, 1) \delta(\tilde{c}, 0).
\end{aligned}
$$

For Term(7),

$$
T_7(k) \equiv \varpi_k(\mu_{13}, M_{13}; G_{131}; \tilde{a} + 2, \tilde{b} + b^{(4)}(i), \tilde{c} - 7; \tilde{\alpha}, \tilde{\beta})
$$

$$
\begin{aligned}
& + \quad \varpi_k(\mu_{33}, M_{33}; G_{331}; \tilde{a}+1, \tilde{b}+b^{(4)}(i)+1, \tilde{c}-7; \tilde{\alpha}, \tilde{\beta}) \\
\text{Term}(7) &= \sum_{i=1}^{2} \text{coe}(A_i^{(4)})\Delta_7(i) \\
\Delta_7(i) &= T_7(0), \quad \tilde{c} \geq 5 \\
\Delta_7(i) &= T_7(1), \quad 3 \leq \tilde{c} < 5 \\
\Delta_7(i) &= T_7(2) + \gamma_{13}\text{Dif}(\tilde{a}+1, \tilde{b}+b^{(4)}(i)-1; \tilde{a}, \tilde{b}+b^{(4)}(i); \\
& \quad \tilde{c}-5, \tilde{\alpha}, \tilde{\beta}; \omega(\mu_{11})-2, \omega(\mu_{11}+1)-2), \quad \tilde{c} < 3.
\end{aligned}
$$

For Term(8),

$$
\begin{aligned}
T_8(k) &\equiv \varpi_k(\mu_{24}, M_{24}; G_{241}; \tilde{a}+a^{(5)}(i), \tilde{b}+2, \tilde{c}-7; \tilde{\alpha}, \tilde{\beta}) \\
& + \quad \varpi_k(\mu_{44}, M_{44}; G_{441}; \tilde{a}+a^{(5)}(i)+1, \tilde{b}+1, \tilde{c}-7; \tilde{\alpha}, \tilde{\beta}) \\
\text{Term}(8) &= \sum_{i=1}^{2} \text{coe}(A_i^{(5)})\Delta_8(i) \\
\Delta_8(i) &= T_8(0), \quad \tilde{c} \geq 5 \\
\Delta_8(i) &= T_8(1), \quad 3 \leq \tilde{c} < 5 \\
\Delta_8(i) &= T_8(2) + \gamma_{15}\text{Dif}(\tilde{a}+a^{(5)}(i)-1, \tilde{b}+1; \tilde{a}+a^{(5)}(i), \tilde{b}; \\
& \quad \tilde{c}-5, \tilde{\alpha}, \tilde{\beta}; \omega(\mu_{11})-2, \omega(\mu_{11}+1)-2), \quad \tilde{c} < 3.
\end{aligned}
$$

Also,

$$
\begin{aligned}
M_{11} &= \min(l_1 + l_1' + 3, l_2 + l_2' + 1) \\
M_{12} &= \min(l_1 + l_1' + 3, l_2 + l_2' + 1) \\
M_{13} &= \min(l_1 + l_1' + 2, l_2 + l_2' + 2) \\
M_{14} &= \min(l_1 + l_1' + 4, l_2 + l_2') \\
M_{21} &= \min(l_1 + l_1' + 1, l_2 + l_2' + 3) \\
M_{22} &= \min(l_1 + l_1' + 1, l_2 + l_2' + 3) \\
M_{23} &= \min(l_1 + l_1', l_2 + l_2' + 4) \\
M_{24} &= \min(l_1 + l_1' + 2, l_2 + l_2' + 2) \\
M_{31} &= \min(l_1 + l_1' + 2, l_2 + l_2' + 2) \\
M_{32} &= \min(l_1 + l_1' + 2, l_2 + l_2' + 2) \\
M_{33} &= \min(l_1 + l_1' + 1, l_2 + l_2' + 3)
\end{aligned}
$$

$$
\begin{aligned}
M_{34} &= \min(l_1 + l_1' + 3, l_2 + l_2' + 1) \\
M_{41} &= \min(l_1 + l_1' + 2, l_2 + l_2' + 2) \\
M_{42} &= \min(l_1 + l_1' + 2, l_2 + l_2' + 2) \\
M_{43} &= \min(l_1 + l_1' + 1, l_2 + l_2' + 3) \\
M_{44} &= \min(l_1 + l_1' + 3, l_2 + l_2' + 1) \\
\mu_{ij} &= \omega(M_{ij}) - 2, \quad i, j = 1, \cdots, 4
\end{aligned}
$$

coe($A_i^{(1)}$)	$a^{(1)}(i)$	$b^{(1)}(i)$	$c^{(1)}(i)$
ab	-1	-1	0
$-a\beta$	-1	0	0
$-b\alpha$	0	-1	0
$\alpha\beta$	0	0	0
ac	-1	1	-2
bc	1	-1	-2
$-c\alpha$	0	1	-2
$-c\beta$	1	0	-2
$c(c-2)$	1	1	-4

coe($A_i^{(2)}$)	$b^{(2)}(i)$	$c^{(2)}(i)$
b	-1	0
$-\beta$	0	0
c	1	-2

coe($A_i^{(3)}$)	$a^{(3)}(i)$	$c^{(2)}(i)$
a	-1	0
$-\alpha$	0	0
c	1	-2

coe($A_i^{(4)}$)	$b^{(4)}(i)$	$c^{(4)}(i)$
bc	0	-2
$-\beta c$	1	-2
$c(c-2)$	2	-4

coe($A_i^{(5)}$)	$a^{(5)}(i)$	$c^{(5)}(i)$
$c(a+1)$	0	-2
$-\alpha c$	1	-2
$c(c-2)$	2	-4

$$
\begin{aligned}
A &\equiv \tilde{a} + a^{(1)}(i) \\
B &\equiv \tilde{b} + b^{(1)}(i) \\
C &\equiv \tilde{c} + c^{(1)}(i).
\end{aligned}
$$

The angular coefficients are:

$$
\begin{aligned}
G_{112}(\Omega) &= \sum_{\Lambda PTN} (\Lambda, P, T, N, \Omega) G(J_{11}, 0) \tilde{G}(J_{11}) b(l_1; N) \\
G_{114}(\Omega) &= \sum_{\Lambda PTN} (\Lambda, P, T, N, \Omega) G(J_{11}, 0) \tilde{G}(J_{11}) b(l_1; N) b(l_2; T) \\
G_{12}(\Omega) &= \sum_{\Lambda PTN} (\Lambda, P, T, N, \Omega) G(J_{12}, 0) \tilde{G}(J_{12}) \\
G_{131}(\Omega) &= \sum_{\Lambda PTN} (\Lambda, P, T, N, \Omega) G(J_{13}, 0) \tilde{G}(J_{13}) \\
G_{132}(\Omega) &= \sum_{\Lambda PTN} (\Lambda, P, T, N, \Omega) G(J_{13}, 0) \tilde{G}(J_{13}) b(l_2; T) \\
G_{142}(\Omega) &= \sum_{\Lambda PTN} (\Lambda, P, T, N, \Omega) G(J_{14}, 0) \tilde{G}(J_{14}) b(T; N) \\
G_{211}(\Omega) &= \sum_{\Lambda PTN} (\Lambda, P, T, N, \Omega) G(J_{21}, 0) \tilde{G}(J_{21}) \\
G_{212}(\Omega) &= \sum_{\Lambda PTN} (\Lambda, P, T, N, \Omega) G(J_{21}, 0) \tilde{G}(J_{21}) b(l_1; N) \\
G_{241}(\Omega) &= \sum_{\Lambda PTN} (\Lambda, P, T, N, \Omega) G(J_{24}, 0) \tilde{G}(J_{24}) \\
G_{242}(\Omega) &= \sum_{\Lambda PTN} (\Lambda, P, T, N, \Omega) G(J_{24}, 0) \tilde{G}(J_{24}) b(T; N) \\
G_{312}(\Omega) &= \sum_{\Lambda PTN} (\Lambda, P, T, N, \Omega) G(J_{31}, 0) \tilde{G}(J_{31}) b(l_1; N) \\
G_{32}(\Omega) &= \sum_{\Lambda PTN} (\Lambda, P, T, N, \Omega) G(J_{32}, 0) \tilde{G}(J_{32}) \\
G_{331}(\Omega) &= \sum_{\Lambda PTN} (\Lambda, P, T, N, \Omega) G(J_{33}, 0) \tilde{G}(J_{33}) \\
G_{342}(\Omega) &= \sum_{\Lambda PTN} (\Lambda, P, T, N, \Omega) G(J_{34}, 0) \tilde{G}(J_{34}) b(T; N) \\
G_{411}(\Omega) &= \sum_{\Lambda PTN} (\Lambda, P, T, N, \Omega) G(J_{41}, 0) \tilde{G}(J_{41}) \\
G_{412}(\Omega) &= \sum_{\Lambda PTN} (\Lambda, P, T, N, \Omega) G(J_{41}, 0) \tilde{G}(J_{41}) b(l_1; N) \\
G_{413}(\Omega) &= \sum_{\Lambda PTN} (\Lambda, P, T, N, \Omega) G(J_{41}, 0) \tilde{G}(J_{41}) b(l_2; T) \\
G_{414}(\Omega) &= \sum_{\Lambda PTN} (\Lambda, P, T, N, \Omega) G(J_{41}, 0) \tilde{G}(J_{41}) b(l_1; N) b(l_2; T) \\
G_{441}(\Omega) &= \sum_{\Lambda PTN} (\Lambda, P, T, N, \Omega) G(J_{44}, 0) \tilde{G}(J_{44})
\end{aligned}
$$

$$G_{442}(\Omega) = \sum_{\Lambda PTN} (\Lambda, P, T, N, \Omega) G(J_{44}, 0) \tilde{G}(J_{44}) b(T; N)$$

with

$$
\begin{aligned}
G(J_{11},0) &= \begin{pmatrix} 1 & 1 & \Lambda \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1' & \Lambda & P \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & l_1 & N \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & l_2 & T \\ 0 & 0 & 0 \end{pmatrix} \\
&\times \begin{pmatrix} P & N & \Omega \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2' & T & \Omega \\ 0 & 0 & 0 \end{pmatrix} \\
\tilde{G}(J_{11}) &= (-1)^{1+L+L'} \sum_{\lambda_1 \lambda_2} (-1)^{\lambda_2} (\lambda_1, \lambda_2) \begin{Bmatrix} l_2 & 1 & T \\ \lambda_2 & L & l_1 \end{Bmatrix} \begin{Bmatrix} L & \lambda_2 & T \\ \lambda_1 & L' & 1 \end{Bmatrix} \\
&\times \begin{Bmatrix} T & \Omega & l_2' \\ l_1' & L' & \lambda_1 \end{Bmatrix} \begin{Bmatrix} \Omega & N & P \\ \Lambda & l_1' & \lambda_1 \end{Bmatrix} \begin{Bmatrix} \lambda_2 & l_1 & 1 \\ \lambda_1 & N & \Lambda \\ 1 & 1 & 1 \end{Bmatrix} \\
G(J_{12},0) &= \begin{pmatrix} 1 & 1 & \Lambda \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1' & \Lambda & P \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & l_1 & N \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & l_2 & T \\ 0 & 0 & 0 \end{pmatrix} \\
&\times \begin{pmatrix} P & N & \Omega \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2' & T & \Omega \\ 0 & 0 & 0 \end{pmatrix} \\
\tilde{G}(J_{12}) &= (-1)^{L+L'} \sum_{\lambda_1} (-1)^{\lambda_1} (2\lambda_1 + 1) \begin{Bmatrix} l_1 & 1 & N \\ \Lambda & \lambda_1 & 1 \end{Bmatrix} \begin{Bmatrix} T & \Omega & l_2' \\ l_1' & L' & \lambda_1 \end{Bmatrix} \\
&\times \begin{Bmatrix} \Omega & N & P \\ \Lambda & l_1' & \lambda_1 \end{Bmatrix} \begin{Bmatrix} L & l_1 & l_2 \\ 1 & 1 & 1 \\ L' & \lambda_1 & T \end{Bmatrix}
\end{aligned}
$$

$$
\begin{aligned}
G(J_{13},0) &= \begin{pmatrix} 1 & 1 & \Lambda \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1' & \Lambda & P \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & l_2 & T \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} T & 1 & N \\ 0 & 0 & 0 \end{pmatrix} \\
&\times \begin{pmatrix} P & l_1 & \Omega \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2' & N & \Omega \\ 0 & 0 & 0 \end{pmatrix} \\
\tilde{G}(J_{13}) &= (-1)^{L'} \sum_{\lambda_1 \lambda_2} (-1)^{\lambda_1} (\lambda_1, \lambda_2) \begin{Bmatrix} l_2 & l_1 & L \\ \lambda_2 & T & 1 \end{Bmatrix} \begin{Bmatrix} \lambda_2 & 1 & l_1 \\ \Lambda & \lambda_1 & 1 \end{Bmatrix} \\
&\times \begin{Bmatrix} N & \Omega & l_2' \\ l_1' & L' & \lambda_1 \end{Bmatrix} \begin{Bmatrix} \Omega & l_1 & P \\ \Lambda & l_1' & \lambda_1 \end{Bmatrix} \begin{Bmatrix} L & \lambda_2 & T \\ 1 & 1 & 1 \\ L' & \lambda_1 & N \end{Bmatrix} \\
G(J_{14},0) &= \begin{pmatrix} 1 & 1 & \Lambda \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1' & \Lambda & P \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & l_1 & T \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & T & N \\ 0 & 0 & 0 \end{pmatrix} \\
&\times \begin{pmatrix} P & N & \Omega \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2' & l_2 & \Omega \\ 0 & 0 & 0 \end{pmatrix} \\
\tilde{G}(J_{14}) &= (-1)^{1+l_2+L+L'} \sum_{\lambda_1} (2\lambda_1 + 1) \begin{Bmatrix} L & l_1 & l_2 \\ \lambda_1 & L' & 1 \end{Bmatrix} \begin{Bmatrix} l_2 & \Omega & l_2' \\ l_1' & L' & \lambda_1 \end{Bmatrix} \\
&\times \begin{Bmatrix} \Omega & N & P \\ \Lambda & l_1' & \lambda_1 \end{Bmatrix} \begin{Bmatrix} l_1 & 1 & T \\ 1 & 1 & 1 \\ \lambda_1 & \Lambda & N \end{Bmatrix}
\end{aligned}
$$

$$G(J_{21},0) = \begin{pmatrix} 1 & 1 & \Lambda \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & \Lambda & P \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_1 & N \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_2 & T \\ 0 & 0 & 0 \end{pmatrix}$$
$$\times \begin{pmatrix} l_1' & N & \Omega \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} P & T & \Omega \\ 0 & 0 & 0 \end{pmatrix}$$
$$\tilde{G}(J_{21}) = (-1)^{1+L}\sum_{\lambda_1\lambda_2}(-1)^{\lambda_2}(\lambda_1,\lambda_2)\begin{Bmatrix} L & l_1 & l_2 \\ \lambda_2 & L' & 1 \end{Bmatrix}\begin{Bmatrix} L' & \lambda_2 & l_2 \\ 1 & T & \lambda_1 \end{Bmatrix}$$
$$\times \begin{Bmatrix} \lambda_2 & 1 & l_1 \\ 1 & N & 1 \end{Bmatrix}\begin{Bmatrix} 1 & \lambda_2 & \lambda_1 \\ N & \Lambda & 1 \end{Bmatrix}\begin{Bmatrix} T & \Omega & P \\ \lambda_1 & N & \Lambda \\ L' & l_1' & l_2' \end{Bmatrix}$$
$$G(J_{22},0) = \begin{pmatrix} 1 & 1 & \Lambda \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & \Lambda & P \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_1 & N \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_2 & T \\ 0 & 0 & 0 \end{pmatrix}$$
$$\times \begin{pmatrix} l_1' & N & \Omega \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} P & T & \Omega \\ 0 & 0 & 0 \end{pmatrix}$$
$$\tilde{G}(J_{22}) = (-1)^{1+l_1+L'}\sum_{\lambda_1}(2\lambda_1+1)\begin{Bmatrix} l_1 & 1 & N \\ \Lambda & \lambda_1 & 1 \end{Bmatrix}\begin{Bmatrix} L & l_1 & l_2 \\ 1 & 1 & 1 \\ L' & \lambda_1 & T \end{Bmatrix}\begin{Bmatrix} T & \Omega & P \\ \lambda_1 & N & \Lambda \\ L' & l_1' & l_2' \end{Bmatrix}$$

$$G(J_{23},0) = \begin{pmatrix} 1 & 1 & \Lambda \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & \Lambda & P \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_2 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} T & 1 & N \\ 0 & 0 & 0 \end{pmatrix}$$
$$\times \begin{pmatrix} l_1' & l_1 & \Omega \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} P & N & \Omega \\ 0 & 0 & 0 \end{pmatrix}$$
$$\tilde{G}(J_{23}) = (-1)^{L+L'+l_1}\sum_{\lambda_1\lambda_2}(\lambda_1,\lambda_2)\begin{Bmatrix} L & l_1 & l_2 \\ 1 & T & \lambda_2 \end{Bmatrix}\begin{Bmatrix} l_1 & \lambda_1 & \Lambda \\ 1 & 1 & \lambda_2 \end{Bmatrix}$$
$$\times \begin{Bmatrix} L & \lambda_2 & T \\ 1 & 1 & 1 \\ L' & \lambda_1 & N \end{Bmatrix}\begin{Bmatrix} L' & \lambda_1 & N \\ l_2' & \Lambda & P \\ l_1' & l_1 & \Omega \end{Bmatrix}$$
$$G(J_{24},0) = \begin{pmatrix} 1 & 1 & \Lambda \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & \Lambda & P \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_1 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & T & N \\ 0 & 0 & 0 \end{pmatrix}$$
$$\times \begin{pmatrix} l_1' & N & \Omega \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} P & l_2 & \Omega \\ 0 & 0 & 0 \end{pmatrix}$$
$$\tilde{G}(J_{24}) = (-1)^{1+L+L'}\sum_{\lambda_1}(-1)^{\lambda_1}(2\lambda_1+1)\begin{Bmatrix} L & l_1 & l_2 \\ \lambda_1 & L' & 1 \end{Bmatrix}\begin{Bmatrix} l_1 & 1 & T \\ 1 & 1 & 1 \\ \lambda_1 & \Lambda & N \end{Bmatrix}$$
$$\times \begin{Bmatrix} \lambda_1 & \Lambda & N \\ l_2 & P & \Omega \\ L' & l_2' & l_1' \end{Bmatrix}$$

$$G(J_{31},0) = \begin{pmatrix} l_1' & 1 & \Lambda \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & 1 & P \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_1 & N \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_2 & T \\ 0 & 0 & 0 \end{pmatrix}$$
$$\times \begin{pmatrix} \Lambda & N & \Omega \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} P & T & \Omega \\ 0 & 0 & 0 \end{pmatrix}$$

$$\tilde{G}(J_{31}) = (-1)^{1+l_1'+l_2+L+L'}\sum_{\lambda_1}(2\lambda_1+1)\begin{Bmatrix} L & l_1 & l_2 \\ \lambda_1 & L' & 1 \end{Bmatrix}\begin{Bmatrix} l_1 & 1 & N \\ 1 & \lambda_1 & 1 \end{Bmatrix}$$

$$\times \begin{Bmatrix} \lambda_1 & N & 1 \\ \Lambda & l_1' & \Omega \end{Bmatrix}\begin{Bmatrix} \lambda_1 & l_2 & L' \\ l_2' & l_1' & \Omega \end{Bmatrix}\begin{Bmatrix} l_2 & T & 1 \\ P & l_2' & \Omega \end{Bmatrix}$$

$$G(J_{32},0) = \begin{pmatrix} l_1' & 1 & \Lambda \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & 1 & P \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_1 & N \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times \begin{pmatrix} 1 & l_2 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} \Lambda & N & \Omega \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} P & T & \Omega \\ 0 & 0 & 0 \end{pmatrix}$$

$$\tilde{G}(J_{32}) = (-1)^{1+l_2+L+L'}\sum_{\lambda_1,\lambda_2,\lambda_3}(-1)^{\lambda_3}(\lambda_1\lambda_2\lambda_3)\begin{Bmatrix} L & l_1 & l_2 \\ \lambda_1 & L' & 1 \end{Bmatrix}\begin{Bmatrix} L' & \lambda_1 & l_2 \\ 1 & T & \lambda_2 \end{Bmatrix}$$

$$\times \begin{Bmatrix} \lambda_1 & l_1 & 1 \\ 1 & 1 & \lambda_2 \end{Bmatrix}\begin{Bmatrix} T & \Omega & P \\ \lambda_3 & L' & \lambda_2 \end{Bmatrix}\begin{Bmatrix} L' & \lambda_3 & P \\ 1 & l_2' & l_1' \end{Bmatrix}\begin{Bmatrix} \lambda_2 & l_1 & 1 \\ \Omega & N & \Lambda \\ \lambda_3 & 1 & l_1' \end{Bmatrix}$$

$$G(J_{33},0) = \begin{pmatrix} l_1' & 1 & \Lambda \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & 1 & P \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_2 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} T & 1 & N \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times \begin{pmatrix} \Lambda & l_1 & \Omega \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} P & N & \Omega \\ 0 & 0 & 0 \end{pmatrix}$$

$$\tilde{G}(J_{33}) = (-1)^{l_1'+l_2+L}\sum_{\lambda_1\lambda_2\lambda_3}(-1)^{\lambda_1+\lambda_2}(\lambda_1,\lambda_2,\lambda_3)\begin{Bmatrix} 1 & 1 & 1 \\ l_1 & \lambda_2 & \lambda_1 \end{Bmatrix}\begin{Bmatrix} \lambda_2 & l_1 & 1 \\ \Lambda & l_1' & \Omega \end{Bmatrix}$$

$$\times \begin{Bmatrix} L & l_1 & l_2 \\ \lambda_1 & L' & 1 \end{Bmatrix}\begin{Bmatrix} L' & \lambda_1 & l_2 \\ N & 1 & T \\ \lambda_3 & \lambda_2 & 1 \end{Bmatrix}\begin{Bmatrix} \lambda_3 & 1 & \lambda_2 \\ N & P & \Omega \\ L' & l_2' & l_1' \end{Bmatrix}$$

$$G(J_{34},0) = \begin{pmatrix} l_1' & 1 & \Lambda \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & 1 & P \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_1 & T \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times \begin{pmatrix} 1 & T & N \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} \Lambda & N & \Omega \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} P & l_2 & \Omega \\ 0 & 0 & 0 \end{pmatrix}$$

$$\tilde{G}(J_{34}) = (-1)^{l_1}\sum_{\lambda_1}(-1)^{\lambda_1}(2\lambda_1+1)\begin{Bmatrix} L & \lambda_1 & l_2' \\ l_1' & L' & 1 \end{Bmatrix}\begin{Bmatrix} \lambda_1 & T & \Omega \\ N & \Lambda & 1 \end{Bmatrix}$$

$$\times \begin{Bmatrix} \lambda_1 & \Lambda & 1 \\ 1 & 1 & l_1' \end{Bmatrix}\begin{Bmatrix} L & l_1 & l_2 \\ l_2' & 1 & P \\ \lambda_1 & T & \Omega \end{Bmatrix}$$

$$G(J_{41},0) = \begin{pmatrix} l_1' & 1 & \Lambda \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & 1 & P \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_1 & N \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_2 & T \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times \begin{pmatrix} \Lambda & N & \Omega \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} P & T & \Omega \\ 0 & 0 & 0 \end{pmatrix}$$

$$\tilde{G}(J_{41}) = (-1)^{l_1'+L}\sum_{\lambda_1\lambda_2\lambda_3}(-1)^{\lambda_1+\lambda_2+\lambda_3}(\lambda_1,\lambda_2,\lambda_3)\begin{Bmatrix} L & l_1 & l_2 \\ \lambda_1 & L' & 1 \end{Bmatrix}\begin{Bmatrix} l_1 & 1 & N \\ 1 & \lambda_1 & 1 \end{Bmatrix}$$

$$\times\ \begin{Bmatrix} \lambda_2 & \lambda_1 & \Omega \\ N & \Lambda & 1 \end{Bmatrix}\begin{Bmatrix} \lambda_3 & \lambda_2 & 1 \\ \Lambda & l_1' & 1 \end{Bmatrix}\begin{Bmatrix} P & \lambda_3 & L' \\ l_1' & l_2' & 1 \end{Bmatrix}\begin{Bmatrix} L' & \lambda_1 & l_2 \\ P & \Omega & T \\ \lambda_3 & \lambda_2 & 1 \end{Bmatrix}$$

$$G(J_{42},0) = \begin{pmatrix} l_1' & 1 & \Lambda \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & 1 & P \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_1 & N \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times\ \begin{pmatrix} 1 & l_2 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} \Lambda & N & \Omega \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} P & T & \Omega \\ 0 & 0 & 0 \end{pmatrix}$$

$$\tilde{G}(J_{42}) = (-1)^{1+l_1+l_2'}\sum_{\lambda_1}(2\lambda_1+1)\begin{Bmatrix} l_1 & N & 1 \\ \Lambda & l_1' & \Omega \end{Bmatrix}\begin{Bmatrix} L & l_1 & l_2 \\ 1 & 1 & 1 \\ L' & \lambda_1 & T \end{Bmatrix}\begin{Bmatrix} \lambda_1 & l_1 & 1 \\ T & \Omega & P \\ L' & l_1' & l_2' \end{Bmatrix}$$

$$G(J_{43},0) = \begin{pmatrix} l_1' & 1 & \Lambda \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & 1 & P \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_2 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} T & 1 & N \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times\ \begin{pmatrix} \Lambda & l_1 & \Omega \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} P & N & \Omega \\ 0 & 0 & 0 \end{pmatrix}$$

$$\tilde{G}(J_{43}) = (-1)^{1+l_2'+L}\sum_{\lambda_1\lambda_2}(-1)^{\lambda_1}(\lambda_1,\lambda_2)\begin{Bmatrix} l_2 & l_1 & L \\ \lambda_1 & T & 1 \end{Bmatrix}\begin{Bmatrix} l_1 & \Lambda & \Omega \\ l_1' & \lambda_1 & 1 \end{Bmatrix}$$

$$\times\ \begin{Bmatrix} L & \lambda_1 & T \\ 1 & 1 & 1 \\ L' & \lambda_2 & N \end{Bmatrix}\begin{Bmatrix} \lambda_2 & \lambda_1 & 1 \\ N & \Omega & P \\ L' & l_1' & l_2' \end{Bmatrix}$$

$$G(J_{44},0) = \begin{pmatrix} l_1' & 1 & \Lambda \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & 1 & P \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_1 & T \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times\ \begin{pmatrix} 1 & T & N \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} \Lambda & N & \Omega \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} P & l_2 & \Omega \\ 0 & 0 & 0 \end{pmatrix}$$

$$\tilde{G}(J_{44}) = (-1)^{1+l_2'+L}\sum_{\lambda_1\lambda_2}(-1)^{\lambda_1}(\lambda_1,\lambda_2)\begin{Bmatrix} L & l_1 & l_2 \\ \lambda_2 & L' & 1 \end{Bmatrix}\begin{Bmatrix} l_1 & 1 & \lambda_1 \\ 1 & \lambda_2 & 1 \end{Bmatrix}$$

$$\times\ \begin{Bmatrix} 1 & l_1 & \lambda_1 \\ 1 & N & T \end{Bmatrix}\begin{Bmatrix} N & 1 & \lambda_1 \\ l_1' & \Omega & \Lambda \end{Bmatrix}\begin{Bmatrix} \lambda_2 & \lambda_1 & 1 \\ l_2 & \Omega & P \\ L' & l_1' & l_2' \end{Bmatrix}.$$

We have also defined:

$$\gamma_1(l_1'l_2'l_1l_2;\tilde{c}) = J_2(\mu_{11},M_{11};G_{114};\tilde{c}-5)$$

$$\gamma_2(l_1'l_2'l_1l_2;\tilde{c}) = J_2(\mu_{41},M_{41};G_{414};\tilde{c}-5)$$

$$\gamma_3(l_1'l_2'l_1l_2;\tilde{c}) = J_2(\mu_{11},M_{11};G_{112};\tilde{c}-7) + J_2(\mu_{34},M_{34};G_{342};\tilde{c}-7)$$
$$+\ J_2(\mu_{44},M_{44};G_{442};\tilde{c}-7) - J_1(\mu_{11},M_{11};G_{112})\eta(\mu_{11}+1,\tilde{c}-2)$$

$$\gamma_4(l_1'l_2'l_1l_2;\tilde{c}) = J_2(\mu_{13},M_{13};G_{132};\tilde{c}-7) + J_2(\mu_{14},M_{14};G_{142};\tilde{c}-7)$$
$$+\ J_2(\mu_{41},M_{41};G_{413};\tilde{c}-7)$$

$$
\begin{aligned}
\gamma_5(l_1'l_2'l_1l_2;\tilde{c}) &= J_2(\mu_{24},M_{24};G_{242};\tilde{c}-7)+J_2(\mu_{31},M_{31};G_{312};\tilde{c}-7)\\
&+ J_2(\mu_{41},M_{41};G_{412};\tilde{c}-7)+J_1(\mu_{11},M_{11};G_{112})\eta(\mu_{11},\tilde{c}-2)\\
\gamma_6(l_1'l_2'l_1l_2;\tilde{c}) &= J_2(\mu_{21},M_{21};G_{212};\tilde{c}-7)\\
\gamma_7(l_1'l_2'l_1l_2;C) &= J_2(\mu_{21},M_{21};G_{211};C-5)\\
\gamma_8(l_1'l_2'l_1l_2;C) &= J_2(\mu_{41},M_{41};G_{411};C-5)\\
\gamma_9(l_1'l_2'l_1l_2;\tilde{c}) &= J_2(\mu_{11},M_{11};G_{112};\tilde{c}-5)\\
\gamma_{10}(l_1'l_2'l_1l_2;\tilde{c}) &= J_2(\mu_{21},M_{21};G_{212};\tilde{c}-5)\\
\gamma_{11}(l_1'l_2'l_1l_2;\tilde{c}) &= J_2(\mu_{31},M_{31};G_{312};\tilde{c}-5)+J_2(\mu_{41},M_{41};G_{412};\tilde{c}-5)\\
&+ J_1(\mu_{11},M_{11};G_{112})\eta(\mu_{11},\tilde{c})\\
\gamma_{12}(l_1'l_2'l_1l_2;\tilde{c}) &= J_2(\mu_{41},M_{41};G_{413};\tilde{c}-5)\\
\gamma_{13}(l_1'l_2'l_1l_2;\tilde{c}) &= J_2(\mu_{13},M_{13};G_{131};\tilde{c}-7)\\
\gamma_{14}(l_1'l_2'l_1l_2;\tilde{c}) &= J_2(\mu_{33},M_{33};G_{331};\tilde{c}-7)\\
\gamma_{15}(l_1'l_2'l_1l_2;\tilde{c}) &= J_2(\mu_{24},M_{24};G_{241};\tilde{c}-7)\\
\gamma_{16}(l_1'l_2'l_1l_2;\tilde{c}) &= J_2(\mu_{44},M_{44};G_{441};\tilde{c}-7)\\
S_5(l_1'l_2'l_1l_2;\tilde{c}) &= \gamma_9(l_1'l_2'l_1l_2;\tilde{c})+\gamma_{10}(l_1'l_2'l_1l_2;\tilde{c})+\gamma_{11}(l_1'l_2'l_1l_2;\tilde{c}).
\end{aligned}
$$

(10) H_D^{10}:

$$
\begin{aligned}
\Delta E_D^{10} &= -\frac{3}{2}\alpha^4\delta_{JJ'}\delta_{M_JM_{J'}}\sum_K(-1)^{K+L+S'+J}\begin{Bmatrix} L' & S' & J\\ S & L & K\end{Bmatrix}\\
&\times \langle\gamma'L'\|R^{(K)}\|\gamma L\rangle\langle S'\|[\vec{\sigma}_1\otimes\vec{\sigma}_2]^{(K)}\|S\rangle
\end{aligned}
$$

with

$$R^{(K)}=\nabla_1^2\frac{1}{r^5}[\vec{r}\otimes\vec{r}]^{(K)}.$$

The orbital part is

$$\langle F'\mathcal{Y}^{M'}_{l_1'l_2'L'}|R_Q^{(K)}|F\mathcal{Y}^{M}_{l_1l_2L}\rangle = (-1)^{L'-M'}\begin{pmatrix} L' & K & L\\ -M' & Q & M\end{pmatrix}U(10)D,$$

where

$$U(10)=\frac{1}{2}\sqrt{2K+1}(l_1,l_2,L,l_1',l_2',L')^{1/2},$$

$$
\begin{aligned}
D &= \sum_{i=1}^{7}\Delta_1(i) + 2c'\tilde{\Delta}_2 \\
\Delta_1(i) &= \mathrm{coe}(S_i)[\varpi_0(\mu_{11}, M_{11}; G_{11}; A+2, B, C; \tilde{\alpha}, \tilde{\beta}) \\
&+ \varpi_0(\mu_{12}, M_{12}; G_{12}; A, B+2, C; \tilde{\alpha}, \tilde{\beta}) \\
&+ 2\varpi_0(\mu_{13}, M_{13}; G_{13}; A+1, B+1, C; \tilde{\alpha}, \tilde{\beta})], \quad C = -2 \\
\Delta_1(i) &= \mathrm{coe}(S_i)[\varpi_1(\mu_{11}, M_{11}; G_{11}; A+2, B, C; \tilde{\alpha}, \tilde{\beta}) \\
&+ \varpi_1(\mu_{12}, M_{12}; G_{12}; A, B+2, C; \tilde{\alpha}, \tilde{\beta}) \\
&+ 2\varpi_1(\mu_{13}, M_{13}; G_{13}; A+1, B+1, C; \tilde{\alpha}, \tilde{\beta})] \\
&+ J_1(\mu_{11}, M_{11}; G_{11})\eta(\mu_{11}, C+5)I_{\omega(\mu_{11})-2}(A, B, C+2)], \quad C = -4 \\
\Delta_1(i) &= \mathrm{coe}(S_i)[\varpi_2(\mu_{11}, M_{11}; G_{11}; A+2, B, C; \tilde{\alpha}, \tilde{\beta}) \\
&+ \varpi_2(\mu_{12}, M_{12}; G_{12}; A, B+2, C; \tilde{\alpha}, \tilde{\beta}) \\
&+ 2\varpi_2(\mu_{13}, M_{13}; G_{13}; A+1, B+1, C; \tilde{\alpha}, \tilde{\beta})] \\
&+ \gamma_1 \mathrm{Dif}(A+1, B-1; A, B; C+2, \tilde{\alpha}, \tilde{\beta}; \omega(\mu_{11}+1)-2, \omega(\mu_{11})-2) \\
&+ \gamma_2 \mathrm{Dif}(A-1, B+1; A, B; C+2, \tilde{\alpha}, \tilde{\beta}; \omega(\mu_{11}+1)-2, \omega(\mu_{11})-2)] \\
&+ [\mathrm{coe}(S_i)\gamma(l_1' l_2' l_1 l_2)\mathrm{Can}(\tilde{a}+a'(i), \tilde{b}+b'(i), \tilde{\alpha}, \tilde{\beta}; \tilde{a}'+b'(i), \tilde{b}'+a'(i), \tilde{\alpha}', \tilde{\beta}'; \\
&\quad C+2; \omega(\mu_{11})-2, \omega(\mu_{11}+L)-2) \\
&+ \mathrm{coe}(S_i)'\gamma(l_2' l_1' l_2 l_1)\mathrm{Can}(\tilde{a}+b'(i), \tilde{b}+a'(i), \tilde{\alpha}, \tilde{\beta}; \tilde{a}'+a'(i), \tilde{b}'+b'(i), \tilde{\alpha}', \tilde{\beta}'; \\
&\quad C+2; \omega(\mu_{11})-2, \omega(\mu_{11}+L)-2)]\delta(X_R, 1)\delta(X_L, 1), \quad C \neq -2, -4 \\
\tilde{\Delta}_2 &= \varpi_0(\mu_{21}, M_{21}; G_{21}; \tilde{a}+1, \tilde{b}+1, \tilde{c}-7; \tilde{\alpha}, \tilde{\beta}) \\
&+ \varpi_0(\mu_{22}, M_{22}; G_{22}; \tilde{a}-1, \tilde{b}+3, \tilde{c}-7; \tilde{\alpha}, \tilde{\beta}) \\
&+ 2\varpi_0(\mu_{23}, M_{23}; G_{23}; \tilde{a}, \tilde{b}+2, \tilde{c}-7; \tilde{\alpha}, \tilde{\beta}), \quad \tilde{c} = 5 \\
\tilde{\Delta}_2 &= \varpi_1(\mu_{21}, M_{21}; G_{21}; \tilde{a}+1, \tilde{b}+1, \tilde{c}-7; \tilde{\alpha}, \tilde{\beta}) \\
&+ \varpi_1(\mu_{22}, M_{22}; G_{22}; \tilde{a}-1, \tilde{b}+3, \tilde{c}-7; \tilde{\alpha}, \tilde{\beta}) \\
&+ 2\varpi_1(\mu_{23}, M_{23}; G_{23}; \tilde{a}, \tilde{b}+2, \tilde{c}-7; \tilde{\alpha}, \tilde{\beta}) \\
&+ J_1(\mu_{21}, M_{21}; G_{21})\eta(\mu_{11}+1, \tilde{c}-2)I_{\omega(\mu_{11}+1)-2}(\tilde{a}-1, \tilde{b}+1, \tilde{c}-5), \quad \tilde{c} = 3 \\
\tilde{\Delta}_2 &= \varpi_2(\mu_{21}, M_{21}; G_{21}; \tilde{a}+1, \tilde{b}+1, \tilde{c}-7; \tilde{\alpha}, \tilde{\beta}) \\
&+ \varpi_2(\mu_{22}, M_{22}; G_{22}; \tilde{a}-1, \tilde{b}+3, \tilde{c}-7; \tilde{\alpha}, \tilde{\beta}) \\
&+ 2\varpi_2(\mu_{23}, M_{23}; G_{23}; \tilde{a}, \tilde{b}+2, \tilde{c}-7; \tilde{\alpha}, \tilde{\beta})
\end{aligned}
$$

$$
\begin{aligned}
&+ \quad \eta_1 \mathrm{Dif}(\tilde{a}, \tilde{b}; \tilde{a}-1, \tilde{b}+1; \tilde{c}-5, \tilde{\alpha}, \tilde{\beta}; \omega(\mu_{11})-2, \omega(\mu_{11}+1)-2) \\
&+ \quad \eta_2 \mathrm{Dif}(\tilde{a}-2, \tilde{b}+2; \tilde{a}-1, \tilde{b}+1; \tilde{c}-5, \tilde{\alpha}, \tilde{\beta}; \omega(\mu_{11})-2, \omega(\mu_{11}+1)-2) \\
&+ \quad [\eta(l_1'l_2'l_1l_2)\mathrm{Can}(\tilde{a}-1, \tilde{b}+1, \tilde{\alpha}, \tilde{\beta}; \tilde{a}'+1, \tilde{b}'-1, \tilde{\alpha}', \tilde{\beta}'; \\
&\quad\quad \tilde{c}-5; \omega(\mu_{11}+1)-2, \omega(\mu_{11}+1+L)-2) \\
&+ \quad \eta(l_2'l_1'l_2l_1)\mathrm{Can}(\tilde{a}+1, \tilde{b}-1, \tilde{\alpha}, \tilde{\beta}; \tilde{a}'-1, \tilde{b}'+1, \tilde{\alpha}', \tilde{\beta}'; \\
&\quad\quad \tilde{c}-5; \omega(\mu_{11}+1)-2, \omega(\mu_{11}+1+L)-2)]\delta(X_R,1)\delta(X_L,1), \quad \tilde{c} \neq 3,5.
\end{aligned}
$$

Also,

$$
\begin{aligned}
M_{11} &= \min(l_1+l_1'+K, l_2+l_2') \\
M_{12} &= \min(l_1+l_1', l_2+l_2'+K) \\
M_{13} &= \min(l_1+l_1'+1, l_2+l_2'+1) \\
M_{21} &= \min(l_1+l_1'+K+1, l_2+l_2'+1) \\
M_{22} &= \min(l_1+l_1'+1, l_2+l_2'+K+1) \\
M_{23} &= \min(l_1+l_1'+2, l_2+l_2'+2) \\
\mu_{ij} &= \omega(M_{ij})-2, \quad i=1,2, \quad j=1,2,3
\end{aligned}
$$

$$
\begin{aligned}
A &\equiv \tilde{a}+a'(i) \\
B &\equiv \tilde{b}+b'(i) \\
C &\equiv \tilde{c}+c'(i)
\end{aligned}
$$

coe(S_i)	$a'(i)$	$b'(i)$	$c'(i)$
$a'(a'+1+c')-l_1'(l_1'+1)$	-2	0	-5
$-\alpha'[2(a'+1)+c']$	-1	0	-5
α'^2	0	0	-5
$c'(c'+1+a')$	0	0	-7
$-a'c'$	-2	2	-7
$-\alpha'c'$	1	0	-7
$\alpha'c'$	-1	2	-7

The angular coefficients are:

$$
\begin{aligned}
G_{11}(E) &= \sum_N (N,E)G(T_{11},0)\tilde{G}(T_{11}) \\
G_{12}(E) &= \sum_N (N,E)G(T_{12},0)\tilde{G}(T_{12})
\end{aligned}
$$

$$
\begin{aligned}
G_{13}(E) &= \sum_{HN}(H,N,E)G(T_{13},0)\tilde{G}(T_{13}) \\
G_{21}(E) &= \sum_{N'H'N}(N',H',N,E)G(T_{21},0)\tilde{G}(T_{21})b(l_1';N') \\
G_{22}(E) &= \sum_{N'H'N}(N',H',N,E)G(T_{22},0)\tilde{G}(T_{22})b(l_1';N') \\
G_{23}(E) &= \sum_{N'H'HN}(N',H',H,N,E)G(T_{23},0)\tilde{G}(T_{23})b(l_1';N')
\end{aligned}
$$

with

$$
\begin{aligned}
G(T_{11},0) &= \begin{pmatrix}1 & 1 & K\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}K & l_1 & N\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_1' & N & E\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_2' & l_2 & E\\ 0 & 0 & 0\end{pmatrix} \\
\tilde{G}(T_{11}) &= (-1)^{L'+L+l_2'}\begin{Bmatrix}L & l_1 & l_2\\ N & L' & K\end{Bmatrix}\begin{Bmatrix}L' & l_1' & l_2'\\ E & l_2 & N\end{Bmatrix} \\
G(T_{12},0) &= \begin{pmatrix}1 & 1 & K\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}K & l_2 & N\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_1' & l_1 & E\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_2' & N & E\\ 0 & 0 & 0\end{pmatrix} \\
\tilde{G}(T_{12}) &= (-1)^{l_1'}\begin{Bmatrix}L & l_1 & l_2\\ N & K & L'\end{Bmatrix}\begin{Bmatrix}L' & l_1' & l_2'\\ E & N & l_1\end{Bmatrix} \\
G(T_{13},0) &= \begin{pmatrix}1 & l_1 & H\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}1 & l_2 & N\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_1' & H & E\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_2' & N & E\\ 0 & 0 & 0\end{pmatrix} \\
\tilde{G}(T_{13}) &= (-1)^{L'+l_1+l_2'}\begin{Bmatrix}L' & l_1' & l_2'\\ E & N & H\end{Bmatrix}\begin{Bmatrix}L & l_1 & l_2\\ K & 1 & 1\\ L' & H & N\end{Bmatrix} \\
G(T_{21},0) &= \begin{pmatrix}l_1' & 1 & N'\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_2' & 1 & H'\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}1 & 1 & K\\ 0 & 0 & 0\end{pmatrix} \\
&\times \begin{pmatrix}K & l_1 & N\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}N' & N & E\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}H' & l_2 & E\\ 0 & 0 & 0\end{pmatrix} \\
\tilde{G}(T_{21}) &= (-1)^{1+L+l_2'}\begin{Bmatrix}L & l_1 & l_2\\ N & L' & K\end{Bmatrix}\begin{Bmatrix}L' & l_1' & l_2'\\ 1 & H' & N'\end{Bmatrix}\begin{Bmatrix}L' & N & l_2\\ E & H' & N'\end{Bmatrix} \\
G(T_{22},0) &= \begin{pmatrix}l_1' & 1 & N'\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_2' & 1 & H'\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}1 & 1 & K\\ 0 & 0 & 0\end{pmatrix} \\
&\times \begin{pmatrix}K & l_2 & N\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}N' & l_1 & E\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}H' & N & E\\ 0 & 0 & 0\end{pmatrix} \\
\tilde{G}(T_{22}) &= (-1)^{1+L'+l_1'}\begin{Bmatrix}L & l_1 & l_2\\ N & K & L'\end{Bmatrix}\begin{Bmatrix}L' & l_1' & l_2'\\ 1 & H' & N'\end{Bmatrix}\begin{Bmatrix}L' & l_1 & N\\ E & H' & N'\end{Bmatrix} \\
G(T_{23},0) &= \begin{pmatrix}l_1' & 1 & N'\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_2' & 1 & H'\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}1 & l_1 & H\\ 0 & 0 & 0\end{pmatrix} \\
&\times \begin{pmatrix}1 & l_2 & N\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}N' & H & E\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}H' & N & E\\ 0 & 0 & 0\end{pmatrix} \\
\tilde{G}(T_{23}) &= (-1)^{1+l_1+l_2'}\begin{Bmatrix}L' & l_1' & l_2'\\ 1 & H' & N'\end{Bmatrix}\begin{Bmatrix}L' & H & N\\ E & H' & N'\end{Bmatrix}\begin{Bmatrix}L & l_1 & l_2\\ K & 1 & 1\\ L' & H & N\end{Bmatrix}
\end{aligned}
$$

We have also defined:

$$\begin{aligned}
\gamma_1(l_1'l_2'l_1l_2) &= J_2(\mu_{11}, M_{11}; G_{11}; C) \\
\gamma_2(l_1'l_2'l_1l_2) &= J_2(\mu_{12}, M_{12}; G_{12}; C) \\
\gamma_3(l_1'l_2'l_1l_2) &= 2J_2(\mu_{13}, M_{13}; G_{13}; C) + J_1(\mu_{11}, M_{11}; G_{11})\eta(\mu_{11}, C+5) \\
\gamma(l_1'l_2'l_1l_2) &= \gamma_1(l_1'l_2'l_1l_2) + \gamma_2(l_1'l_2'l_1l_2) + \gamma_3(l_1'l_2'l_1l_2) \\
\eta_1(l_1'l_2'l_1l_2) &= J_2(\mu_{21}, M_{21}; G_{21}; \tilde{c}-7) \\
\eta_2(l_1'l_2'l_1l_2) &= J_2(\mu_{22}, M_{22}; G_{22}; \tilde{c}-7) \\
\eta_3(l_1'l_2'l_1l_2) &= 2J_2(\mu_{23}, M_{23}; G_{23}; \tilde{c}-7) + J_1(\mu_{21}, M_{21}; G_{21})\eta(\mu_{11}+1, \tilde{c}-2) \\
\eta(l_1'l_2'l_1l_2) &= \eta_1(l_1'l_2'l_1l_2) + \eta_2(l_1'l_2'l_1l_2) + \eta_3(l_1'l_2'l_1l_2).
\end{aligned}$$

If

$$\mathrm{coe}(S_i) = f_i(l_1', a', \alpha'),$$

then

$$\mathrm{coe}(S_i)' = f_i(l_2', b', \beta').$$

(11) H_D^{11}:

$$\begin{aligned}
\Delta E_D^{11} &= \frac{1}{4}\alpha^4 \delta_{JJ'}\delta_{M_JM_{J'}} \sum_K (-1)^{K+L+S'+J} \begin{Bmatrix} L' & S' & J \\ S & L & K \end{Bmatrix} \\
&\times \langle \gamma' L' \| R^{(K)} \| \gamma L \rangle \langle S' \| [\vec{\sigma}_1 \otimes \vec{\sigma}_2]^{(K)} \| S \rangle
\end{aligned}$$

with

$$R^{(K)} = \nabla_1^2 \frac{1}{r^3} [\vec{r} \otimes \vec{\nabla}_1]^{(K)}.$$

The orbital part is

$$\langle F' \mathcal{Y}^{M'}_{l_1'l_2'L'} | R_Q^{(K)} | F \mathcal{Y}^{M}_{l_1l_2L} \rangle = (-1)^{L'-M'} \begin{pmatrix} L' & K & L \\ -M' & Q & M \end{pmatrix} U(11)D,$$

where

$$U(11) = \frac{1}{2}\sqrt{2K+1}(l_1, l_2, L, l_1', l_2', L')^{1/2}$$

$$D = \sum_{i=1}^{6} \mathrm{Term}(i)$$

$$\begin{aligned}
\mathrm{Term}(1) &= \sum_{i=1}^{7}\sum_{j=1}^{2} O_{ij}^{(1)}[\varpi_1(\mu_{11}, M_{11}; G_{111}; \tilde{a} + a_{ij}^{(1)} + 1, \tilde{b} + b'(i), \tilde{c} + c'(i); \tilde{\alpha}, \tilde{\beta}) \\
&+ \varpi_1(\mu_{12}, M_{12}; G_{121}; \tilde{a} + a_{ij}^{(1)}, \tilde{b} + b'(i) + 1, \tilde{c} + c'(i); \tilde{\alpha}, \tilde{\beta}) \\
&+ J_1(\mu_{11}, M_{11}; G_{111})\mathrm{Dif}(\tilde{a} + a_{ij}^{(1)} + 1, \tilde{b} + b'(i); \tilde{a} + a_{ij}^{(1)}, \tilde{b} + b'(i) + 1; \\
&\tilde{c} + c'(i), \tilde{\alpha}, \tilde{\beta}; \omega(\mu_{11}) - 2, \omega(\mu_{11} + 1) - 2)] \\
\mathrm{Term}(2) &= \sum_{i=1}^{7} \mathrm{coe}(S_i)[\varpi_1(\mu_{11}, M_{11}; G_{112}; \tilde{a} + a'(i), \tilde{b} + b'(i), \tilde{c} + c'(i); \tilde{\alpha}, \tilde{\beta}) \\
&+ \varpi_1(\mu_{12}, M_{12}; G_{122}; \tilde{a} + a'(i) - 1, \tilde{b} + b'(i) + 1, \tilde{c} + c'(i); \tilde{\alpha}, \tilde{\beta}) \\
&+ J_1(\mu_{11}, M_{11}; G_{112})\mathrm{Dif}(\tilde{a} + a'(i), \tilde{b} + b'(i); \tilde{a} + a'(i) - 1, \tilde{b} + b'(i) + 1; \\
&\tilde{c} + c'(i), \tilde{\alpha}, \tilde{\beta}; \omega(\mu_{11}) - 2, \omega(\mu_{11} + 1) - 2)]
\end{aligned}$$

$$\begin{aligned}
\mathrm{Term}(3) &= \sum_{i=1}^{7} \mathrm{coe}(S_i) c \Delta_3(i) \\
\Delta_3(i) &= \varpi_0(\mu_{11}, M_{11}; G_{111}; A + 2, B, C - 2; \tilde{\alpha}, \tilde{\beta}) \\
&+ 2\varpi_0(\mu_{12}, M_{12}; G_{121}; A + 1, B + 1, C - 2; \tilde{\alpha}, \tilde{\beta}) \\
&+ \varpi_0(\mu_{13}, M_{13}; G_{13}; A, B + 2, C - 2; \tilde{\alpha}, \tilde{\beta}), \quad C = 0 \\
\Delta_3(i) &= \varpi_1(\mu_{11}, M_{11}; G_{111}; A + 2, B, C - 2; \tilde{\alpha}, \beta) \\
&+ 2\varpi_1(\mu_{12}, M_{12}; G_{121}; A + 1, B + 1, C - 2; \tilde{\alpha}, \tilde{\beta}) \\
&+ \varpi_1(\mu_{13}, M_{13}; G_{13}; A, B + 2, C - 2; \tilde{\alpha}, \tilde{\beta}) \\
&+ J_1(\mu_{11}, M_{11}; G_{111})\eta(\mu_{11}, C + 3) I_{\omega(\mu_{11})-2}(A, B, C), \quad C = -2 \\
\Delta_3(i) &= \varpi_2(\mu_{11}, M_{11}; G_{111}; A + 2, B, C - 2; \tilde{\alpha}, \tilde{\beta}) \\
&+ 2\varpi_2(\mu_{12}, M_{12}; G_{121}; A + 1, B + 1, C - 2; \tilde{\alpha}, \tilde{\beta}) \\
&+ \varpi_2(\mu_{13}, M_{13}; G_{13}; A, B + 2, C - 2; \tilde{\alpha}, \tilde{\beta}) \\
&+ \gamma_1 \mathrm{Dif}(A + 1, B - 1; A, B; C, \tilde{\alpha}, \tilde{\beta}; \omega(\mu_{11} + 1) - 2, \omega(\mu_{11}) - 2) \\
&+ \gamma_2 \mathrm{Dif}(A - 1, B + 1; A, B; C, \tilde{\alpha}, \tilde{\beta}; \omega(\mu_{11} + 1) - 2, \omega(\mu_{11}) - 2) \\
&+ \gamma I_{\omega(\mu_{11})-2}(A, B, C), \quad C \neq -2, 0
\end{aligned}$$

$$\begin{aligned}
\text{Term}(4) &= \sum_{i=1}^{2} \text{coe}(Q_i)c'[\varpi_1(\mu_{21}, M_{21}; G_{211}; \tilde{a} + a(i), \tilde{b}+1, \tilde{c}-5; \tilde{\alpha}, \tilde{\beta}) \\
&+ \varpi_1(\mu_{22}, M_{22}; G_{221}; \tilde{a} + a(i) - 1, \tilde{b}+2, \tilde{c}-5; \tilde{\alpha}, \tilde{\beta}) \\
&+ J_1(\mu_{21}, M_{21}; G_{211})\text{Dif}(\tilde{a} + a(i), \tilde{b}+1; \tilde{a} + a(i) - 1, \tilde{b}+2; \\
&\quad \tilde{c}-5, \tilde{\alpha}, \tilde{\beta}; \omega(\mu_{11}+1) - 2, \omega(\mu_{11}) - 2)]
\end{aligned}$$

$$\begin{aligned}
\text{Term}(5) &= c'\varpi_1(\mu_{21}, M_{21}; G_{212}; \tilde{a} - 1, \tilde{b}+1, \tilde{c}-5; \tilde{\alpha}, \tilde{\beta}) \\
&+ c'\varpi_1(\mu_{22}, M_{22}; G_{222}; \tilde{a} - 2, \tilde{b}+2, \tilde{c}-5; \tilde{\alpha}, \tilde{\beta}) \\
&+ c'J_1(\mu_{21}, M_{21}; G_{212})\text{Dif}(\tilde{a} - 1, \tilde{b}+1; \tilde{a} - 2, \tilde{b}+2; \\
&\quad \tilde{c}-5, \tilde{\alpha}, \tilde{\beta}; \omega(\mu_{11}+1) - 2, \omega(\mu_{11}) - 2)]
\end{aligned}$$

$$\begin{aligned}
\text{Term}(6) &= cc'\Delta_6 \\
\Delta_6 &= \varpi_0(\mu_{21}, M_{21}; G_{211}; \tilde{a}+1, \tilde{b}+1, \tilde{c}-7; \tilde{\alpha}, \tilde{\beta}) \\
&+ 2\varpi_0(\mu_{22}, M_{22}; G_{221}; \tilde{a}, \tilde{b}+2, \tilde{c}-7; \tilde{\alpha}, \tilde{\beta}) \\
&+ \varpi_0(\mu_{23}, M_{23}; G_{231}; \tilde{a}-1, \tilde{b}+3, \tilde{c}-7; \tilde{\alpha}, \tilde{\beta}), \quad \tilde{c} = 5 \\
\Delta_6 &= \varpi_1(\mu_{21}, M_{21}; G_{211}; \tilde{a}+1, \tilde{b}+1, \tilde{c}-7; \tilde{\alpha}, \tilde{\beta}) \\
&+ 2\varpi_1(\mu_{22}, M_{22}; G_{221}; \tilde{a}, \tilde{b}+2, \tilde{c}-7; \tilde{\alpha}, \tilde{\beta}) \\
&+ \varpi_1(\mu_{23}, M_{23}; G_{231}; \tilde{a}-1, \tilde{b}+3, \tilde{c}-7; \tilde{\alpha}, \tilde{\beta}) \\
&+ J_1(\mu_{21}, M_{21}; G_{211})\eta(\mu_{11}+1, \tilde{c}-2)I_{\omega(\mu_{11}+1)-2}(\tilde{a}-1, \tilde{b}+1, \tilde{c}-5), \\
&\qquad \tilde{c} = 3 \\
\Delta_6 &= \varpi_2(\mu_{21}, M_{21}; G_{211}; \tilde{a}+1, \tilde{b}+1, \tilde{c}-7; \tilde{\alpha}, \tilde{\beta}) \\
&+ 2\varpi_2(\mu_{22}, M_{22}; G_{221}; \tilde{a}, \tilde{b}+2, \tilde{c}-7; \tilde{\alpha}, \tilde{\beta}) \\
&+ \varpi_2(\mu_{23}, M_{23}; G_{231}; \tilde{a}-1, \tilde{b}+3, \tilde{c}-7; \tilde{\alpha}, \tilde{\beta}) \\
&+ \gamma_4\text{Dif}(\tilde{a}, \tilde{b}; \tilde{a}-1, \tilde{b}+1; \tilde{c}-5, \tilde{\alpha}, \tilde{\beta}; \omega(\mu_{11}) - 2, \omega(\mu_{11}+1) - 2) \\
&+ \gamma_5\text{Dif}(\tilde{a}-2, \tilde{b}+2; \tilde{a}-1, \tilde{b}+1; \tilde{c}-5, \tilde{\alpha}, \tilde{\beta}; \omega(\mu_{11}) - 2, \omega(\mu_{11}+1) - 2) \\
&+ \tilde{\gamma}I_{\omega(\mu_{11}+1)-2}(\tilde{a}-1, \tilde{b}+1, \tilde{c}-5), \quad \tilde{c} \neq 3, 5.
\end{aligned}$$

Also,

$$M_{11} = \min(l_1 + l_1' + 2, l_2 + l_2')$$

$$
\begin{aligned}
M_{12} &= \min(l_1 + l_1' + 1, l_2 + l_2' + 1) \\
M_{13} &= \min(l_1 + l_1', l_2 + l_2' + 2) \\
M_{21} &= \min(l_1 + l_1' + 3, l_2 + l_2' + 1) \\
M_{22} &= \min(l_1 + l_1' + 2, l_2 + l_2' + 2) \\
M_{23} &= \min(l_1 + l_1' + 1, l_2 + l_2' + 3) \\
\mu_{ij} &= \omega(M_{ij}) - 2, \quad i = 1,2, \quad j = 1,2,3
\end{aligned}
$$

$$
\begin{aligned}
A &\equiv \tilde{a} + a'(i) \\
B &\equiv \tilde{b} + b'(i) \\
C &\equiv \tilde{c} + c'(i)
\end{aligned}
$$

$\mathrm{coc}(S_i)$	$a'(i)$	$b'(i)$	$c'(i)$
$a'(a'+1+c') - l_1'(l_1'+1)$	-2	0	-3
$-\alpha'[2(a'+1)+c']$	-1	0	-3
α'^2	0	0	-3
$c'(c'+1+a')$	0	0	-5
$-a'c'$	-2	2	-5
$-\alpha'c'$	1	0	-5
$\alpha'c'$	-1	2	-5

$\mathrm{coc}(Q_i)$	$a(i)$	$b(i)$	$c(i)$
a	-1	0	0
$-\alpha$	0	0	0
c	1	0	-2

$$
\begin{aligned}
a_{ij}^{(1)} &= a'(i) + a(j) \\
b_{ij}^{(1)} &= b'(i) + b(j) \\
c_{ij}^{(1)} &= c'(i) + c(j) \\
O_{ij}^{(1)} &= \mathrm{coc}(S_i)\mathrm{coc}(Q_j).
\end{aligned}
$$

The angular coefficients are:

$$
\begin{aligned}
G_{111}(E) &= \sum_{TN}(T,N,E)G(T_{11},0)\tilde{G}(T_{11}) \\
G_{112}(E) &= \sum_{TN}(T,N,E)G(T_{11},0)\tilde{G}(T_{11})b(l_1;T)
\end{aligned}
$$

$$
\begin{aligned}
G_{121}(E) &= \sum_{TN}(T,N,E)G(T_{12},0)\tilde{G}(T_{12}) \\
G_{122}(E) &= \sum_{TN}(T,N,E)G(T_{12},0)\tilde{G}(T_{12})b(l_1;N) \\
G_{13}(E) &= \sum_{TN}(T,N,E)G(T_{13},0)\tilde{G}(T_{13}) \\
G_{211}(E) &= 2\sum_{N'H'TN}(N',H',T,N,E)G(T_{21},0)\tilde{G}(T_{21})b(l_1';N') \\
G_{212}(E) &= 2\sum_{N'H'TN}(N',H',T,N,E)G(T_{21},0)\tilde{G}(T_{21})b(l_1';N')b(l_1;T) \\
G_{221}(E) &= 2\sum_{N'H'TN}(N',H',T,N,E)G(T_{22},0)\tilde{G}(T_{22})b(l_1';N') \\
G_{222}(E) &= 2\sum_{N'H'TN}(N',H',T,N,E)G(T_{22},0)\tilde{G}(T_{22})b(l_1';N')b(l_1;N) \\
G_{231}(E) &= 2\sum_{N'H'TN}(N',H',T,N,E)G(T_{23},0)\tilde{G}(T_{23})b(l_1';N')
\end{aligned}
$$

with

$$
\begin{aligned}
G(T_{11},0) &= \begin{pmatrix} 1 & l_1 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & T & N \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_1' & N & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & l_2 & E \\ 0 & 0 & 0 \end{pmatrix} \\
\tilde{G}(T_{11}) &= (-1)^{1+L+L'+l_1+l_2'}\begin{Bmatrix} L & l_1 & l_2 \\ N & L' & K \end{Bmatrix}\begin{Bmatrix} L' & l_1' & l_2' \\ E & l_2 & N \end{Bmatrix}\begin{Bmatrix} 1 & 1 & K \\ l_1 & N & T \end{Bmatrix} \\
G(T_{12},0) &= \begin{pmatrix} 1 & l_1 & N \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2 & 1 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_1' & N & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & T & E \\ 0 & 0 & 0 \end{pmatrix} \\
\tilde{G}(T_{12}) &= (-1)^{L'+l_1+l_2'}\begin{Bmatrix} L' & l_1' & l_2' \\ E & T & N \end{Bmatrix}\begin{Bmatrix} L & l_1 & l_2 \\ K & 1 & 1 \\ L' & N & T \end{Bmatrix} \\
G(T_{13},0) &= \begin{pmatrix} l_2 & 1 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & T & N \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_1' & l_1 & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & N & E \\ 0 & 0 & 0 \end{pmatrix} \\
\tilde{G}(T_{13}) &= (-1)^{1+l_1+l_2'}\begin{Bmatrix} L & l_1 & l_2 \\ N & K & L' \end{Bmatrix}\begin{Bmatrix} L' & l_1' & l_2' \\ E & N & l_1 \end{Bmatrix}\begin{Bmatrix} 1 & 1 & K \\ l_2 & N & T \end{Bmatrix} \\
G(T_{21},0) &= \begin{pmatrix} l_1' & 1 & N' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & 1 & H' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_1 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & T & N \\ 0 & 0 & 0 \end{pmatrix} \\
&\times \begin{pmatrix} N' & N & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} H' & l_2 & E \\ 0 & 0 & 0 \end{pmatrix} \\
\tilde{G}(T_{21}) &= (-1)^{L+l_1+l_2'}\begin{Bmatrix} L & l_1 & l_2 \\ N & L' & K \end{Bmatrix}\begin{Bmatrix} L' & l_1' & l_2' \\ 1 & H' & N' \end{Bmatrix}\begin{Bmatrix} 1 & 1 & K \\ l_1 & N & T \end{Bmatrix} \\
&\times \begin{Bmatrix} L' & N & l_2 \\ E & H' & N' \end{Bmatrix} \\
G(T_{22},0) &= \begin{pmatrix} l_1' & 1 & N' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & 1 & H' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_1 & N \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2 & 1 & T \\ 0 & 0 & 0 \end{pmatrix} \\
&\times \begin{pmatrix} N' & N & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} H' & T & E \\ 0 & 0 & 0 \end{pmatrix}
\end{aligned}
$$

$$\tilde{G}(T_{22}) = (-1)^{1+l_1+l_2'}\begin{Bmatrix} L' & l_1' & l_2' \\ 1 & H' & N' \end{Bmatrix}\begin{Bmatrix} L' & N & T \\ E & H' & N' \end{Bmatrix}\begin{Bmatrix} L & l_1 & l_2 \\ K & 1 & 1 \\ L' & N & T \end{Bmatrix}$$

$$G(T_{23}, 0) = \begin{pmatrix} l_1' & 1 & N' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & 1 & H' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2 & 1 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & T & N \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times \begin{pmatrix} N' & l_1 & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} H' & N & E \\ 0 & 0 & 0 \end{pmatrix}$$

$$\tilde{G}(T_{23}) = (-1)^{L'+l_1+l_2'}\begin{Bmatrix} L & l_1 & l_2 \\ N & K & L' \end{Bmatrix}\begin{Bmatrix} L' & l_1' & l_2' \\ 1 & H' & N' \end{Bmatrix}\begin{Bmatrix} 1 & 1 & K \\ l_2 & N & T \end{Bmatrix}$$

$$\times \begin{Bmatrix} L' & l_1 & N \\ E & H' & N' \end{Bmatrix}.$$

We have also defined:

$$\gamma_1 = J_2(\mu_{11}, M_{11}; G_{111}; \tilde{c} + c'(i) - 2)$$

$$\gamma_2 = J_2(\mu_{13}, M_{13}; G_{13}; \tilde{c} + c'(i) - 2)$$

$$\gamma_3 = 2J_2(\mu_{12}, M_{12}; G_{121}; \tilde{c} + c'(i) - 2) + J_1(\mu_{11}, M_{11}; G_{111})\eta(\mu_{11}, \tilde{c} + c'(i) + 3)$$

$$\gamma = \gamma_1 + \gamma_2 + \gamma_3$$

$$\gamma_4 = J_2(\mu_{21}, M_{21}; G_{211}; \tilde{c} - 7)$$

$$\gamma_5 = J_2(\mu_{23}, M_{23}; G_{231}; \tilde{c} - 7)$$

$$\gamma_6 = 2J_2(\mu_{22}, M_{22}; G_{221}; \tilde{c} - 7) + J_1(\mu_{21}, M_{21}; G_{211})\eta(\mu_{11} + 1, \tilde{c} - 2)$$

$$\tilde{\gamma} = \gamma_4 + \gamma_5 + \gamma_6.$$

(12) H_D^{12}:

We split H_D^{12} into two parts:

$$H_D^{12} = H_D^{121} + H_D^{122},$$

where

$$H_D^{121} = -i\frac{1}{8}\alpha^4\nabla_1^2\frac{1}{r^3}[(\vec{\sigma}_1 \cdot \vec{r})(\vec{\sigma}_2 \cdot \vec{p}_2) + (\vec{\sigma}_2 \cdot \vec{r})(\vec{\sigma}_1 \cdot \vec{p}_2)]$$

$$H_D^{122} = i\frac{3}{8}\alpha^4\nabla_1^2\frac{1}{r^5}(\vec{\sigma}_1 \cdot \vec{r})(\vec{\sigma}_2 \cdot \vec{r})(\vec{r} \cdot \vec{p}_2).$$

(a) H_D^{121}:

$$\Delta E_D^{121} = -\frac{1}{8}\alpha^4\delta_{JJ'}\delta_{M_JM_{J'}}\sum_K(1 + (-1)^K)(-1)^{L+S'+J}\begin{Bmatrix} L' & S' & J \\ S & L & K \end{Bmatrix}$$

$$\times \langle\gamma' L'\|R^{(K)}\|\gamma L\rangle\langle S'\|[\vec{\sigma}_1 \otimes \vec{\sigma}_2]^{(K)}\|S\rangle$$

with

$$R^{(K)} = \nabla_1^2 \frac{1}{r^3}[\vec{r} \otimes \vec{\nabla}_2]^{(K)}.$$

The orbital part is

$$\langle F' \mathcal{Y}^{M'}_{l_1' l_2' L'} | R^{(K)}_Q | F \mathcal{Y}^{M}_{l_1 l_2 L} \rangle = (-1)^{L'-M'} \begin{pmatrix} L' & K & L \\ -M' & Q & M \end{pmatrix} U(121) D,$$

where

$$U(121) = \frac{1}{2}\sqrt{2K+1}(l_1, l_2, L, l_1', l_2', L')^{1/2}$$

$$D = \sum_{i=1}^{7} \mathrm{Term}(i)$$

$$\begin{aligned}
\mathrm{Term}(1) &= \sum_{i=1}^{7} \mathrm{coe}(S_i) b[\varpi_1(\mu_{11}, M_{11}; G_{111}; A+1, B-1, C; \tilde{\alpha}, \tilde{\beta}) \\
&+ \varpi_1(\mu_{13}, M_{13}; G_{131}; A, B, C; \tilde{\alpha}, \tilde{\beta}) \\
&+ J_1(\mu_{11}, M_{11}; G_{111}) \mathrm{Dif}(A+1, B-1; A, B; \\
&\quad C, \tilde{\alpha}, \tilde{\beta}; \omega(\mu_{11}) - 2, \omega(\mu_{11}+1) - 2)]
\end{aligned}$$

$$\begin{aligned}
\mathrm{Term}(2) &= -\beta \sum_{i=1}^{7} \mathrm{coe}(S_i)[\varpi_1(\mu_{11}, M_{11}; G_{111}; A+1, B, C; \tilde{\alpha}, \tilde{\beta}) \\
&+ \varpi_1(\mu_{13}, M_{13}; G_{131}; A, B+1, C; \tilde{\alpha}, \tilde{\beta}) \\
&+ J_1(\mu_{11}, M_{11}; G_{111}) \mathrm{Dif}(A+1, B; A, B+1; \\
&\quad C, \tilde{\alpha}, \tilde{\beta}; \omega(\mu_{11}) - 2, \omega(\mu_{11}+1) - 2)]
\end{aligned}$$

$$\begin{aligned}
\mathrm{Term}(3) &= \sum_{i=1}^{7} \mathrm{coe}(S_i) c \Delta_3(i) \\
\Delta_3(i) &= 2\varpi_0(\mu_{11}, M_{11}; G_{111}; A+1, B+1, C-2; \tilde{\alpha}, \tilde{\beta}) \\
&+ \varpi_0(\mu_{12}, M_{12}; G_{12}; A+2, B, C-2; \tilde{\alpha}, \tilde{\beta}) \\
&+ \varpi_0(\mu_{13}, M_{13}; G_{131}; A, B+2, C-2; \tilde{\alpha}, \tilde{\beta}), \quad C = 0 \\
\Delta_3(i) &= 2\varpi_1(\mu_{11}, M_{11}; G_{111}; A+1, B+1, C-2; \tilde{\alpha}, \tilde{\beta}) \\
&+ \varpi_1(\mu_{12}, M_{12}; G_{12}; A+2, B, C-2; \tilde{\alpha}, \tilde{\beta})
\end{aligned}$$

$$
\begin{aligned}
&+ \quad \varpi_1(\mu_{13}, M_{13}; G_{131}; A, B+2, C-2; \tilde{\alpha}, \tilde{\beta}) \\
&- \quad J_1(\mu_{11}, M_{11}; G_{111})\eta(\mu_{11}+1, C+3) I_{\omega(\mu_{11}+1)-2}(A, B, C), \quad C = -2 \\
\Delta_3(i) &= 2\varpi_2(\mu_{11}, M_{11}; G_{111}; A+1, B+1, C-2; \tilde{\alpha}, \tilde{\beta}) \\
&+ \quad \varpi_2(\mu_{12}, M_{12}; G_{12}; A+2, B, C-2; \tilde{\alpha}, \tilde{\beta}) \\
&+ \quad \varpi_2(\mu_{13}, M_{13}; G_{131}; A, B+2, C-2; \tilde{\alpha}, \tilde{\beta}) \\
&+ \quad \gamma_2 \mathrm{Dif}(A+1, B-1; A, B; C, \tilde{\alpha}, \tilde{\beta}; \omega(\mu_{11})-2, \omega(\mu_{11}+1)-2) \\
&+ \quad \gamma_3 \mathrm{Dif}(A-1, B+1; A, B; C, \tilde{\alpha}, \tilde{\beta}; \omega(\mu_{11})-2, \omega(\mu_{11}+1)-2) \\
&+ \quad (\gamma_1+\gamma_2+\gamma_3) I_{\omega(\mu_{11}+1)-2}(A, B, C), \quad C \neq -2, 0
\end{aligned}
$$

$$
\begin{aligned}
\mathrm{Term}(4) &= \sum_{i=1}^{7} \mathrm{coe}(S_i)[\varpi_1(\mu_{11}, M_{11}; G_{112}; A+1, B-1, C; \tilde{\alpha}, \tilde{\beta}) \\
&+ \quad \varpi_1(\mu_{13}, M_{13}; G_{132}; A, B, C; \tilde{\alpha}, \tilde{\beta}) \\
&+ \quad J_1(\mu_{11}, M_{11}; G_{112}) \mathrm{Dif}(A+1, B-1; A, B; \\
&\quad\quad C, \tilde{\alpha}, \tilde{\beta}; \omega(\mu_{21})-2, \omega(\mu_{11}+1)-2)]
\end{aligned}
$$

$$
\begin{aligned}
\mathrm{Term}(5) &= bc'\varpi_1(\mu_{21}, M_{21}; G_{211}; \tilde{a}, \tilde{b}, \tilde{c}-5; \tilde{\alpha}, \tilde{\beta}) \\
&- \quad \beta c'\varpi_1(\mu_{21}, M_{21}; G_{211}; \tilde{a}, \tilde{b}+1, \tilde{c}-5; \tilde{\alpha}, \tilde{\beta}) \\
&+ \quad bc'\varpi_1(\mu_{23}, M_{23}; G_{231}; \tilde{a}-1, \tilde{b}+1, \tilde{c}-5; \tilde{\alpha}, \tilde{\beta}) \\
&- \quad \beta c'\varpi_1(\mu_{23}, M_{23}; G_{231}; \tilde{a}-1, \tilde{b}+2, \tilde{c}-5; \tilde{\alpha}, \tilde{\beta})
\end{aligned}
$$

$$
\begin{aligned}
\mathrm{Term}(6) &= c'\varpi_1(\mu_{21}, M_{21}; G_{212}; \tilde{a}, \tilde{b}, \tilde{c}-5; \tilde{\alpha}, \tilde{\beta}) \\
&+ \quad c'\varpi_1(\mu_{23}, M_{23}; G_{232}; \tilde{a}-1, \tilde{b}+1, \tilde{c}-5; \tilde{\alpha}, \tilde{\beta})
\end{aligned}
$$

$$
\begin{aligned}
\mathrm{Term}(7) &= cc'\Delta_7 \\
\Delta_7 &= 2\varpi_2(\mu_{21}, M_{21}; G_{211}; \tilde{a}, \tilde{b}+2, \tilde{c}-7; \tilde{\alpha}, \tilde{\beta}) \\
&+ \quad \varpi_2(\mu_{22}, M_{22}; G_{221}; \tilde{a}+1, \tilde{b}+1, \tilde{c}-7; \tilde{\alpha}, \tilde{\beta}) \\
&+ \quad \varpi_2(\mu_{23}, M_{23}; G_{231}; \tilde{a}-1, \tilde{b}+3, \tilde{c}-7; \tilde{\alpha}, \tilde{\beta}) \\
&+ \quad \gamma_5 \mathrm{Dif}(\tilde{a}, \tilde{b}; \tilde{a}-1, \tilde{b}+1; \tilde{c}-5, \tilde{\alpha}, \tilde{\beta}; \omega(\mu_{11}+1)-2, \omega(\mu_{11})-2) \\
&+ \quad \gamma_6 \mathrm{Dif}(\tilde{a}-2, \tilde{b}+2; \tilde{a}-1, \tilde{b}+1; \tilde{c}-5, \tilde{\alpha}, \tilde{\beta}; \omega(\mu_{11}+1)-2, \omega(\mu_{11})-2)
\end{aligned}
$$

$$+ \quad (\gamma_4+\gamma_5+\gamma_6) I_{\omega(\mu_{11})-2}(\tilde{a}-1,\tilde{b}+1,\tilde{c}-5), \quad \tilde{c}\neq 3,5$$

$$\Delta_7 = 2\varpi_1(\mu_{21}, M_{21}; G_{211}; \tilde{a}, \tilde{b}+2, \tilde{c}-7; \tilde{\alpha}, \tilde{\beta})$$

$$+ \quad \varpi_1(\mu_{22}, M_{22}; G_{221}; \tilde{a}+1, \tilde{b}+1, \tilde{c}-7; \tilde{\alpha}, \tilde{\beta})$$

$$+ \quad \varpi_1(\mu_{23}, M_{23}; G_{231}; \tilde{a}-1, \tilde{b}+3, \tilde{c}-7; \tilde{\alpha}, \tilde{\beta}), \quad \tilde{c}=3,5.$$

Also,

$$M_{11} = \min(l_1+l_1'+1, l_2+l_2'+1)$$
$$M_{12} = \min(l_1+l_1'+2, l_2+l_2')$$
$$M_{13} = \min(l_1+l_1', l_2+l_2'+2)$$
$$M_{21} = \min(l_1+l_1'+2, l_2+l_2'+2)$$
$$M_{22} = \min(l_1+l_1'+3, l_2+l_2'+1)$$
$$M_{23} = \min(l_1+l_1'+1, l_2+l_2'+3)$$
$$\mu_{ij} = \omega(M_{ij})-2, \quad i=1,2, \quad j=1,2,3$$

$$A \equiv \tilde{a}+a'(i)$$
$$B \equiv \tilde{b}+b'(i)$$
$$C \equiv \tilde{c}+c'(i)$$

$\mathrm{coe}(S_i)$	$a'(i)$	$b'(i)$	$c'(i)$
$a'(a'+1+c')-l_1'(l_1'+1)$	-2	0	-3
$-\alpha'[2(a'+1)+c']$	-1	0	-3
α'^2	0	0	-3
$c'(c'+1+a')$	0	0	-5
$-a'c'$	-2	2	-5
$-\alpha'c'$	1	0	-5
$\alpha'c'$	-1	2	-5

The angular coefficients are:

$$G_{111}(E) = \sum_{TH}(T,H,E)G(T_{11},0)\tilde{G}(T_{11})$$
$$G_{112}(E) = \sum_{TH}(T,H,E)G(T_{11},0)\tilde{G}(T_{11})b(l_2;T)$$
$$G_{12}(E) = \sum_{TH}(T,H,E)G(T_{12},0)\tilde{G}(T_{12})$$

$$
\begin{aligned}
G_{131}(E) &= \sum_{TH}(T,H,E)G(T_{13},0)\tilde{G}(T_{13}) \\
G_{132}(E) &= \sum_{TH}(T,H,E)G(T_{13},0)\tilde{G}(T_{13})b(l_2;T) \\
G_{211}(E) &= \sum_{N'H'TH}(N',H',T,H,E)G(T_{21},0)\tilde{G}(T_{21})2b(l_1';N') \\
G_{212}(E) &= \sum_{N'H'TH}(N',H',T,H,E)G(T_{21},0)\tilde{G}(T_{21})2b(l_1';N')b(l_2;T) \\
G_{221}(E) &= \sum_{N'H'TH}(N',H',T,H,E)G(T_{22},0)\tilde{G}(T_{22})2b(l_1';N') \\
G_{231}(E) &= \sum_{N'H'TH}(N',H',T,H,E)G(T_{23},0)\tilde{G}(T_{23})2b(l_1';N') \\
G_{232}(E) &= \sum_{N'H'TH}(N',H',T,H,E)G(T_{23},0)\tilde{G}(T_{23})2b(l_1';N')b(l_2;T)
\end{aligned}
$$

with

$$
\begin{aligned}
G(T_{11},0) &= \begin{pmatrix}1 & l_1 & H\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}1 & l_2 & T\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_1' & H & E\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_2' & T & E\\ 0 & 0 & 0\end{pmatrix} \\
\tilde{G}(T_{11}) &= (-1)^{1+L'+l_1+l_2'}\begin{Bmatrix}L' & l_1' & l_2'\\ E & T & H\end{Bmatrix}\begin{Bmatrix}L & l_1 & l_2\\ K & 1 & 1\\ L' & H & T\end{Bmatrix} \\
G(T_{12},0) &= \begin{pmatrix}1 & l_1 & T\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}1 & T & H\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_1' & H & E\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_2' & l_2 & E\\ 0 & 0 & 0\end{pmatrix} \\
\tilde{G}(T_{12}) &= (-1)^{L+L'+l_1+l_2'}\begin{Bmatrix}L & l_1 & l_2\\ H & L' & K\end{Bmatrix}\begin{Bmatrix}L' & l_1' & l_2'\\ E & l_2 & H\end{Bmatrix}\begin{Bmatrix}1 & 1 & K\\ l_1 & H & T\end{Bmatrix} \\
G(T_{13},0) &= \begin{pmatrix}1 & l_2 & T\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}1 & T & H\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_1' & l_1 & E\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_2' & H & E\\ 0 & 0 & 0\end{pmatrix} \\
\tilde{G}(T_{13}) &= (-1)^{l_1+l_2'}\begin{Bmatrix}L & l_1 & l_2\\ H & K & L'\end{Bmatrix}\begin{Bmatrix}L' & l_1' & l_2'\\ E & H & l_1\end{Bmatrix}\begin{Bmatrix}1 & 1 & K\\ l_2 & H & T\end{Bmatrix} \\
G(T_{21},0) &= \begin{pmatrix}l_1' & 1 & N'\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_2' & 1 & H'\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}1 & l_1 & H\\ 0 & 0 & 0\end{pmatrix} \\
&\times \begin{pmatrix}1 & l_2 & T\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}N' & H & E\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}H' & T & E\\ 0 & 0 & 0\end{pmatrix} \\
\tilde{G}(T_{21}) &= (-1)^{l_1+l_2'}\begin{Bmatrix}L' & l_1' & l_2'\\ 1 & H' & N'\end{Bmatrix}\begin{Bmatrix}L' & H & T\\ E & H' & N'\end{Bmatrix}\begin{Bmatrix}L & l_1 & l_2\\ K & 1 & 1\\ L' & H & T\end{Bmatrix} \\
G(T_{22},0) &= \begin{pmatrix}l_1' & 1 & N'\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_2' & 1 & H'\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}1 & l_1 & T\\ 0 & 0 & 0\end{pmatrix} \\
&\times \begin{pmatrix}1 & T & H\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}N' & H & E\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}H' & l_2 & E\\ 0 & 0 & 0\end{pmatrix} \\
\tilde{G}(T_{22}) &= (-1)^{1+L+l_1+l_2'}\begin{Bmatrix}L & l_1 & l_2\\ H & L' & K\end{Bmatrix}\begin{Bmatrix}L' & l_1' & l_2'\\ 1 & H' & N'\end{Bmatrix}\begin{Bmatrix}1 & 1 & K\\ l_1 & H & T\end{Bmatrix}
\end{aligned}
$$

$$
\begin{aligned}
& \times \begin{Bmatrix} L' & H & l_2 \\ E & H' & N' \end{Bmatrix} \\
G(T_{23},0) &= \begin{pmatrix} l_1' & 1 & N' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & 1 & H' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_2 & T \\ 0 & 0 & 0 \end{pmatrix} \\
& \times \begin{pmatrix} 1 & T & H \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} N' & l_1 & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} H' & H & E \\ 0 & 0 & 0 \end{pmatrix} \\
\tilde{G}(T_{23}) &= (-1)^{1+L'+l_1+l_2'}\begin{Bmatrix} L & l_1 & l_2 \\ H & K & L' \end{Bmatrix}\begin{Bmatrix} L' & l_1' & l_2' \\ 1 & H' & N' \end{Bmatrix}\begin{Bmatrix} 1 & 1 & K \\ l_2 & H & T \end{Bmatrix} \\
& \times \begin{Bmatrix} L' & l_1 & H \\ E & H' & N' \end{Bmatrix}.
\end{aligned}
$$

We have also defined:

$$
\begin{aligned}
\gamma_1 &= 2J_2(\mu_{11}, M_{11}; G_{111}; C-2) - J_1(\mu_{11}, M_{11}; G_{111})\eta(\mu_{11}+1, C+3) \\
\gamma_2 &= J_2(\mu_{12}, M_{12}; G_{12}; C-2) \\
\gamma_3 &= J_2(\mu_{13}, M_{13}; G_{131}; C-2) \\
\gamma_4 &= 2J_2(\mu_{21}, M_{21}; G_{211}; \tilde{c}-7) \\
\gamma_5 &= J_2(\mu_{22}, M_{22}; G_{221}; \tilde{c}-7) \\
\gamma_6 &= J_2(\mu_{23}, M_{23}; G_{231}; \tilde{c}-7).
\end{aligned}
$$

(b) H_D^{122}:

$$
\begin{aligned}
\Delta E_D^{122} &= \frac{3}{8}\alpha^4\delta_{JJ'}\delta_{M_JM_{J'}}\sum_K(-1)^{K+L+S'+J}\begin{Bmatrix} L' & S' & J \\ S & L & K \end{Bmatrix} \\
& \times \langle\gamma' L'\|R^{(K)}\|\gamma L\rangle\langle S'\|[\vec{\sigma}_1\otimes\vec{\sigma}_2]^{(K)}\|S\rangle
\end{aligned}
$$

with

$$
R^{(K)} = \nabla_1^2\frac{1}{r^5}[\vec{r}\otimes\vec{r}]^{(K)}(\vec{r}\cdot\vec{\nabla}_2)
$$

The orbital part is

$$
\langle F'\mathcal{Y}^{M'}_{l_1'l_2'L'}|R_Q^{(K)}|F\mathcal{Y}^{M}_{l_1l_2L}\rangle = (-1)^{L'-M'}\begin{pmatrix} L' & K & L \\ -M' & Q & M \end{pmatrix}U(122)D,
$$

where

$$
U(122) = \frac{1}{2}\sqrt{2K+1}(l_1, l_2, L, l_1', l_2', L')^{1/2}
$$

and

$$
\begin{aligned}
D &= \sum_{i=1}^{7}\sum_{j=1}^{2} O_{ij}^{(1)} \Delta_{ij}(1) + \sum_{i=1}^{7} \mathrm{coe}(S_i)\Delta_2(i) + c\sum_{i=1}^{7} \mathrm{coe}(S_i)\Delta_3(i) \\
&+ cc'\Delta_4 + c'\sum_{i=1}^{2} \mathrm{coe}(Q_i)\Delta_5 + c'\Delta_6.
\end{aligned}
$$

For $\Delta_{ij}(1)$,

$$
\begin{aligned}
T_1(k) &\equiv \varpi_k(\mu_{11}, M_{11}; G_{111}; A_1+3, B_1, C_1; \tilde{\alpha}, \tilde{\beta}) \\
&+ \varpi_k(\min(\mu_{12}, \mu_{15}), \max(M_{12}, M_{15}); G_{121}+G_{151}; A_1+2, B_1+1, C_1; \tilde{\alpha}, \tilde{\beta}) \\
&+ \varpi_k(\mu_{14}, M_{14}; G_{141}; A_1, B_1+3, C_1; \tilde{\alpha}, \tilde{\beta}) \\
&+ \varpi_k(\min(\mu_{13}, \mu_{16}), \max(M_{13}, M_{16}); G_{131}+G_{161}; A_1+1, B_1+2, C_1; \tilde{\alpha}, \tilde{\beta}) \\
\Delta_{ij}(1) &= T_1(0), \quad C_1 = -2 \\
\Delta_{ij}(1) &= T_1(1) + J_1(\mu_{11}, M_{11}; G_{111})[\eta(\mu_{11}, C_1+5) I_{\omega(\mu_{11})-2}(A_1+1, B_1, C_1+2) \\
&- \eta(\mu_{11}+1, C_1+5) I_{\omega(\mu_{11}+1)-2}(A_1, B_1+1, C_1+2)], \quad C_1 = -4 \\
\Delta_{ij}(1) &= T_1(2) \\
&+ \gamma_1 \mathrm{Dif}(A_1+2, B_1-1; A_1+1, B_1; C_1+2, \tilde{\alpha}, \tilde{\beta}; \omega(\mu_{11}+1)-2, \omega(\mu_{11})-2) \\
&+ \gamma_4 \mathrm{Dif}(A_1-1, B_1+2; A_1, B_1+1; C_1+2, \tilde{\alpha}, \tilde{\beta}; \omega(\mu_{11})-2, \omega(\mu_{11}+1)-2) \\
&+ (\gamma_1+\gamma_2+\gamma_5)\mathrm{Dif}(A_1+1, B_1; A_1, B_1+1; \\
&\quad C_1+2, \tilde{\alpha}, \tilde{\beta}; \omega(\mu_{11})-2, \omega(\mu_{11}+1)-2), \quad C_1 \neq -4, -2
\end{aligned}
$$

For $\Delta_2(i)$,

$$
\begin{aligned}
T_2(k) &\equiv \varpi_k(\mu_{11}, M_{11}; G_{112}; A+3, B-1, C; \tilde{\alpha}, \tilde{\beta}) \\
&+ \varpi_k(\min(\mu_{12}, \mu_{15}), \max(M_{12}, M_{15}); G_{122}+G_{152}; A+2, B, C; \tilde{\alpha}, \tilde{\beta}) \\
&+ \varpi_k(\min(\mu_{13}, \mu_{16}), \max(M_{13}, M_{16}); G_{132}+G_{162}; A+1, B+1, C; \tilde{\alpha}, \tilde{\beta}) \\
&+ \varpi_k(\mu_{14}, M_{14}; G_{142}; A, B+2, C; \tilde{\alpha}, \tilde{\beta}) \\
\Delta_2(i) &= T_2(1), \quad C = -4, -2 \\
\Delta_2(i) &= T_2(2) \\
&+ \gamma_7 \mathrm{Dif}(A+2, B-2; A+1, B-1; C+2, \tilde{\alpha}, \tilde{\beta}; \omega(\mu_{11}+1)-2, \omega(\mu_{11})-2) \\
&+ \gamma_{10} \mathrm{Dif}(A-1, B+1; A, B; C+2, \tilde{\alpha}, \tilde{\beta}; \omega(\mu_{11})-2, \omega(\mu_{11}+1)-2)
\end{aligned}
$$

$$
\begin{aligned}
&+ \quad (\gamma_7+\gamma_8+\gamma_{11})\mathrm{Dif}(A+1,B-1;A,B;\\
&\qquad C+2,\tilde{\alpha},\tilde{\beta};\omega(\mu_{11})-2,\omega(\mu_{11}+1)-2), \quad C\neq -4,-2
\end{aligned}
$$

For $\Delta_3(i)$,

$$
\begin{aligned}
T_3(k) &\equiv \varpi_k(\min(\mu_{11},\mu_{18},\mu_{111}),\max(M_{11},M_{18},M_{111});G_{111}+G_{18}+G_{1,11};\\
&\quad A+3,B+1,C-2;\tilde{\alpha},\tilde{\beta})\\
&+ \varpi_k(\min(\mu_{12},\mu_{15},\mu_{19},\mu_{112}),\max(M_{12},M_{15},M_{19},M_{112});G_{121}+G_{151}\\
&+ G_{19}+G_{1,12};A+2,B+2,C-2;\tilde{\alpha},\tilde{\beta})\\
&+ \varpi_k(\min(\mu_{13},\mu_{16},\mu_{110}),\max(M_{13},M_{16},M_{110});G_{131}+G_{161}+G_{1,10};\\
&\quad A+1,B+3,C-2;\tilde{\alpha},\tilde{\beta})\\
&+ \varpi_k(\mu_{14},M_{14};G_{141};A,B+4,C-2;\tilde{\alpha},\tilde{\beta})\\
&+ \varpi_k(\mu_{17},M_{17};G_{17};A+4,B,C-2;\tilde{\alpha},\tilde{\beta})\\
\Delta_3(i) &= T_3(0), \quad C=0\\
\Delta_3(i) &= T_3(1)+2J_1(\mu_{11},M_{11};G_{111})\eta(\mu_{11},C+3)I_{\omega(\mu_{11})-2}(A+1,B+1,C)\\
&- J_1(\mu_{11},M_{11};G_{111})\eta(\mu_{11}+1,C+3)I_{\omega(\mu_{11}+1)-2}(A,B+2,C)\\
&- J_1(\mu_{11},M_{11};G_{111})\eta(\mu_{11}+1,C+3)I_{\omega(\mu_{11}+1)-2}(A+2,B,C), \quad C=-2\\
\Delta_3(i) &= T_3(2)+\gamma_{16}\eta(\mu_{11},C+5)I_{\omega(\mu_{11})-2}(A-1,B+1,C+2)\\
&+ \gamma_{17}\eta(\mu_{11},C+5)I_{\omega(\mu_{11})-2}(A+1,B-1,C+2)\\
&+ (\gamma_{15}+2\gamma_{16})\eta(\mu_{11}+1,C+5)I_{\omega(\mu_{11}+1)-2}(A,B,C+2), \quad C=-4\\
\Delta_3(i) &= T_3(3)\\
&+ \xi_5\mathrm{Dif}(A+2,B-2;A+1,B-1;C+2,\tilde{\alpha},\tilde{\beta};\omega(\mu_{11}+1)-2,\omega(\mu_{11})-2)\\
&+ (\xi_1+\xi_5)\mathrm{Dif}(A+1,B-1;A,B;C+2,\tilde{\alpha},\tilde{\beta};\omega(\mu_{11})-2,\omega(\mu_{11}+1)-2)\\
&+ (\xi_1+\xi_2+\xi_5)\mathrm{Dif}(A,B;A-1,B+1;C+2,\tilde{\alpha},\tilde{\beta};\\
&\quad \omega(\mu_{11}+1)-2,\omega(\mu_{11})-2)\\
&+ (\xi_1+\xi_2+\xi_3+\xi_5)\mathrm{Dif}(A-1,B+1;A-2,B+2;C+2,\tilde{\alpha},\tilde{\beta};\\
&\quad \omega(\mu_{11})-2,\omega(\mu_{11}+1)-2)\\
&+ (\sum_{i=1}^{5}\xi_i)I_{\omega(\mu_{11}+1)-2}(A-2,B+2,C+2), \quad C\neq 0,-2,-4
\end{aligned}
$$

For Δ_4,

$$\begin{aligned}
T_4(k) &\equiv \varpi_k(\min(\mu_{21},\mu_{28},\mu_{211}),\max(M_{21},M_{28},M_{211}); G_{211}+G_{28}+G_{2,11};\\
&\quad \tilde{a}+2,\tilde{b}+2,\tilde{c}-9;\tilde{\alpha},\tilde{\beta})\\
&+ \varpi_k(\min(\mu_{22},\mu_{25},\mu_{29},\mu_{212}),\max(M_{22},M_{25},M_{29},M_{212}); G_{221}+G_{251}\\
&+ G_{29}+G_{2,12};\tilde{a}+1,\tilde{b}+3,\tilde{c}-9;\tilde{\alpha},\tilde{\beta})\\
&+ \varpi_k(\min(\mu_{23},\mu_{26},\mu_{210}),\max(M_{23},M_{26},M_{210}); G_{231}+G_{261}+G_{2,10};\\
&\quad \tilde{a},\tilde{b}+4,\tilde{c}-9;\tilde{\alpha},\tilde{\beta})\\
&+ \varpi_k(\mu_{24},M_{24};G_{241};\tilde{a}-1,\tilde{b}+5,\tilde{c}-9;\tilde{\alpha},\tilde{\beta})\\
&+ \varpi_k(\mu_{27},M_{27};G_{27};\tilde{a}+3,\tilde{b}+1,\tilde{c}-9;\tilde{\alpha},\tilde{\beta})\\
\Delta_4 &= T_4(1), \quad \tilde{c}=5,7\\
\Delta_4 &= T_4(2)+\gamma_{21}\eta(\mu_{11}+1,\tilde{c}-2)I_{\omega(\mu_{11}+1)-2}(\tilde{a}-2,\tilde{b}+2,\tilde{c}-5)\\
&+ \gamma_{22}\eta(\mu_{11}+1,\tilde{c}-2)I_{\omega(\mu_{11}+1)-2}(\tilde{a},\tilde{b},\tilde{c}-5)\\
&+ (\gamma_{20}+2\gamma_{21})\eta(\mu_{11},\tilde{c}-2)I_{\omega(\mu_{11})-2}(\tilde{a}-1,\tilde{b}+1,\tilde{c}-5), \quad \tilde{c}=3\\
\Delta_4 &= T_4(3)\\
&+ \xi_{10}\mathrm{Dif}(\tilde{a}+1,\tilde{b}-1;\tilde{a},\tilde{b};\tilde{c}-5,\tilde{\alpha},\tilde{\beta};\omega(\mu_{11})-2,\omega(\mu_{11}+1)-2)\\
&+ (\xi_6+\xi_{10})\mathrm{Dif}(\tilde{a},\tilde{b};\tilde{a}-1,\tilde{b}+1;\tilde{c}-5,\tilde{\alpha},\tilde{\beta};\omega(\mu_{11}+1)-2,\omega(\mu_{11})-2)\\
&+ (\xi_6+\xi_7+\xi_{10})\mathrm{Dif}(\tilde{a}-1,\tilde{b}+1;\tilde{a}-2,\tilde{b}+2;\tilde{c}-5,\tilde{\alpha},\tilde{\beta};\\
&\quad \omega(\mu_{11})-2,\omega(\mu_{11}+1)-2)\\
&+ (\xi_6+\xi_7+\xi_8+\xi_{10})\mathrm{Dif}(\tilde{a}-2,\tilde{b}+2;\tilde{a}-3,\tilde{b}+3;\tilde{c}-5,\tilde{\alpha},\tilde{\beta};\\
&\quad \omega(\mu_{11}+1)-2,\omega(\mu_{11})-2), \quad \tilde{c}\neq 3,5,7
\end{aligned}$$

For Δ_5,

$$\begin{aligned}
T_5(k) &\equiv \varpi_k(\mu_{21},M_{21};G_{211};\tilde{a}+2,\tilde{b}+b(i)+1,\tilde{c}-7;\tilde{\alpha},\tilde{\beta})\\
&+ \varpi_k(\min(\mu_{22},\mu_{25}),\max(M_{22},M_{25}); G_{221}+G_{251};\tilde{a}+1,\tilde{b}+b(i)+2,\\
&\quad \tilde{c}-7;\tilde{\alpha},\tilde{\beta})\\
&+ \varpi_k(\min(\mu_{23},\mu_{26}),\max(M_{23},M_{26}); G_{231}+G_{261};\tilde{a},\tilde{b}+b(i)+3,\\
&\quad \tilde{c}-7;\tilde{\alpha},\tilde{\beta})\\
&+ \varpi_k(\mu_{24},M_{24};G_{241};\tilde{a}-1,\tilde{b}+b(i)+4,\tilde{c}-7;\tilde{\alpha},\tilde{\beta})
\end{aligned}$$

$$\Delta_5 = T_5(1), \quad \tilde{c} = 3, 5$$

$$\begin{aligned}
\Delta_5 &= T_5(2) \\
&+ \gamma_{23}\mathrm{Dif}(\tilde{a}+1, \tilde{b}+b(i); \tilde{a}, \tilde{b}+b(i)+1; \\
&\quad \tilde{c}-5, \tilde{\alpha}, \tilde{\beta}; \omega(\mu_{11})-2, \omega(\mu_{11}+1)-2) \\
&+ (\gamma_{23}+\gamma_{24})\mathrm{Dif}(\tilde{a}, \tilde{b}+b(i)+1; \tilde{a}-1, \tilde{b}+b(i)+2; \\
&\quad \tilde{c}-5, \tilde{\alpha}, \tilde{\beta}; \omega(\mu_{11}+1)-2, \omega(\mu_{11})-2) \\
&+ (\gamma_{23}+\gamma_{24}+\gamma_{25})\mathrm{Dif}(\tilde{a}-1, \tilde{b}+b(i)+2; \tilde{a}-2, \tilde{b}+b(i)+3; \tilde{c}-5, \tilde{\alpha}, \tilde{\beta}; \\
&\quad \omega(\mu_{11})-2, \omega(\mu_{11}+1)-2), \quad \tilde{c} \neq 3, 5
\end{aligned}$$

For Δ_6,

$$\begin{aligned}
T_6(k) &\equiv \varpi_k(\mu_{21}, M_{21}; G_{212}; \tilde{a}+2, \tilde{b}, \tilde{c}-7; \tilde{\alpha}, \tilde{\beta}) \\
&+ \varpi_k(\min(\mu_{22}, \mu_{25}), \max(M_{22}, M_{25}); G_{222}+G_{252}; \tilde{a}+1, \tilde{b}+1, \\
&\quad \tilde{c}-7; \tilde{\alpha}, \tilde{\beta}) \\
&+ \varpi_k(\min(\mu_{23}, \mu_{26}), \max(M_{23}, M_{26}); G_{232}+G_{262}; \tilde{a}, \tilde{b}+2, \\
&\quad \tilde{c}-7; \tilde{\alpha}, \tilde{\beta}) \\
&+ \varpi_k(\mu_{24}, M_{24}; G_{242}; \tilde{a}-1, \tilde{b}+3, \tilde{c}-7; \tilde{\alpha}, \tilde{\beta}) \\
\Delta_6 &= T_6(1), \quad \tilde{c} = 3, 5 \\
\Delta_6 &= T_6(2) \\
&+ \gamma_{27}\mathrm{Dif}(\tilde{a}+1, \tilde{b}-1; \tilde{a}, \tilde{b}; \tilde{c}-5, \tilde{\alpha}, \tilde{\beta}; \omega(\mu_{11})-2, \omega(\mu_{11}+1)-2) \\
&+ (\gamma_{27}+\gamma_{28})\mathrm{Dif}(\tilde{a}, \tilde{b}; \tilde{a}-1, \tilde{b}+1; \tilde{c}-5, \tilde{\alpha}, \tilde{\beta}; \\
&\quad \omega(\mu_{11}+1)-2, \omega(\mu_{11})-2) \\
&+ (\gamma_{27}+\gamma_{28}+\gamma_{29})\mathrm{Dif}(\tilde{a}-1, \tilde{b}+1; \tilde{a}-2, \tilde{b}+2; \tilde{c}-5, \tilde{\alpha}, \tilde{\beta}; \\
&\quad \omega(\mu_{11})-2, \omega(\mu_{11}+1)-2), \quad \tilde{c} \neq 3, 5.
\end{aligned}$$

Also,

$$\begin{aligned}
M_{11} &= \min(l_1 + l_1' + K + 1, l_2 + l_2' + 1) \\
M_{12} &= \min(l_1 + l_1' + K, l_2 + l_2') \\
M_{13} &= \min(l_1 + l_1' + 1, l_2 + l_2' + K + 1)
\end{aligned}$$

$$
\begin{aligned}
M_{14} &= \min(l_1 + l_1', l_2 + l_2' + K + 2) \\
M_{15} &= \min(l_1 + l_1' + 2, l_2 + l_2' + 2) \\
M_{16} &= \min(l_1 + l_1' + 1, l_2 + l_2' + 3) \\
M_{17} &= \min(l_1 + l_1' + K + 2, l_2 + l_2') \\
M_{18} &= \min(l_1 + l_1' + K + 1, l_2 + l_2' + 1) \\
M_{19} &= \min(l_1 + l_1', l_2 + l_2' + K) \\
M_{110} &= \min(l_1 + l_1' + 1, l_2 + l_2' + K + 1) \\
M_{111} &= \min(l_1 + l_1' + 3, l_2 + l_2' + 1) \\
M_{112} &= \min(l_1 + l_1' + 2, l_2 + l_2' + 2) \\
M_{21} &= \min(l_1 + l_1' + K + 2, l_2 + l_2' + 2) \\
M_{22} &= \min(l_1 + l_1' + K + 1, l_2 + l_2' + 1) \\
M_{23} &= \min(l_1 + l_1' + 2, l_2 + l_2' + K + 2) \\
M_{24} &= \min(l_1 + l_1' + 1, l_2 + l_2' + K + 3) \\
M_{25} &= \min(l_1 + l_1' + 3, l_2 + l_2' + 3) \\
M_{26} &= \min(l_1 + l_1' + 2, l_2 + l_2' + 4) \\
M_{27} &= \min(l_1 + l_1' + K + 3, l_2 + l_2' + 1) \\
M_{28} &= \min(l_1 + l_1' + K + 2, l_2 + l_2' + 2) \\
M_{29} &= \min(l_1 + l_1' + 1, l_2 + l_2' + K + 1) \\
M_{210} &= \min(l_1 + l_1' + 2, l_2 + l_2' + K + 2) \\
M_{211} &= \min(l_1 + l_1' + 4, l_2 + l_2' + 2) \\
M_{212} &= \min(l_1 + l_1' + 3, l_2 + l_2' + 3) \\
\mu_{ij} &= \omega(M_{ij}) - 2, \quad i = 1, 2, \quad j = 1, \cdots, 12
\end{aligned}
$$

$$
\begin{aligned}
A &\equiv \tilde{a} + a'(i) \\
B &\equiv \tilde{b} + b'(i) \\
C &\equiv \tilde{c} + c'(i) \\
A_1 &\equiv \tilde{a} + a'(i) \\
B_1 &\equiv \tilde{b} + b'(i) + b(j)
\end{aligned}
$$

$$
\begin{aligned}
C_1 &\equiv \tilde{c} + c'(i) \\
O_{ij}^{(1)} &\equiv \mathrm{coc}(S_i)\mathrm{coc}(Q_j)
\end{aligned}
$$

$\mathrm{coc}(S_i)$	$a'(i)$	$b'(i)$	$c'(i)$
$a'(a'+1+c') - l_1'(l_1'+1)$	-2	0	-5
$-\alpha'[2(a'+1)+c']$	-1	0	-5
α'^2	0	0	-5
$c'(c'+1+a')$	0	0	-7
$-a'c'$	-2	2	-7
$-\alpha'c'$	1	0	-7
$\alpha'c'$	-1	2	-7

$\mathrm{coc}(Q_i)$	$b(i)$	$c(i)$
b	-1	0
$-\beta$	0	0
c	1	-2

The angular coefficients are:

$$
\begin{aligned}
G_{111}(E) &= \sum_{TN\Lambda}(T,N,\Lambda,E)G(T_{11},0)\tilde{G}(T_{11}) \\
G_{112}(E) &= \sum_{TN\Lambda}(T,N,\Lambda,E)G(T_{11},0)\tilde{G}(T_{11})b(l_2;T)
\end{aligned}
$$

$$
G_{121}(E) = \sum_{TN}(T,N,E)G(T_{12},0)\tilde{G}(T_{12})
$$

$$
\begin{aligned}
G_{131}(E) &= \sum_{TN\Lambda}(T,N,\Lambda,E)G(T_{13},0)\tilde{G}(T_{13}) \\
G_{132}(E) &= \sum_{TN\Lambda}(T,N,\Lambda,E)G(T_{13},0)\tilde{G}(T_{13})b(l_2;T)
\end{aligned}
$$

$$
\begin{aligned}
G_{141}(E) &= \sum_{TN\Lambda}(T,N,\Lambda,E)G(T_{14},0)\tilde{G}(T_{14}) \\
G_{142}(E) &= \sum_{TN\Lambda}(T,N,\Lambda,E)G(T_{14},0)\tilde{G}(T_{14})b(l_2;T)
\end{aligned}
$$

$$
\begin{aligned}
G_{151}(E) &= \sum_{TN\Lambda H}(T,N,\Lambda,H,E)G(T_{15},0)\tilde{G}(T_{15})2 \\
G_{152}(E) &= \sum_{TN\Lambda H}(T,N,\Lambda,H,E)G(T_{15},0)\tilde{G}(T_{15})2b(l_2;T)
\end{aligned}
$$

$$G_{161}(E) = \sum_{TN\Lambda H} (T, N, \Lambda, H, E) G(T_{16}, 0) \tilde{G}(T_{16}) 2$$
$$G_{162}(E) = \sum_{TN\Lambda H} (T, N, \Lambda, H, E) G(T_{16}, 0) \tilde{G}(T_{16}) 2 b(l_2; T)$$

$$G_{17}(E) = \sum_{TN\Lambda} (T, N, \Lambda, E) G(T_{17}, 0) \tilde{G}(T_{17})$$

$$G_{18}(E) = \sum_{TN\Lambda} (T, N, \Lambda, E) G(T_{18}, 0) \tilde{G}(T_{18})$$

$$G_{19}(E) = \sum_{N} (N, E) G(T_{19}, 0) \tilde{G}(T_{19})$$

$$G_{1,10}(E) = \sum_{TN\Lambda} (T, N, \Lambda, E) G(T_{1,10}, 0) \tilde{G}(T_{1,10})$$

$$G_{1,11}(E) = \sum_{TN\Lambda H} (T, N, \Lambda, H, E) G(T_{1,11}, 0) \tilde{G}(T_{1,11}) 2$$

$$G_{1,12}(E) = \sum_{TN\Lambda H} (T, N, \Lambda, H, E) G(T_{1,12}, 0) \tilde{G}(T_{1,12}) 2$$

$$G_{211}(E) = \sum_{N'H'TN\Lambda} (N', H', T, N, \Lambda, E) G(T_{21}, 0) \tilde{G}(T_{21}) 2 b(l_1'; N')$$
$$G_{212}(E) = \sum_{N'H'TN\Lambda} (N', H', T, N, \Lambda, E) G(T_{21}, 0) \tilde{G}(T_{21}) 2 b(l_1'; N') b(l_2; T)$$

$$G_{221}(E) = \sum_{N'H'TN} (N', H', T, N, E) G(T_{22}, 0) \tilde{G}(T_{22}) 2 b(l_1'; N')$$

$$G_{231}(E) = \sum_{N'H'TN\Lambda} (N', H', T, N, \Lambda, E) G(T_{23}, 0) \tilde{G}(T_{23}) 2 b(l_1'; N')$$
$$G_{232}(E) = \sum_{N'H'TN\Lambda} (N', H', T, N, \Lambda, E) G(T_{23}, 0) \tilde{G}(T_{23}) 2 b(l_1'; N') b(l_2; T)$$

$$G_{241}(E) = \sum_{N'H'TN\Lambda} (N', H', T, N, \Lambda, E) G(T_{24}, 0) \tilde{G}(T_{24}) 2 b(l_1'; N')$$
$$G_{242}(E) = \sum_{N'H'TN\Lambda} (N', H', T, N, \Lambda, E) G(T_{24}, 0) \tilde{G}(T_{24}) 2 b(l_1'; N') b(l_2; T)$$

$$G_{251}(E) = \sum_{N'H'TN\Lambda H} (N', H', T, N, \Lambda, H, E) G(T_{25}, 0) \tilde{G}(T_{25}) 4b(l_1'; N')$$

$$G_{252}(E) = \sum_{N'H'TN\Lambda H} (N', H', T, N, \Lambda, H, E) G(T_{25}, 0) \tilde{G}(T_{25}) 4b(l_1'; N') b(l_2; T)$$

$$G_{261}(E) = \sum_{N'H'TN\Lambda H} (N', H', T, N, \Lambda, H, E) G(T_{26}, 0) \tilde{G}(T_{26}) 4b(l_1'; N')$$

$$G_{262}(E) = \sum_{N'H'TN\Lambda H} (N', H', T, N, \Lambda, H, E) G(T_{26}, 0) \tilde{G}(T_{26}) 4b(l_1'; N') b(l_2; T)$$

$$G_{27}(E) = \sum_{N'H'TN\Lambda} (N', H', T, N, \Lambda, E) G(T_{27}, 0) \tilde{G}(T_{27}) 2b(l_1'; N')$$

$$G_{28}(E) = \sum_{N'H'TN\Lambda} (N', H', T, N, \Lambda, E) G(T_{28}, 0) \tilde{G}(T_{28}) 2b(l_1'; N')$$

$$G_{29}(E) = \sum_{N'H'N} (N', H', N, E) G(T_{29}, 0) \tilde{G}(T_{29}) 2b(l_1'; N')$$

$$G_{2,10}(E) = \sum_{N'H'TN\Lambda} (N', H', T, N, \Lambda, E) G(T_{2,10}, 0) \tilde{G}(T_{2,10}) 2b(l_1'; N')$$

$$G_{2,11}(E) = \sum_{N'H'TN\Lambda H} (N', H', T, N, \Lambda, H, E) G(T_{2,11}, 0) \tilde{G}(T_{2,11}) 4b(l_1'; N')$$

$$G_{2,12}(E) = \sum_{N'H'TN\Lambda H} (N', H', T, N, \Lambda, H, E) G(T_{2,12}, 0) \tilde{G}(T_{2,12}) 4b(l_1'; N')$$

with

$$\begin{aligned}
G(T_{11}, 0) &= \begin{pmatrix} 1 & 1 & K \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & l_2 & T \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} K & 1 & N \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & N & \Lambda \\ 0 & 0 & 0 \end{pmatrix} \\
&\times \begin{pmatrix} l_1' & \Lambda & E \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2' & T & E \\ 0 & 0 & 0 \end{pmatrix} \\
\tilde{G}(T_{11}) &= (-1)^{1+L'+l_1+l_2'} \begin{Bmatrix} L' & l_1' & l_2' \\ E & T & \Lambda \end{Bmatrix} \begin{Bmatrix} L & l_1 & l_2 \\ K & N & 1 \\ L' & \Lambda & T \end{Bmatrix} \\
G(T_{12}, 0) &= \begin{pmatrix} 1 & 1 & K \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & K & N \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & l_2 & T \\ 0 & 0 & 0 \end{pmatrix}^2 \begin{pmatrix} l_1' & N & E \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2' & l_2 & E \\ 0 & 0 & 0 \end{pmatrix} \\
\tilde{G}(T_{12}) &= (-1)^{1+L+L'+l_2'} \begin{Bmatrix} L & l_1 & l_2 \\ N & L' & K \end{Bmatrix} \begin{Bmatrix} L' & l_1' & l_2' \\ E & l_2 & N \end{Bmatrix}
\end{aligned}$$

$$G(T_{13},0) = \begin{pmatrix} 1 & 1 & K \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_2 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_1 & 1 & N \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} T & K & \Lambda \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times \begin{pmatrix} l_1' & N & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & \Lambda & E \\ 0 & 0 & 0 \end{pmatrix}$$

$$\tilde{G}(T_{13}) = (-1)^{1+L+l_1'}\begin{Bmatrix} L & l_1 & l_2 \\ 1 & T & N \end{Bmatrix}\begin{Bmatrix} L' & l_1' & l_2' \\ E & \Lambda & N \end{Bmatrix}\begin{Bmatrix} L & K & L' \\ \Lambda & N & T \end{Bmatrix}$$

$$G(T_{14},0) = \begin{pmatrix} 1 & 1 & K \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_2 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & K & N \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} T & N & \Lambda \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times \begin{pmatrix} l_1' & l_1 & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & \Lambda & E \\ 0 & 0 & 0 \end{pmatrix}$$

$$\tilde{G}(T_{14}) = (-1)^{l_1+l_2'}\begin{Bmatrix} L & l_1 & l_2 \\ \Lambda & K & L' \end{Bmatrix}\begin{Bmatrix} L' & l_1' & l_2' \\ E & \Lambda & l_1 \end{Bmatrix}\begin{Bmatrix} l_2 & 1 & T \\ N & \Lambda & K \end{Bmatrix}$$

$$G(T_{15},0) = \begin{pmatrix} 1 & 1 & N \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_2 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_1 & N & H \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} T & 1 & \Lambda \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times \begin{pmatrix} l_1' & H & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & \Lambda & E \\ 0 & 0 & 0 \end{pmatrix}$$

$$\tilde{G}(T_{15}) = (-1)^{1+L+L'+l_2'}\begin{Bmatrix} L' & l_1' & l_2' \\ E & \Lambda & H \end{Bmatrix}\sum_{\lambda_1}(\lambda_1)\begin{Bmatrix} L & l_1 & l_2 \\ 1 & T & \lambda_1 \end{Bmatrix}$$

$$\times \begin{Bmatrix} N & 1 & 1 \\ \lambda_1 & H & l_1 \end{Bmatrix}\begin{Bmatrix} L & \lambda_1 & T \\ K & 1 & 1 \\ L' & H & \Lambda \end{Bmatrix}$$

$$G(T_{16},0) = \begin{pmatrix} 1 & 1 & N \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_2 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_1 & 1 & H \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} T & N & \Lambda \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times \begin{pmatrix} l_1' & H & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & \Lambda & E \\ 0 & 0 & 0 \end{pmatrix}$$

$$\tilde{G}(T_{16}) = (-1)^{1+L'+l_1'}\begin{Bmatrix} L' & l_1' & l_2' \\ E & \Lambda & H \end{Bmatrix}\begin{Bmatrix} N & 1 & 1 \\ l_2 & \Lambda & T \end{Bmatrix}\sum_{\lambda_1}(\lambda_1)\begin{Bmatrix} L & l_1 & l_2 \\ 1 & \Lambda & \lambda_1 \end{Bmatrix}$$

$$\times \begin{Bmatrix} 1 & 1 & K \\ H & \lambda_1 & l_1 \end{Bmatrix}\begin{Bmatrix} L & L' & K \\ H & \lambda_1 & \Lambda \end{Bmatrix}$$

$$G(T_{17},0) = \begin{pmatrix} 1 & 1 & K \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_1 & 1 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} K & 1 & N \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} T & N & \Lambda \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times \begin{pmatrix} l_1' & \Lambda & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & l_2 & E \\ 0 & 0 & 0 \end{pmatrix}$$

$$\tilde{G}(T_{17}) = (-1)^{L+L'+l_1+l_2'}\begin{Bmatrix} L & l_1 & l_2 \\ \Lambda & L' & K \end{Bmatrix}\begin{Bmatrix} L' & l_1' & l_2' \\ E & l_2 & \Lambda \end{Bmatrix}\begin{Bmatrix} l_1 & 1 & T \\ N & \Lambda & K \end{Bmatrix}$$

$$G(T_{18},0) = \begin{pmatrix} 1 & 1 & K \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_1 & 1 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} T & K & N \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2 & 1 & \Lambda \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times \begin{pmatrix} l_1' & N & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & \Lambda & E \\ 0 & 0 & 0 \end{pmatrix}$$

$$\tilde{G}(T_{18}) = (-1)^{1+L'+l_2'}\begin{Bmatrix} L & l_1 & l_2 \\ 1 & \Lambda & T \end{Bmatrix}\begin{Bmatrix} L' & l_1' & l_2' \\ E & \Lambda & N \end{Bmatrix}\begin{Bmatrix} L & L' & K \\ N & T & \Lambda \end{Bmatrix}$$

$$G(T_{19},0) = \begin{pmatrix} 1 & 1 & K \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2 & K & N \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_1' & l_1 & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & N & E \\ 0 & 0 & 0 \end{pmatrix}$$

$$\tilde{G}(T_{19}) = (-1)^{1+l_1'}\begin{Bmatrix} L & l_1 & l_2 \\ N & K & L' \end{Bmatrix}\begin{Bmatrix} L' & l_1' & l_2' \\ E & N & l_1 \end{Bmatrix}$$

$$G(T_{1,10},0) = \begin{pmatrix} 1 & 1 & K \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_1 & 1 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & K & N \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2 & N & \Lambda \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times \begin{pmatrix} l_1' & T & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & \Lambda & E \\ 0 & 0 & 0 \end{pmatrix}$$

$$\tilde{G}(T_{1,10}) = (-1)^{1+L'+l_1+l_2'}\begin{Bmatrix} L' & l_1' & l_2' \\ E & \Lambda & T \end{Bmatrix}\begin{Bmatrix} L & l_1 & l_2 \\ K & 1 & N \\ L' & T & \Lambda \end{Bmatrix}$$

$$G(T_{1,11},0) = \begin{pmatrix} l_1 & 1 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & 1 & N \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} T & N & H \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2 & 1 & \Lambda \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times \begin{pmatrix} l_1' & H & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & \Lambda & E \\ 0 & 0 & 0 \end{pmatrix}$$

$$\tilde{G}(T_{1,11}) = (-1)^{1+L'+l_2'}\begin{Bmatrix} L' & l_1' & l_2' \\ E & \Lambda & H \end{Bmatrix}\begin{Bmatrix} N & 1 & 1 \\ l_1 & H & T \end{Bmatrix}\begin{Bmatrix} L & l_1 & l_2 \\ K & 1 & 1 \\ L' & H & \Lambda \end{Bmatrix}$$

$$G(T_{1,12},0) = \begin{pmatrix} l_1 & 1 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & 1 & N \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} T & 1 & H \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2 & N & \Lambda \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times \begin{pmatrix} l_1' & H & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & \Lambda & E \\ 0 & 0 & 0 \end{pmatrix}$$

$$\tilde{G}(T_{1,12}) = (-1)^{1+L'+l_1+l_2'}\begin{Bmatrix} L' & l_1' & l_2' \\ E & \Lambda & H \end{Bmatrix}\sum_{\lambda_1}(-1)^{\lambda_1}(\lambda_1)\begin{Bmatrix} L & l_1 & l_2 \\ N & \Lambda & \lambda_1 \end{Bmatrix}$$

$$\times \begin{Bmatrix} 1 & 1 & N \\ l_1 & \lambda_1 & T \end{Bmatrix}\begin{Bmatrix} \lambda_1 & T & 1 \\ 1 & K & H \end{Bmatrix}\begin{Bmatrix} L & \lambda_1 & \Lambda \\ H & L' & K \end{Bmatrix}$$

$$G(T_{21},0) = \begin{pmatrix} l_1' & 1 & N' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & 1 & H' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & 1 & K \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_2 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} K & 1 & N \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times \begin{pmatrix} l_1 & N & \Lambda \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} N' & \Lambda & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} H' & T & E \\ 0 & 0 & 0 \end{pmatrix}$$

$$\tilde{G}(T_{21}) = (-1)^{l_1+l_2'}\begin{Bmatrix} L' & l_1' & l_2' \\ 1 & H' & N' \end{Bmatrix}\begin{Bmatrix} L' & \Lambda & T \\ E & H' & N' \end{Bmatrix}\begin{Bmatrix} L & l_1 & l_2 \\ K & N & 1 \\ L' & \Lambda & T \end{Bmatrix}$$

$$G(T_{22},0) = \begin{pmatrix} l_1' & 1 & N' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & 1 & H' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & 1 & K \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_2 & T \\ 0 & 0 & 0 \end{pmatrix}^2$$

$$\times \begin{pmatrix} l_1 & K & N \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} N' & N & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} H' & l_2 & E \\ 0 & 0 & 0 \end{pmatrix}$$

$$\tilde{G}(T_{22}) = (-1)^{L+l_2'}\begin{Bmatrix} L & l_1 & l_2 \\ N & L' & K \end{Bmatrix}\begin{Bmatrix} L' & l_1' & l_2' \\ 1 & H' & N' \end{Bmatrix}\begin{Bmatrix} L' & N & l_2 \\ E & H' & N' \end{Bmatrix}$$

$$G(T_{23},0) = \begin{pmatrix} l_1' & 1 & N' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & 1 & H' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & 1 & K \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_2 & T \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times \begin{pmatrix} l_1 & 1 & N \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} T & K & \Lambda \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} N' & N & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} H' & \Lambda & E \\ 0 & 0 & 0 \end{pmatrix}$$

$$\tilde{G}(T_{23}) = (-1)^{L+L'+l_1'}\begin{Bmatrix} L & l_1 & l_2 \\ 1 & T & N \end{Bmatrix}\begin{Bmatrix} L' & l_1' & l_2' \\ 1 & H' & N' \end{Bmatrix}\begin{Bmatrix} L & K & L' \\ \Lambda & N & T \end{Bmatrix}$$

$$\times \begin{Bmatrix} L' & N & \Lambda \\ E & H' & N' \end{Bmatrix}$$

$$G(T_{24},0) = \begin{pmatrix} l_1' & 1 & N' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & 1 & H' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & 1 & K \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_2 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & K & N \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times \begin{pmatrix} T & N & \Lambda \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} N' & l_1 & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} H' & \Lambda & E \\ 0 & 0 & 0 \end{pmatrix}$$

$$\tilde{G}(T_{24}) = (-1)^{1+L'+l_1+l_2'}\begin{Bmatrix} L & l_1 & l_2 \\ \Lambda & K & L' \end{Bmatrix}\begin{Bmatrix} L' & l_1' & l_2' \\ 1 & H' & N' \end{Bmatrix}$$

$$\times \begin{Bmatrix} l_2 & 1 & T \\ N & \Lambda & K \end{Bmatrix}\begin{Bmatrix} L' & l_1 & \Lambda \\ E & H' & N' \end{Bmatrix}$$

$$G(T_{25},0) = \begin{pmatrix} l_1' & 1 & N' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & 1 & H' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & 1 & N \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_2 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_1 & N & H \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times \begin{pmatrix} T & 1 & \Lambda \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} N' & H & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} H' & \Lambda & E \\ 0 & 0 & 0 \end{pmatrix}$$

$$\tilde{G}(T_{25}) = (-1)^{L+l_2'}\begin{Bmatrix} L' & H & \Lambda \\ E & H' & N' \end{Bmatrix}\begin{Bmatrix} L' & l_1' & l_2' \\ 1 & H' & N' \end{Bmatrix}\sum_{\lambda_1}(\lambda_1)\begin{Bmatrix} L & l_1 & l_2 \\ 1 & T & \lambda_1 \end{Bmatrix}$$

$$\times \begin{Bmatrix} N & 1 & 1 \\ \lambda_1 & H & l_1 \end{Bmatrix}\begin{Bmatrix} L & \lambda_1 & T \\ K & 1 & 1 \\ L' & H & \Lambda \end{Bmatrix}$$

$$G(T_{26},0) = \begin{pmatrix} l_1' & 1 & N' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & 1 & H' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & 1 & N \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_2 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_1 & 1 & H \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times \begin{pmatrix} T & N & \Lambda \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} N' & H & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} H' & \Lambda & E \\ 0 & 0 & 0 \end{pmatrix}$$

$$\tilde{G}(T_{26}) = (-1)^{l_1'}\begin{Bmatrix} N & 1 & 1 \\ l_2 & \Lambda & T \end{Bmatrix}\begin{Bmatrix} L' & H & \Lambda \\ E & H' & N' \end{Bmatrix}\begin{Bmatrix} L' & l_1' & l_2' \\ 1 & H' & N' \end{Bmatrix}$$

$$\times \sum_{\lambda_1}(\lambda_1)\begin{Bmatrix} L & l_1 & l_2 \\ 1 & \Lambda & \lambda_1 \end{Bmatrix}\begin{Bmatrix} L & L' & K \\ H & \lambda_1 & \Lambda \end{Bmatrix}\begin{Bmatrix} 1 & 1 & K \\ H & \lambda_1 & l_1 \end{Bmatrix}$$

$$
\begin{aligned}
G(T_{27},0) &= \begin{pmatrix} l_1' & 1 & N' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & 1 & H' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & 1 & K \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_1 & 1 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} K & 1 & N \\ 0 & 0 & 0 \end{pmatrix} \\
&\times \begin{pmatrix} T & N & \Lambda \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} N' & \Lambda & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} H' & l_2 & E \\ 0 & 0 & 0 \end{pmatrix} \\
\tilde{G}(T_{27}) &= (-1)^{1+L+l_1+l_2'}\begin{Bmatrix} L & l_1 & l_2 \\ \Lambda & L' & K \end{Bmatrix}\begin{Bmatrix} L' & l_1' & l_2' \\ 1 & H' & N' \end{Bmatrix}\begin{Bmatrix} l_1 & 1 & T \\ N & \Lambda & K \end{Bmatrix} \\
&\times \begin{Bmatrix} L' & \Lambda & l_2 \\ E & H' & N' \end{Bmatrix} \\
G(T_{28},0) &= \begin{pmatrix} l_1' & 1 & N' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & 1 & H' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & 1 & K \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_1 & 1 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} T & K & N \\ 0 & 0 & 0 \end{pmatrix} \\
&\times \begin{pmatrix} l_2 & 1 & \Lambda \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} N' & N & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} H' & \Lambda & E \\ 0 & 0 & 0 \end{pmatrix} \\
\tilde{G}(T_{28}) &= (-1)^{l_2'}\begin{Bmatrix} L & l_1 & l_2 \\ 1 & \Lambda & T \end{Bmatrix}\begin{Bmatrix} L' & l_1' & l_2' \\ 1 & H' & N' \end{Bmatrix}\begin{Bmatrix} L & L' & K \\ N & T & \Lambda \end{Bmatrix} \\
&\times \begin{Bmatrix} L' & N & \Lambda \\ E & H' & N' \end{Bmatrix}
\end{aligned}
$$

$$
\begin{aligned}
G(T_{29},0) &= \begin{pmatrix} l_1' & 1 & N' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & 1 & H' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & 1 & K \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2 & K & N \\ 0 & 0 & 0 \end{pmatrix} \\
&\times \begin{pmatrix} N' & l_1 & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} H' & N & E \\ 0 & 0 & 0 \end{pmatrix} \\
\tilde{G}(T_{29}) &= (-1)^{L'+l_1'}\begin{Bmatrix} L & l_1 & l_2 \\ N & K & L' \end{Bmatrix}\begin{Bmatrix} L' & l_1' & l_2' \\ 1 & H' & N' \end{Bmatrix}\begin{Bmatrix} L' & l_1 & N \\ E & H' & N' \end{Bmatrix}
\end{aligned}
$$

$$
\begin{aligned}
G(T_{2,10},0) &= \begin{pmatrix} l_1' & 1 & N' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & 1 & H' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & 1 & K \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_1 & 1 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & K & N \\ 0 & 0 & 0 \end{pmatrix} \\
&\times \begin{pmatrix} l_2 & N & \Lambda \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} N' & T & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} H' & \Lambda & E \\ 0 & 0 & 0 \end{pmatrix} \\
\tilde{G}(T_{2,10}) &= (-1)^{l_1+l_2'}\begin{Bmatrix} L' & l_1' & l_2' \\ 1 & H' & N' \end{Bmatrix}\begin{Bmatrix} L' & T & \Lambda \\ E & H' & N' \end{Bmatrix}\begin{Bmatrix} L & l_1 & l_2 \\ K & 1 & N \\ L' & T & \Lambda \end{Bmatrix}
\end{aligned}
$$

$$
\begin{aligned}
G(T_{2,11},0) &= \begin{pmatrix} l_1' & 1 & N' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & 1 & H' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_1 & 1 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & 1 & N \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} T & N & H \\ 0 & 0 & 0 \end{pmatrix} \\
&\times \begin{pmatrix} l_2 & 1 & \Lambda \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} N' & H & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} H' & \Lambda & E \\ 0 & 0 & 0 \end{pmatrix} \\
\tilde{G}(T_{2,11}) &= (-1)^{l_2'}\begin{Bmatrix} L' & l_1' & l_2' \\ 1 & H' & N' \end{Bmatrix}\begin{Bmatrix} N & 1 & 1 \\ l_1 & H & T \end{Bmatrix}\begin{Bmatrix} L' & H & \Lambda \\ E & H' & N' \end{Bmatrix} \\
&\times \begin{Bmatrix} L & l_1 & l_2 \\ K & 1 & 1 \\ L' & H & \Lambda \end{Bmatrix}
\end{aligned}
$$

$$
\begin{aligned}
G(T_{2,12},0) &= \begin{pmatrix} l_1' & 1 & N' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & 1 & H' \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_1 & 1 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & 1 & N \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} T & 1 & H \\ 0 & 0 & 0 \end{pmatrix} \\
&\times \begin{pmatrix} l_2 & N & \Lambda \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} N' & H & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} H' & \Lambda & E \\ 0 & 0 & 0 \end{pmatrix} \\
\tilde{G}(T_{2,12}) &= (-1)^{l_1+l_2'}\begin{Bmatrix} L' & l_1' & l_2' \\ 1 & H' & N' \end{Bmatrix}\begin{Bmatrix} L' & H & \Lambda \\ E & H' & N' \end{Bmatrix}\sum_{\lambda_1}(-1)^{\lambda_1}(\lambda_1) \\
&\times \begin{Bmatrix} L & l_1 & l_2 \\ N & \Lambda & \lambda_1 \end{Bmatrix}\begin{Bmatrix} 1 & 1 & N \\ l_1 & \lambda_1 & T \end{Bmatrix}\begin{Bmatrix} \lambda_1 & T & 1 \\ 1 & K & H \end{Bmatrix}\begin{Bmatrix} L & \lambda_1 & \Lambda \\ H & L' & K \end{Bmatrix}.
\end{aligned}
$$

We have also defined:

$$
\begin{aligned}
\gamma_1 &= J_2(\mu_{11}, M_{11}; G_{111}; C) \\
\gamma_2 &= J_2(\mu_{12}, M_{12}; G_{121}; C) + J_1(\mu_{11}, M_{11}; G_{111})\eta(\mu_{11}, C+5) \\
\gamma_3 &= J_2(\mu_{13}, M_{13}; G_{131}; C) - J_1(\mu_{11}, M_{11}; G_{111})\eta(\mu_{11}+1, C+5) \\
\gamma_4 &= J_2(\mu_{14}, M_{14}; G_{141}; C) \\
\gamma_5 &= J_2(\mu_{15}, M_{15}; G_{151}; C) \\
\gamma_6 &= J_2(\mu_{16}, M_{16}; G_{161}; C)
\end{aligned}
$$

$$
\begin{aligned}
\gamma_7 &= J_2(\mu_{11}, M_{11}; G_{112}; C) \\
\gamma_8 &= J_2(\mu_{12}, M_{12}; G_{122}; C) \\
\gamma_9 &= J_2(\mu_{13}, M_{13}; G_{132}; C) \\
\gamma_{10} &= J_2(\mu_{14}, M_{14}; G_{142}; C) \\
\gamma_{11} &= J_2(\mu_{15}, M_{15}; G_{152}; C) \\
\gamma_{12} &= J_2(\mu_{16}, M_{16}; G_{162}; C)
\end{aligned}
$$

$$
\begin{aligned}
\gamma_{13} &= J_2(\mu_{11}, M_{11}; G_{111}; C-2) + J_2(\mu_{111}, M_{111}; G_{1,11}; C-2) \\
&+ J_2(\mu_{18}, M_{18}; G_{18}; C-2) - J_1(\mu_{11}, M_{11}; G_{111})\eta(\mu_{11}+1, C+3) \\
\gamma_{14} &= J_2(\mu_{12}, M_{12}; G_{121}; C-2) + J_2(\mu_{15}, M_{15}; G_{151}; C-2) \\
&+ J_2(\mu_{19}, M_{19}; G_{19}; C-2) + J_2(\mu_{112}, M_{112}; G_{1,12}; C-2) \\
&+ 2J_1(\mu_{11}, M_{11}; G_{111})\eta(\mu_{11}, C+3) \\
\gamma_{15} &= J_2(\mu_{13}, M_{13}; G_{131}; C-2) + J_2(\mu_{16}, M_{16}; G_{161}; C-2) \\
&+ J_2(\mu_{110}, M_{110}; G_{1,10}; C-2) - J_1(\mu_{11}, M_{11}; G_{111})\eta(\mu_{11}+1, C+3)
\end{aligned}
$$

$$\gamma_{16} = J_2(\mu_{14}, M_{14}; G_{141}; C-2)$$

$$\gamma_{17} = J_2(\mu_{17}, M_{17}; G_{17}; C-2)$$

$$\begin{aligned}
\gamma_{18} &= J_2(\mu_{21}, M_{21}; G_{211}; \tilde{c}-9) + J_2(\mu_{28}, M_{28}; G_{28}; \tilde{c}-9) \\
&+ J_2(\mu_{211}, M_{211}; G_{2,11}; \tilde{c}-9) \\
\gamma_{19} &= J_2(\mu_{22}, M_{22}; G_{221}; \tilde{c}-9) + J_2(\mu_{25}, M_{25}; G_{251}; \tilde{c}-9) \\
&+ J_2(\mu_{29}, M_{29}; G_{29}; \tilde{c}-9) + J_2(\mu_{212}, M_{212}; G_{2,12}; \tilde{c}-9) \\
\gamma_{20} &= J_2(\mu_{23}, M_{23}; G_{231}; \tilde{c}-9) + J_2(\mu_{26}, M_{26}; G_{261}; \tilde{c}-9) \\
&+ J_2(\mu_{210}, M_{210}; G_{2,10}; \tilde{c}-9) \\
\gamma_{21} &= J_2(\mu_{24}, M_{24}; G_{241}; \tilde{c}-9) \\
\gamma_{22} &= J_2(\mu_{27}, M_{27}; G_{27}; \tilde{c}-9)
\end{aligned}$$

$$\begin{aligned}
\gamma_{23} &= J_2(\mu_{21}, M_{21}; G_{211}; \tilde{c}-7) \\
\gamma_{24} &= J_2(\mu_{22}, M_{22}; G_{221}; \tilde{c}-7) + J_2(\mu_{25}, M_{25}; G_{251}; \tilde{c}-7) \\
\gamma_{25} &= J_2(\mu_{23}, M_{23}; G_{231}; \tilde{c}-7) + J_2(\mu_{26}, M_{26}; G_{261}; \tilde{c}-7) \\
\gamma_{26} &= J_2(\mu_{24}, M_{24}; G_{241}; \tilde{c}-7)
\end{aligned}$$

$$\begin{aligned}
\gamma_{27} &= J_2(\mu_{21}, M_{21}; G_{212}; \tilde{c}-7) \\
\gamma_{28} &= J_2(\mu_{22}, M_{22}; G_{222}; \tilde{c}-7) + J_2(\mu_{25}, M_{25}; G_{252}; \tilde{c}-7) \\
\gamma_{29} &= J_2(\mu_{23}, M_{23}; G_{232}; \tilde{c}-7) + J_2(\mu_{26}, M_{26}; G_{262}; \tilde{c}-7) \\
\gamma_{30} &= J_2(\mu_{24}, M_{24}; G_{242}; \tilde{c}-7)
\end{aligned}$$

$$\begin{aligned}
\xi_1 &= J_3(\mu_{11}, M_{11}; G_{111}; C-2) + J_3(\mu_{18}, M_{18}; G_{18}; C-2) \\
&+ J_3(\mu_{111}, M_{111}; G_{1,11}; C-2) + \gamma_{17}\eta(\mu_{11}, C+5) \\
\xi_2 &= J_3(\mu_{12}, M_{12}; G_{121}; C-2) + J_3(\mu_{15}, M_{15}; G_{151}; C-2) \\
&+ J_3(\mu_{19}, M_{19}; G_{19}; C-2) + J_3(\mu_{112}, M_{112}; G_{1,12}; C-2) \\
&+ (\gamma_{15} + 2\gamma_{16})\eta(\mu_{11}+1, C+5) \\
\xi_3 &= J_3(\mu_{13}, M_{13}; G_{131}; C-2) + J_3(\mu_{16}, M_{16}; G_{161}; C-2)
\end{aligned}$$

$$
\begin{aligned}
&+ \quad J_3(\mu_{110}, M_{110}; G_{1,10}; C-2) + \gamma_{16}\eta(\mu_{11}, C+5) \\
\xi_4 &= J_3(\mu_{14}, M_{14}; G_{141}; C-2) \\
\xi_5 &= J_3(\mu_{17}, M_{17}; G_{17}; C-2)
\end{aligned}
$$

$$
\begin{aligned}
\xi_6 &= J_3(\mu_{21}, M_{21}; G_{211}; \tilde{c}-9) + J_3(\mu_{28}, M_{28}; G_{28}; \tilde{c}-9) \\
&+ J_3(\mu_{211}, M_{211}; G_{2,11}; \tilde{c}-9) + \gamma_{22}\eta(\mu_{11}+1, \tilde{c}-2) \\
\xi_7 &= J_3(\mu_{22}, M_{22}; G_{221}; \tilde{c}-9) + J_3(\mu_{25}, M_{25}; G_{251}; \tilde{c}-9) \\
&+ J_3(\mu_{29}, M_{29}; G_{29}; \tilde{c}-9) + J_3(\mu_{212}, M_{212}; G_{2,12}; \tilde{c}-9) \\
&+ (\gamma_{20}+2\gamma_{21})\eta(\mu_{11}, \tilde{c}-2) \\
\xi_8 &= J_3(\mu_{23}, M_{23}; G_{231}; \tilde{c}-9) + J_3(\mu_{26}, M_{26}; G_{261}; \tilde{c}-9) \\
&+ J_3(\mu_{210}, M_{210}; G_{2,10}; \tilde{c}-9) + \gamma_{21}\eta(\mu_{11}+1, \tilde{c}-2) \\
\xi_9 &= J_3(\mu_{24}, M_{24}; G_{241}; \tilde{c}-9) \\
\xi_{10} &= J_3(\mu_{27}, M_{27}; G_{27}; \tilde{c}-9).
\end{aligned}
$$

(13) H_D^{13}:

$$
\begin{aligned}
\Delta E_D^{13} &= \frac{1}{16}\alpha^4 \delta_{JJ'}\delta_{M_J M_{J'}} \sum_K (-1)^{K+L+S'+J} \begin{Bmatrix} L' & S' & J \\ S & L & K \end{Bmatrix} \\
&\times \langle \gamma' L' \| R^{(K)} \| \gamma L \rangle \langle S' \| [\vec{\sigma}_1 \otimes \vec{\sigma}_2]^{(K)} \| S \rangle
\end{aligned}
$$

with

$$
R^{(K)} = \frac{1}{r^3}[\vec{\nabla}_2 \otimes \vec{\nabla}_1]^{(K)}
$$

The orbital part is

$$
\langle F' \mathcal{Y}^{M'}_{l_1' l_2' L'} | R_Q^{(K)} | F \mathcal{Y}^{M}_{l_1 l_2 L} \rangle = (-1)^{L'-M'} \begin{pmatrix} L' & K & L \\ -M' & Q & M \end{pmatrix} U(13) D,
$$

where

$$
U(13) = \frac{1}{2}(-1)^K \sqrt{2K+1}(l_1, l_2, L, l_1', l_2', L')^{1/2}
$$

$$
D = \sum_{i=1}^{7} \text{Term}(i)
$$

$$\begin{aligned}\mathrm{Term}(1) &= c(c-2)[2\varpi_0(\mu_1, M_1; G_{11}; \tilde{a}+1, \tilde{b}+1, \tilde{c}-7; \tilde{\alpha}, \tilde{\beta}) \\ &+ \varpi_0(\mu_2, M_2; G_{21}; \tilde{a}+2, \tilde{b}, \tilde{c}-7; \tilde{\alpha}, \tilde{\beta}) \\ &+ \varpi_0(\mu_3, M_3; G_{31}; \tilde{a}, \tilde{b}+2, \tilde{c}-7; \tilde{\alpha}, \tilde{\beta})], \quad \tilde{c}=5\end{aligned}$$

$$\begin{aligned}\mathrm{Term}(1) &= c(c-2)[2\varpi_1(\mu_1, M_1; G_{11}; \tilde{a}+1, \tilde{b}+1, \tilde{c}-7; \tilde{\alpha}, \tilde{\beta}) \\ &+ \varpi_1(\mu_2, M_2; G_{21}; \tilde{a}+2, \tilde{b}, \tilde{c}-7; \tilde{\alpha}, \tilde{\beta}) \\ &+ \varpi_1(\mu_3, M_3; G_{31}; \tilde{a}, \tilde{b}+2, \tilde{c}-7; \tilde{\alpha}, \tilde{\beta}) \\ &- J_1(\mu_1, M_1; G_{11})\eta(\mu_1+1, \tilde{c}-2) I_{\omega(\mu_1+1)-2}(\tilde{a}, \tilde{b}, \tilde{c}-5)], \quad \tilde{c}=3\end{aligned}$$

$$\begin{aligned}\mathrm{Term}(1) &= c(c-2)[2\varpi_2(\mu_1, M_1; G_{11}; \tilde{a}+1, \tilde{b}+1, \tilde{c}-7; \tilde{\alpha}, \tilde{\beta}) \\ &+ \varpi_2(\mu_2, M_2; G_{21}; \tilde{a}+2, \tilde{b}, \tilde{c}-7; \tilde{\alpha}, \tilde{\beta}) \\ &+ \varpi_2(\mu_3, M_3; G_{31}; \tilde{a}, \tilde{b}+2, \tilde{c}-7; \tilde{\alpha}, \tilde{\beta}) \\ &+ \gamma_2 \mathrm{Dif}(\tilde{a}+1, \tilde{b}-1; \tilde{a}, \tilde{b}; \tilde{c}-5, \tilde{\alpha}, \tilde{\beta}; \omega(\mu_1)-2, \omega(\mu_1+1)-2) \\ &+ \gamma_3 \mathrm{Dif}(\tilde{a}-1, \tilde{b}+1; \tilde{a}, \tilde{b}; \tilde{c}-5, \tilde{\alpha}, \tilde{\beta}; \omega(\mu_1)-2, \omega(\mu_1+1)-2)] \\ &+ c(c-2)[\tilde{\gamma}(l_1' l_2' l_1 l_2)\mathrm{Can}(\tilde{a}, \tilde{b}, \tilde{\alpha}, \tilde{\beta}; \tilde{a}', \tilde{b}', \tilde{\alpha}', \tilde{\beta}'; \\ &\quad \tilde{c}-5; \omega(\mu_1+1)-2, \omega(\mu_1+1+L)-2) \\ &+ (\tilde{\gamma}(l_1' l_2' l_1 l_2) - \tilde{\gamma}(l_2' l_1' l_1 l_2)) I_{\omega(\mu_1+1+L)-2}(\tilde{a}', \tilde{b}', \tilde{c}-5; \tilde{\alpha}', \tilde{\beta}')] \\ &\times \delta(X_R, 1)\delta(X_L, 1), \quad \tilde{c} \neq 3, 5\end{aligned}$$

$$\begin{aligned}\mathrm{Term}(2) &= bc[\varpi_1(\mu_1, M_1; G_{11}; \tilde{a}+1, \tilde{b}-1, \tilde{c}-5; \tilde{\alpha}, \tilde{\beta}) \\ &+ \varpi_1(\mu_3, M_3; G_{31}; \tilde{a}, \tilde{b}, \tilde{c}-5; \tilde{\alpha}, \tilde{\beta}) \\ &+ J_1(\mu_1, M_1; G_{11})\mathrm{Dif}(\tilde{a}+1, \tilde{b}-1; \tilde{a}, \tilde{b}; \tilde{c}-5, \tilde{\alpha}, \tilde{\beta}; \\ &\quad \omega(\mu_1)-2, \omega(\mu_1+1)-2)]\end{aligned}$$

$$\begin{aligned}\mathrm{Term}(3) &= ac[\varpi_1(\mu_1, M_1; G_{11}; \tilde{a}-1, \tilde{b}+1, \tilde{c}-5; \tilde{\alpha}, \tilde{\beta}) \\ &+ \varpi_1(\mu_2, M_2; G_{21}; \tilde{a}, \tilde{b}, \tilde{c}-5; \tilde{\alpha}, \tilde{\beta}) \\ &+ J_1(\mu_1, M_1; G_{11})\mathrm{Dif}(\tilde{a}-1, \tilde{b}+1; \tilde{a}, \tilde{b}; \tilde{c}-5, \tilde{\alpha}, \tilde{\beta}; \\ &\quad \omega(\mu_1)-2, \omega(\mu_1+1)-2)]\end{aligned}$$

$$
\begin{aligned}
\text{Term}(4) &= -\alpha c[\varpi_1(\mu_1, M_1; G_{11}; \tilde{a}, \tilde{b}+1, \tilde{c}-5; \tilde{\alpha}, \tilde{\beta}) \\
&+ \varpi_1(\mu_2, M_2; G_{21}; \tilde{a}+1, \tilde{b}, \tilde{c}-5; \tilde{\alpha}, \tilde{\beta}) \\
&+ J_1(\mu_1, M_1; G_{11})\text{Dif}(\tilde{a}, \tilde{b}+1; \tilde{a}+1, \tilde{b}; \tilde{c}-5, \tilde{\alpha}, \tilde{\beta}; \\
&\quad \omega(\mu_1)-2, \omega(\mu_1+1)-2)]
\end{aligned}
$$

$$
\begin{aligned}
\text{Term}(5) &= -\beta c[\varpi_1(\mu_1, M_1; G_{11}; \tilde{a}+1, \tilde{b}, \tilde{c}-5; \tilde{\alpha}, \tilde{\beta}) \\
&+ \varpi_1(\mu_3, M_3; G_{31}; \tilde{a}, \tilde{b}+1, \tilde{c}-5; \tilde{\alpha}, \tilde{\beta}) \\
&+ J_1(\mu_1, M_1; G_{11})\text{Dif}(\tilde{a}+1, \tilde{b}; \tilde{a}, \tilde{b}+1; \tilde{c}-5, \tilde{\alpha}, \tilde{\beta}; \\
&\quad \omega(\mu_1)-2, \omega(\mu_1+1)-2)]
\end{aligned}
$$

$$
\begin{aligned}
\text{Term}(6) &= c\varpi_1(\mu_1, M_1; G_{12}; \tilde{a}-1, \tilde{b}+1, \tilde{c}-5; \tilde{\alpha}, \tilde{\beta}) \\
&+ c\varpi_1(\mu_1, M_1; G_{13}; \tilde{a}+1, \tilde{b}-1, \tilde{c}-5; \tilde{\alpha}, \tilde{\beta}) \\
&+ c\varpi_1(\min(\mu_2, \mu_3), \max(M_2, M_3); G_{22}+G_{31}+G_{32}; \tilde{a}, \tilde{b}, \tilde{c}-5; \tilde{\alpha}, \tilde{\beta}) \\
&+ cJ_1(\mu_1, M_1; G_{12})\text{Dif}(\tilde{a}-1, \tilde{b}+1; \tilde{a}, \tilde{b}; \tilde{c}-5, \tilde{\alpha}, \tilde{\beta}; \\
&\quad \omega(\mu_1)-2, \omega(\mu_1+1)-2) \\
&+ cJ_1(\mu_1, M_1; G_{13})\text{Dif}(\tilde{a}+1, \tilde{b}-1; \tilde{a}, \tilde{b}; \tilde{c}-5, \tilde{\alpha}, \tilde{\beta}; \\
&\quad \omega(\mu_1)-2, \omega(\mu_1+1)-2) \\
&+ c\tilde{\xi}(l_1'l_2'l_1l_2)\text{Can}(\tilde{a}, \tilde{b}, \tilde{\alpha}, \tilde{\beta}; \tilde{a}', \tilde{b}', \tilde{\alpha}', \tilde{\beta}'; \tilde{c}-5; \\
&\quad \omega(\mu_1+1)-2, \omega(\mu_1+1+L)-2)\delta(X_R, 1)\delta(X_L, 1)
\end{aligned}
$$

$$
\begin{aligned}
\text{Term}(7) &= \varpi_1(\mu_1, M_1; abG_{11}+bG_{12}+aG_{13}+G_{14}; \tilde{a}-1, \tilde{b}-1, \tilde{c}-3; \tilde{\alpha}, \tilde{\beta}) \\
&- \varpi_1(\mu_1, M_1; a\beta G_{11}+\beta G_{12}; \tilde{a}-1, \tilde{b}, \tilde{c}-3; \tilde{\alpha}, \tilde{\beta}) \\
&- \varpi_1(\mu_1, M_1; b\alpha G_{11}+\alpha G_{13}; \tilde{a}, \tilde{b}-1, \tilde{c}-3; \tilde{\alpha}, \tilde{\beta}) \\
&+ \varpi_1(\mu_1, M_1; \alpha\beta G_{11}; \tilde{a}, \tilde{b}, \tilde{c}-3; \tilde{\alpha}, \tilde{\beta}) \\
&+ [\tau_1(l_1'l_2'l_1l_2; ab)\text{Can}(\tilde{a}-1, \tilde{b}-1, \tilde{\alpha}, \tilde{\beta}; \tilde{a}'-1, \tilde{b}'-1, \tilde{\alpha}', \tilde{\beta}'; \tilde{c}-3; \\
&\quad \omega(\mu_1)-2, \omega(\mu_1+L)-2) \\
&+ \tau_2(l_1'l_2'l_1l_2; a\beta)\text{Can}(\tilde{a}-1, \tilde{b}, \tilde{\alpha}, \tilde{\beta}; \tilde{a}'-1, \tilde{b}', \tilde{\alpha}', \tilde{\beta}'; \tilde{c}-3; \\
&\quad \omega(\mu_1)-2, \omega(\mu_1+L)-2)
\end{aligned}
$$

$$
\begin{aligned}
+ \quad & \tau_3(l_1'l_2'l_1l_2;b\alpha)\mathrm{Can}(\tilde{a},\tilde{b}-1,\tilde{\alpha},\tilde{\beta};\tilde{a}',\tilde{b}'-1,\tilde{\alpha}',\tilde{\beta}';\tilde{c}-3; \\
& \omega(\mu_1)-2,\omega(\mu_1+L)-2) \\
+ \quad & \tau_4(l_1'l_2'l_1l_2;\alpha\beta)\mathrm{Can}(\tilde{a},\tilde{b},\tilde{\alpha},\tilde{\beta};\tilde{a}',\tilde{b}',\tilde{\alpha}',\tilde{\beta}';\tilde{c}-3; \\
& \omega(\mu_1)-2,\omega(\mu_1+L)-2)]\delta(X_R,1)\delta(X_L,1).
\end{aligned}
$$

Also,

$$
\begin{aligned}
M_1 &= \min(l_1+l_1'+1,l_2+l_2'+1) \\
M_2 &= \min(l_1+l_1'+2,l_2+l_2') \\
M_3 &= \min(l_1+l_1',l_2+l_2'+2) \\
\mu_i &= \omega(M_i)-2, \quad i=1,2,3
\end{aligned}
$$

The angular coefficients are:

$$
\begin{aligned}
G_{11}(E) &= \sum_{T\Lambda}(T,\Lambda,E)G(T_1,0)\tilde{G}(T_1) \\
G_{12}(E) &= \sum_{T\Lambda}(T,\Lambda,E)G(T_1,0)\tilde{G}(T_1)b(l_1;T) \\
G_{13}(E) &= \sum_{T\Lambda}(T,\Lambda,E)G(T_1,0)\tilde{G}(T_1)b(l_2;\Lambda) \\
G_{14}(E) &= \sum_{T\Lambda}(T,\Lambda,E)G(T_1,0)\tilde{G}(T_1)b(l_1;T)b(l_2;\Lambda)
\end{aligned}
$$

$$
\begin{aligned}
G_{21}(E) &= \sum_{T\Lambda}(T,\Lambda,E)G(T_2,0)\tilde{G}(T_2) \\
G_{22}(E) &= \sum_{T\Lambda}(T,\Lambda,E)G(T_2,0)\tilde{G}(T_2)b(l_1;T)
\end{aligned}
$$

$$
\begin{aligned}
G_{31}(E) &= \sum_{T\Lambda}(T,\Lambda,E)G(T_3,0)\tilde{G}(T_3) \\
G_{32}(E) &= \sum_{T\Lambda}(T,\Lambda,E)G(T_3,0)\tilde{G}(T_3)b(T;\Lambda)
\end{aligned}
$$

with

$$
\begin{aligned}
G(T_1,0) &= \begin{pmatrix} 1 & l_1 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_2 & \Lambda \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_1' & T & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & \Lambda & E \\ 0 & 0 & 0 \end{pmatrix} \\
\tilde{G}(T_1) &= (-1)^{1+L'+l_1+l_2'}\begin{Bmatrix} L' & l_1' & l_2' \\ E & \Lambda & T \end{Bmatrix}\begin{Bmatrix} L & l_1 & l_2 \\ K & 1 & 1 \\ L' & T & \Lambda \end{Bmatrix}
\end{aligned}
$$

$$
\begin{aligned}
G(T_2,0) &= \begin{pmatrix} 1 & l_1 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & T & \Lambda \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_1' & \Lambda & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & l_2 & E \\ 0 & 0 & 0 \end{pmatrix} \\
\tilde{G}(T_2) &= (-1)^{L+L'+l_1+l_2'+K}\begin{Bmatrix} L & l_1 & l_2 \\ \Lambda & L' & K \end{Bmatrix}\begin{Bmatrix} L' & l_1' & l_2' \\ E & l_2 & \Lambda \end{Bmatrix}\begin{Bmatrix} 1 & 1 & K \\ l_1 & \Lambda & T \end{Bmatrix}
\end{aligned}
$$

$$
\begin{aligned}
G(T_3,0) &= \begin{pmatrix} 1 & l_2 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & T & \Lambda \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_1' & l_1 & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & \Lambda & E \\ 0 & 0 & 0 \end{pmatrix} \\
\tilde{G}(T_3) &= (-1)^{l_1+l_2'+K}\begin{Bmatrix} L & l_1 & l_2 \\ \Lambda & K & L' \end{Bmatrix}\begin{Bmatrix} L' & l_1' & l_2' \\ E & \Lambda & l_1 \end{Bmatrix}\begin{Bmatrix} 1 & 1 & K \\ l_2 & \Lambda & T \end{Bmatrix}
\end{aligned}
$$

We have also defined:

$$
\begin{aligned}
\gamma_1(l_1'l_2'l_1l_2) &= 2J_2(\mu_1, M_1; G_{11}; \tilde{c}-7) - J_1(\mu_1, M_1; G_{11})\eta(\mu_1+1, \tilde{c}-2) \\
\gamma_2(l_1'l_2'l_1l_2) &= J_2(\mu_2, M_2; G_{21}; \tilde{c}-7) \\
\gamma_3(l_1'l_2'l_1l_2) &= J_2(\mu_3, M_3; G_{31}; \tilde{c}-7) \\
\gamma &= \gamma_1+\gamma_2+\gamma_3 \\
\tilde{\gamma}(l_1'l_2'l_1l_2) &= \gamma(l_1'l_2'l_1l_2)+\gamma(l_2'l_1'l_2l_1) \\
\xi(l_1'l_2'l_1l_2) &= J_1(\mu_1, M_1; G_{12}) + J_1(\mu_1, M_1; G_{13}) + J_1(\mu_2, M_2; G_{22}) \\
&+ J_1(\mu_3, M_3; G_{31}) + J_1(\mu_3, M_3; G_{32}) \\
\tilde{\xi}(l_1'l_2'l_1l_2) &= \xi(l_1'l_2'l_1l_2)+\xi(l_2'l_1'l_2l_1)
\end{aligned}
$$

$$
\begin{aligned}
\sigma_1(l_1'l_2'l_1l_2; ab) &= abJ_1(\mu_1, M_1; G_{11}) + bJ_1(\mu_1, M_1; G_{12}) \\
&+ aJ_1(\mu_1, M_1; G_{13}) + J_1(\mu_1, M_1; G_{14}) \\
\sigma_2(l_1'l_2'l_1l_2; a\beta) &= -a\beta J_1(\mu_1, M_1; G_{11}) - \beta J_1(\mu_1, M_1; G_{12}) \\
\sigma_3(l_1'l_2'l_1l_2; b\alpha) &= -b\alpha J_1(\mu_1, M_1; G_{11}) - \alpha J_1(\mu_1, M_1; G_{13}) \\
\sigma_4(l_1'l_2'l_1l_2; \alpha\beta) &= \alpha\beta J_1(\mu_1, M_1; G_{11}) \\
\tau_1(l_1'l_2'l_1l_2; ab) &= \sigma_1(l_1'l_2'l_1l_2; ab) + \sigma_1(l_2'l_1'l_2l_1; ba) \\
\tau_2(l_1'l_2'l_1l_2; a\beta) &= \sigma_2(l_1'l_2'l_1l_2; a\beta) + \sigma_3(l_2'l_1'l_2l_1; a\beta) \\
\tau_3(l_1'l_2'l_1l_2; b\alpha) &= \sigma_3(l_1'l_2'l_1l_2; b\alpha) + \sigma_2(l_2'l_1'l_2l_1; b\alpha) \\
\tau_4(l_1'l_2'l_1l_2; \alpha\beta) &= \sigma_4(l_1'l_2'l_1l_2; \alpha\beta) + \sigma_4(l_2'l_1'l_2l_1; \beta\alpha).
\end{aligned}
$$

(14) H_D^{14}:

First of all, one should decouple the spin part from the original operator because it is not in the form of $(\vec{\sigma}_1 \cdot O_1)(\vec{\sigma}_2 \cdot O_2)$. Let

$$A \equiv \vec{\sigma}_2 \cdot \{\vec{r} \times [\vec{\sigma}_1 \cdot (\vec{r} \times \vec{\nabla}_1)]\vec{\nabla}_2\}. \tag{A.1}$$

Since

$$\begin{aligned}
A &= \vec{\sigma}_2 \cdot \{\vec{r} \times [\vec{\sigma}_1 \cdot (\vec{r}_1 \times \vec{\nabla}_1)]\vec{\nabla}_2\} - \vec{\sigma}_2 \cdot \{\vec{r} \times [\vec{\sigma}_1 \cdot (\vec{r}_2 \times \vec{\nabla}_1)]\vec{\nabla}_2\} \\
&= \vec{\sigma}_2 \cdot \{(\vec{r} \times \vec{\nabla}_2)[\vec{\sigma}_1 \cdot (\vec{r}_1 \times \vec{\nabla}_1)]\} - \vec{\sigma}_2 \cdot \{\vec{r}_1 \times [\vec{\sigma}_1 \cdot (\vec{r}_2 \times \vec{\nabla}_1)]\vec{\nabla}_2\} \\
&+ \vec{\sigma}_2 \cdot \{\vec{r}_2 \times [\vec{\sigma}_1 \cdot (\vec{r}_2 \times \vec{\nabla}_1)]\vec{\nabla}_2\} \\
&= [\vec{\sigma}_2 \cdot (\vec{r} \times \vec{\nabla}_2)][\vec{\sigma}_1 \cdot (\vec{r}_1 \times \vec{\nabla}_1)] - \vec{\sigma}_2 \cdot \{\vec{r}_1 \times [\vec{\sigma}_1 \cdot (\vec{r}_2 \times \vec{\nabla}_1)]\vec{\nabla}_2\} \\
&+ [\vec{\sigma}_1 \cdot (\vec{r}_2 \times \vec{\nabla}_1)][\vec{\sigma}_2 \cdot (\vec{r}_2 \times \vec{\nabla}_2)],
\end{aligned}$$

thus, one only needs to consider the following operator:

$$\begin{aligned}
B &\equiv \vec{\sigma}_2 \cdot \{\vec{r}_1 \times [\vec{\sigma}_1 \cdot (\vec{r}_2 \times \vec{\nabla}_1)]\vec{\nabla}_2\} = \sigma_{2i}\epsilon_{ijk}r_{1j}\sigma_{1s}\epsilon_{slm}r_{2l}\partial_{1m}\partial_{2k} \\
&= \sigma_{2i}\sigma_{1s}\epsilon_{ijk}\epsilon_{slm}r_{2l}(r_{1j}\partial_{1m})\partial_{2k} = \sigma_{2i}\sigma_{1s}\epsilon_{ijk}\epsilon_{slm}r_{2l}(\partial_{1m}r_{1j} - \delta_{mj})\partial_{2k} \\
&= (\sigma_{1s}\epsilon_{slm}r_{2l}\partial_{1m})(\sigma_{2i}\epsilon_{ijk}r_{1j}\partial_{2k}) - \sigma_{2i}\sigma_{1s}r_{2l}\partial_{2k}(\delta_{ks}\delta_{il} - \delta_{kl}\delta_{is}) \\
&= [\vec{\sigma}_1 \cdot (\vec{r}_2 \times \vec{\nabla}_1)][\vec{\sigma}_2 \cdot (\vec{r}_1 \times \vec{\nabla}_2)] - (\vec{\sigma}_2 \cdot \vec{r}_2)(\vec{\sigma}_1 \cdot \vec{\nabla}_2) + (\vec{\sigma}_1 \cdot \vec{\sigma}_2)(\vec{r}_2 \cdot \vec{\nabla}_2).
\end{aligned}$$

Substituting the above expression into Eq. (A.1) and using $\vec{r} = \vec{r}_1 - \vec{r}_2$, one obtains

$$\begin{aligned}
A &= [\vec{\sigma}_2 \cdot (\vec{r} \times \vec{\nabla}_2)][\vec{\sigma}_1 \cdot (\vec{r}_1 \times \vec{\nabla}_1)] - [\vec{\sigma}_1 \cdot (\vec{r}_2 \times \vec{\nabla}_1)][\vec{\sigma}_2 \cdot (\vec{r} \times \vec{\nabla}_2)] \\
&+ (\vec{\sigma}_2 \cdot \vec{r}_2)(\vec{\sigma}_1 \cdot \vec{\nabla}_2) - (\vec{\sigma}_1 \cdot \vec{\sigma}_2)(\vec{r}_2 \cdot \vec{\nabla}_2).
\end{aligned}$$

After interchanging $\vec{r}_1$ and $\vec{r}_2$, and $\vec{\sigma}_1$ and $\vec{\sigma}_2$ in the first and third terms and neglecting the last term which is proportional to $\vec{\sigma}_1 \cdot \vec{\sigma}_2$, one arrives at the expression of

$$\begin{aligned}
A &\cong -[\vec{\sigma}_1 \cdot (\vec{r} \times \vec{\nabla}_1)][\vec{\sigma}_2 \cdot (\vec{r}_2 \times \vec{\nabla}_2)] - [\vec{\sigma}_1 \cdot (\vec{r}_2 \times \vec{\nabla}_1)][\vec{\sigma}_2 \cdot (\vec{r} \times \vec{\nabla}_2)] \\
&+ (\vec{\sigma}_1 \cdot \vec{r}_1)(\vec{\sigma}_2 \cdot \vec{\nabla}_1),
\end{aligned} \tag{A.2}$$

where $\cong$ means that Eq. (A.2) is used only in the calculation of the energy splittings. Finally,

$$H_D^{14} = H_D^{141} + H_D^{142} + H_D^{143}, \tag{A.3}$$

where

$$
\begin{aligned}
H_D^{141} &= -\frac{3}{16}\alpha^4\frac{1}{r^5}[\vec{\sigma}_1\cdot(\vec{r}\times\vec{\nabla}_1)][\vec{\sigma}_2\cdot(\vec{r}_2\times\vec{\nabla}_2)] \\
H_D^{142} &= -\frac{3}{16}\alpha^4\frac{1}{r^5}[\vec{\sigma}_1\cdot(\vec{r}_2\times\vec{\nabla}_1)][\vec{\sigma}_2\cdot(\vec{r}\times\vec{\nabla}_2)] \\
H_D^{143} &= \frac{3}{16}\alpha^4\frac{1}{r^5}(\vec{\sigma}_1\cdot\vec{r}_1)(\vec{\sigma}_2\cdot\vec{\nabla}_1).
\end{aligned}
$$

Thus,

$$
\begin{aligned}
\Delta E_D^{14} &= -\frac{3}{16}\alpha^4\delta_{JJ'}\delta_{M_JM_{J'}}\sum_K(-1)^{K+L+S'+J}\begin{Bmatrix} L' & S' & J \\ S & L & K \end{Bmatrix}\langle S'\|[\vec{\sigma}_1\otimes\vec{\sigma}_2]^{(K)}\|S\rangle \\
&\times\ (\langle\gamma'L'\|R^{(K)}(1)\|\gamma L\rangle+\langle\gamma'L'\|R^{(K)}(2)\|\gamma L\rangle+\langle\gamma'L'\|R^{(K)}(3)\|\gamma L\rangle)
\end{aligned}
$$

with

$$
\begin{aligned}
R^{(K)}(1) &= \frac{1}{r^5}[(\vec{r}\times\vec{\nabla}_1)\otimes(\vec{r}_2\times\vec{\nabla}_2)]^{(K)} \\
R^{(K)}(2) &= \frac{1}{r^5}[(\vec{r}_2\times\vec{\nabla}_1)\otimes(\vec{r}\times\vec{\nabla}_2)]^{(K)} \\
R^{(K)}(3) &= -\frac{1}{r^5}[\vec{r}_1\otimes\vec{\nabla}_1)]^{(K)}.
\end{aligned}
$$

The orbital part is

$$
\langle F'\mathcal{Y}^{M'}_{l_1'l_2'L'}|\sum_{i=1}^{3}R_Q^{(K)}(i)|F\mathcal{Y}^{M}_{l_1l_2L}\rangle = (-1)^{L'-M'}\begin{pmatrix} L' & K & L \\ -M' & Q & M \end{pmatrix}U(14)D,
$$

where

$$
U(14)=3\sqrt{2K+1}(l_1,l_2,L,l_1',l_2',L')^{1/2},
$$

and

$$
D = \sum_{i=1}^{7}\mathrm{Term}(i).
$$

For Term(1),

$$
\begin{aligned}
T_1(k) \equiv\ & \varpi_k(\omega(M(l_1+l_1'))-2,M(l_1+l_1');\tilde{\Omega}_1(l_1'l_2'l_1l_2;E); \\
& \tilde{a},\tilde{b},\tilde{c}-5;\tilde{\alpha},\tilde{\beta}) \\
+\ & \varpi_k(\omega(M(l_1+l_1'+1))-2,M(l_1+l_1'+1);\Omega_2(l_1'l_2'l_1l_2;E);
\end{aligned}
$$

$$
\begin{aligned}
& \tilde{a}-1,\tilde{b}+1,\tilde{c}-5;\tilde{\alpha},\tilde{\beta}) \\
+ \quad & \varpi_k(\omega(M(l_1+l_1'+1))-2,M(l_1+l_1'+1);\Omega_2(l_2'l_1'l_2l_1;E); \\
& \tilde{a}+1,\tilde{b}-1,\tilde{c}-5;\tilde{\alpha},\tilde{\beta}) \\
- \quad & \varpi_k(\omega(M(l_1+l_2'))-2,M(l_1+l_2');\hat{\Omega}_1(l_2'l_1'l_1l_2;E); \\
& \tilde{a}',\tilde{b}',\tilde{c}-5;\tilde{\alpha}',\tilde{\beta}') \\
- \quad & \varpi_k(\omega(M(l_1+l_2'+1))-2,M(l_1+l_2'+1);\Omega_2(l_2'l_1'l_1l_2;E); \\
& \tilde{a}'-1,\tilde{b}'+1,\tilde{c}-5;\tilde{\alpha}',\tilde{\beta}') \\
- \quad & \varpi_k(\omega(M(l_1+l_2'+1))-2,M(l_1+l_2'+1);\Omega_2(l_1'l_2'l_2l_1;E); \\
& \tilde{a}'+1,\tilde{b}'-1,\tilde{c}-5;\tilde{\alpha}',\tilde{\beta}')
\end{aligned}
$$

$$
\begin{aligned}
\text{Term}(1) &= T_1(0)\delta(X_R,1)\delta(X_L,1), \quad \tilde{c}\geq 3 \\
\text{Term}(1) &= [T_1(1)-2\sum_{E}^{M(l_1+l_1'+1)} GA_{1134}(l_1'l_2'l_1l_2)\eta(l_1+l_1'+1,\tilde{c}) \\
&\times\ I_{\omega(l_1+l_1'+1)-2}(\tilde{a}-1,\tilde{b}-1,\tilde{c}-3) \\
&+\ 2\sum_{E}^{M(l_1+l_2'+1)} GA_{1134}(l_2'l_1'l_1l_2)\eta(l_1+l_2'+1,\tilde{c}) \\
&\times\ I_{\omega(l_1+l_2'+1)-2}(\tilde{a}'-1,\tilde{b}'-1,\tilde{c}-3)]\delta(X_R,1)\delta(X_L,1), \quad 1\leq\tilde{c}\leq 2
\end{aligned}
$$

$$
\begin{aligned}
\text{Term}(1) &= \{T_1(2)+\gamma_2(l_2'l_1'l_2l_1)\text{Dif}(\tilde{a},\tilde{b}-2;\tilde{a}-1,\tilde{b}-1;\tilde{c}-3,\tilde{\alpha},\tilde{\beta}; \\
&\quad \omega(l_1+l_1')-2,\omega(l_1+l_1'+1)-2) \\
&+\ [\gamma_2(l_2'l_1'l_2l_1)+\gamma_1(l_1'l_2'l_1l_2)]\text{Dif}(\tilde{a}-1,\tilde{b}-1;\tilde{a}-2,\tilde{b};\tilde{c}-3,\tilde{\alpha},\tilde{\beta}; \\
&\quad \omega(l_1+l_1'+1)-2,\omega(l_1+l_1')-2) \\
&-\ \gamma_2(l_1'l_2'l_2l_1)\text{Dif}(\tilde{a}',\tilde{b}'-2;\tilde{a}'-1,\tilde{b}'-1;\tilde{c}-3,\tilde{\alpha}',\tilde{\beta}'; \\
&\quad \omega(l_1+l_2')-2,\omega(l_1+l_2'+1)-2) \\
&-\ [\gamma_2(l_1'l_2'l_2l_1)+\gamma_1(l_2'l_1'l_1l_2)]\text{Dif}(\tilde{a}'-1,\tilde{b}'-1;\tilde{a}'-2,\tilde{b}';\tilde{c}-3,\tilde{\alpha}',\tilde{\beta}'; \\
&\quad \omega(l_1+l_2'+1)-2,\omega(l_1+l_2')-2) \\
&+\ [\gamma_1(l_1'l_2'l_1l_2)+\gamma_2(l_1'l_2'l_1l_2)+\gamma_2(l_2'l_1'l_2l_1)]\text{Can}(\tilde{a}-2,\tilde{b},\tilde{\alpha},\tilde{\beta}; \\
&\quad \tilde{a}'-2,\tilde{b}',\tilde{\alpha}',\tilde{\beta}';\tilde{c}-3;\omega(l_1+l_1')-2,\omega(l_1+l_2')-2)\} \\
&\times\ \delta(X_R,1)\delta(X_L,1), \quad \tilde{c}=0.
\end{aligned}
$$

$$\text{Term}(2) = 0.$$

For Term(3),

$$\begin{aligned}
T_3(k) &\equiv c\varpi_k(\omega(M(l_1+l_1')) - 2, M(l_1+l_1'); \Omega_3; \tilde{a}+2, \tilde{b}, \tilde{c}-7; \tilde{\alpha}, \tilde{\beta}) \\
&+ c\varpi_k(\omega(M(l_1+l_1'+1)) - 2, M(l_1+l_1'+1); \Omega_4; \tilde{a}+1, \tilde{b}+1, \tilde{c}-7; \tilde{\alpha}, \tilde{\beta}) \\
&+ c\varpi_k(\omega(M(l_1+l_1')) - 2, M(l_1+l_1'); \Omega_5; \tilde{a}, \tilde{b}+2, \tilde{c}-7; \tilde{\alpha}, \tilde{\beta}) \\
\text{Term}(3) &= T_3(0), \quad \tilde{c} \geq 5 \\
\text{Term}(3) &= T_3(1) - c(\sum_E GA_{1,l2})\eta(l_1+l_1', \tilde{c}-2) I_{\omega(l_1+l_1')-2}(\tilde{a}, \tilde{b}, \tilde{c}-5), \\
&\qquad\qquad\qquad\qquad\qquad 3 \leq \tilde{c} \leq 4 \\
\text{Term}(3) &= T_3(2) + c\gamma_3 \text{Dif}(\tilde{a}+1, \tilde{b}-1; \tilde{a}, \tilde{b}; \tilde{c}-5, \tilde{\alpha}, \tilde{\beta}; \\
&\quad \omega(l_1+l_1'+1) - 2, \omega(l_1+l_1') - 2) \\
&+ c(\gamma_3+\gamma_4)\text{Dif}(\tilde{a}, \tilde{b}; \tilde{a}-1, \tilde{b}+1; \tilde{c}-5, \tilde{\alpha}, \tilde{\beta}; \\
&\quad \omega(l_1+l_1') - 2, \omega(l_1+l_1'+1) - 2) \\
&+ [cS_1(l_1'l_2'l_1l_2)\text{Can}(\tilde{a}-1, \tilde{b}+1, \tilde{\alpha}, \tilde{\beta}; \tilde{a}'-1, \tilde{b}'+1, \tilde{\alpha}', \tilde{\beta}'; \\
&\quad \tilde{c}-5; \omega(l_1+l_1'+1) - 2, \omega(l_1+l_2'+1) - 2) \\
&+ cS_1(l_2'l_1'l_2l_1)\text{Can}(\tilde{a}+1, \tilde{b}-1, \tilde{\alpha}, \tilde{\beta}; \tilde{a}'+1, \tilde{b}'-1, \tilde{\alpha}', \tilde{\beta}'; \\
&\quad \tilde{c}-5; \omega(l_1+l_1'+1) - 2, \omega(l_1+l_2'+1) - 2)]\delta(X_R, 1)\delta(X_L, 1), \\
&\qquad\qquad\qquad\qquad\qquad \tilde{c} \leq 2.
\end{aligned}$$

For Term(4) + Term(5),

$$T_{45}(k) = \Xi(l_1', l_2', a', b'; \alpha', \beta') - \Xi(l_2', l_1', b', a'; \beta', \alpha')$$

with

$$\begin{aligned}
&\Xi(l_1', l_2', a', b'; \alpha', \beta') \equiv \\
&a\varpi_k(\omega(M(l_1+l_1'+1)) - 2, M(l_1+l_1'+1); \Omega_6(l_1'l_2'l_1l_2); \tilde{a}-1, \tilde{b}+1, \tilde{c}-5; \tilde{\alpha}, \tilde{\beta}) \\
&-\alpha\varpi_k(\omega(M(l_1+l_1'+1)) - 2, M(l_1+l_1'+1); \Omega_6(l_1'l_2'l_1l_2); \tilde{a}, \tilde{b}+1, \tilde{c}-5; \tilde{\alpha}, \tilde{\beta}) \\
&+b\varpi_k(\omega(M(l_1+l_1')) - 2, M(l_1+l_1'); \Omega_7(l_1'l_2'l_1l_2); \tilde{a}, \tilde{b}, \tilde{c}-5; \tilde{\alpha}, \tilde{\beta}) \\
&-\beta\varpi_k(\omega(M(l_1+l_1')) - 2, M(l_1+l_1'); \Omega_7(l_1'l_2'l_1l_2); \tilde{a}, \tilde{b}+1, \tilde{c}-5; \tilde{\alpha}, \tilde{\beta})
\end{aligned}$$

$$+a\varpi_k(\omega(M(l_1+l_1'))-2,M(l_1+l_1');\Omega_8(l_1'l_2'l_1l_2);\tilde{a},\tilde{b},\tilde{c}-5;\tilde{\alpha},\tilde{\beta})$$
$$-\alpha\varpi_k(\omega(M(l_1+l_1'))-2,M(l_1+l_1');\Omega_8(l_1'l_2'l_1l_2);\tilde{a}+1,\tilde{b},\tilde{c}-5;\tilde{\alpha},\tilde{\beta})+$$
$$b\varpi_k(\omega(M(l_1+l_1'+1))-2,M(l_1+l_1'+1);\Omega_6(l_2'l_1'l_2l_1);\tilde{a}+1,\tilde{b}-1,\tilde{c}-5;\tilde{\alpha},\tilde{\beta})$$
$$-\beta\varpi_k(\omega(M(l_1+l_1'+1))-2,M(l_1+l_1'+1);\Omega_6(l_2'l_1'l_2l_1);\tilde{a}+1,\tilde{b},\tilde{c}-5;\tilde{\alpha},\tilde{\beta})$$
$$+a\varpi_k(\omega(M(l_1+l_1'))-2,M(l_1+l_1');\Omega_7(l_2'l_1'l_2l_1);\tilde{a},\tilde{b},\tilde{c}-5;\tilde{\alpha},\tilde{\beta})$$
$$-\alpha\varpi_k(\omega(M(l_1+l_1'))-2,M(l_1+l_1');\Omega_7(l_2'l_1'l_2l_1);\tilde{a}+1,\tilde{b},\tilde{c}-5;\tilde{\alpha},\tilde{\beta})$$
$$+b\varpi_k(\omega(M(l_1+l_1'))-2,M(l_1+l_1');\Omega_8(l_2'l_1'l_2l_1);\tilde{a},\tilde{b},\tilde{c}-5;\tilde{\alpha},\tilde{\beta})$$
$$-\beta\varpi_k(\omega(M(l_1+l_1'))-2,M(l_1+l_1');\Omega_8(l_2'l_1'l_2l_1);\tilde{a},\tilde{b}+1,\tilde{c}-5;\tilde{\alpha},\tilde{\beta}).$$

$$\begin{aligned}
\text{Term}(45) &= T_{45}(0)\delta(X_R,1)\delta(X_L,1), \quad \tilde{c}\geq 3\\
\text{Term}(45) &= T_{45}(1)\delta(X_R,1)\delta(X_L,1), \quad 1\leq\tilde{c}\leq 2\\
\text{Term}(45) &= \{T_{45}(2)+a\gamma_8(l_1'l_2'l_1l_2)\text{Dif}(\tilde{a}-2,\tilde{b};\tilde{a}-1,\tilde{b}-1;\tilde{c}-3,\tilde{\alpha},\tilde{\beta};\\
&\quad \omega(l_1+l_1')-2,\omega(l_1+l_1'+1)-2)\\
&- \alpha\gamma_8(l_1'l_2'l_1l_2)\text{Dif}(\tilde{a}-1,\tilde{b};\tilde{a},\tilde{b}-1;\tilde{c}-3,\tilde{\alpha},\tilde{\beta};\\
&\quad \omega(l_1+l_1')-2,\omega(l_1+l_1'+1)-2)\\
&+ b\gamma_8(l_2'l_1'l_2l_1)\text{Dif}(\tilde{a},\tilde{b}-2;\tilde{a}-1,\tilde{b}-1;\tilde{c}-3,\tilde{\alpha},\tilde{\beta};\\
&\quad \omega(l_1+l_1')-2,\omega(l_1+l_1'+1)-2)\\
&- \beta\gamma_8(l_2'l_1'l_2l_1)\text{Dif}(\tilde{a},\tilde{b}-1;\tilde{a}-1,\tilde{b};\tilde{c}-3,\tilde{\alpha},\tilde{\beta};\\
&\quad \omega(l_1+l_1')-2,\omega(l_1+l_1'+1)-2)\\
&- a\gamma_8(l_2'l_1'l_1l_2)\text{Dif}(\tilde{a}'-2,\tilde{b}';\tilde{a}'-1,\tilde{b}'-1;\tilde{c}-3,\tilde{\alpha}',\tilde{\beta}';\\
&\quad \omega(l_1+l_2')-2,\omega(l_1+l_2'+1)-2)\\
&+ \alpha\gamma_8(l_2'l_1'l_1l_2)\text{Dif}(\tilde{a}'-1,\tilde{b}';\tilde{a}',\tilde{b}'-1;\tilde{c}-3,\tilde{\alpha}',\tilde{\beta}';\\
&\quad \omega(l_1+l_2')-2,\omega(l_1+l_2'+1)-2)\\
&- b\gamma_8(l_1'l_2'l_2l_1)\text{Dif}(\tilde{a}',\tilde{b}'-2;\tilde{a}'-1,\tilde{b}'-1;\tilde{c}-3,\tilde{\alpha}',\tilde{\beta}';\\
&\quad \omega(l_1+l_2')-2,\omega(l_1+l_2'+1)-2)\\
&+ \beta\gamma_8(l_1'l_2'l_2l_1)\text{Dif}(\tilde{a}',\tilde{b}'-1;\tilde{a}'-1,\tilde{b}';\tilde{c}-3,\tilde{\alpha}',\tilde{\beta}';\\
&\quad \omega(l_1+l_2')-2,\omega(l_1+l_2'+1)-2)\\
&+ [aH(l_1'l_2'l_1l_2)+bH(l_2'l_1'l_2l_1)]\text{Can}(\tilde{a}-1,\tilde{b}-1,\tilde{\alpha},\tilde{\beta};
\end{aligned}$$

$$\tilde{a}' - 1, \tilde{b}' - 1, \tilde{\alpha}', \tilde{\beta}'; \tilde{c} - 3; \omega(l_1 + l_1' + 1) - 2, \omega(l_1 + l_2' + 1) - 2)$$
$$- \quad \alpha H(l_1'l_2'l_1l_2)\mathrm{Can}(\tilde{a}, \tilde{b} - 1, \tilde{\alpha}, \tilde{\beta}; \tilde{a}', \tilde{b}' - 1, \tilde{\alpha}', \tilde{\beta}'; \tilde{c} - 3;$$
$$\omega(l_1 + l_1' + 1) - 2, \omega(l_1 + l_2' + 1) - 2)$$
$$- \quad \beta H(l_2'l_1'l_2l_1)\mathrm{Can}(\tilde{a} - 1, \tilde{b}, \tilde{\alpha}, \tilde{\beta}; \tilde{a}' - 1, \tilde{b}', \tilde{\alpha}', \tilde{\beta}'; \tilde{c} - 3;$$
$$\omega(l_1 + l_1' + 1) - 2, \omega(l_1 + l_2' + 1) - 2)\}\delta(X_R, 1)\delta(X_L, 1), \quad \tilde{c} = 0.$$

For Term(6),

$$\begin{aligned}
T_6(k) &= \alpha c\varpi_k(\omega(M(l_1 + l_1')) - 2, M(l_1 + l_1'); GA_{231}; \tilde{a}, \tilde{b} + 2, \tilde{c} - 7; \tilde{\alpha}, \tilde{\beta}) \\
&- \alpha c\varpi_k(\omega(M(l_1 + l_1')) - 2, M(l_1 + l_1'); GA_{231}; \tilde{a} + 1, \tilde{b} + 2, \tilde{c} - 7; \tilde{\alpha}, \tilde{\beta}) \\
&+ (a + 1)c\varpi_k(\omega(M(l_1 + l_1')) - 2, M(l_1 + l_1'); GB_{71}; \tilde{a}, \tilde{b} + 2, \tilde{c} - 7; \tilde{\alpha}, \tilde{\beta}) \\
&- \alpha c\varpi_k(\omega(M(l_1 + l_1')) - 2, M(l_1 + l_1'); GB_{71}; \tilde{a} + 1, \tilde{b} + 2, \tilde{c} - 7; \tilde{\alpha}, \tilde{\beta})
\end{aligned}$$

$$\begin{aligned}
\mathrm{Term}(6) &= T_6(0), \quad \tilde{c} \geq 5 \\
\mathrm{Term}(6) &= T_6(1), \quad 3 \leq \tilde{c} \leq 4 \\
\mathrm{Term}(6) &= T_6(2) + [(2a + 1)c\gamma_{11}(l_1'l_2'l_1l_2)\mathrm{Can}(\tilde{a} - 1, \tilde{b} + 1, \tilde{\alpha}, \tilde{\beta}; \tilde{a}' - 1, \tilde{b}' + 1, \\
&\quad \tilde{\alpha}', \tilde{\beta}'; \tilde{c} - 5; \omega(l_1 + l_1' + 1) - 2, \omega(l_1 + l_2' + 1) - 2) \\
&\quad - 2\alpha c\gamma_{11}(l_1'l_2'l_1l_2)\mathrm{Can}(\tilde{a}, \tilde{b} + 1, \tilde{\alpha}, \tilde{\beta}; \tilde{a}', \tilde{b}' + 1, \tilde{\alpha}', \tilde{\beta}'; \\
&\quad \tilde{c} - 5; \omega(l_1 + l_1' + 1) - 2, \omega(l_1 + l_2' + 1) - 2) \\
&\quad + (2b + 1)c\gamma_{11}(l_2'l_1'l_2l_1)\mathrm{Can}(\tilde{a} + 1, \tilde{b} - 1, \tilde{\alpha}, \tilde{\beta}; \tilde{a}' + 1, \tilde{b}' - 1, \tilde{\alpha}', \tilde{\beta}'; \\
&\quad \tilde{c} - 5; \omega(l_1 + l_1' + 1) - 2, \omega(l_1 + l_2' + 1) - 2) \\
&\quad - 2\beta c\gamma_{11}(l_2'l_1'l_2l_1)\mathrm{Can}(\tilde{a} + 1, \tilde{b}, \tilde{\alpha}, \tilde{\beta}; \tilde{a}' + 1, \tilde{b}', \tilde{\alpha}', \tilde{\beta}'; \tilde{c} - 5; \\
&\quad \omega(l_1 + l_1' + 1) - 2, \omega(l_1 + l_2' + 1) - 2)]\delta(X_R, 1)\delta(X_L, 1), \quad \tilde{c} \leq 2.
\end{aligned}$$

For Term(7),

$$\begin{aligned}
T_7(k) &= \varpi_k(\omega(M(l_1 + l_1')) - 2, M(l_1 + l_1'); GB_{11}; A, B, C; \tilde{\alpha}, \tilde{\beta}) \\
\mathrm{Term}(7) &= \sum_{i=1}^{8} \mathrm{coe}(A_i^{(6)})\Delta_7(i) + \sum_{i=1}^{8} \tilde{\Delta}_7 \\
\Delta_7(i) &= T_7(0), \quad C \geq -2 \\
\Delta_7(i) &= T_7(1), \quad -4 \leq C \leq -3
\end{aligned}$$

$$
\begin{aligned}
\Delta_7(i) &= T_7(2), \quad C \leq -5 \\
\tilde{\Delta}_7 &= [\Lambda(a,b,\alpha,\beta;i)\gamma_{13}(l_1{}'l_2{}'l_1l_2)\mathrm{Can}(A-1,B-1,\tilde{\alpha},\tilde{\beta};\tilde{a}'+a^{(6)}(i)-1, \\
&\quad \tilde{b}'+b^{(6)}(i)-1,\tilde{\alpha}',\tilde{\beta}';C+2;\omega(l_1+l_1{}'+1)-2,\omega(l_1+l_2{}'+1)-2) \\
&+ \Lambda(b,a,\beta,\alpha;i)\gamma_{13}(l_2{}'l_1{}'l_2l_1)\mathrm{Can}(\tilde{a}+b^{(6)}(i)-1,\tilde{b}+a^{(6)}(i)-1,\tilde{\alpha},\tilde{\beta}; \\
&\quad \tilde{a}'+b^{(6)}(i)-1,\tilde{b}'+a^{(6)}(i)-1,\tilde{\alpha}',\tilde{\beta}';C+2; \\
&\quad \omega(l_1+l_1{}'+1)-2,\omega(l_1+l_2{}'+1)-2)]\delta(X_R,1)\delta(X_L,1), \quad C \leq -5 \\
\tilde{\Delta}_7 &= 0, \quad \text{otherwise.}
\end{aligned}
$$

Here,

$$
\begin{aligned}
M(i) &= 20, \quad i = \text{even} \\
&= 19, \quad i = \text{odd}
\end{aligned}
$$

$$
\begin{aligned}
A &\equiv \tilde{a}+a^{(6)}(i) \\
B &\equiv \tilde{b}+b^{(6)}(i) \\
C &\equiv \tilde{c}+c^{(6)}(i)
\end{aligned}
$$

coe($A_i^{(1)}$)	$a^{(1)}(i)$	$b^{(1)}(i)$	$c^{(1)}(i)$
ab	-1	-1	0
$-a\beta$	-1	0	0
$-b\alpha$	0	-1	0
$\alpha\beta$	0	0	0
ca	-1	1	-2
cb	1	-1	-2
$-c\alpha$	0	1	-2
$-c\beta$	1	0	-2
$c(c-2)$	1	1	-4

coe($A_i^{(2)}$)	$b^{(2)}(i)$	$c^{(2)}(i)$
b	-1	0
$-\beta$	0	0
c	1	-2

coe($A_i^{(3)}$)	$a^{(3)}(i)$	$c^{(3)}(i)$
a	-1	0
$-\alpha$	0	0
c	1	-2

$coe(A_i^{(4)})$	$a^{(4)}(i)$	$c^{(4)}(i)$
ac	0	-2
$-c\alpha$	1	-2
$c(c-2)$	2	-4

$coe(A_i^{(5)})$	$b^{(5)}(i)$	$c^{(5)}(i)$
$(b+1)c$	0	-2
$-c\beta$	1	-2
$c(c-2)$	2	-4

$coe(A_i^{(6)})$	$a^{(6)}(i)$	$b^{(6)}(i)$	$c^{(6)}(i)$
$(a+1)b$	0	0	-5
$-b\alpha$	1	0	-5
$-(a+1)\beta$	0	1	-5
$\alpha\beta$	1	1	-5
cb	2	0	-7
$(a+1)c$	0	2	-7
$-c\alpha$	1	2	-7
$-c\beta$	2	1	-7
$c(c-2)$	2	2	-9

$coe(A_i^{(7)})$	$b^{(7)}(i)$	$c^{(7)}(i)$
b	0	-5
$-\beta$	1	-5
c	2	-7

$coe(A_i^{(8)})$	$a^{(8)}(i)$	$c^{(8)}(i)$
$a+1$	0	-5
$-\alpha$	1	-5
c	2	-7

$coe(A_i^{(9)})$	$b^{(9)}(i)$	$c^{(9)}(i)$
bc	1	-7
$-\beta c$	2	-7
$c(c-2)$	3	-9

$coe(A_i^{(10)})$	$a^{(10)}(i)$	$c^{(10)}(i)$
$(a+2)c$	1	-7
$-\alpha c$	2	-7
$c(c-2)$	3	-9

$\text{coe}(A_i^{(11)})$	$a^{(11)}(i)$	$b^{(11)}(i)$	$c^{(11)}(i)$
ab	-1	1	-5
$-b\alpha$	0	1	-5
$-a\beta$	-1	2	-5
$\alpha\beta$	0	2	-5
cb	1	1	-7
ca	-1	3	-7
$-c\alpha$	0	3	-7
$-c\beta$	1	2	-7
$c(c-2)$	1	3	-9

$\text{coe}(A_i^{(12)})$	$b^{(12)}(i)$	$c^{(12)}(i)$
b	1	-5
$-\beta$	2	-5
c	3	-7

$\text{coe}(A_i^{(13)})$	$a^{(13)}(i)$	$c^{(13)}(i)$
a	-1	-5
$-\alpha$	0	-5
c	1	-7

$\text{coe}(A_i^{(14)})$	$b^{(14)}(i)$	$c^{(14)}(i)$
bc	2	-7
$-\beta c$	3	-7
$c(c-2)$	4	-9

$\text{coe}(A_i^{(15)})$	$a^{(15)}(i)$	$c^{(15)}(i)$
$(a+1)c$	0	-7
$-\alpha c$	1	-7
$c(c-2)$	2	-9

$\text{coe}(A_i^{(0)})$	$a^{(0)}(i)$	$c^{(0)}(i)$
a	0	-5
$-\alpha$	1	-5
c	2	-7

The angular coefficients are:

$$GA_{114}(E) = \sum_{HNT\Lambda}(H,N,T,\Lambda,E)G(TA_{11},0)\tilde{G}(TA_{11})b(l_1;T)b(l_2;\Lambda)$$

$$GA_{12}(E) = \sum_{HNT\Lambda}(H,N,T,\Lambda,E)G(TA_{12},0)\tilde{G}(TA_{12})$$

$$GA_{132}(E) = \sum_{HNT\Lambda} (H,N,T,\Lambda,E)G(TA_{13},0)\tilde{G}(TA_{13})b(l_1;T)$$

$$GA_{142}(E) = \sum_{HNT\Lambda} (H,N,T,\Lambda,E)G(TA_{14},0)\tilde{G}(TA_{14})b(T;\Lambda)$$

$$GA_{213}(E) = \sum_{HNT\Lambda} (H,N,T,\Lambda,E)G(TA_{21},0)\tilde{G}(TA_{21})b(l_2;\Lambda)$$

$$GA_{214}(E) = \sum_{HNT\Lambda} (H,N,T,\Lambda,E)G(TA_{21},0)\tilde{G}(TA_{21})b(l_1;T)b(l_2;\Lambda)$$

$$GA_{231}(E) = \sum_{HNT\Lambda} (H,N,T,\Lambda,E)G(TA_{23},0)\tilde{G}(TA_{23})$$

$$GA_{232}(E) = \sum_{HNT\Lambda} (H,N,T,\Lambda,E)G(TA_{23},0)\tilde{G}(TA_{23})b(l_1;T)$$

$$GA_{242}(E) = \sum_{HNT\Lambda} (H,N,T,\Lambda,E)G(TA_{24},0)\tilde{G}(TA_{24})b(T;\Lambda)$$

$$GB_{11}(E) = \sum_{HNT\Lambda} (H,N,T,\Lambda,E)G(TB_1,0)\tilde{G}(TB_1)$$

$$GB_{12}(E) = \sum_{HNT\Lambda} (H,N,T,\Lambda,E)G(TB_1,0)\tilde{G}(TB_1)b(H;\Lambda)$$

$$GB_{13}(E) = \sum_{HNT\Lambda} (H,N,T,\Lambda,E)G(TB_1,0)\tilde{G}(TB_1)b(l_2;T)$$

$$GB_{14}(E) = \sum_{HNT\Lambda} (H,N,T,\Lambda,E)G(TB_1,0)\tilde{G}(TB_1)b(H;\Lambda)b(l_2;T)$$

$$GB_{53}(E) = \sum_{HNT\Lambda} (H,N,T,\Lambda,E)G(TB_5,0)\tilde{G}(TB_5)b(l_2;T)$$

$$GB_{54}(E) = \sum_{HNT\Lambda} (H,N,T,\Lambda,E)G(TB_5,0)\tilde{G}(TB_5)b(l_1;\Lambda)b(l_2;T)$$

$$GB_{71}(E) = \sum_{HNT\Lambda} (H,N,T,\Lambda,E)G(TB_7,0)\tilde{G}(TB_7)$$

$$GB_{72}(E) = \sum_{HNT\Lambda} (H,N,T,\Lambda,E)G(TB_7,0)\tilde{G}(TB_7)b(T;\Lambda)$$

$$GC_{11}(E) = \frac{1}{6}\sum_{TH}(T,H,E)G(TC_1,0)\tilde{G}(TC_1)$$

$$GC_{12}(E) = \frac{1}{6}\sum_{TH}(T,H,E)G(TC_1,0)\tilde{G}(TC_1)b(l_1;T)$$

$$GC_2(E) = \frac{1}{6}\sum_{TH}(T,H,E)G(TC_2,0)\tilde{G}(TC_2)$$

We first define the following operator:

$$\uplus \equiv \sum_{m_1m_2}\sum_{m_1'm_2'}\sum_{\mu_1\mu_2}\sum_{\sigma_1\sigma_2}\sum_{\theta_1\theta_2}\sum_{\eta\nu}\sum_{\tau\lambda\epsilon}\begin{pmatrix} l_1 & l_2 & L \\ m_1 & m_2 & -M \end{pmatrix}\begin{pmatrix} l_1' & l_2' & L' \\ m_1' & m_2' & -M' \end{pmatrix}$$
$$\times \begin{pmatrix} 1 & 1 & K \\ \mu_1 & \mu_2 & 0 \end{pmatrix}\begin{pmatrix} 1 & 1 & 1 \\ \sigma_1 & \sigma_2 & -\mu_1 \end{pmatrix}\begin{pmatrix} 1 & 1 & 1 \\ \theta_1 & \theta_2 & -\mu_2 \end{pmatrix},$$

then,

$$G(TA_{11},0) = \begin{pmatrix} l_1' & 1 & H \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & 1 & N \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_1 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_2 & \Lambda \\ 0 & 0 & 0 \end{pmatrix}$$
$$\times \begin{pmatrix} H & T & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} N & \Lambda & E \\ 0 & 0 & 0 \end{pmatrix}$$
$$G(TA_{11}) = \uplus(-1)^{M+M'+m_1'+m_2'+1+\epsilon}\begin{pmatrix} l_1' & 1 & H \\ -m_1' & \sigma_1 & \eta \end{pmatrix}\begin{pmatrix} l_2' & 1 & N \\ -m_2' & \theta_1 & \nu \end{pmatrix}$$
$$\times \begin{pmatrix} 1 & l_1 & T \\ \sigma_2 & m_1 & \tau \end{pmatrix}\begin{pmatrix} 1 & l_2 & \Lambda \\ \theta_2 & m_2 & \lambda \end{pmatrix}\begin{pmatrix} H & T & E \\ \eta & \tau & \epsilon \end{pmatrix}\begin{pmatrix} N & \Lambda & E \\ \nu & \lambda & -\epsilon \end{pmatrix}$$

$$G(TA_{12},0) = \begin{pmatrix} l_1' & 1 & H \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & 1 & N \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_1 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_2 & \Lambda \\ 0 & 0 & 0 \end{pmatrix}$$
$$\times \begin{pmatrix} H & T & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} N & \Lambda & E \\ 0 & 0 & 0 \end{pmatrix}$$
$$G(TA_{12}) = \uplus(-1)^{M+M'+m_1'+m_2'+1+\epsilon}\begin{pmatrix} l_1' & 1 & H \\ -m_1' & \sigma_1 & \eta \end{pmatrix}\begin{pmatrix} l_2' & 1 & N \\ -m_2' & \theta_1 & \nu \end{pmatrix}$$
$$\times \begin{pmatrix} 1 & l_1 & T \\ \theta_2 & m_1 & \tau \end{pmatrix}\begin{pmatrix} 1 & l_2 & \Lambda \\ \sigma_2 & m_2 & \lambda \end{pmatrix}\begin{pmatrix} H & T & E \\ \eta & \tau & \epsilon \end{pmatrix}\begin{pmatrix} N & \Lambda & E \\ \nu & \lambda & -\epsilon \end{pmatrix}$$

$$G(TA_{13},0) = \begin{pmatrix} l_1' & 1 & H \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & 1 & N \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_1 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & T & \Lambda \\ 0 & 0 & 0 \end{pmatrix}$$
$$\times \begin{pmatrix} H & \Lambda & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} N & l_2 & E \\ 0 & 0 & 0 \end{pmatrix}$$
$$G(TA_{13}) = \uplus(-1)^{M+M'+m_1'+m_2'+\tau+\nu}\begin{pmatrix} l_1' & 1 & H \\ -m_1' & \sigma_1 & \eta \end{pmatrix}\begin{pmatrix} l_2' & 1 & N \\ -m_2' & \theta_1 & \nu \end{pmatrix}$$
$$\times \begin{pmatrix} 1 & l_1 & T \\ \sigma_2 & m_1 & \tau \end{pmatrix}\begin{pmatrix} 1 & T & \Lambda \\ \theta_2 & -\tau & \lambda \end{pmatrix}\begin{pmatrix} H & \Lambda & E \\ \eta & \lambda & \epsilon \end{pmatrix}\begin{pmatrix} N & l_2 & E \\ -\nu & m_2 & \epsilon \end{pmatrix}$$

$$G(TA_{14},0) = \begin{pmatrix} l_1' & 1 & H \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & 1 & N \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_2 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & T & \Lambda \\ 0 & 0 & 0 \end{pmatrix}$$
$$\times \begin{pmatrix} H & l_1 & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} N & \Lambda & E \\ 0 & 0 & 0 \end{pmatrix}$$

$$
\begin{aligned}
G(TA_{14}) &= \biguplus(-1)^{M+M'+m_1'+m_2'+\tau+\eta}\begin{pmatrix} l_1' & 1 & H \\ -m_1' & \sigma_1 & \eta \end{pmatrix}\begin{pmatrix} l_2' & 1 & N \\ -m_2' & \theta_1 & \nu \end{pmatrix} \\
&\times \begin{pmatrix} 1 & l_2 & T \\ \sigma_2 & m_2 & \tau \end{pmatrix}\begin{pmatrix} 1 & T & \Lambda \\ \theta_2 & -\tau & \lambda \end{pmatrix}\begin{pmatrix} H & l_1 & E \\ -\eta & m_1 & \epsilon \end{pmatrix}\begin{pmatrix} N & \Lambda & E \\ \nu & \lambda & \epsilon \end{pmatrix}
\end{aligned}
$$

$$
\begin{aligned}
G(TA_{21},0) &= \begin{pmatrix} 1 & 1 & H \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & H & N \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_1 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_2 & \Lambda \\ 0 & 0 & 0 \end{pmatrix} \\
&\times \begin{pmatrix} l_1' & T & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} N & \Lambda & E \\ 0 & 0 & 0 \end{pmatrix} \\
G(TA_{21}) &= \biguplus(-1)^{M+M'+\lambda}\begin{pmatrix} 1 & 1 & H \\ \sigma_1 & \theta_1 & \eta \end{pmatrix}\begin{pmatrix} l_2' & H & N \\ m_2' & \eta & \nu \end{pmatrix} \\
&\times \begin{pmatrix} 1 & l_1 & T \\ \sigma_2 & m_1 & \tau \end{pmatrix}\begin{pmatrix} 1 & l_2 & \Lambda \\ \theta_2 & m_2 & \lambda \end{pmatrix}\begin{pmatrix} l_1' & T & E \\ m_1' & \tau & \epsilon \end{pmatrix}\begin{pmatrix} N & \Lambda & E \\ \nu & -\lambda & \epsilon \end{pmatrix}
\end{aligned}
$$

$$
\begin{aligned}
G(TA_{22},0) &= \begin{pmatrix} 1 & 1 & H \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & H & N \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_1 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_2 & \Lambda \\ 0 & 0 & 0 \end{pmatrix} \\
&\times \begin{pmatrix} l_1' & T & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} N & \Lambda & E \\ 0 & 0 & 0 \end{pmatrix} \\
G(TA_{22}) &= \biguplus(-1)^{M+M'+\lambda}\begin{pmatrix} 1 & 1 & H \\ \sigma_1 & \theta_1 & \eta \end{pmatrix}\begin{pmatrix} l_2' & H & N \\ m_2' & \eta & \nu \end{pmatrix} \\
&\times \begin{pmatrix} 1 & l_1 & T \\ \theta_2 & m_1 & \tau \end{pmatrix}\begin{pmatrix} 1 & l_2 & \Lambda \\ \sigma_2 & m_2 & \lambda \end{pmatrix}\begin{pmatrix} l_1' & T & E \\ m_1' & \tau & \epsilon \end{pmatrix}\begin{pmatrix} N & \Lambda & E \\ \nu & -\lambda & \epsilon \end{pmatrix}
\end{aligned}
$$

$$
\begin{aligned}
G(TA_{23},0) &= \begin{pmatrix} 1 & 1 & H \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & H & N \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_1 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & T & \Lambda \\ 0 & 0 & 0 \end{pmatrix} \\
&\times \begin{pmatrix} l_1' & \Lambda & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} N & l_2 & E \\ 0 & 0 & 0 \end{pmatrix} \\
G(TA_{23}) &= \biguplus(-1)^{M+M'+\tau+1}\begin{pmatrix} 1 & 1 & H \\ \sigma_1 & \theta_1 & \eta \end{pmatrix}\begin{pmatrix} l_2' & H & N \\ m_2' & \eta & \nu \end{pmatrix} \\
&\times \begin{pmatrix} 1 & l_1 & T \\ \sigma_2 & m_1 & \tau \end{pmatrix}\begin{pmatrix} 1 & T & \Lambda \\ \theta_2 & -\tau & \lambda \end{pmatrix}\begin{pmatrix} l_1' & \Lambda & E \\ m_1' & \lambda & \epsilon \end{pmatrix}\begin{pmatrix} N & l_2 & E \\ \nu & m_2 & \epsilon \end{pmatrix}
\end{aligned}
$$

$$
\begin{aligned}
G(TA_{24},0) &= \begin{pmatrix} 1 & 1 & H \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & H & N \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_2 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & T & \Lambda \\ 0 & 0 & 0 \end{pmatrix} \\
&\times \begin{pmatrix} l_1' & l_1 & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} N & \Lambda & E \\ 0 & 0 & 0 \end{pmatrix} \\
G(TA_{24}) &= \biguplus(-1)^{M+M'+\tau+1+m_1+\lambda}\begin{pmatrix} 1 & 1 & H \\ \sigma_1 & \theta_1 & \eta \end{pmatrix}\begin{pmatrix} l_2' & H & N \\ m_2' & \eta & \nu \end{pmatrix} \\
&\times \begin{pmatrix} 1 & l_2 & T \\ \sigma_2 & m_2 & \tau \end{pmatrix}\begin{pmatrix} 1 & T & \Lambda \\ \theta_2 & -\tau & \lambda \end{pmatrix}\begin{pmatrix} l_1' & l_1 & E \\ m_1' & -m_1 & \epsilon \end{pmatrix}\begin{pmatrix} N & \Lambda & E \\ \nu & -\lambda & \epsilon \end{pmatrix}
\end{aligned}
$$

$$
\begin{aligned}
G(TB_1,0) &= \begin{pmatrix} 1 & l_1 & H \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_2 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & T & N \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & H & \Lambda \\ 0 & 0 & 0 \end{pmatrix} \\
&\times \begin{pmatrix} l_1' & \Lambda & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & N & E \\ 0 & 0 & 0 \end{pmatrix} \\
G(TB_1) &= \biguplus(-1)^{M+M'+1+\tau+\eta+\epsilon}\begin{pmatrix} 1 & l_1 & H \\ \theta_1 & m_1 & \eta \end{pmatrix}\begin{pmatrix} 1 & l_2 & T \\ \theta_2 & m_2 & \tau \end{pmatrix} \\
&\times \begin{pmatrix} 1 & T & N \\ \sigma_1 & -\tau & \nu \end{pmatrix}\begin{pmatrix} 1 & H & \Lambda \\ \sigma_2 & -\eta & \lambda \end{pmatrix}\begin{pmatrix} l_1' & \Lambda & E \\ m_1' & \lambda & \epsilon \end{pmatrix}\begin{pmatrix} l_2' & N & E \\ m_2' & \nu & -\epsilon \end{pmatrix}
\end{aligned}
$$

$$
\begin{aligned}
G(TB_2,0) &= \begin{pmatrix} 1 & l_1 & H \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_2 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & T & N \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} N & 1 & \Lambda \\ 0 & 0 & 0 \end{pmatrix} \\
&\times \begin{pmatrix} l_1' & H & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & \Lambda & E \\ 0 & 0 & 0 \end{pmatrix} \\
G(TB_2) &= \biguplus(-1)^{M+M'+\tau+\nu+\epsilon}\begin{pmatrix} 1 & l_1 & H \\ \theta_1 & m_1 & \eta \end{pmatrix}\begin{pmatrix} 1 & l_2 & T \\ \theta_2 & m_2 & \tau \end{pmatrix} \\
&\times \begin{pmatrix} 1 & T & N \\ \sigma_1 & -\tau & \nu \end{pmatrix}\begin{pmatrix} N & 1 & \Lambda \\ -\nu & \sigma_2 & \lambda \end{pmatrix}\begin{pmatrix} l_1' & H & E \\ m_1' & \eta & \epsilon \end{pmatrix}\begin{pmatrix} l_2' & \Lambda & E \\ m_2' & \lambda & -\epsilon \end{pmatrix}
\end{aligned}
$$

$$
\begin{aligned}
G(TB_3,0) &= \begin{pmatrix} 1 & l_1 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_2 & N \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & T & H \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & H & \Lambda \\ 0 & 0 & 0 \end{pmatrix} \\
&\times \begin{pmatrix} l_1' & \Lambda & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & N & E \\ 0 & 0 & 0 \end{pmatrix} \\
G(TB_3) &= \biguplus(-1)^{M+M'+\tau+\eta+\epsilon}\begin{pmatrix} 1 & l_1 & T \\ \theta_2 & m_1 & \tau \end{pmatrix}\begin{pmatrix} 1 & l_2 & N \\ \sigma_1 & m_2 & \nu \end{pmatrix} \\
&\times \begin{pmatrix} 1 & T & H \\ \theta_1 & -\tau & \eta \end{pmatrix}\begin{pmatrix} 1 & H & \Lambda \\ \sigma_2 & -\eta & \lambda \end{pmatrix}\begin{pmatrix} l_1' & \Lambda & E \\ m_1' & \lambda & \epsilon \end{pmatrix}\begin{pmatrix} l_2' & N & E \\ m_2' & \nu & -\epsilon \end{pmatrix}
\end{aligned}
$$

$$
\begin{aligned}
G(TB_4,0) &= \begin{pmatrix} 1 & l_1 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_2 & N \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & T & H \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} N & 1 & \Lambda \\ 0 & 0 & 0 \end{pmatrix} \\
&\times \begin{pmatrix} l_1' & H & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & \Lambda & E \\ 0 & 0 & 0 \end{pmatrix} \\
G(TB_4) &= \biguplus(-1)^{M+M'+1+\tau+\nu+\epsilon}\begin{pmatrix} 1 & l_1 & T \\ \theta_2 & m_1 & \tau \end{pmatrix}\begin{pmatrix} 1 & l_2 & N \\ \sigma_1 & m_2 & \nu \end{pmatrix} \\
&\times \begin{pmatrix} 1 & T & H \\ \theta_1 & -\tau & \eta \end{pmatrix}\begin{pmatrix} N & 1 & \Lambda \\ -\nu & \sigma_2 & \lambda \end{pmatrix}\begin{pmatrix} l_1' & H & E \\ m_1' & \eta & \epsilon \end{pmatrix}\begin{pmatrix} l_2' & \Lambda & E \\ m_2' & \lambda & -\epsilon \end{pmatrix}
\end{aligned}
$$

$$
\begin{aligned}
G(TB_5,0) &= \begin{pmatrix} 1 & l_2 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & 1 & H \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} H & T & N \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_1 & \Lambda \\ 0 & 0 & 0 \end{pmatrix} \\
&\times \begin{pmatrix} l_1' & \Lambda & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & N & E \\ 0 & 0 & 0 \end{pmatrix}
\end{aligned}
$$

$$
\begin{aligned}
G(TB_5) &= \biguplus(-1)^{M+M'+m_2'}\begin{pmatrix}1 & l_2 & T\\ \theta_2 & m_2 & \tau\end{pmatrix}\begin{pmatrix}1 & 1 & H\\ \sigma_1 & \theta_1 & \eta\end{pmatrix}\\
&\times \begin{pmatrix}H & T & N\\ \eta & \tau & \nu\end{pmatrix}\begin{pmatrix}1 & l_1 & \Lambda\\ \sigma_2 & m_1 & \lambda\end{pmatrix}\begin{pmatrix}l_1' & \Lambda & E\\ m_1' & \lambda & \epsilon\end{pmatrix}\begin{pmatrix}l_2' & N & E\\ -m_2' & \nu & \epsilon\end{pmatrix}
\end{aligned}
$$

$$
\begin{aligned}
G(TB_6,0) &= \begin{pmatrix}1 & l_2 & T\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}1 & 1 & H\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}H & T & N\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}N & 1 & \Lambda\\ 0 & 0 & 0\end{pmatrix}\\
&\times \begin{pmatrix}l_1' & l_1 & E\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_2' & \Lambda & E\\ 0 & 0 & 0\end{pmatrix}\\
G(TB_6) &= \biguplus(-1)^{M+M'+1+m_1'}\begin{pmatrix}1 & l_2 & T\\ \theta_2 & m_2 & \tau\end{pmatrix}\begin{pmatrix}1 & 1 & H\\ \sigma_1 & \theta_1 & \eta\end{pmatrix}\\
&\times \begin{pmatrix}H & T & N\\ \eta & \tau & \nu\end{pmatrix}\begin{pmatrix}N & 1 & \Lambda\\ \nu & \sigma_2 & \lambda\end{pmatrix}\begin{pmatrix}l_1' & l_1 & E\\ -m_1' & m_1 & \epsilon\end{pmatrix}\begin{pmatrix}l_2' & \Lambda & E\\ m_2' & \lambda & \epsilon\end{pmatrix}
\end{aligned}
$$

$$
\begin{aligned}
G(TB_7,0) &= \begin{pmatrix}1 & l_1 & T\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}1 & 1 & H\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}H & l_2 & N\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}1 & T & \Lambda\\ 0 & 0 & 0\end{pmatrix}\\
&\times \begin{pmatrix}l_1' & \Lambda & E\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_2' & N & E\\ 0 & 0 & 0\end{pmatrix}\\
G(TB_7) &= \biguplus(-1)^{M+M'+1+\eta+\tau+\epsilon}\begin{pmatrix}1 & l_1 & T\\ \theta_2 & m_1 & \tau\end{pmatrix}\begin{pmatrix}1 & 1 & H\\ \sigma_1 & \theta_1 & \eta\end{pmatrix}\\
&\times \begin{pmatrix}H & l_2 & N\\ -\eta & m_2 & \nu\end{pmatrix}\begin{pmatrix}1 & T & \Lambda\\ \sigma_2 & -\tau & \lambda\end{pmatrix}\begin{pmatrix}l_1' & \Lambda & E\\ m_1' & \lambda & \epsilon\end{pmatrix}\begin{pmatrix}l_2' & N & E\\ m_2' & \nu & -\epsilon\end{pmatrix}
\end{aligned}
$$

$$
\begin{aligned}
G(TB_8,0) &= \begin{pmatrix}1 & l_1 & T\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}1 & 1 & H\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}H & l_2 & N\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}N & 1 & \Lambda\\ 0 & 0 & 0\end{pmatrix}\\
&\times \begin{pmatrix}l_1' & T & E\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_2' & \Lambda & E\\ 0 & 0 & 0\end{pmatrix}\\
G(TB_8) &= \biguplus(-1)^{M+M'+\eta+\nu+\epsilon}\begin{pmatrix}1 & l_1 & T\\ \theta_2 & m_1 & \tau\end{pmatrix}\begin{pmatrix}1 & 1 & H\\ \sigma_1 & \theta_1 & \eta\end{pmatrix}\\
&\times \begin{pmatrix}H & l_2 & N\\ -\eta & m_2 & \nu\end{pmatrix}\begin{pmatrix}N & 1 & \Lambda\\ -\nu & \sigma_2 & \lambda\end{pmatrix}\begin{pmatrix}l_1' & T & E\\ m_1' & \tau & \epsilon\end{pmatrix}\begin{pmatrix}l_2' & \Lambda & E\\ m_2' & \lambda & -\epsilon\end{pmatrix}
\end{aligned}
$$

$$
\begin{aligned}
G(TC_1,0) &= \begin{pmatrix}1 & l_1 & T\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}1 & T & H\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_1' & H & E\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_2' & l_2 & E\\ 0 & 0 & 0\end{pmatrix}\\
\tilde{G}(TC_1) &= (-1)^{L+L'+l_1+l_2'}\begin{Bmatrix}L & l_1 & l_2\\ H & L' & K\end{Bmatrix}\begin{Bmatrix}L' & l_1' & l_2'\\ E & l_2 & H\end{Bmatrix}\begin{Bmatrix}1 & 1 & K\\ l_1 & H & T\end{Bmatrix}
\end{aligned}
$$

$$
\begin{aligned}
G(TC_2,0) &= \begin{pmatrix}l_2 & 1 & T\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}1 & l_1 & H\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_1' & H & E\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_2' & T & E\\ 0 & 0 & 0\end{pmatrix}\\
\tilde{G}(TC_2) &= (-1)^{1+L'+l_1+l_2'}\begin{Bmatrix}L' & l_1' & l_2'\\ E & T & H\end{Bmatrix}\begin{Bmatrix}L & l_1 & l_2\\ K & 1 & 1\\ L' & H & T\end{Bmatrix}
\end{aligned}
$$

$$
\begin{aligned}
\Omega_1(l_1'l_2'l_1l_2) &= GA_{114}(l_1'l_2'l_1l_2) + GB_{14}(l_1'l_2'l_1l_2) + GC_{12}(l_1'l_2'l_1l_2) \\
&+ GB_{13}(l_1'l_2'l_1l_2) \\
\Omega_2(l_1'l_2'l_1l_2) &= GA_{214}(l_1'l_2'l_1l_2) + GB_{54}(l_1'l_2'l_1l_2) \\
\tilde{\Omega}_1(l_1'l_2'l_1l_2) &= \Omega_1(l_1'l_2'l_1l_2) + \Omega_1(l_2'l_1'l_2l_1) \\
\Omega_3(l_1'l_2'l_1l_2) &= GB_{13}(l_1'l_2'l_1l_2) + GC_{11}(l_1'l_2'l_1l_2) \\
\Omega_4(l_1'l_2'l_1l_2) &= GA_{132}(l_1'l_2'l_1l_2) + GA_{142}(l_1'l_2'l_1l_2) \\
&+ GA_{213}(l_1'l_2'l_1l_2) + GB_{53}(l_1'l_2'l_1l_2) + GC_2(l_1'l_2'l_1l_2) \\
\Omega_5(l_1'l_2'l_1l_2) &= GA_{232}(l_1'l_2'l_1l_2) + GA_{242}(l_1'l_2'l_1l_2) \\
&+ GB_{12}(l_1'l_2'l_1l_2) + GB_{72}(l_1'l_2'l_1l_2) \\
\Omega_6(l_1'l_2'l_1l_2) &= GA_{213}(l_1'l_2'l_1l_2) + GB_{53}(l_1'l_2'l_1l_2) \\
\Omega_7(l_1'l_2'l_1l_2) &= GB_{12}(l_1'l_2'l_1l_2) \\
\Omega_8(l_1'l_2'l_1l_2) &= GB_{13}(l_1'l_2'l_1l_2) + GC_{11}(l_1'l_2'l_1l_2)
\end{aligned}
$$

We have also defined:

$$
\begin{aligned}
\gamma_1(l_1'l_2'l_1l_2) &= J_2(\omega(M(l_1+l_1')) - 2, M(l_1+l_1'); \tilde{\Omega}_1(l_1'l_2'l_1l_2); \tilde{c}-5) \\
&+ (\sum_E \Omega_2(l_1'l_2'l_1l_2))\eta(l_1+l_1'+1, \tilde{c}) \\
\gamma_2(l_1'l_2'l_1l_2) &= J_2(\omega(M(l_1+l_1'+1)) - 2, M(l_1+l_1'+1); \Omega_2(l_1'l_2'l_1l_2); \tilde{c}-5) \\
\gamma_3(l_1'l_2'l_1l_2) &= J_2(\omega(M(l_1+l_1')) - 2, M(l_1+l_1'); \Omega_3(l_1'l_2'l_1l_2); \tilde{c}-7) \\
\gamma_4(l_1'l_2'l_1l_2) &= J_2(\omega(M(l_1+l_1'+1)) - 2, M(l_1+l_1'+1); \Omega_4(l_1'l_2'l_1l_2); \tilde{c}-7) \\
&- (\sum_E GA_{142})\eta(l_1+l_1', \tilde{c}-2) \\
\gamma_5(l_1'l_2'l_1l_2) &= J_2(\omega(M(l_1+l_1')) - 2, M(l_1+l_1'); \Omega_5(l_1'l_2'l_1l_2); \tilde{c}-7) \\
S_1(l_1'l_2'l_1l_2) &= \gamma_3(l_1'l_2'l_1l_2) + \gamma_4(l_1'l_2'l_1l_2) + \gamma_5(l_1'l_2'l_1l_2) \\
\gamma_6(l_1'l_2'l_1l_2) &= J_2(\omega(M(l_1+l_1'+1)) - 2, M(l_1+l_1'+1); \Omega_6(l_1'l_2'l_1l_2); \tilde{c}-5) \\
\gamma_7(l_1'l_2'l_1l_2) &= \sum_E GA_{142}(l_1'l_2'l_1l_2) \\
\gamma_8(l_1'l_2'l_1l_2) &= J_2(\omega(M(l_1+l_1'+1)) - 2, M(l_1+l_1'+1); \Omega_6(l_1'l_2'l_1l_2); \tilde{c}-5) \\
\gamma_9(l_1'l_2'l_1l_2) &= J_2(\omega(M(l_1+l_1')) - 2, M(l_1+l_1'); \Omega_7(l_1'l_2'l_1l_2); \tilde{c}-5) \\
\gamma_{10}(l_1'l_2'l_1l_2) &= J_2(\omega(M(l_1+l_1')) - 2, M(l_1+l_1'); \Omega_8(l_1'l_2'l_1l_2); \tilde{c}-5) \\
H(l_1'l_2'l_1l_2) &= \gamma_8(l_1'l_2'l_1l_2) + \gamma_{10}(l_1'l_2'l_1l_2) + \gamma_9(l_2'l_1'l_2l_1)
\end{aligned}
$$

$$
\begin{aligned}
\gamma_{11}(l_1'l_2'l_1l_2) &= J_2(\omega(M(l_1+l_1'))-2, M(l_1+l_1'); GA_{231}(l_1'l_2'l_1l_2); \tilde{c}-7) \\
\gamma_{12}(l_1'l_2'l_1l_2) &= J_2(\omega(M(l_1+l_1'))-2, M(l_1+l_1'); GB_{71}(l_1'l_2'l_1l_2); \tilde{c}-7) \\
\gamma_{13}(l_1'l_2'l_1l_2) &= J_2(\omega(M(l_1+l_1'))-2, M(l_1+l_1'); GB_{11}(l_1'l_2'l_1l_2); \tilde{c}+c^{(6)}(i))
\end{aligned}
$$

$$
\Lambda(a, b, \alpha, \beta; i) = \mathrm{coe}(A_i^{(6)}).
$$

(15) H_{eso}:

$$
\begin{aligned}
\Delta E_{eso} &= \frac{3}{2} i\alpha^2 \delta_{JJ'}\delta_{M_J M_{J'}}(-1)^{L+S'+J}\begin{Bmatrix} L' & S' & J \\ S & L & 1 \end{Bmatrix} \\
&\times \langle \gamma' L' \| R^{(1)} \| \gamma L\rangle \langle S' \| \vec{\sigma}_1 \| S\rangle
\end{aligned}
$$

with

$$
\mathbf{R} = \frac{\vec{r}}{r^3} \times \vec{\nabla}_1.
$$

The orbital part is

$$
\langle F' \mathcal{Y}^{M'}_{l_1'l_2'L'} | R_0^{(1)} | F \mathcal{Y}^{M}_{l_1 l_2 L}\rangle = (-1)^{L'-M'}\begin{pmatrix} L' & 1 & L \\ -M' & 0 & M \end{pmatrix} U(15) D,
$$

where

$$
U(15) = -i\frac{\sqrt{6}}{2}(l_1, l_2, L, l_1', l_2', L')^{1/2}
$$

$$
\begin{aligned}
D &= \varpi_1(\mu_1, M_1; G_{12}; \tilde{a}, \tilde{b}, \tilde{c}-3; \tilde{\alpha}, \tilde{\beta}) \\
&- \varpi_1(\mu_2, M_2; aG_{21} + G_{22}; \tilde{a}-1, \tilde{b}+1, \tilde{c}-3; \tilde{\alpha}, \tilde{\beta}) \\
&+ \alpha\varpi_1(\mu_2, M_2; G_{21}; \tilde{a}, \tilde{b}+1, \tilde{c}-3; \tilde{\alpha}, \tilde{\beta}) \\
&+ J_1(\mu_1, M_1; G_{12})\mathrm{Dif}(\tilde{a}, \tilde{b}; \tilde{a}-1, \tilde{b}+1; \tilde{c}-3, \tilde{\alpha}, \tilde{\beta}; \omega(\mu_1)-2, \omega(\mu_1+1)-2).
\end{aligned}
$$

Also,

$$
\begin{aligned}
M_1 &= \min(l_1 + l_1' + 2, l_2 + l_2') \\
M_2 &= \min(l_1 + l_1' + 1, l_2 + l_2' + 1) \\
\mu_i &= \omega(M_i) - 2, \quad i = 1, 2.
\end{aligned}
$$

The angular coefficients are:

$$
\begin{aligned}
G_{12}(E) &= \sum_{TH}(T,H,E)G(T_1,0)\tilde{G}(T_1)b(l_1;T) \\
G_{21}(E) &= \sum_{TH}(T,H,E)G(T_2,0)\tilde{G}(T_2) \\
G_{22}(E) &= \sum_{TH}(T,H,E)G(T_2,0)\tilde{G}(T_2)b(l_1;H)
\end{aligned}
$$

with

$$
\begin{aligned}
G(T_1,0) &= \begin{pmatrix} 1 & l_1 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & T & H \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_1' & H & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & l_2 & E \\ 0 & 0 & 0 \end{pmatrix} \\
\tilde{G}(T_1) &= (-1)^{1+L+L'+l_1+l_2'}\begin{Bmatrix} L & l_1 & l_2 \\ H & L' & 1 \end{Bmatrix}\begin{Bmatrix} L' & l_1' & l_2' \\ E & l_2 & H \end{Bmatrix}\begin{Bmatrix} 1 & 1 & 1 \\ l_1 & H & T \end{Bmatrix}
\end{aligned}
$$

$$
\begin{aligned}
G(T_2,0) &= \begin{pmatrix} 1 & l_1 & H \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & l_2 & T \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_1' & H & E \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & T & E \\ 0 & 0 & 0 \end{pmatrix} \\
\tilde{G}(T_2) &= (-1)^{L'+l_1+l_2'}\begin{Bmatrix} L' & l_1' & l_2' \\ E & T & H \end{Bmatrix}\begin{Bmatrix} L & l_1 & l_2 \\ 1 & 1 & 1 \\ L' & H & T \end{Bmatrix}.
\end{aligned}
$$

(16) H_{Zso}:

$$
\begin{aligned}
\Delta E_{Zso} &= -\frac{1}{2}iZ\alpha^2\delta_{JJ'}\delta_{M_JM_{J'}}(-1)^{L+S'+J}\begin{Bmatrix} L' & S' & J \\ S & L & 1 \end{Bmatrix} \\
&\times \langle\gamma'L'\|R^{(1)}\|\gamma L\rangle\langle S'\|\vec{\sigma}_1\|S\rangle
\end{aligned}
$$

with

$$\mathbf{R} = \frac{\vec{r}_1}{r_1^3} \times \vec{\nabla}_1.$$

The orbital part is

$$\langle F'\mathcal{Y}^{M'}_{l_1'l_2'L'}|R^{(1)}_0|F\mathcal{Y}^{M}_{l_1l_2L}\rangle = (-1)^{L'-M'}\begin{pmatrix} L' & 1 & L \\ -M' & 0 & M \end{pmatrix}U(16)D,$$

where

$$U(16) = -i\frac{\sqrt{6}}{2}(l_1,l_2,L,l_1',l_2',L')^{1/2}$$

$$
\begin{aligned}
D &= \varpi_0(\mu_1,M_1;G_{12};\tilde{a}-3,\tilde{b},\tilde{c};\tilde{\alpha},\tilde{\beta}) \\
&+ c\varpi_0(\mu_2,M_2;G_2;\tilde{a}-2,\tilde{b}+1,\tilde{c}-2;\tilde{\alpha},\tilde{\beta}).
\end{aligned}
$$

Also,

$$
\begin{aligned}
M_1 &= \min(l_1 + l_1' + 2, l_2 + l_2') \\
M_2 &= \min(l_1 + l_1' + 1, l_2 + l_2' + 1) \\
\mu_i &= \omega(M_i) - 2, \quad i = 1, 2.
\end{aligned}
$$

The angular coefficients are:

$$
\begin{aligned}
G_{12}(E) &= \sum_{TH} (T, H, E) G(T_1, 0) \tilde{G}(T_1) b(l_1; T) \\
G_2(E) &= \sum_{TH} (T, H, E) G(T_2, 0) \tilde{G}(T_2)
\end{aligned}
$$

with

$$
\begin{aligned}
G(T_1, 0) &= \begin{pmatrix} 1 & l_1 & T \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & T & H \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1' & H & E \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2' & l_2 & E \\ 0 & 0 & 0 \end{pmatrix} \\
\tilde{G}(T_1) &= (-1)^{1+L+L'+l_1+l_2'} \begin{Bmatrix} L & l_1 & l_2 \\ H & L' & 1 \end{Bmatrix} \begin{Bmatrix} L' & l_1' & l_2' \\ E & l_2 & H \end{Bmatrix} \begin{Bmatrix} 1 & 1 & 1 \\ l_1 & H & T \end{Bmatrix}
\end{aligned}
$$

$$
\begin{aligned}
G(T_2, 0) &= \begin{pmatrix} 1 & l_1 & H \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2 & 1 & T \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1' & H & E \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2' & T & E \\ 0 & 0 & 0 \end{pmatrix} \\
\tilde{G}(T_2) &= (-1)^{L'+l_1+l_2'} \begin{Bmatrix} L' & l_1' & l_2' \\ E & T & H \end{Bmatrix} \begin{Bmatrix} L & l_1 & l_2 \\ 1 & 1 & 1 \\ L' & H & T \end{Bmatrix}.
\end{aligned}
$$

(17) H_{ess}:

$$
\begin{aligned}
\Delta E_{ess} &= -\frac{3}{4}\alpha^2 \delta_{JJ'} \delta_{M_J M_{J'}} \sum_K (-1)^{K+L+S'+J} \begin{Bmatrix} L' & S' & J \\ S & L & K \end{Bmatrix} \\
&\times \langle \gamma' L' \| R^{(K)} \| \gamma L \rangle \langle S' \| [\vec{\sigma}_1 \otimes \vec{\sigma}_2]^{(K)} \| S \rangle
\end{aligned}
$$

with

$$
R^{(K)} = \frac{1}{r^5} [\vec{r} \otimes \vec{r}]^{(K)}.
$$

The orbital part is

$$
\langle F' \mathcal{Y}^{M'}_{l_1' l_2' L'} | R^{(K)}_Q | F \mathcal{Y}^{M}_{l_1 l_2 L} \rangle = (-1)^{L'-M'} \begin{pmatrix} L' & K & L \\ -M' & Q & M \end{pmatrix} U(17) D,
$$

where

$$
U(17) = \frac{1}{2}\sqrt{2K+1}(l_1, l_2, L, l_1', l_2', L')^{1/2}
$$

$$
\begin{aligned}
T(k) &\equiv \varpi_k(\mu_1, M_1; G_1; \tilde{a}+2, \tilde{b}, \tilde{c}-5; \tilde{\alpha}, \tilde{\beta}) \\
&+ \varpi_k(\mu_2, M_2; G_2; \tilde{a}, \tilde{b}+2, \tilde{c}-5; \tilde{\alpha}, \tilde{\beta}) \\
&+ \varpi_k(\mu_3, M_3; G_3; \tilde{a}+1, \tilde{b}+1, \tilde{c}-5; \tilde{\alpha}, \tilde{\beta}) \\
D &= T(0), \quad \tilde{c} \geq 3 \\
D &= T(1) + J_1(\mu_1, M_1; G_1)\eta(\mu_1, \tilde{c}) I_{\omega(\mu_1)-2}(\tilde{a}, \tilde{b}, \tilde{c}-3), \quad 1 \leq \tilde{c} \leq 2 \\
D &= T(2) + \gamma_1 \mathrm{Dif}(\tilde{a}+1, \tilde{b}-1; \tilde{a}, \tilde{b}; \tilde{c}-3, \tilde{\alpha}, \tilde{\beta}; \omega(\mu_1+1)-2, \omega(\mu_1)-2) \\
&+ \gamma_2 \mathrm{Dif}(\tilde{a}-1, \tilde{b}+1; \tilde{a}, \tilde{b}; \tilde{c}-3, \tilde{\alpha}, \tilde{\beta}; \omega(\mu_1+1)-2, \omega(\mu_1)-2), \quad \tilde{c} = 0.
\end{aligned}
$$

Also,

$$
\begin{aligned}
M_1 &= \min(l_1 + l_1' + 2, l_2 + l_2') \\
M_2 &= \min(l_1 + l_1', l_2 + l_2' + 2) \\
M_3 &= \min(l_1 + l_1' + 1, l_2 + l_2' + 1) \\
\mu_i &= \omega(M_i) - 2, \quad i = 1, 2, 3.
\end{aligned}
$$

The angular coefficients are:

$$
\begin{aligned}
G_1(E) &= \sum_N (N, E) G(T_1, 0) \tilde{G}(T_1) \\
G_2(E) &= \sum_N (N, E) G(T_2, 0) \tilde{G}(T_2) \\
G_3(E) &= 2 \sum_{HN} (H, N, E) G(T_3, 0) \tilde{G}(T_3)
\end{aligned}
$$

with

$$
\begin{aligned}
G(T_1, 0) &= \begin{pmatrix} 1 & 1 & K \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} K & l_1 & N \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1' & N & E \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2' & l_2 & E \\ 0 & 0 & 0 \end{pmatrix} \\
\tilde{G}(T_1) &= (-1)^{L+L'+l_2'} \begin{Bmatrix} L & l_1 & l_2 \\ N & L' & K \end{Bmatrix} \begin{Bmatrix} L' & l_1' & l_2' \\ E & l_2 & N \end{Bmatrix} \\
G(T_2, 0) &= \begin{pmatrix} 1 & 1 & K \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} K & l_2 & N \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1' & l_1 & E \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2' & N & E \\ 0 & 0 & 0 \end{pmatrix} \\
\tilde{G}(T_2) &= (-1)^{l_1'} \begin{Bmatrix} L & l_1 & l_2 \\ N & K & L' \end{Bmatrix} \begin{Bmatrix} L' & l_1' & l_2' \\ E & N & l_1 \end{Bmatrix} \\
G(T_3, 0) &= \begin{pmatrix} 1 & l_1 & H \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & l_2 & N \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1' & H & E \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2' & N & E \\ 0 & 0 & 0 \end{pmatrix} \\
\tilde{G}(T_3) &= (-1)^{L'+l_1+l_2'} \begin{Bmatrix} L' & l_1' & l_2' \\ E & N & H \end{Bmatrix} \begin{Bmatrix} L & l_1 & l_2 \\ K & 1 & 1 \\ L' & H & N \end{Bmatrix}.
\end{aligned}
$$

We have also defined:

$$\gamma_1 = J_2(\mu_1, M_1; G_1; \tilde{c} - 5)$$
$$\gamma_2 = J_2(\mu_2, M_2; G_2; \tilde{c} - 5).$$

(18) $\tilde{\Delta}_3$:

$$\tilde{\Delta}_3 = -iZ\alpha^2 \delta_{JJ'} \delta_{M_J M_{J'}} (-1)^{L+S'+J} \begin{Bmatrix} L' & S' & J \\ S & L & 1 \end{Bmatrix}$$
$$\times \langle \gamma' L' \| R^{(1)} \| \gamma L \rangle \langle S' \| \vec{\sigma}_1 \| S \rangle$$

with

$$\mathbf{R} = \frac{\vec{r}_1}{r_1^3} \times \vec{\nabla}_2.$$

The orbital part is

$$\langle F' \mathcal{Y}^{M'}_{l_1' l_2' L'} | R^{(1)}_0 | F \mathcal{Y}^{M}_{l_1 l_2 L} \rangle = (-1)^{L'-M'} \begin{pmatrix} L' & 1 & L \\ -M' & 0 & M \end{pmatrix} U(18) D,$$

where

$$U(18) = i\frac{\sqrt{r}}{2}(l_1, l_2, L, l_1', l_2', L')^{1/2}$$

$$D = \varpi_0(\mu_1, M_1; bG_{11} + G_{12}; \tilde{a} - 2, \tilde{b} - 1, \tilde{c}; \tilde{\alpha}, \tilde{\beta})$$
$$- \beta \varpi_0(\mu_1, M_1; G_{11}; \tilde{a} - 2, \tilde{b}, \tilde{c}; \tilde{\alpha}, \tilde{\beta})$$
$$+ c\varpi_0(\mu_1, M_1; G_{11}; \tilde{a} - 2, \tilde{b} + 1, \tilde{c} - 2; \tilde{\alpha}, \tilde{\beta}).$$

Also,

$$M_1 = \min(l_1 + l_1' + 1, l_2 + l_2' + 1)$$
$$\mu_1 = \omega(M_1) - 2.$$

The angular coefficients are:

$$G_{11}(E) = \sum_{TH} (T, H, E) G(T_1, 0) \tilde{G}(T_1)$$
$$G_{12}(E) = \sum_{TH} (T, H, E) G(T_1, 0) \tilde{G}(T_1) b(l_2; T)$$

with

$$G(T_1, 0) = \begin{pmatrix} 1 & l_1 & H \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & l_2 & T \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1' & H & E \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2' & T & E \\ 0 & 0 & 0 \end{pmatrix}$$
$$\tilde{G}(T_1) = (-1)^{L'+l_1+l_2'} \begin{Bmatrix} L' & l_1' & l_2' \\ E & T & H \end{Bmatrix} \begin{Bmatrix} L & l_1 & l_2 \\ 1 & 1 & 1 \\ L' & H & T \end{Bmatrix}.$$

Vita Auctoris

Zong-Chao Yan was born on Oct. 8, 1957 in Shanghai, China. He graduated from Shanghai Teachers University in 1981 with a B.Sc. degree in Physics. Then he went to Tongji University in the same city where he obtained a M.Sc. degree in elementary particle physics in 1984. From 1985 to 1988, he was a lecturer in the Physics Department of Shanghai Teachers University. In September, 1988, he began his second M.Sc. program at the Physics Department of Memorial University of Newfoundland, working on atomic collision problems, under the supervision of Dr. T. T. Gien. After receiving his second M.Sc. degree from Memorial University in the fall of 1990, he entered the Ph.D. program at the Physics Department, University of Windsor, working on atomic fine structure problems, under the supervision of Dr. Gordon Drake. He expects to graduate in the spring of 1994.