PHYSICAL REVIEW B VOLUME 26, NUMBER 8 15 OCTOBER 1982

Intermediate-coupling scheme for many-electron systems of the complexes of the transition-metal ions

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(Received 8 October 1981; revised manuscript received 10 March 1982)

The generalized theory of the intermediate-coupling scheme has been developed for the many-electron systems of the second and third series of the transition-metal-ion octahedral complexes. The theory has been developed for the general configuration, kd^n ($k=3,4,5$; $n=2,\ldots,9$) but has been presented up to $n=5$. The transformation matrices for the remaining $d^{10-n}(n<5)$ configurations can be easily found from those of $d^n(n<5)$ by using the well-known principle of electron-hole complimentarity. To show the enormous simplicity and great advantage over the strong-field coupling scheme so long used in such cases, the d^3 configuration has been treated by this method as an application. At the end some typical magnitudes of the parameters like Dq, ζ, B, and C have been used to find the energy levels and the paramagnetic susceptibility for K_2ReCl_6. The beauty and importance of this scheme lies in the fact that as one switches off the spin-orbit interaction one gets results identical with those of Tanabe and Sugano, and further, if one also switches off the crystal field but retains only the interelectronic repulsion term one gets the results coinciding with those of Racah in atomic spectroscopy.

I. INTRODUCTION

It is well known that in order to adequately describe the magnetic and optical properties of the complexes of the rare earths and the first transition series it is sufficient to use the weak-field and the strong-field coupling schemes, respectively. But for the complexes of the transition-metal ions in the second and third series, the above schemes are grossly inadequate since the crystal-field as well as the spin-orbit interaction are much stronger than the interelectronic-repulsion term. In fact, in going through the Periodic Table, we notice that the interelectronic repulsion among the outer-shell electrons gets weaker while the spin-orbit interaction becomes stronger. In atomic spectroscopy this situation is known as the breakdown of the Russell-Saunders scheme. The appropriate coupling scheme to use in such cases is the jj-coupling scheme, also known as the intermediate-coupling scheme. This exact situation is encountered in the compounds of the palladium ($4d^n$) and platinum ($5d^n$) groups of ions. Taking the Racah parameter B, the spin-orbit interaction constant ζ, and the octahedral ligand-field parameter Dq as the indicators of the respective interactions, it is easy to realize that while the applicability of the weak-field scheme for the ions of the palladium and platinum groups is of doubtful validity, any calculation based on the strong-field scheme should include the configuration mixing due to the strong spin-orbit interaction. Alternatively, one may inquire whether it is possible to develop a scheme analogous to the jj-coupling scheme in atomic spectroscopy. Such a procedure has been developed in this paper and is outlined below.

The fact that the strong spin-orbit interaction can change the magnetic behavior of the $4d^n$ and $5d^n$ compounds was pointed out by Van Vleck[1] as far back as in 1932. While studying the anomalous magnetic properties of the palladium and platinum series of ions, he showed by qualitative arguments that the large spin-orbit interaction is responsible for the complicated behavior of these ions. He also showed that, just as the electrostatic field quenches the orbital angular momentum of the ion, the combined action of the electrostatic and the spin-orbit interaction can quench the total angular momentum. Later, Liehr[2] and Moffitt and his co-workers[3,4] studied the cases where the spin-orbit interaction is strong. Liehr considered an ion with a single electron; he treated the electrostatic (the cubic field and the lower symmetric crystal fields) and the spin-orbit interactions on the same footing and stressed the importance of the role of the spin-orbit interaction in the properties of the $4d^n$ and $5d^n$ ions. Moffitt and his co-workers, from a similar point of view, analyzed the absorption spectra of the hexafluorides of the $5d^n$ ($n=2$, 3, and 4) ions. These studies may be said to have used the intermediate-coupling scheme in the true sense of the word, where a number of authors still use the strong-field coupling scheme but take into account the configuration interaction due to the spin-orbit interaction. Contrary to the claims that are made, such calculations cannot be considered as truly based on the intermediate-coupling scheme for the following reasons.

Since the wave functions belonging to different coupling schemes are related by a unitary transformation, diagonalization of the complete matrices using any of the schemes will give identical results. However, the appropriateness of a particular scheme lies in its ability to give "good" results when only a few terms or configurations are included in the calculation. In this sense, the basic orbitals used to build the many-electron functions are of importance.

The three schemes use different starting orbitals. In the weak-field scheme, the starting orbital is d and the zeroth-order wave functions are $|d,m_l=2\rangle$, $|d,1\rangle$, $|d,0\rangle$, $|d,-1\rangle$, and $|d,-2\rangle$. The zeroth-order Hamiltonian consists of the free-ion Hamiltonian, given by

$$\mathscr{H}_w=\mathscr{H}_{\text{core}}-\sum_i \frac{Ze^2}{r_i}+\sum_{i\neq j}\frac{e^2}{r_{ij}}\ , \qquad (1.1)$$

where the summation is over all the d electrons. Here $\mathscr{H}_{\text{core}}$ involves the electrons in the closed shells. In the strong-field scheme, the starting orbitals[5–7] are t_2 and e. The zeroth-order functions are $|t_2\xi\rangle$, $|t_2\eta\rangle$, $|t_2\zeta\rangle$, $|e\theta\rangle$, and $|e\epsilon\rangle$. The zeroth-order Hamiltonian is given by

$$\mathscr{H}_S=\mathscr{H}_{\text{core}}-\sum_i \frac{Ze^2}{r_i}+\sum_i V_c(\vec{r}_i)\ . \qquad (1.2)$$

The symmetry group of $\mathscr{H}_S$ is O_h, whereas in the weak-field scheme it is the full-rotation group R_3. In the intermediate-coupling scheme the starting orbitals are γ_{8l}, γ_7, and γ_{8u}, which are explained in the next section. The zeroth-order Hamiltonian now includes the spin-orbit interaction:

$$\mathscr{H}_I=\mathscr{H}_{\text{core}}-\sum_i \frac{Ze^2}{r_i}+\sum_i V_c(\vec{r}_i)$$
$$+\zeta\sum_i \vec{l}_i\cdot\vec{s}_i\ . \qquad (1.3)$$

Owing to the spin operators in the above Hamiltonian, the symmetry group of $\mathscr{H}_I$ is now the octaheral double group, denoted by O_h'.

It follows from what has just been said that although the strong-field calculations, including the configuration mixing via the spin-orbit interaction, can be applied to the $4d^n$ and $5d^n$ ions, the strong-field scheme is not identical with the intermediate-coupling scheme. From the computational point of view, however, the strong-field approach has certain advantages which will be evident later in this paper. The advantage is due to the fact that the relevant transformation matrices are readily available which are very helpful to construct the intermediate-coupling scheme for the many-electron systems. With this introduction we now develop the intermediate-coupling scheme for the many-electron systems.

II. THE INTERMEDIATE-COUPLING SCHEME

We consider a single d electron in the crystal field of octahedral (O_h) symmetry. We include the spin-orbit interaction in the zeroth-order Hamiltonian along with the free-ion Hamiltonian and the crystal-field potential:

$$H_0=H_{\text{free ion}}+V_c+\zeta\vec{l}\cdot\vec{s}\ . \qquad (2.1)$$

Since spin is now included, the full symmetry group of this Hamiltonian is the octahedral double group (O_h').[5,6]

As mentioned earlier in the strong-field scheme, the spin-orbit interaction is not included in the zeroth-order Hamiltonian. In this scheme there are two single-electron energy levels denoted by t_2 (lower level) and e (upper level) whose spatial degeneracies are 3 and 2, respectively. The sets of spatial basis functions for these two levels are (ξ,η,ζ) and (θ,ϵ), respectively,[5,6] which span the T_{2g} and E_g representations of the O_h group. These functions are suitable linear combinations of the five d orbitals $(d_2,d_1,d_0,d_{-1},d_{-2})$.[5,6] The electronic energies for the t_2 and e levels are, respectively, $-4Dq$ and $6Dq$ measured from the free-ion energy level.[5–7] Each of these levels has a spin degeneracy of 2. The complete sets of basis functions are obtained by coupling the spin functions with the spatial t_2 and e basis functions and then symmetry adapting to the irreducible representations Γ_7 and Γ_8 of the double group O_h'. These sets are given as follows:

$$\kappa' = |\gamma_{8t_2}\kappa\rangle = -\frac{i}{\sqrt{6}}\xi^+ - \frac{1}{\sqrt{6}}\eta^+ - i\frac{\sqrt{2}}{\sqrt{3}}\zeta^- ,$$

$$\lambda' = |\gamma_{8t_2}\lambda\rangle = \frac{i}{\sqrt{2}}\xi^- + \frac{1}{\sqrt{2}}\eta^- ,$$

$$\mu' = |\gamma_{8t_2}\mu\rangle = -\frac{i}{\sqrt{2}}\xi^+ + \frac{1}{\sqrt{2}}\eta^+ ,$$

$$\nu' = |\gamma_{8t_2}\nu\rangle = \frac{i}{\sqrt{6}}\xi^- - \frac{1}{\sqrt{6}}\eta^- - i\frac{\sqrt{2}}{\sqrt{3}}\zeta^+ , \tag{2.2}$$

$$\alpha'' = |\gamma_7\alpha''\rangle = \frac{i}{\sqrt{3}}\xi^- - \frac{1}{\sqrt{3}}\eta^- + \frac{i}{\sqrt{3}}\zeta^+ ,$$

$$\beta'' = |\gamma_7\beta''\rangle = \frac{i}{\sqrt{3}}\xi^+ + \frac{1}{\sqrt{3}}\eta^+ - \frac{i}{\sqrt{3}}\zeta^- ,$$

$$\kappa'' = |\gamma_{8e}\kappa\rangle = \epsilon^- ,$$

$$\lambda'' = |\gamma_{8e}\lambda\rangle = -\theta^+ ,$$

$$\mu'' = |\gamma_{8e}\mu\rangle = \theta^- ,$$

$$\nu'' = |\gamma_{8e}\nu\rangle = -\epsilon^+ .$$

We shall use the notations Γ_6, Γ_7, and Γ_8 instead of E', E'', and U, respectively, which appear in Ref. 5.

In deriving the above sets we note that the spin functions $|S=\frac{1}{2}, m_S=+\frac{1}{2}\rangle$ and $|S=\frac{1}{2}, m_S=-\frac{1}{2}\rangle$ span the Γ_6 representation of O_h'. Decomposing the direct product $T_{2g}\otimes\Gamma_6$ we get Γ_8 and Γ_7 which give the first two sets in (2.2). Similarly $E_g\otimes\Gamma_6$ gives Γ_8 corresponding to the last set. The coupling coefficients required here are given in Table A 20 of Ref. 5.

In the presence of the spin-orbit interaction term $\zeta\vec{l}\cdot\vec{s}$ there will be mixing between the γ_{8t_2} and γ_{8e} terms. The matrix of H_0 between these two terms is as follows:

$$H_0 = \begin{array}{c|cc} & \gamma_{8t_2} & \gamma_{8e} \\ \gamma_{8t_2} & -4Dq-\frac{1}{2}\zeta & \sqrt{3/2}\zeta' \\ \gamma_{8e} & \sqrt{3/2}\zeta' & 6Dq \end{array} .$$

Since the radial part of the wave function for a t_2 electron may be slightly different from that for an e electron, we have reasonably taken two different spin-orbit interaction parameters, ζ and ζ'.[8]

Diagonalizing the above matrix we get two eigenvalues:

$$\epsilon_0(\gamma_{8l}) = Dq - \tfrac{1}{4}\zeta - \tfrac{1}{2}[(10Dq+\tfrac{1}{2}\zeta)^2 + 6\zeta'^2]^{1/2} , \tag{2.3}$$

$$\epsilon_0(\gamma_{8u}) = Dq - \tfrac{1}{4}\zeta + \tfrac{1}{2}[(10Dq+\tfrac{1}{2}\zeta)^2 + 6\zeta'^2]^{1/2} ,$$

with the corresponding eigenvectors

$$\begin{bmatrix} \cos\theta \\ -\sin\theta \end{bmatrix}$$

and

$$\begin{bmatrix} \sin\theta \\ \cos\theta \end{bmatrix} ,$$

respectively, where we have set

$$\tan 2\theta = \frac{\sqrt{6}\zeta'}{10Dq+\frac{1}{2}\zeta} . \tag{2.4}$$

Now, the γ_{8l} and γ_{8u} basis sets corresponding to the two fourfold degenerate energy levels in (2.3) are linear combinations of the original γ_{8t_2} and γ_{8e} basis sets:

$$\begin{aligned} a_l &= |\gamma_{8l}a\rangle \\ &= \cos\theta|\gamma_{8t_2}a\rangle - \sin\theta|\gamma_{8e}a\rangle , \\ a_u &= |\gamma_{8u}a\rangle \\ &= \sin\theta|\gamma_{8t_2}a\rangle + \cos\theta|\gamma_{8e}a\rangle . \end{aligned} \tag{2.5}$$

The γ_{8u} level is above the γ_{8l} level and the remaining doubly degenerate γ_7 level lies in between those two. The energy value of the γ_7 level is

$$\begin{aligned} \epsilon_0(\gamma_7) &= \langle\gamma_7 a|H_0|\gamma_7 a\rangle \\ &= -4Dq+\zeta . \end{aligned} \tag{2.6}$$

For a many-electron transition-metal ion $\mathrm{N}d^n$, we can make use of these three single-electron energy levels (γ_{8l}, γ_{8u}, and γ_7) as obtained above—the task then is to accommodate the n d electrons in these levels in various ways and to construct the symmetry adapted wave functions for each configuration; $\gamma_{8l}^{n_1}\gamma_{8u}^{n_2}\gamma_7^{n_3}$ ($n_1,n_2\le 4$; $n_3\le 2$; $n_1+n_2+n_3=n$). This configuration gives a ${}^4C_{n_1}{}^4C_{n_2}{}^2C_{n_3}$-fold degenerate level, the associated unperturbed energy (in the absence of electron-electron interactions and external magnetic fields) being

$$\begin{aligned} E_0(n_1,n_2,n_3) &= n_1\epsilon_0(\gamma_{8l}) + n_2\epsilon_0(\gamma_{8u}) \\ &\quad + n_3\epsilon_0(\gamma_7) . \end{aligned} \tag{2.7}$$

The method of construction of determinantal (antisymmetric) wave functions for the different configurations in the present case is very similar to the analogous procedure for the strong-field scheme.[5–7] The main difference here is that we are dealing with three basic single-electron levels instead of two. The coupling coefficients used in this construction are given in Table A 20 of Ref. 5. However, the sets of coefficients for the decomposition of $\Gamma_8\otimes\Gamma_8$, $\Gamma_8\otimes\Gamma_7$, and $\Gamma_7\otimes\Gamma_7$ are not found ready made; these are easily constructed by using the Wigner coefficients[9] in conjunction with the Table A 19 of Ref. 5. We give below only a few examples of the determinantal wave functions constructed according to the present scheme:

$$\begin{aligned}
&|\gamma_{8l}^2{:}A_1a_1\rangle=\frac{1}{\sqrt{2}}(\,|\kappa_l\nu_l|-|\lambda_l\mu_l|\,)\,,\\
&|\gamma_{8u}^3{:}\Gamma_8\kappa\rangle=-|\kappa_u\lambda_u\mu_u|\,,\\
&|\gamma_7^2{:}A_1a_1\rangle=|\alpha''\beta''|\,,\\
&|\gamma_{8l}^2(E)\gamma_{8u}{:}\Gamma_6\alpha'\rangle=\tfrac{1}{2}(\,|\kappa_l\nu_l\lambda_u|+|\lambda_lu_l\lambda_u|+|\kappa_l\lambda_l\nu_u|+|\mu_l\nu_l\nu_u|\,)\,,\\
&|\gamma_{8l}^3\underline{\gamma_7\gamma_{8u}}(T_1){:}\tfrac{3}{2}\Gamma_8\kappa\rangle=\frac{\sqrt{3}}{\sqrt{10}}(-|\kappa_l\lambda_l\mu_l\alpha''\kappa_u|+|\kappa_l\lambda_l\mu_l\beta''\nu_u|+|\kappa_l\lambda_l\nu_l\beta''\mu_u|\,)+\frac{1}{\sqrt{10}}|\kappa_l\lambda_l\nu_l\alpha''\nu_u|\,,\\
&|\underline{\gamma_{8l}^2(T_2)\gamma_7}((\Gamma_8))\underline{\gamma_{8u}^2}(T_2){:}\tfrac{5}{2}\Gamma_8\kappa\rangle=\frac{1}{\sqrt{10}}(-|\kappa_l\lambda_l\alpha''\kappa_u\mu_u|+|\mu_l\nu_l\alpha''\kappa_u\mu_u|-|\lambda_l\nu_l\beta''\kappa_u\mu_u|\\
&\qquad -|\kappa_l\mu_l\beta''\lambda_u\nu_u|-|\kappa_l\mu_l\alpha''\kappa_u\lambda_u|+|\kappa_l\mu_l\alpha''\mu_u\nu_u|\\
&\qquad +|\kappa_l\lambda_l\beta''\kappa_u\lambda_u|-|\kappa_l\lambda_l\beta''\mu_u\nu_u|-|\mu_l\nu_l\beta''\kappa_u\lambda_u|\\
&\qquad +|\mu_l\nu_l\beta''\mu_u\nu_u|\,)\,.
\end{aligned}\tag{2.8}$$

The notations used here to designate a state are quite obvious and clearly show the steps contained in the construction of the state. Thus, for example, the construction of the state $|\underline{\gamma_{8l}^2(T_2)\gamma_7}((\Gamma_8))\underline{\gamma_{8u}^2}(T_2){:}\tfrac{5}{2}\Gamma_8\kappa\rangle$ consists of the following steps:

(i) T_2 states are obtained from the two-electron configuration γ_{8l}^2.

(ii) These two-electron T_2 states are combined with the one-electron γ_7 states to get three-electron (note the first underline) Γ_8 states (indicated by Γ_8 within the double parentheses).

(iii) These three-electron Γ_8 states are finally combined with the T_2 states of the two-electron (note the second underline) configuration γ_{8u}^2 to give the κ component state of one of the two Γ_8 levels (the direct product $\Gamma_8\otimes T_2$ gives two Γ_8 representations denoted by $\frac{3}{2}\Gamma_8$ and $\frac{5}{2}\Gamma_8$).[5]

By using Eq. (2.5) we can express these wave functions in terms of determinants involving $\kappa',\lambda',\mu',\nu'$; α'',β''; $\kappa'',\lambda'',\mu'',\nu''$. Thus, for example, the fourth wave function in (2.8) becomes

$$\begin{aligned}
|\gamma_{8l}^2(E)\gamma_{8u}{:}\Gamma_6\alpha'\rangle=&\tfrac{1}{2}C_{30}(\,|\kappa'\nu'\lambda''|+|\lambda'\mu'\lambda''|+|\kappa'\lambda'\nu''|+|\mu'\nu'\nu''|\,)\\
&+\tfrac{1}{2}C_{21}(\,|\kappa''\lambda''\nu'|+|\lambda''\mu''\lambda'|+|\kappa''\nu''\lambda'|+|\mu''\nu''\nu'|\,)\\
&+\tfrac{1}{2}C_{12}(\,|\kappa'\lambda'\nu''|+|\lambda'\mu'\lambda''|+|\kappa'\nu'\lambda''|+|\mu'\nu'\nu''|\,)\\
&+\tfrac{1}{2}C_{03}(\,|\kappa''\nu''\lambda'|+|\lambda''\mu''\lambda'|+|\kappa''\lambda''\nu'|+|\mu''\nu''\nu'|\,)\,,
\end{aligned}\tag{2.9}$$

where

$$C_{mn}=\cos^m\theta\sin^n\theta\,.$$

After this step we can express the $\gamma_{8l}^{n_1}\gamma_{8u}^{n_2}\gamma_7^{n_3}$ wave functions in terms of the $\gamma_{8t_2}^{m_1}\gamma_{8e}^{m_2}\gamma_7^{m_3}$ wave functions:

$$|\gamma_{8l}^{n_1}\gamma_{8u}^{n_2}\gamma_7^{n_3}{:}i\Gamma\alpha\rangle=\sum_{\substack{j,m_1,m_2\\(m_1+m_2=n_1+n_2)}}a^{\Gamma}(i,n_1,n_2,n_3;j,m_1,m_2)\,|\gamma_{8t_2}^{m_1}\gamma_{8e}^{m_2}\gamma_7^{n_3}{:}j\Gamma\alpha\rangle\,,\tag{2.10}$$

where

$$a^{\Gamma}(i,n_1,n_2,n_3;j,m_1,m_2)=\langle\gamma_{8t_2}^{m_1}\gamma_{8e}^{m_2}\gamma_7^{n_3}{:}j\Gamma\alpha\,|\,\gamma_{8l}^{n_1}\gamma_{8u}^{n_2}\gamma_7^{n_3}{:}i\Gamma\alpha\rangle\,.$$

We note that by making the replacements $l\to t_2$, $u\to e$, κ_l, etc.$\to\kappa'$, etc., κ_u, etc.$\to\kappa''$, etc., in the original expression [such as those in (2.8)] for a $\gamma_{8l}^{n_1}\gamma_{8u}^{n_2}\gamma_7^{n_3}$ wave function we get the corresponding $\gamma_{8t_2}^{n_1}\gamma_{8e}^{n_2}\gamma_7^{n_3}$ wave function. Thus, for example, the fourth wave function in (2.8) gives

$$|\gamma_{8t_2}^2(E)\gamma_{8e}:\Gamma_6\alpha'\rangle=\tfrac{1}{2}(\,|\kappa'\nu'\lambda''|+|\lambda'\mu'\lambda''|+|\kappa'\lambda'\nu''|+|\mu'\nu'\nu''|\,)\,. \tag{2.11}$$

As an example of the transformation (2.10), we find that Eq. (2.9) gives

$$|\gamma_{8l}^2(E)\gamma_{8u}:\Gamma_6 a\rangle=C_{10}\,|\gamma_{8t_2}^2(E)\gamma_{8e}:\Gamma_6 a\rangle+C_{01}\,|\gamma_{8e}^2(E)\gamma_{8t_2}:\Gamma_6 a\rangle\,. \tag{2.12}$$

These transformations for all the wave functions of d^2, d^3, d^4, and d^5 ions are given in matrix form in Tables I A, II A, III A, and IV A, respectively in Ref. 27 (Appendix B). We note that these transformation matrices are unitary.

Next, we use Eq. (2.2) to express the $\gamma_{8t_2}^{n_1}\gamma_{8e}^{n_2}\gamma_7^{n_3}$ wave functions in terms of determinants involving $\xi^+,\eta^+,\zeta^+,\xi^-,\eta^-,\zeta^-,\theta^+,\epsilon^+,\theta^-,\epsilon^-$. For example, Eq. (2.11) gives

$$\begin{aligned}|\gamma_{8t_2}^2(E)\gamma_{8e}:\Gamma_6\alpha'\rangle=\tfrac{1}{6}(&\,|\xi^+\xi^-\theta^+|-2i\,|\xi^+\eta^-\theta^+|+2i\,|\eta^+\xi^-\theta^+|+|\eta^+\eta^-\theta^+|\\&+|\xi^+\zeta^+\theta^+|-i\,|\eta^+\zeta^+\theta^+|-|\zeta^-\xi^-\theta^+|-i\,|\zeta^-\eta^-\theta^+|+2\,|\zeta^-\zeta^+\theta^+|\,)\\&+\frac{1}{2\sqrt{3}}(-|\xi^+\xi^-\epsilon^+|+|\eta^+\eta^-\epsilon^+|-|\zeta^-\xi^-\epsilon^+|+i\,|\zeta^-\eta^-\epsilon^+|\\&+|\xi^+\zeta^+\epsilon^+|+i\,|\eta^+\zeta^+\epsilon^+|\,)\,.\end{aligned} \tag{2.13}$$

Finally we couple the space and spin parts of the usual strong-field-scheme wave functions (given in Ref. 5) to correspond to the representations of the double group O_h' and express the $\gamma_{8t_2}^{n_1}\gamma_{8e}^{n_2}\gamma_7^{n_3}$ wave functions in terms of these symmetry adapted strong-field wave functions:

$$|\gamma_{8t_2}^{n_1}\gamma_{8e}^{n_2}\gamma_7^{n_3}:i\Gamma\alpha\rangle=\sum_{\substack{j,k,m\\(m=n_1+n_3)}} b^{\Gamma}(i,n_1,n_2,n_3;k,m,n_2)\,|t_2^m e^{n_2};(j^{2s+1}D):k\Gamma\alpha\rangle\,, \tag{2.14}$$

where

$$b^{\Gamma}(i,n_1,n_2,n_3;j,k,m,n_2)=\langle t_2^m e^{n_2};(j^{2S+1}D):k\Gamma\alpha\,|\,\gamma_{8t_2}^{n_1}\gamma_{8e}^{n_2}\gamma_7^{n_3};i\Gamma\alpha\rangle\,.$$

For example, by using the coupling coefficients for the decomposition, $\Gamma_8\otimes T_1\rightarrow\Gamma_6+\Gamma_7+\frac{3}{2}\Gamma_8+\frac{5}{2}\Gamma_8$, we can form linear combinations of the twelve strong-field wave functions $|t_2^2(^3T_1)e;^4T_1 m_s\alpha\rangle$ ($m_s=\frac{3}{2},\frac{1}{2},-\frac{1}{2},-\frac{3}{2}$; $\alpha=1,0,-1$) to correspond to the irreducible representations of the O_h' group:

$$\begin{aligned}|t_2^2(^3T_1)e;(^4T_1):\Gamma_6\alpha'\rangle&=\frac{1}{\sqrt{2}}\,|t_2^2(^3T_1)e;^4T_1\tfrac{3}{2}-1\rangle-\frac{1}{\sqrt{3}}\,|t_2^2(^3T_1)e;^4T_1\tfrac{1}{2}0\rangle+\frac{1}{\sqrt{6}}\,|t_2^2(^3T_1)e;^4T_1-\tfrac{1}{2}1\rangle\\&=\frac{i}{2}\left[-\frac{1}{2}|\zeta^+\eta^+\theta^+|+\frac{\sqrt{3}}{2}|\zeta^+\eta^+\epsilon^+|\right]+\frac{1}{2}\left[-\frac{1}{2}|\xi^+\zeta^+\theta^+|-\frac{\sqrt{3}}{2}|\xi^+\zeta^+\epsilon^+|\right]\\&\quad-\frac{i}{3}(\,|\eta^+\xi^+\theta^-|+|\eta^+\xi^-\theta^+|+|\eta^-\xi^+\theta^+|\,)\\&\quad+\frac{i}{12}(\,|\zeta^+\eta^-\theta^-|+|\zeta^-\eta^+\theta^-|+|\zeta^-\eta^-\theta^+|\,)\\&\quad-\frac{i}{4\sqrt{3}}(\,|\zeta^+\eta^-\epsilon^-|+|\zeta^-\eta^+\epsilon^-|+|\zeta^-\eta^-\epsilon^+|\,)\\&\quad-\frac{1}{12}(\,|\xi^+\zeta^-\theta^-|+|\xi^-\zeta^+\theta^-|+|\xi^-\zeta^-\theta^+|\,)\\&\quad-\frac{1}{4\sqrt{3}}(\,|\xi^+\zeta^-\epsilon^-|+|\xi^-\zeta^+\epsilon^-|+|\xi^-\zeta^-\epsilon^+|\,)\,,\end{aligned} \tag{2.15a}$$

$$|t_2^2(^3T_1)e;(^4T_1):\Gamma_7\alpha''\rangle=\frac{1}{\sqrt{6}}\,|t_2^2(^3T_1)e;{}^4T_1\tfrac{3}{2}1\rangle-\frac{1}{\sqrt{2}}\,|t_2^2(^3T_1)e;{}^4T_1-\tfrac{1}{2}-1\rangle-\frac{1}{\sqrt{3}}\,|t_2^2(^3T_1)e;{}^4T_1-\tfrac{3}{2}0\rangle$$

$$=-\frac{i}{2\sqrt{3}}\left[-\frac{1}{2}\,|\zeta^+\eta^+\theta^+|+\frac{\sqrt{3}}{2}\,|\zeta^+\eta^+\epsilon^+|\right]$$

$$+\frac{1}{2\sqrt{3}}\left[-\frac{1}{2}\,|\xi^+\zeta^+\theta^+|-\frac{\sqrt{3}}{2}\,|\xi^+\zeta^+\epsilon^+|\right]$$

$$+\frac{i}{4\sqrt{3}}(|\zeta^+\eta^-\theta^-|+|\zeta^-\eta^+\theta^-|+|\zeta^-\eta^-\theta^+|)$$

$$-\frac{i}{4}(|\zeta^+\eta^-\epsilon^-|+|\zeta^-\eta^+\epsilon^-|+|\zeta^-\eta^-\epsilon^+|)$$

$$+\frac{1}{4\sqrt{3}}(|\xi^+\zeta^-\theta^-|+|\xi^-\zeta^+\theta^-|+|\xi^-\zeta^-\theta^+|)$$

$$+\tfrac{1}{4}(|\xi^+\zeta^-\epsilon^-|+|\xi^-\zeta^+\epsilon^-|+|\xi^-\zeta^-\epsilon^+|)-\frac{i}{\sqrt{3}}\,|\eta^-\xi^-\theta^-|\;, \tag{2.15b}$$

$$|t_2^2(^3T_1)e;(^4T_1):\tfrac{3}{2}\Gamma_8\kappa\rangle=\frac{\sqrt{3}}{\sqrt{5}}\,|t_2^2(^3T_1)e;{}^4T_1\tfrac{3}{2}0\rangle-\frac{\sqrt{2}}{\sqrt{5}}\,|t_2^2(^3T_1)e;{}^4T_1\tfrac{1}{2}1\rangle$$

$$=\frac{i\sqrt{3}}{\sqrt{5}}\,|\eta^+\xi^+\theta^+|-\frac{i}{2\sqrt{15}}(|\zeta^+\eta^+\theta^-|+|\zeta^+\eta^-\theta^+|+|\zeta^-\eta^+\theta^+|)$$

$$+\frac{i}{2\sqrt{5}}(|\zeta^+\eta^+\epsilon^-|+|\zeta^+\eta^-\epsilon^+|+|\zeta^-\eta^+\epsilon^+|)$$

$$+\frac{1}{2\sqrt{15}}(|\xi^+\zeta^+\theta^-|+|\xi^+\zeta^-\theta^+|+|\xi^-\zeta^+\theta^+|)$$

$$+\frac{1}{2\sqrt{5}}(|\xi^+\zeta^+\epsilon^-|+|\xi^+\zeta^-\epsilon^+|+|\xi^-\zeta^+\epsilon^+|)\;, \tag{2.15c}$$

$$|t_2^2(^3T_1)e;(^4T_1):\tfrac{5}{2}\Gamma_8\kappa\rangle=-\frac{1}{\sqrt{15}}\,|t_2^2(^3T_1)e;{}^4T_1)e;{}^4T_1\tfrac{3}{2}0\rangle-\frac{1}{\sqrt{10}}\,|t_2^2(^3T_1)e;{}^4T_1\tfrac{1}{2}1\rangle$$

$$-\frac{\sqrt{5}}{\sqrt{6}}\,|t_2^2(^3T_1)e;{}^4T_1-\tfrac{3}{2}-1\rangle$$

$$=-\frac{i}{\sqrt{15}}\,|\eta^+\xi^+\theta^+|-\frac{i}{4\sqrt{15}}(|\zeta^+\eta^+\theta^-|+|\zeta^+\eta^-\theta^+|+|\zeta^-\eta^+\theta^+|)$$

$$+\frac{i}{4\sqrt{5}}(|\zeta^+\eta^+\epsilon^-|+|\zeta^+\eta^-\epsilon^+|+|\zeta^-\eta^+\epsilon^+|)$$

$$+\frac{1}{4\sqrt{15}}(|\xi^+\zeta^+\theta^-|+|\xi^+\zeta^-\theta^+|+|\xi^-\zeta^+\theta^+|)$$

$$+\frac{1}{4\sqrt{5}}(|\xi^+\zeta^+\epsilon^-|+|\xi^+\zeta^-\epsilon^+|+|\xi^-\zeta^+\epsilon^+|)$$

$$+\frac{i\sqrt{5}}{4}\left[\frac{1}{\sqrt{3}}\,|\zeta^-\eta^-\theta^-|-|\zeta^-\eta^-\epsilon^-|\right]+\frac{\sqrt{5}}{4}\left[\frac{1}{\sqrt{3}}\,|\xi^-\zeta^-\theta^-|+|\xi^-\zeta^-\epsilon^-|\right]. \tag{2.15d}$$

As an example of the transformation (2.14), we find that

$$|\gamma_{8t_2}^2(E)\gamma_{8e}:\Gamma_6 a\rangle = \frac{1}{\sqrt{3}}\,|t_2^2(^1E)e;(^2A_1):\Gamma_6 a\rangle - \frac{2}{3}\,|t_2^2(^3T_1)e;(^4T_1):\Gamma_6 a\rangle - \frac{\sqrt{2}}{3}\,|t_2^2(^3T_1)e;(^2T_1):\Gamma_6 a\rangle\ , \tag{2.16}$$

where the transformation coefficients are as given in (2.14). Thus, for example, using Eq. (2.13) and Eq. (2.15a) we find

$$\langle t_2^2(^3T_1)e;(^4T_1):\Gamma_6\alpha'\,|\,\gamma_{8t_2}^2(E)\gamma_{8e}:\Gamma_6\alpha'\rangle = -\tfrac{1}{24}-\tfrac{1}{8}-\tfrac{1}{24}-\tfrac{1}{8}-\tfrac{1}{9}-\tfrac{1}{9}-\tfrac{1}{72}-\tfrac{1}{24}-\tfrac{1}{72}-\tfrac{1}{24}=-\tfrac{2}{3}\ .$$

The other coefficients in (2.16) are similarly evaluated:

$$\langle t_2^2(^1E)e;(^2A_1):\Gamma_6\alpha'\,|\,\gamma_{8t_2}^2(E)\gamma_{8e}:\Gamma_6\alpha'\rangle = \frac{1}{\sqrt{3}}\ ,$$

$$\langle t_2^2(^1T_2)e;(^2T_1):\Gamma_6\alpha'\,|\,\gamma_{8t_2}^2(E)\gamma_{8e}:\Gamma_6\alpha'\rangle = 0\ ,$$

$$\langle t_2^2(^3T_1)e;(^4T_2):\Gamma_6\alpha'\,|\,\gamma_{8t_2}^2(E)\gamma_{8e}:\Gamma_6\alpha'\rangle = 0\ ,$$

$$\langle t_2^2(^3T_1)e;(^2T_1):\Gamma_6\alpha'\,|\,\gamma_{8t_2}^2(E)\gamma_{8e}:\Gamma_6\alpha'\rangle = -\frac{\sqrt{2}}{3}\ .$$

These transformations (2.14) for the wave functions of the d^2, d^3, d^4, and d^5 ions are presented in matrix form in Tables I B, II B, III B, and IV B respectively, in Ref. 27 (Appendix B). These transformation matrices are unitary as they should be.

After going through these two successive transformations (2.10) and (2.14), the original $\gamma_{8l}^{n_1}\gamma_{8u}^{n_2}\gamma_7^{n_3}$ wave functions of our intermediate-coupling scheme will be expressed in terms of the wave functions of the usual strong-field coupling scheme and thus the matrices of $\mathscr{H}_e$ in the intermediate-coupling scheme can be directly evaluated in terms of those in the strong-field scheme. This method of taking recourse to the strong-field-scheme results is advantageous because the matrices of $\mathscr{H}_e$ in the strong-field scheme have been fully tabulated in terms of the usual Racah parameters, A, B, C (Tables A 26 – A 30 in Ref. 5).

We have presented the transformation matrices of our scheme up to the d^5 transition-metal ion. Similar results for the remaining ions are not given explicitly since according to the principle of electron-hole complementarity, the scheme can be easily extended to embrace those ions also—the terms and matrices for the d^{10-n} ion follow from those of the d^n ion ($n=2,3,4$).

III. APPLICABILITY OF THE SCHEME

As already stated, the intermediate-coupling scheme developed here will be very helpful for the ions of the second and third transition-metal series. In this case ($\mathscr{H}_e \ll V_c \simeq \mathscr{H}_{so}$), according to the configurations of the different unperturbed states, we can classify these states into several groups such that the energy separation between two unperturbed states belonging to different groups will be considerably large compared to the perturbations which these states would acquire on addition of $\mathscr{H}_e$ to the unperturbed Hamiltonian containing V_c and $\mathscr{H}_{so}$. Then, as a first approximation, we may neglect the "mixing" (through $\mathscr{H}_e$) of states in different groups. Of course, we can always improve the accuracy by taking into account the effects coming from configurations located energetically higher and higher above the low-lying group of states. Thus, the Hamiltonian matrix block for any given representation of O_h' will break into smaller sub blocks, each of which can be diagonalized with very little computational labor. Thus the major part of the approach consists of straightforward and easy analytical calculations based on the well-tabulated results given here.

Chakravarty and Desai[6,10] undertook the theoretical study of the optical and magnetic properties of osmium fluoride (OsF_6) to illustrate the usefulness of the intermediate-coupling scheme. Here Os^{6+} is a $4d^2$ ion situated in the octahedral field due to the six F^- ligands. The results of this study are in good agreement with the available experimental data.[3,4,11] The merit of their investigation is that the results obtained in the first approximation only are sufficiently close to the experimental data and that these are easily derived in simple analytical forms. Earlier Eisenstein[12] tackled the same problem by using the conventional strong-field coupling scheme. Naturally he had to consider all configuration interactions through $\mathscr{H}_e + \mathscr{H}_{so}$ and the matrices to be diagonalized were of huge dimensions. Hence, although the results of Eisenstein are exact, his solution fully depends on numerical computations and there is hardly any scope for obtaining results in analytical forms.

The complex K_2ReCl_6 was similarly treated by Eisenstein[13] on the basis of the strong-field scheme. We shall apply the intermediate-coupling scheme for the same complex and use the same set of values for the parameters as employed by Eisenstein to show that the results obtained in the first approximation of our scheme are very close to the exact results of Eisenstein. Further, it will be evident that our procedure involves simple analytical steps and the amount of numerical computation necessary is very small compared to that encountered in Eisenstein's work. Here lies the importance of our present investigation.

Re^{4+} in K_2ReCl_6 is a $5d^3$ ion situated in the octahedral ligand field. To investigate the ordinary properties of the system we need only a few lower states. So we start with the six low-lying unperturbed levels,

$$|\Gamma_8^1\rangle=|\gamma_{8l}^3{:}\Gamma_8\rangle,\ |\Gamma_8^2\rangle=|\gamma_{8l}^2(E)\gamma_7{:}\Gamma_8\rangle\ ,\ |\Gamma_8^3\rangle=|\gamma_{8l}^2(T_2)\gamma_7{:}\Gamma_8\rangle\ ,$$

$$|\Gamma_8^4\rangle=|\gamma_{8l}\gamma_7^2{:}\Gamma_8\rangle,\ |\Gamma_6\rangle=|\gamma_{8l}^2(T_2)\gamma_7{:}\Gamma_6\rangle,\ |\Gamma_7\rangle=|\gamma_{8l}^2(A_1)\gamma_7{:}\Gamma_7\rangle\ .$$

Usually $\epsilon_0(\gamma_{8u})$ is much greater than $\epsilon_0(\gamma_{8l})$ and $\epsilon_0(\gamma_7)$ so that the states coming from the configurations $\gamma_{8l}\gamma_7\gamma_{8u}, \gamma_{8l}\gamma_{8u}^2, \gamma_7^2\gamma_{8u}, \gamma_7\gamma_{8u}^2, \gamma_{8u}^3$ are situated much higher in energy scale and therefore can be omitted. Thus, for the values $Dq=3350\ \mathrm{cm}^{-1}$, $\zeta=\zeta'=2300\ \mathrm{cm}^{-1}$, as used by Eisenstein for K_2ReCl_6, we get $\epsilon_0(\gamma_{8l})=-14\,777\ \mathrm{cm}^{-1}$, $\epsilon_0(\gamma_7)=-11\,100\ \mathrm{cm}^{-1}$, and $\epsilon_0(\gamma_{8u})=20\,327\ \mathrm{cm}^{-1}$. Using Tables II A(3) and II B(3) given in Ref. 27 (Appendix B), we express the unperturbed states considered in terms of the strong-field-scheme wave functions. Then, using the known electrostatic matrices in the strong-field scheme, we can easily construct the required matrix elements of the Hamiltonian ($\mathscr{H}_e$ being the only perturbation included), with respect to these states of the present scheme. For the electrostatic matrices in the strong-field scheme one may use Table A 28 of Ref. 5, where the matrix elements are given in terms of three Racah parameters A, B, and C. However, because of the covalency effects (which are more prominent in the complexes of $4d^n$ and $5d^n$ ions), there arises the inequivalence of the $5dt_2$ and the $5de$ orbitals so that it would be reasonable to introduce several different sets of Racah parameters A_i, B_i, C_i, where i refers to the number of times $(0-4)$ that the $5de$ radial function occurs in the Coulomb integrals. The electrostatic matrix elements used by Eisenstein[13] are in terms of such Racah parameters. However, we cannot use those elements directly here since our wave functions have been constructed in accordance with Griffith's phase convention[5] which is slightly different from that in Ref. 13. The proper electrostatic matrices to be used in our case are given in Appendix C.

The perturbed energies for the Γ_6 and Γ_7 levels, with the use of Appendixes B and C are simply

$$\begin{aligned}E_1(\Gamma_6)&=\langle\gamma_{8l}^2(T_2)\gamma_7{:}\Gamma_6\alpha'\,|\,\mathscr{H}\,|\,\gamma_{8l}^2(T_2)\gamma_7{:}\Gamma_6\alpha'\rangle\\&=2\epsilon_0(\gamma_{8l})+\epsilon_0(\gamma_7)\\&\quad+\left[(3A_0-6B_0+3C_0)C_{40}+(2\sqrt{6}B_1)C_{31}+(2A_0+4A_2-3B_0-14B_2+\tfrac{7}{3}C_0+\tfrac{5}{3}C_2)C_{22}\right.\\&\quad\left.+\left[\frac{10\sqrt{6}}{3}B_1\right]C_{13}+(2A_2+A_4-\tfrac{10}{3}B_2-8B_4+\tfrac{1}{3}C_2)C_{04}\right]\ ,\end{aligned}\tag{3.1}$$

and

$$\begin{aligned}E_1(\Gamma_7)&=\langle\gamma_{8l}^2(A_1)\gamma_7{:}\Gamma_7\alpha''\,|\,\mathscr{H}\,|\,\gamma_{8l}^2(A_1)\gamma_7{:}\Gamma_7\alpha''\rangle\\&=2\epsilon_0(\gamma_{8l})+\epsilon_0(\gamma_7)\\&\quad+[(3A_0+5C_0)C_{40}+(6\sqrt{6}B_1)C_{31}+(2A_0+4A_2-5B_0+12B_2+\tfrac{5}{3}C_0+5C_2)C_{22}\\&\quad+(2\sqrt{6}B_1)C_{13}+(2A_2+A_4-2B_2+8B_4+C_2+4C_4)C_{04}]\ .\end{aligned}\tag{3.2}$$

The corresponding wave functions are the original unperturbed functions $|\Gamma_6\rangle$ and $|\Gamma_7\rangle$, respectively.

The energies and wave functions for the four Γ_8 levels are obtained by diagonalizing the 4×4 matrix of the Hamiltonian with respect to the four unperturbed Γ_8 states considered. This matrix is

$$\mathscr{H}=\begin{array}{c|cccc|} & \Gamma_8^1 & \Gamma_8^2 & \Gamma_8^3 & \Gamma_8^4 \\ \Gamma_8^1 & E_{11} & E_{12} & E_{13} & E_{14} \\ \Gamma_8^2 & E_{12} & E_{22} & E_{23} & E_{24} \\ \Gamma_8^3 & E_{13} & E_{23} & E_{33} & E_{34} \\ \Gamma_8^4 & E_{14} & E_{24} & E_{34} & E_{44} \end{array}, \tag{3.3}$$

where the matrix elements are

$$E_{11}=3\epsilon_0(\gamma_{8l})+[(3A_0-5B_0+\tfrac{10}{3}C_0)C_{40}-(4\sqrt{6}B_1)C_{31}+(6A_2-16B_2+4C_2)C_{22} +(3A_4-8B_4+4C_4)C_{04}]\ , \tag{3.4}$$

$$E_{12}=[(2B_0+\tfrac{2}{3}C_0)C_{30}+(4B_2)C_{12}]\ , \tag{3.5}$$

$$E_{13}=\left[\left[\sqrt{6}B_0+\frac{\sqrt{6}}{3}C_0\right]C_{30}+(2B_1)C_{21}-\left[\frac{4\sqrt{6}}{3}B_2+\frac{\sqrt{6}}{3}C_2\right]C_{12}\right]\ , \tag{3.6}$$

$$E_{14}=[(5B_0+\tfrac{5}{3}C_0)C_{21}-(2\sqrt{6}B_1)C_{11}+(2B_2+C_2)C_{02}]\ , \tag{3.7}$$

$$E_{22}=2\epsilon_0(\gamma_{8l})+\epsilon_0(\gamma_7) +[(3A_0-8B_0+\tfrac{7}{3}C_0)C_{40}-(2\sqrt{6}B_1)C_{31}+(2A_0+4A_2-5B_0-10B_2+\tfrac{5}{3}C_0+C_2)C_{22} +(2\sqrt{6}B_1)C_{13}+(2A_2+A_4-2B_2+C_2+2C_4)C_{04}]\ , \tag{3.8}$$

$$E_{23}=-\left[\sqrt{6}B_0+\frac{\sqrt{6}}{3}C_0\right]C_{20}+(4B_1)C_{11}-\left[\frac{2\sqrt{6}}{3}B_2\right]C_{02}\ , \tag{3.9}$$

$$E_{24}=-(2B_0+\tfrac{2}{3}C_0)C_{30}-(4B_2)C_{12}\ , \tag{3.10}$$

$$E_{34}=-\left[\sqrt{6}B_0+\frac{\sqrt{6}}{3}C_0\right]C_{30}-(2B_1)C_{21}+\left[\frac{4\sqrt{6}}{3}B_2-\frac{2\sqrt{6}}{3}B_0+\frac{\sqrt{6}}{3}C_2\right]C_{12}\ , \tag{3.11}$$

$$E_{44}=\epsilon_0(\gamma_{8l})+2\epsilon_0(\gamma_7)+(3A_0-5B_0+\tfrac{10}{3}C_0)C_{20}+(2\sqrt{6}B_1)C_{11}+(A_0+2A_2-2B_2+\tfrac{5}{3}C_0+C_2)C_{02}\ . \tag{3.12}$$

The above matrix elements can be easily derived by using the tables cited in Appendix C.

With the following choice of the values of the parameters, Eisenstein[13] got good agreement with the observed energy levels of the system:

$$\begin{aligned} &D_q=3350,\\ &A_0=A_2=A_4=0,\\ &B_0=380,\\ &B_1=335,\\ &B_2=305,\\ &B_4=260,\\ &C_0=1760,\\ &C_2=1520,\\ &C_4=1300,\\ &\zeta=\zeta'=2300\ . \end{aligned}$$

With the use of the same values in our case we obtain the following numerical results:

$$\begin{aligned} &E_1(\Gamma_6)=6778.8\ ,\\ &E_1(\Gamma_7)=12\,836.7\ , \end{aligned} \tag{3.13}$$

and

$$\begin{aligned} &E_{11}=3661.6,\\ &E_{12}=1922.5,\\ &E_{13}=2384.0,\\ &E_{14}=4684.1,\\ &E_{22}=4597.4,\\ &E_{23}=-2248.2,\\ &E_{24}=-1922.5,\\ &E_{33}=3779.7,\\ &E_{34}=-2388.0,\\ &E_{44}=11\,452.6\ , \end{aligned} \tag{3.14}$$

where Dq and all the A's, B's, C's, and E's are in cm^{-1} and the energy levels in (3.13) and the diagonal matrix elements in (3.14) have been measured from the value $3\epsilon_0(\gamma_{8l})=-44\,332.5$ cm^{-1}. Diagonalization of the matrix (3.3) gives the following four Γ_8 energy levels in cm^{-1}:

$$\begin{aligned} &E_1(\Gamma_8^a)=-2460.4,\\ &E_1(\Gamma_8^b)=5621.0,\\ &E_1(\Gamma_8^c)=6476.1,\\ &E_1(\Gamma_8^d)=13\,854.5\,. \end{aligned} \tag{3.15}$$

Relative to the lowest level Γ_8^a, the positions of the levels in order of increasing magnitude are, in cm^{-1},

$$\begin{aligned} &E_1(\Gamma_8^a)=0,\\ &E_1(\Gamma_8^b)\simeq 8081,\\ &E_1(\Gamma_8^c)\simeq 8936,\\ &E_1(\Gamma_6)\simeq 9239,\\ &E_1(\Gamma_7)\simeq 15\,297,\\ &E_1(\Gamma_8^d)\simeq 16\,315\,. \end{aligned} \tag{3.16}$$

We note that these levels almost coincide with the corresponding levels by Eisenstein (again, in cm^{-1}):

$$\begin{aligned} &{}^4A_2(\Gamma_8):\ 0,\\ &{}^2T_1(\Gamma_8):\ 7895,\\ &{}^2E(\Gamma_8):\ 8798,\\ &{}^2T_1(\Gamma_6):\ 9176,\\ &{}^2T_2(\Gamma_7):\ 14\,653,\\ &{}^2T_2(\Gamma_8):\ 15\,723\,. \end{aligned} \tag{3.17}$$

Obviously, the coincidence would be exact if we take into account the interactions with the higher levels also. The number of higher levels whose interactions with the six lower levels were neglected is 33. The fair agreement between the two sets of levels [our set of (3.16) and Eisenstein's set in (3.17)] clearly indicates that this group of higher levels, although very large in number, have very little interactions with the six lower levels. Of course, this situation was evident at the very beginning of the calculation in our scheme and simplifications in the subsequent steps were based on this aspect. We note that the positions of the levels in (3.16) are slightly higher than the corresponding exact positions in (3.17). This is expected because the effects of the higher levels which we neglected here are to "depress" the lower levels, the depression of the lowest level being smaller than those of the others. The wave functions corresponding to the four Γ_8 levels in (3.15) are, respectively,

$$\begin{aligned} &|\Gamma_8^a\gamma\rangle=-0.623\,78\,|\Gamma_8^1\gamma\rangle+0.439\,19\,|\Gamma_8^2\gamma\rangle+0.535\,30\,|\Gamma_8^3\gamma\rangle+0.362\,58\,|\Gamma_8^4\gamma\rangle\,,\\ &|\Gamma_8^b\gamma\rangle=-0.682\,25\,|\Gamma_8^1\gamma\rangle-0.493\,62\,|\Gamma_8^2\gamma\rangle-0.509\,61\,|\Gamma_8^3\gamma\rangle+0.1765\,65\,|\Gamma_8^4\gamma\rangle\,,\\ &|\Gamma_8^c\gamma\rangle=-0.040\,76\,|\Gamma_8^1\gamma\rangle+0.745\,88\,|\Gamma_8^2\gamma\rangle-0.664\,78\,|\Gamma_8^3\gamma\rangle+0.007\,72\,|\Gamma_8^4\gamma\rangle\,,\\ &|\Gamma_8^d\gamma\rangle=0.379\,17\,|\Gamma_8^1\gamma\rangle-0.085\,01\,|\Gamma_8^2\gamma\rangle-0.108\,20\,|\Gamma_8^3\gamma\rangle+0.915\,04\,|\Gamma_8^4\gamma\rangle\quad(\gamma=\kappa,\lambda,\mu,\nu)\,. \end{aligned} \tag{3.18}$$

We now proceed further to find the paramagnetic susceptibility of the system. The magnetic-moment operator of the system is

$$\begin{aligned} \vec{\mu}&=\beta(K\vec{L}+2\vec{S})\\ &=\beta\sum_i(K\vec{l}_i+2\vec{s}_i)\,, \end{aligned} \tag{3.19}$$

where β is the usual Bohr magneton and K is the orbital reduction factor arising out of the covalency effect.[14–21] Since the system has cubic symmetry, it is sufficient to evaluate the z component of susceptibility. In the present case, the appropriate formula to use is

$$\chi=\frac{N\beta^2}{4k_BT}\sum_i|\langle\Gamma_{8i}^a|N_z|\Gamma_{8i}^a\rangle|^2+2N\beta^2\sum_{i,j}\frac{|\langle\psi_j|N_z|\Gamma_{8i}^a\rangle|^2}{E_j}\,, \tag{3.20}$$

where N is the Avogadro number and k_B is the Boltzmann constant. Here, the first sum over the index i, is required to distinguish the four degenerate ground-state wave functions. The second sum is over i and also over all excited states; E_j is the excitation energy for the state whose wave function is ψ_j. Thus we require the matrix elements of the operator

$$N_z = KL_z + 2S_z = \sum_i (Kl_{iz} + 2s_{iz}) .$$

First we evaluate the matrix elements of the single-electron operator $\eta_z = Kl_z + 2s_z$ with respect to the single-electron states $\kappa_l, \lambda_l, \mu_l, \nu_l, \alpha'', \beta''$. The nonzero elements are as given below:

$$\begin{aligned}
\langle \kappa_l | \eta_z | \kappa_l \rangle &= -\langle \nu_l | \eta_z | \nu_l \rangle \\
&= -\tfrac{1}{3}(1-K_2)C_{20} + \frac{4\sqrt{2}}{\sqrt{3}} K_1 C_{11} - C_{02} , \\
\langle \lambda_l | \eta_z | \lambda_l \rangle &= -\langle \mu_l | \eta_z | \mu_l \rangle \\
&= -(1-K_2)C_{20} + C_{02} , \\
\langle \kappa_l | \eta_z | \beta'' \rangle &= \langle \nu_l | \eta_z | \alpha'' \rangle \\
&= -\frac{\sqrt{2}}{3}(K_2+2)C_{10} + \frac{2}{\sqrt{3}} K_1 C_{01} , \\
\langle \alpha'' | \eta_z | \alpha'' \rangle &= -\langle \beta'' | \eta_z | \beta'' \rangle \\
&= -\tfrac{1}{3}(2K_2+1) .
\end{aligned} \tag{3.21}$$

Here, in view of the inequivalence of the $5dt_2$ and the $5de$ orbitals we have used two different orbital reduction factors—we have put $K = K_1$ when η_z has nonvanishing matrix elements between a t_2 orbital and an e orbital and $K = K_2$ when η_z has nonvanishing matrix elements between two t_2 orbitals.

With the use of these results in (3.21) and the determinantal expressions (given in Appendix A) for the wave functions

$$\begin{aligned}
|\gamma_1\rangle &= |\gamma_{8l}^3 : \Gamma_8 \gamma\rangle , \\
|\gamma_2\rangle &= |\gamma_{8l}^2(E)\gamma_7 : \Gamma_8 \gamma\rangle , \\
|\gamma_3\rangle &= |\gamma_{8l}^2(T_2)\gamma_7 : \Gamma_8 \gamma\rangle , \\
|\gamma_4\rangle &= |\gamma_{8l}\gamma_7^2 : \Gamma_8 \gamma\rangle , \\
|a_1\rangle &= |\gamma_{8l}^2(T_2)\gamma_7 : \Gamma_6 a\rangle ,
\end{aligned}$$

and

$$|b_1\rangle = |\gamma_{8l}^2(A_1)\gamma_7 : \Gamma_7 b\rangle ,$$

where $\gamma = \kappa, \lambda, \mu, \nu$; $a = \alpha', \beta'$; $b = \alpha'', \beta''$, we can easily obtain the matrix elements of the operator $N_z = \sum_i \eta_{iz}$ with respect to these unperturbed many-electron wave functions. The nonvanishing matrix elements required in Eq. (3.20) are given in the following:

$$\begin{aligned}
\langle \kappa_1 | N_z | \kappa_1 \rangle &= -\langle \nu_1 | N_z | \nu_1 \rangle \\
&= -\frac{1}{3}(1-K_2)C_{20} + \frac{4\sqrt{2}}{\sqrt{3}} K_1 C_{11} - C_{02} , \\
\langle \lambda_1 | N_z | \lambda_1 \rangle &= -\langle \mu_1 | N_z | \mu_1 \rangle \\
&= -(1-K_2)C_{20} + C_{02} , \\
\langle \kappa_1 | N_z | \kappa_2 \rangle &= -\langle \nu_1 | N_z | \nu_2 \rangle \\
&= \frac{1}{3}(K_2+2)C_{10} - \frac{\sqrt{2}}{\sqrt{3}} K_1 C_{01} , \\
\langle \lambda_1 | N_z | \lambda_2 \rangle &= -\langle \mu_1 | N_z | \mu_2 \rangle \\
&= \frac{1}{3}(K_2+2)C_{10} - \frac{\sqrt{2}}{\sqrt{3}} K_1 C_{01} , \\
\langle \lambda_1 | N_z | \lambda_3 \rangle &= -\langle \mu_1 | N_z | \mu_3 \rangle \\
&= \frac{2\sqrt{2}}{3\sqrt{3}}(K_2+2)C_{10} - \tfrac{4}{3} K_1 C_{01} , \\
\langle \kappa_1 | N_z | \beta_1'' \rangle &= \langle \nu_1 | N_z | \alpha_1'' \rangle \\
&= -\frac{1}{3}(K_2+2)C_{10} + \frac{\sqrt{2}}{\sqrt{3}} K_1 C_{01} , \\
\langle \lambda_1 | N_z | \alpha_1' \rangle &= \langle \mu_1 | N_z | \beta_1' \rangle \\
&= -\frac{1}{3\sqrt{3}}(K_2+2)C_{10} + \frac{\sqrt{2}}{3} K_1 C_{01} , \\
\langle \lambda_2 | N_z | \alpha_1' \rangle &= \langle \mu_2 | N_z | \beta_1' \rangle \\
&= -\frac{4}{3\sqrt{3}}(1-K_2)C_{20} + \frac{4\sqrt{2}}{3} K_1 C_{11} , \\
\langle \lambda_3 | N_z | \alpha_1' \rangle &= \langle \mu_3 | N_z | \beta_1' \rangle \\
&= \frac{2\sqrt{2}}{9}(1-K_2)C_{20} + \frac{8}{3\sqrt{3}} K_1 C_{11} \\
&\quad - \frac{2\sqrt{2}}{3} C_{02} - \frac{2\sqrt{2}}{9}(2K_2+1) , \\
\langle \kappa_4 | N_z | \beta_1'' \rangle &= \langle \nu_4 | N_z | \alpha_1'' \rangle \\
&= -\frac{1}{3}(K_2+2)C_{10} + \frac{\sqrt{2}}{\sqrt{3}} K_1 C_{01} , \\
\langle \lambda_4 | N_z | \alpha_1' \rangle &= \langle \mu_4 | N_z | \beta_1' \rangle \\
&= \frac{1}{3\sqrt{3}}(K_2+2)C_{10} - \frac{\sqrt{2}}{3} K_1 C_{01} .
\end{aligned} \tag{3.22}$$

Finally, using the energy values in (3.16), the wave functions in (3.18), and the matrix elements in (3.22), we find that Eq. (3.20) reduces to the following expression:

$$\chi=(0.375\,23/2T)(9.361\,08-1.504\,56K_1-0.231\,70K_2+0.062\,27K_1^2+0.018\,61K_1K_2+0.001\,43K_2^2)+1.043\,32\times 10^{-4}(0.2168+0.0123K_1+0.2170K_2+0.0949K_1^2+0.0211K_1K_2+0.0544K_2^2)\,. \tag{3.23}$$

This expression almost coincides with the corresponding expression obtained by Eisenstein.[13] In Eisenstein's paper the notations $\alpha\equiv(\kappa_\gamma\kappa_\epsilon)^{1/2}$ and κ_ϵ appear in place of K_1 and K_2, respectively.

IV. CONCLUDING REMARKS

In this paper we have worked out in full detail the intermediate-coupling scheme and its relation with the strong-field scheme. A truncated intermediate-coupling scheme especially meant for the ions of the second and third transition-metal series was earlier developed by Moffitt and others[3,11] in a different way. They neglected the γ_{8u} orbital and used the fact that the $j=\frac{3}{2}$ state of spherical symmetry (for example, $^2P_{3/2}$ state or $^2D_{3/2}$ state in a free ion) transforms as a Γ_8 representation in O_h' and also that the product of a function transforming as A_2 in O_h, with a spherically symmetric $j=\frac{1}{2}$ state, transforms as Γ_7 in O_h'. Then, denoting the γ_{8u} and γ_7 orbitals by $t_{3/2}$ and $t_{1/2}$, they reduced the intermediate-coupling scheme for a d^n ion in a crystal field to that of a j-j coupling scheme for a free p^n atom. This is similar to t_2-p isomorphism first discussed by Abragam and Pryce[15] and more rigorously shown later by Griffith.[16]

Here we have constructed the intermediate-coupling scheme for the octahedral transition-metal complexes purely from the crystal-field approach in that only the metal d orbitals have been considered. It is now well established[17,18] that some form of allowance for covalency is usually necessary; the d electrons are somewhat delocalized from the central metal ion and participate in the formation of chemical bonds. This has given way to modern ligand-field theory. We have incorporated this covalency effect phenomenologically: It has been shown on the basis of the molecular orbital theory[7,18–25] that we need not change the basic model (i.e., we can still use the pure d orbitals), and the effects of covalency may be almost fully reflected in the usual key parameters Dq,ζ, A,B,C and in the orbital reduction factor K. Dq now has a somewhat different interpretation and the values of ζ, A,B,C usually get reduced from the corresponding free-ion values. As we have seen in the preceding section, it is reasonable to use more parameters in order to take account of the inequivalence of the dt_2 and the de orbitals, this inequivalence being also a consequence of the covalency effects.

The scheme developed here is meant for the transition-metal ions ($4d^n$ and $5d^n$) in perfect octahedral stereochemistry. By changing the sign of Dq it can also be applied to the tetrahedral complexes.[5–7] In reality, however, for a number of reasons, amongst which are the Jahn-Teller effect and crystal-packing considerations,[5,6] it is almost impossible to have complexes with perfect octahedral or tetrahedral stereochemistries. The deviation from perfect cubic symmetry can be treated as a perturbation over the ideal situation. Thus, for example, De, Desai, and Chakravarty[26] took account of the axial distortion (reflected by the parameters Ds, Dt) in investigating the magnetic properties of Mo^{5+} ($4d^1$ ion) in $RbMoF_6$, $KMoF_6$, $CsMoF_6$, $NaMoF_6$, and also of Mo^{5+} impurity in $CaWO_4$. Such departure from the cubic symmetry is also found in the case of hexachlororhenium compounds.[13]

In condensed systems there may be the presence of superexchange interactions leading to deviations from strict-paramagnetic behavior which could be observed in the corresponding dilute systems. Thus, for example, the superexchange interaction in K_2ReCl_6 leads, at sufficiently low temperatures, to antiferromagnetism of the compound. Also, because of the same effect, the temperature-dependent susceptibility of K_2ReCl_6 in its paramagnetic phase obeys the Curie-Weiss law rather than the Curie law. The susceptibility calculated here and also in Ref. 13 applies only to a magnetically dilute system; for example, to K_2ReCl_6 in K_2PtCl_6. In subsequent papers we shall deal with the individual cases of the $4d^n$ and $5d^n$ complexes in order to understand their complicated optical and magnetic properties, which are not well understood at present.

APPENDIX A

The wave functions in the intermediate-coupling scheme are given below.

1. d^2 system

Configuration $\gamma_{8p}^2 (p=l \text{ or } p=u)$

$$|\gamma_{8p}^2{:}A_1a_1\rangle=\frac{1}{\sqrt{2}}(|\kappa_p\nu_p|-|\lambda_p\mu_p|)$$

$$|\gamma_{8p}^2{:}E\theta\rangle=\frac{1}{\sqrt{2}}(|\kappa_p\nu_p|+|\lambda_p\mu_p|)$$

$$|\gamma_{8p}^2{:}E\epsilon\rangle=\frac{1}{\sqrt{2}}(|\kappa_p\lambda_p|+|\mu_p\nu_p|)$$

$$|\gamma_{8p}^2{:}T_2 1\rangle=|\lambda_p\nu_p|$$

$$|\gamma_{8p}^2{:}T_2 0\rangle=\frac{1}{\sqrt{2}}(|\kappa_p\lambda_p|-|\mu_p\nu_p|)$$

$$|\gamma_{8p}^2{:}T_2-1\rangle=-|\kappa_p\mu_p|$$

Configuration γ_7^2

$$|\gamma_7^2{:}A_1a_1\rangle=|\alpha''\beta''|$$

Configuration $\gamma_{8l}\gamma_{8u}$

$$|\gamma_{8l}\gamma_{8u}{:}A_1a_1\rangle=\tfrac{1}{2}(|\kappa_l\nu_u|-|\nu_l\kappa_u|-|\lambda_l\mu_u|+|\mu_l\lambda_u|)$$

$$|\gamma_{8l}\gamma_{8u}{:}A_2a_2\rangle=\tfrac{1}{2}(|\kappa_l\lambda_u|+|\lambda_l\kappa_u|-|\mu_l\nu_u|-|\nu_l\mu_u|)$$

$$|\gamma_{8l}\gamma_{8u}{:}3{:}T_1 1\rangle=\frac{1}{2\sqrt{10}}(-\sqrt{3}|\kappa_l\mu_u|-\sqrt{3}|\mu_l\kappa_u|-3|\lambda_l\lambda_u|-5|\nu_l\nu_u|)$$

$$|\gamma_{8l}\gamma_{8u}{:}3{:}T_1 0\rangle=\frac{1}{2\sqrt{5}}(|\kappa_l\nu_u|+|\nu_l\kappa_u|+3|\lambda_l\mu_u|+3|\mu_l\lambda_u|)$$

$$|\gamma_{8l}\gamma_{8u}{:}3{:}T_1-1\rangle=\frac{1}{2\sqrt{10}}(-5|\kappa_l\kappa_u|-\sqrt{3}|\lambda_l\nu_u|-\sqrt{3}|\nu_l\lambda_u|-3|\mu_l\mu_u|)$$

$$|\gamma_{8l}\gamma_{8u}{:}3{:}T_2 1\rangle=\frac{1}{2\sqrt{2}}(-\sqrt{3}|\kappa_l\kappa_u|+|\lambda_l\nu_u|+|\nu_l\lambda_u|+\sqrt{3}|\mu_l\mu_u|)$$

$$|\gamma_{8l}\gamma_{8u}{:}3{:}T_2 0\rangle=\tfrac{1}{2}(|\kappa_l\lambda_u|+|\lambda_l\kappa_u|+|\mu_l\nu_u|+|\nu_l\mu_u|)$$

$$|\gamma_{8l}\gamma_{8u}{:}3{:}T_2-1\rangle=\frac{1}{2\sqrt{2}}(|\kappa_l\mu_u|+|\mu_l\kappa_u|+\sqrt{3}|\lambda_l\lambda_u|-\sqrt{3}|\nu_l\nu_u|)$$

$$|\gamma_{8l}\gamma_{8u}{:}E\theta\rangle=\tfrac{1}{2}(|\kappa_l\nu_u|-|\nu_l\kappa_u|+|\lambda_l\mu_u|-|\mu_l\lambda_u|)$$

$$|\gamma_{8l}\gamma_{8u}{:}E\epsilon\rangle=\tfrac{1}{2}(|\kappa_l\lambda_u|-|\lambda_l\kappa_u|+|\mu_l\nu_u|-|\nu_l\mu_u|)$$

$$|\gamma_{8l}\gamma_{8u}:2:T_2 1\rangle=\frac{1}{\sqrt{2}}(\,|\lambda_l\nu_u| - |\nu_l\lambda_u|\,)$$

$$|\gamma_{8l}\gamma_{8u}:2:T_2 0\rangle=\tfrac{1}{2}(\,|\kappa_l\lambda_u| - |\lambda_l\kappa_u| - |\mu_l\nu_u| + |\nu_l\mu_u|\,)$$

$$|\gamma_{8l}\gamma_{8u}:2:T_2 -1\rangle=\frac{1}{\sqrt{2}}(-|\kappa_l\mu_u| + |\mu_l\kappa_u|\,)$$

$$|\gamma_{8l}\gamma_{8u}:1:T_1 1\rangle=\frac{1}{\sqrt{10}}(\sqrt{3}\,|\kappa_l\mu_u| + \sqrt{3}\,|\mu_l\kappa_u| - 2\,|\lambda_l\lambda_u|\,)$$

$$|\gamma_{8l}\gamma_{8u}:1:T_1 0\rangle=\frac{1}{2\sqrt{5}}(3\,|\kappa_l\nu_u| + 3\,|\nu_l\kappa_u| - |\lambda_l\mu_u| - |\mu_l\lambda_u|\,)$$

$$|\gamma_{8l}\gamma_{8u}:1:T_1 -1\rangle=\frac{1}{\sqrt{10}}(\sqrt{3}\,|\lambda_l\nu_u| + \sqrt{3}\,|\nu_l\lambda_u| - 2\,|\mu_l\mu_u|\,)$$

Configuration $\gamma_7\gamma_{8p}$ $(p=l$ or $p=u)$

$$|\gamma_7\gamma_{8p}:T_1 1\rangle=\frac{1}{2}\,|\alpha''\nu_p| + \frac{\sqrt{3}}{2}\,|\beta''\mu_p|$$

$$|\gamma_7\gamma_{8p}:T_1 0\rangle=\frac{1}{\sqrt{2}}\,|\alpha''\kappa_p| - \frac{1}{\sqrt{2}}\,|\beta''\nu_p|$$

$$|\gamma_7\gamma_{8p}:T_1 -1\rangle=-\frac{\sqrt{3}}{2}\,|\alpha''\lambda_p| - \frac{1}{2}\,|\beta''\kappa_p|$$

$$|\gamma_7\gamma_{8p}:T_2 1\rangle=-\frac{1}{2}\,|\alpha''\lambda_p| + \frac{\sqrt{3}}{2}\,|\beta''\kappa_p|$$

$$|\gamma_7\gamma_{8p}:T_2 0\rangle=-\frac{1}{\sqrt{2}}\,|\alpha''\mu_p| + \frac{1}{\sqrt{2}}\,|\beta''\lambda_p|$$

$$|\gamma_7\gamma_{8p}:T_2 -1\rangle=-\frac{\sqrt{3}}{2}\,|\alpha''\nu_p| + \frac{1}{2}\,|\beta''\mu_p|$$

$$|\gamma_7\gamma_{8p}:E\theta\rangle=\frac{1}{\sqrt{2}}\,|\alpha''\kappa_p| + \frac{1}{\sqrt{2}}\,|\beta''\nu_p|$$

$$|\gamma_7\gamma_{8p}:E\epsilon\rangle=-\frac{1}{\sqrt{2}}\,|\alpha''\mu_p| - \frac{1}{\sqrt{2}}\,|\beta''\lambda_p|$$

2. d^3 system

Configuration γ_{8p}^3 $(p=l$ or $p=u)$

$$|\gamma_{8p}^3:\Gamma_8\kappa\rangle=-|\kappa_p\lambda_p\mu_p|$$

$$|\gamma_{8p}^3:\Gamma_8\lambda\rangle=-|\kappa_p\lambda_p\nu_p|$$

$$|\gamma_{8p}^3:\Gamma_8\mu\rangle=-|\kappa_p\mu_p\nu_p|$$

$$|\gamma_{8p}^3:\Gamma_8\nu\rangle=-|\lambda_p\mu_p\nu_p|$$

Configuration $\gamma_{8p}^2\gamma_{8q}$ $(p=l,\ q=u$ or $p=u, q=l)$

$$|\gamma_{8p}^2(A_1)\gamma_{8q}:\Gamma_8\kappa\rangle=\frac{1}{\sqrt{2}}(|\kappa_p\nu_p\kappa_q|-|\lambda_p\mu_p\kappa_q|)$$

$$|\gamma_{8p}^2(A_1)\gamma_{8q}:\Gamma_8\lambda\rangle=\frac{1}{\sqrt{2}}(|\kappa_p\nu_p\lambda_q|-|\lambda_p\mu_p\lambda_q|)$$

$$|\gamma_{8p}^2(A_1)\gamma_{8q}:\Gamma_8\mu\rangle=\frac{1}{\sqrt{2}}(|\kappa_p\nu_p\mu_q|-|\lambda_p\mu_p\mu_q|)$$

$$|\gamma_{8p}^2(A_1)\gamma_{8u}:\Gamma_8\nu\rangle=\frac{1}{\sqrt{2}}(|\kappa_p\nu_p\nu_q|-|\lambda_p\mu_p\nu_q|)$$

$$|\gamma_{8p}^2(E)\gamma_{8q}:\Gamma_6\alpha'\rangle=\tfrac{1}{2}(|\kappa_p\nu_p\lambda_q|+|\lambda_p\mu_p\lambda_q|+|\kappa_p\lambda_p\nu_q|+|\mu_p\nu_p\nu_q|)$$

$$|\gamma_{8p}^2(E)\gamma_{8q}:\Gamma_6\beta'\rangle=-\tfrac{1}{2}(|\kappa_p\nu_p\mu_q|+|\lambda_p\mu_p\mu_q|+|\kappa_p\lambda_p\kappa_q|+|\mu_p\nu_p\kappa_q|)$$

$$|\gamma_{8p}^2(E)\gamma_{8q}:\Gamma_7\alpha''\rangle=\tfrac{1}{2}(-|\kappa_p\nu_p\nu_q|-|\lambda_p\mu_p\nu_q|+|\kappa_p\lambda_p\lambda_q|+|\mu_p\nu_p\lambda_q|)$$

$$|\gamma_{8p}^2(E)\gamma_{8q}:\Gamma_7\beta''\rangle=\tfrac{1}{2}(|\kappa_p\nu_p\kappa_q|+|\lambda_p\mu_p\kappa_q|-|\kappa_p\lambda_p\mu_q|-|\mu_p\nu_p\mu_q|)$$

$$|\gamma_{8p}^2(E)\gamma_{8q}:\Gamma_8\kappa\rangle=\tfrac{1}{2}(|\kappa_p\nu_p\kappa_q|+|\lambda_p\mu_p\kappa_q|+|\kappa_p\lambda_p\mu_q|+|\mu_p\nu_p\mu_q|)$$

$$|\gamma_{8p}^2(E)\gamma_{8q}:\Gamma_8\lambda\rangle=\tfrac{1}{2}(-|\kappa_p\nu_p\lambda_q|-|\lambda_p\mu_p\lambda_q|+|\kappa_p\lambda_p\nu_q|+|\mu_p\nu_p\nu_q|)$$

$$|\gamma_{8p}^2(E)\gamma_{8q}:\Gamma_8\mu\rangle=\tfrac{1}{2}(-|\kappa_p\nu_p\mu_q|-|\lambda_p\mu_p\mu_q|+|\kappa_p\lambda_p\kappa_q|+|\mu_p\nu_p\kappa_q|)$$

$$|\gamma_{8p}^2(E)\gamma_{8q}:\Gamma_8\nu\rangle=\tfrac{1}{2}(|\kappa_p\nu_p\nu_q|+|\lambda_p\mu_p\nu_q|+|\kappa_p\lambda_p\lambda_q|+|\mu_p\nu_p\lambda_q|)$$

$$|\gamma_{8p}^2(T_2)\gamma_{8q}:\Gamma_6\alpha'\rangle=\frac{1}{\sqrt{6}}(|\lambda_p\nu_p\kappa_q|+\sqrt{3}|\kappa_p\mu_p\mu_q|-|\kappa_p\lambda_p\nu_q|+|\mu_p\nu_p\nu_q|)$$

$$|\gamma_{8p}^2(T_2)\gamma_{8q}:\Gamma_6\beta'\rangle=\frac{1}{\sqrt{6}}(-|\kappa_p\lambda_p\kappa_q|+|\mu_p\nu_p\kappa_q|-\sqrt{3}|\lambda_p\nu_p\lambda_q|-|\kappa_p\mu_p\nu_q|)$$

$$|\gamma_{8p}^2(T_2)\gamma_{8q}:\Gamma_7\alpha''\rangle=\frac{1}{\sqrt{6}}(-\sqrt{3}|\kappa_p\mu_p\kappa_q|-|\kappa_p\lambda_p\lambda_q|+|\mu_p\nu_p\lambda_q|+|\lambda_p\nu_p\mu_q|)$$

$$|\gamma_{8p}^2(T_2)\gamma_{8q}:\Gamma_7\beta''\rangle=\frac{1}{\sqrt{6}}(-|\kappa_p\mu_p\lambda_q|-|\kappa_p\lambda_p\mu_q|+|\mu_p\nu_p\mu_q|+\sqrt{3}|\lambda_p\nu_p\nu_q|)$$

$$|\gamma_{8p}^2(T_2)\gamma_{8q}:\tfrac{3}{2}:\Gamma_8\kappa\rangle=\frac{1}{\sqrt{30}}(4|\kappa_p\mu_p\lambda_q|+|\kappa_p\lambda_p\mu_q|-|\mu_p\nu_p\mu_q+2\sqrt{3}|\lambda_p\nu_p\nu_q|)$$

$$|\gamma_{8p}^2(T_2)\gamma_{8q}:\tfrac{3}{2}:\Gamma_8\lambda\rangle=\frac{1}{\sqrt{10}}(-2|\kappa_p\mu_p\mu_q|-\sqrt{3}|\kappa_p\lambda_p\nu_q|+\sqrt{3}|\mu_p\nu_p\nu_q|)$$

$$|\gamma_{8p}^2(T_2)\gamma_{8q}:\tfrac{3}{2}:\Gamma_8\mu\rangle=\frac{1}{\sqrt{10}}(\sqrt{3}|\kappa_p\lambda_p\kappa_q|-\sqrt{3}|\mu_p\nu_p\kappa_q|-2|\lambda_p\nu_p\lambda_q|)$$

$$|\gamma_{8p}^2(T_2)\gamma_{8q}:\tfrac{3}{2}:\Gamma_8\nu\rangle=\frac{1}{\sqrt{30}}(2\sqrt{3}|\kappa_p\mu_p\kappa_q|-|\kappa_p\lambda_p\lambda_q|+|\mu_p\nu_p\lambda_q|+4|\lambda_p\nu_p\mu_q|)$$

$$|\gamma_{8p}^2(T_2)\gamma_{8q}:\tfrac{5}{2}:\Gamma_8\kappa\rangle=\frac{1}{\sqrt{10}}(-\sqrt{3}|\kappa_p\mu_p\lambda_q|+\sqrt{3}|\kappa_p\lambda_p\mu_q|-\sqrt{3}|\mu_p\nu_p\mu_q|+|\lambda_p\nu_p\nu_q|)$$

$$|\gamma_{8p}^2(T_2)\gamma_{8q}:\tfrac{5}{2}:\Gamma_8\lambda\rangle=\frac{1}{\sqrt{30}}(5|\lambda_p\nu_p\kappa_q|-\sqrt{3}|\kappa_p\mu_p\mu_q|+|\kappa_p\lambda_p\nu_q|-|\mu_p\nu_p\nu_q|)$$

$$|\gamma_{8p}^2(T_2)\gamma_{8q}:\tfrac{5}{2}:\Gamma_8\mu\rangle=\frac{1}{\sqrt{30}}(-|\kappa_p\lambda_p\kappa_q|+|\mu_p\nu_p\kappa_q|-\sqrt{3}|\lambda_p\nu_p\lambda_q|+5|\kappa_p\mu_p\nu_q|)$$

$$|\gamma_{8p}^2(T_2)\gamma_{8q}:\tfrac{5}{2}:\Gamma_8\nu\rangle=\frac{1}{\sqrt{10}}(|\kappa_p\mu_p\kappa_q|-\sqrt{3}|\kappa_p\lambda_p\lambda_q|+\sqrt{3}|\mu_p\nu_p\lambda_q|-\sqrt{3}|\lambda_p\nu_p\mu_q|)$$

Configuration $\gamma_{8p}^2\gamma_7$ ($p=l$ or $p=u$)

$$|\gamma_{8p}^2(A_1)\gamma_7{:}\Gamma_7\alpha''\rangle=\frac{1}{\sqrt{2}}(|\kappa_p\nu_p\alpha''|-|\lambda_p\mu_p\alpha''|)$$

$$|\gamma_{8p}^2(A_1)\gamma_7{:}\Gamma_7\beta''\rangle=\frac{1}{\sqrt{2}}(|\kappa_p\nu_p\beta''|-|\lambda_p\mu_p\beta''|)$$

$$|\gamma_{8p}^2(E)\gamma_7{:}\Gamma_8\kappa\rangle=\frac{1}{\sqrt{2}}(|\kappa_p\nu_p\beta''|+|\lambda_p\mu_p\beta''|)$$

$$|\gamma_{8p}^2(E)\gamma_7{:}\Gamma_8\lambda\rangle=\frac{1}{\sqrt{2}}(|\kappa_p\lambda_p\alpha''|+|\mu_p\nu_p\alpha''|)$$

$$|\gamma_{8p}^2(E)\gamma_7{:}\Gamma_8\mu\rangle=-\frac{1}{\sqrt{2}}(|\kappa_p\lambda_p\beta''|+|\mu_p\nu_p\beta''|)$$

$$|\gamma_{8p}^2(E)\gamma_7{:}\Gamma_8\nu\rangle=-\frac{1}{\sqrt{2}}(|\kappa_p\nu_p\alpha''|+|\lambda_p\mu_p\alpha''|)$$

$$|\gamma_{8p}^2(T_2)\gamma_7{:}\Gamma_6\alpha'\rangle=\frac{1}{\sqrt{6}}(|\kappa_p\lambda_p\alpha''|-|\mu_p\nu_p\alpha''|-2|\lambda_p\nu_p\beta''|)$$

$$|\gamma_{8p}^2(T_2)\gamma_7{:}\Gamma_6\beta'\rangle=\frac{1}{\sqrt{6}}(-2|\kappa_p\mu_p\alpha''|-|\kappa_p\lambda_p\beta''|+|\mu_p\nu_p\beta''|)$$

$$|\gamma_{8p}^2(T_2)\gamma_7{:}\Gamma_8\kappa\rangle=|\lambda_p\nu_p\alpha''|$$

$$|\gamma_{8p}^2(T_2)\gamma_7{:}\Gamma_8\lambda\rangle=\frac{1}{\sqrt{3}}(|\kappa_p\lambda_p\alpha''|-|\mu_p\nu_p\alpha''|+|\lambda_p\nu_p\beta''|)$$

$$|\gamma_{8p}^2(T_2)\gamma_7{:}\Gamma_8\mu\rangle=\frac{1}{\sqrt{3}}(-|\kappa_p\mu_p\alpha''|+|\kappa_p\lambda_p\beta''|-|\mu_p\nu_p\beta''|)$$

$$|\gamma_{8p}^2(T_2)\gamma_7{:}\Gamma_8\nu\rangle=-|\kappa_p\mu_p\beta''|$$

Configuration $\gamma_{8p}\gamma_7^2$ ($p=l$ or $p=u$)

$$|\gamma_{8p}\gamma_7^2{:}\Gamma_8\kappa\rangle=|\kappa_p\alpha''\beta''|$$

$$|\gamma_{8p}\gamma_7^2{:}\Gamma_8\lambda\rangle=|\lambda_p\alpha''\beta''|$$

$$|\gamma_{8p}\gamma_7^2{:}\Gamma_8\mu\rangle=|\mu_p\alpha''\beta''|$$

$$|\gamma_{8p}\gamma_7^2{:}\Gamma_8\nu\rangle=|\nu_p\alpha''\beta''|$$

Configuration $\gamma_{8l}\gamma_{8u}\gamma_7$

$$|\underline{\gamma_{8l}\gamma_{8u}}(A_1)\gamma_7{:}\Gamma_7\alpha''\rangle=\tfrac{1}{2}(|\kappa_l\nu_u\alpha''|-|\nu_l\kappa_u\alpha''|-|\lambda_l\mu_u\alpha''|+|\mu_l\lambda_u\alpha''|)$$

$$|\underline{\gamma_{8l}\gamma_{8u}}(A_1)\gamma_7{:}\Gamma_7\beta''\rangle=\tfrac{1}{2}(|\kappa_l\nu_u\beta''|-|\nu_l\kappa_u\beta''|-|\lambda_l\mu_u\beta''|+|\mu_l\lambda_u\beta''|)$$

$$|\underline{\gamma_{8l}\gamma_{8u}}(A_2)\gamma_7{:}\Gamma_6\alpha'\rangle=\tfrac{1}{2}(|\kappa_l\lambda_u\alpha''|+|\lambda_l\kappa_u\alpha''|-|\mu_l\nu_u\alpha''|-|\nu_l\mu_u\alpha''|)$$

$$|\underline{\gamma_{8l}\gamma_{8u}}(A_2)\gamma_7{:}\Gamma_6\beta'\rangle=\tfrac{1}{2}(|\kappa_l\lambda_u\beta''|+|\lambda_l\kappa_u\beta''|-|\mu_l\nu_u\beta''|-|\nu_l\mu_u\beta''|)$$

$$|\underline{\gamma_{8l}\gamma_{8u}}(E)\gamma_7{:}\Gamma_8\kappa\rangle=\tfrac{1}{2}(|\kappa_l\nu_u\beta''|-|\nu_l\kappa_u\beta''|+|\lambda_l\mu_u\beta''|-|\mu_l\lambda_u\beta''|)$$

$$|\underline{\gamma_{8l}\gamma_{8u}}(E)\gamma_7{:}\Gamma_8\lambda\rangle=\tfrac{1}{2}(\,|\kappa_l\lambda_u\alpha''|-|\lambda_l\kappa_u\alpha''|+|\mu_l\nu_u\alpha''|-|\nu_l\mu_u\alpha''|\,)$$

$$|\underline{\gamma_{8l}\gamma_{8u}}(E)\gamma_7{:}\Gamma_8\mu\rangle=-\tfrac{1}{2}(\,|\kappa_l\lambda_u\beta''|-|\lambda_l\kappa_u\beta''|+|\mu_l\nu_u\beta''|-|\nu_l\mu_u\beta''|\,)$$

$$|\underline{\gamma_{8l}\gamma_{8u}}(E)\gamma_7{:}\Gamma_8\nu\rangle=-\tfrac{1}{2}(\,|\kappa_l\nu_u\alpha''|-|\nu_l\kappa_u\alpha''|+|\lambda_l\mu_u\alpha''|-|\mu_l\lambda u\alpha''|\,)$$

$$|\underline{\gamma_{8l}\gamma_{8u}}(3{:}T_1)\gamma_7{:}\Gamma_7\alpha''\rangle=\frac{1}{2\sqrt{15}}(\,|\kappa_l\nu_u\alpha''|+|\nu_l\kappa_u\alpha''|+3\,|\lambda_l\mu_u\alpha''|+3\,|\mu_l\lambda_u\alpha''|$$
$$+\sqrt{3}\,|\kappa_l\mu_u\beta''|+\sqrt{3}\,|\mu_l\kappa_u\beta''|+3\,|\lambda_l\lambda_u\beta''|+5\,|\nu_l\nu_u\beta''|\,)$$

$$|\underline{\gamma_{8l}\gamma_{8u}}(3{:}T_1)\gamma_7{:}\Gamma_7\beta''\rangle=\frac{-1}{2\sqrt{15}}(5\,|\kappa_l\kappa_u\alpha''|+\sqrt{3}\,|\lambda_l\nu_u\alpha''|+\sqrt{3}\,|\nu_l\lambda_u\alpha''|+3\,|\mu_l\mu_u\alpha''|$$
$$+|\kappa_l\nu_u\beta''|+|\nu_l\kappa_\mu\beta''|+3\,|\lambda_l\mu_u\beta''|+3\,|\mu_l\lambda_u\beta''|\,)$$

$$|\underline{\gamma_{8l}\gamma_{8u}}(3{:}T_1)\gamma_7{:}\Gamma_8\kappa\rangle=\frac{1}{2\sqrt{30}}(5\,|\kappa_l\kappa_u\alpha''+\sqrt{3}\,|\lambda_l\nu_u\alpha''|+\sqrt{3}\,|\nu_l\lambda_u\alpha''|+3\,|\mu_l\mu_u\alpha''|$$
$$-2\,|\kappa_l\nu_u\beta''|-2\,|\nu_l\kappa_u\beta''|-6\,|\lambda_l\mu_u\beta''|-6\,|\mu_l\lambda_u\beta''|\,)$$

$$|\underline{\gamma_{8l}\gamma_{8u}}(3{:}T_1)\gamma_7{:}\Gamma_8\lambda\rangle=\frac{1}{2\sqrt{10}}(-5\,|\kappa_l\kappa_u\beta''|-\sqrt{3}\,|\lambda_l\nu_u\beta''|-\sqrt{3}\,|\nu_l\lambda_u\beta''|-3\,|\mu_l\mu_u\beta''|\,)$$

$$|\underline{\gamma_{8l}\gamma_{8u}}(3{:}T_1)\gamma_7{:}\Gamma_8\mu\rangle=\frac{1}{2\sqrt{10}}(-\sqrt{3}\,|\kappa_l\mu_u\alpha''|-\sqrt{3}\,|\mu_l\kappa_u\alpha''|-3\,|\lambda_l\lambda_u\alpha''|-5\,|\nu_l\nu_u\alpha''|\,)$$

$$|\underline{\gamma_{8l}\gamma_{8u}}(3{:}T_1)\gamma_7{:}\Gamma_8\nu\rangle=\frac{1}{2\sqrt{30}}(-2\,|\kappa_l\nu_u\alpha''|-2\,|\nu_l\kappa_u\alpha''|-6\,|\lambda_l\mu_u\alpha''|-6\,|\mu_l\lambda_u\alpha''|$$
$$+\sqrt{3}\,|\kappa_l\mu_u\beta''|+\sqrt{3}\,|\mu_l\kappa_u\beta''|+3\,|\lambda_l\lambda_u\beta''|+5\,|\nu_l\nu_u\beta''|\,)$$

$$|\underline{\gamma_{8l}\gamma_{8u}}(3{:}T_2)\gamma_7{:}\Gamma_6\alpha'\rangle=\frac{1}{2\sqrt{3}}(\,|\kappa_l\lambda_u\alpha''|+|\lambda_l\kappa_u\alpha''|+|\mu_l\nu_u\alpha''|+|\nu_l\mu_u\alpha''|$$
$$+\sqrt{3}\,|\kappa_l\kappa_u\beta''|-|\lambda_l\nu_u\beta''|-|\nu_l\lambda_u\beta''|-\sqrt{3}\,|\mu_l\mu_u\beta''|\,)$$

$$|\underline{\gamma_{8l}\gamma_{8u}}(3{:}T_2)\gamma_7{:}\Gamma_6\beta'\rangle=\frac{1}{2\sqrt{3}}(\,|\kappa_l\mu_u\alpha''|+|\mu_l\kappa_u\alpha''|+\sqrt{3}\,|\lambda_l\lambda_u\alpha''|-\sqrt{3}\,|\nu_l\nu_u\alpha''|$$
$$-|\kappa_l\lambda_u\beta''|-|\lambda_l\kappa_u\beta''|-|\mu_l\nu_u\beta''|-|\nu_l\mu_u\beta''|\,)$$

$$|\underline{\gamma_{8l}\gamma_{8u}}(3{:}T_2)\gamma_7{:}\Gamma_8\kappa\rangle=\frac{1}{2\sqrt{2}}(-\sqrt{3}\,|\kappa_l\kappa_u\alpha''|+|\lambda_l\nu_u\alpha''|+|\nu_l\lambda_u\alpha''|+\sqrt{3}\,|\mu_l\mu_u\alpha''|\,)$$

$$|\underline{\gamma_{8l}\gamma_{8u}}(3{:}T_2)\gamma_7{:}\Gamma_8\lambda\rangle=\frac{1}{2\sqrt{6}}(2\,|\kappa_l\lambda_u\alpha''|+2\,|\lambda_l\kappa_u\alpha''|+2\,|\mu_l\nu_u\alpha''|+2\,|\nu_l\mu_u\alpha''|$$
$$-\sqrt{3}\,|\kappa_l\kappa_u\beta''|+|\lambda_l\nu_u\beta''|+|\nu_l\lambda_u\beta''|+\sqrt{3}\,|\mu_l\mu_u\beta''|\,)$$

$$|\underline{\gamma_{8l}\gamma_{8u}}(3{:}T_2)\gamma_7{:}\Gamma_8\mu\rangle=\frac{1}{2\sqrt{6}}(\,|\kappa_l\mu_u\alpha''|+|\mu_l\kappa_\mu\alpha''|+\sqrt{3}\,|\lambda_l\lambda_u\alpha''|-\sqrt{3}\,|\nu_l\nu_u\alpha''|$$
$$+2\,|\kappa_l\lambda_u\beta''|+2\,|\lambda_l\kappa_u\beta''|+2\,|\mu_l\nu_u\beta''|+2\,|\nu_l\mu_u\beta''|\,)$$

$$|\underline{\gamma_{8l}\gamma_{8u}}(3{:}T_2)\gamma_7{:}\Gamma_8\nu\rangle=\frac{1}{2\sqrt{2}}(\,|\kappa_l\mu_u\beta''|+|\mu_l\kappa_u\beta''|+\sqrt{3}\,|\lambda_l\lambda_u\beta''|-\sqrt{3}\,|\nu_l\nu_u\beta''|\,)$$

$$|\underline{\gamma_{8l}\gamma_{8u}}(2{:}T_2)\gamma_7{:}\Gamma_6\alpha'\rangle=\frac{1}{2\sqrt{3}}(\,|\kappa_l\lambda_u\alpha''|-|\lambda_l\kappa_u\alpha''|-|\mu_l\nu_u\alpha''|+|\nu_l\mu_u\alpha''|$$
$$-2|\lambda_l\nu_u\beta''|+2|\nu_l\lambda_u\beta''|\,)$$

$$|\underline{\gamma_{8l}\gamma_{8u}}(2{:}T_2)\gamma_7{:}\Gamma_6\beta'\rangle=\frac{1}{2\sqrt{3}}(-2|\kappa_l\mu_u\alpha''|+2|\mu_l\kappa_u\alpha''|-|\kappa_l\lambda_u\beta''|+|\lambda_l\kappa_u\beta''|$$
$$+|\mu_l\nu_u\beta''|-|\nu_l\mu_u\beta''|\,)$$

$$|\underline{\gamma_{8l}\gamma_{8u}}(2{:}T_2)\gamma_7{:}\Gamma_8\kappa\rangle=\frac{1}{\sqrt{2}}(\,|\lambda_l\nu_u\alpha''|-|\nu_l\lambda_u\alpha''|\,)$$

$$|\underline{\gamma_{8l}\gamma_{8u}}(2{:}T_2)\gamma_7{:}\Gamma_8\lambda\rangle=\frac{1}{\sqrt{6}}(\kappa_l\lambda_u\alpha''|-|\lambda_l\kappa_u\alpha''|-|\mu_l\nu_u\alpha''|+|\nu_l\mu_u\alpha''|$$
$$+|\lambda_l\nu_u\beta''|-|\nu_l\lambda_u\beta''|\,)$$

$$|\underline{\gamma_{8l}\gamma_{8u}}(2{:}T_2)\gamma_7{:}\Gamma_8\mu\rangle=\frac{1}{\sqrt{6}}(-|\kappa_l\mu_u\alpha''|+|\mu_l\kappa_u\alpha''|+|\kappa_l\lambda_u\beta''|-|\lambda_l\kappa_u\beta''|$$
$$-|\mu_l\nu_u\beta''|+|\nu_l\mu_u\beta''|\,)$$

$$|\underline{\gamma_{8l}\gamma_{8u}}(2{:}T_2)\gamma_7{:}\Gamma_8\nu\rangle=\frac{1}{\sqrt{2}}(-|\kappa_l\mu_u\beta''|+|\mu_l\kappa_u\beta''|\,)$$

$$|\underline{\gamma_{8l}\gamma_{8u}}(1{:}T_1)\gamma_7{:}\Gamma_7\alpha''\rangle=\frac{1}{2\sqrt{15}}(3|\kappa_l\nu_u\alpha''|-|\lambda_l\mu_u\alpha''|-|\mu_l\lambda_u\alpha''|+3|\nu_l\kappa_u\alpha''|$$
$$-2\sqrt{3}|\kappa_l\mu_u\beta''|-2\sqrt{3}|\mu_l\kappa_u\beta''|+4|\lambda_l\lambda_u\beta''|\,)$$

$$|\underline{\gamma_{8l}\gamma_{8u}}(1{:}T_1)\gamma_7{:}\Gamma_7\beta''\rangle=\frac{1}{2\sqrt{15}}(2\sqrt{3}|\lambda_l\nu_u\alpha''|+2\sqrt{3}|\nu_l\lambda_u\alpha''|-4|\mu_l\mu_u\alpha''|-3|\kappa_l\nu_u\beta''|$$
$$-3|\nu_l\kappa_u\beta''|+|\lambda_l\mu_u\beta''|+|\mu_l\lambda_u\beta''|\,)$$

$$|\underline{\gamma_{8l}\gamma_{8u}}(1{:}T_1)\gamma_7{:}\Gamma_8\kappa\rangle=\frac{1}{\sqrt{30}}(-\sqrt{3}|\lambda_l\nu_u\alpha''|-\sqrt{3}|\nu_l\lambda_u\alpha''|+2|\mu_l\mu_u\alpha''|-3|\kappa_l\nu_u\beta''|$$
$$+|\lambda_l\mu_u\beta''|+|\mu_l\lambda_u\beta''|-3|\nu_l\kappa_u\beta''|\,)$$

$$|\underline{\gamma_{8l}\gamma_{8u}}(1{:}T_1)\gamma_7{:}\Gamma_8\lambda\rangle=\frac{1}{\sqrt{10}}(\sqrt{3}|\lambda_l\nu_u\beta''|+\sqrt{3}|\nu_l\lambda_u\beta''|-2|\mu_l\mu_u\beta''|\,)$$

$$|\underline{\gamma_{8l}\gamma_{8u}}(1{:}T_1)\gamma_7{:}\Gamma_8\mu\rangle=\frac{1}{\sqrt{10}}(\sqrt{3}|\kappa_l\mu_u\alpha''|+\sqrt{3}|\mu_l\kappa_u\alpha''|-2|\lambda_l\lambda_u\alpha''|\,)$$

$$|\underline{\gamma_{8l}\gamma_{8u}}(1{:}T_1)\gamma_7{:}\Gamma_8\nu\rangle=\frac{1}{\sqrt{30}}(-3|\kappa_l\nu_u\alpha''|-3|\nu_l\kappa_u\alpha''|+|\lambda_l\mu_u\alpha''|+|\mu_l\lambda_u\alpha''|$$
$$-\sqrt{3}|\kappa_l\mu_u\beta''|-\sqrt{3}|\mu_l\kappa_u\beta''|+2|\lambda_l\lambda_u\beta''|\,)$$

3. d^4 system

The wave function for the first component of each irreducible representation has been given. Other wave functions can be similarly constructed by combining those of the d^1, d^2, and d^3 systems through proper coupling coefficients.

Configuration γ_{8p}^4 *($p=l$ or $p=u$)*

$$|\gamma_{8p}^4\!:\!A_1a_1\rangle = -|\kappa_p\lambda_p\mu_p\nu_p|$$

Configuration $\gamma_{8p}^3\gamma_{8q}$ *($p=l$, $q=u$ or $p=u$, $q=l$)*

$$|\gamma_{8p}^3\gamma_{8q}\!:\!A_1a_1\rangle = \tfrac{1}{2}(-|\kappa_p\lambda_p\mu_p\nu_q| + |\kappa_p\lambda_p\nu_p\mu_q| - |\kappa_p\mu_p\nu_p\lambda_q| + |\lambda_p\mu_p\nu_p\kappa_q|)$$

$$|\gamma_{8p}^3\gamma_{8q}\!:\!A_2a_2\rangle = \tfrac{1}{2}(-|\kappa_p\lambda_p\mu_p\lambda_q| - |\kappa_p\lambda_p\nu_p k_q| + |\kappa_p\mu_p\nu_p\nu_q| + |\lambda_p\mu_p\nu_p\mu_q|)$$

$$|\gamma_{8p}^3\gamma_{8q}\!:\!E\theta\rangle = \tfrac{1}{2}(-|\kappa_p\lambda_p\mu_p\nu_q| - |\kappa_p\lambda_p\nu_p\mu_q| + |\kappa_p\mu_p\nu_p\lambda_q| + |\lambda_p\mu_p\nu_p\kappa_q|)$$

$$|\gamma_{8p}^3\gamma_{8q}\!:\!3\!:\!T_1 1\rangle = \frac{1}{2\sqrt{10}}(\sqrt{3}\,|\kappa_p\lambda_p\mu_p\mu_q| + 3\,|\kappa_p\lambda_p\nu_p\lambda_q| + \sqrt{3}\,|\kappa_p\mu_p\nu_p\kappa_q| + 5\,|\lambda_p\mu_p\nu_p\nu_q|)$$

$$|\gamma_{8p}^3\gamma_{8q}\!:\!3\!:\!T_2 1\rangle = \frac{1}{2\sqrt{2}}(\sqrt{3}\,|\kappa_p\lambda_p\mu_p\kappa_q| - |\kappa_p\lambda_p\nu_p\nu_q| - \sqrt{3}\,|\kappa_p\mu_p\nu_p\mu_q| - |\lambda_p\mu_p\nu_p\lambda_q|)$$

$$|\gamma_{8p}^3\gamma_{8q}\!:\!2\!:\!T_2 1\rangle = \frac{1}{\sqrt{2}}(-|\kappa_p\lambda_p\nu_p\nu_q| + |\lambda_p\mu_p\nu_p\lambda_q|)$$

$$|\gamma_{8p}^3\gamma_{8q}\!:\!1\!:\!T_1 1\rangle = \frac{1}{\sqrt{10}}(-\sqrt{3}\,|\kappa_p\lambda_p\mu_p\mu_q| + 2\,|\kappa_p\lambda_p\nu_p\lambda_q| - \sqrt{3}\,|\kappa_p\mu_p\nu_p\kappa_q|)$$

Configuration $\gamma_{8l}^2\gamma_{8u}^2$

$$|\gamma_{8l}^2(A_1)\gamma_{8u}^2(A_1)\!:\!A_1a_1\rangle = \tfrac{1}{2}(|\kappa_l\nu_l\kappa_u\nu_u| - |\kappa_l\nu_l\lambda_u\mu_u| - |\lambda_l\mu_l\kappa_u\nu_u| + |\lambda_l\mu_l\lambda_u\mu_u|)$$

$$|\gamma_{8l}^2(A_1)\gamma_{8u}^2(E)\!:\!E\theta\rangle = \tfrac{1}{2}(|\kappa_l\nu_l\kappa_u\nu_u| + |\kappa_l\nu_l\lambda_u\mu_u| - |\lambda_l\mu_l\kappa_u\nu_u| - |\lambda_l\mu_l\lambda_u\mu_u|)$$

$$|\gamma_{8l}^2(A_1)\gamma_{8u}^2(T_2)\!:\!T_2 1\rangle = \frac{1}{\sqrt{2}}(|\kappa_l\nu_l\lambda_u\nu_u| - |\lambda_l\mu_l\lambda_u\nu_u|)$$

$$|\gamma_{8l}^2(E)\gamma_{8u}^2(A_1)\!:\!E\theta\rangle = \tfrac{1}{2}(|\kappa_l\nu_l\kappa_u\nu_u| - |\kappa_l\nu_l\lambda_u\mu_u| + |\lambda_l\mu_l\kappa_u\nu_u| - |\lambda_l\mu_l\lambda_u\mu_u|)$$

$$|\gamma_{8l}^2(T_2)\gamma_{8u}^2(E)\!:\!T_1 1\rangle = \frac{1}{2\sqrt{2}}(-\sqrt{3}\,|\kappa_l\mu_l\kappa_\mu\nu_u| - \sqrt{3}\,|\kappa_l\mu_l\lambda_u\mu_u| - |\lambda_l\nu_l\kappa_u\lambda_u| - |\lambda_l\nu_l\mu_u\nu_u|)$$

$$|\gamma_{8l}^2(T_2)\gamma_{8u}^2(E)\!:\!T_2 1\rangle = \frac{1}{2\sqrt{2}}(-|\lambda_l\nu_l\kappa_u\nu_u| - |\lambda_l\nu_l\lambda_u\mu_u| + \sqrt{3}\,|\kappa_l\mu_l\kappa_u\lambda_u| + \sqrt{3}\,|\kappa_l\mu_l\mu_u\nu_u|)$$

$$|\gamma_{8l}^2(T_2)\gamma_{8u}^2(T_2)\!:\!A_1a_1\rangle = \frac{1}{2\sqrt{3}}(-2\,|\lambda_l\nu_l\kappa_u\mu_u| - |\kappa_l\lambda_l\kappa_u\lambda_u| + |\kappa_l\lambda_l\mu_u\nu_u| + |\mu_l\nu_l\kappa_u\lambda_u|$$
$$-|\mu_l\nu_l\mu_u\nu_u| - 2\,|\kappa_l\mu_l\lambda_u\nu_u|)$$

$$|\gamma_{8l}^2(T_2)\gamma_{8u}^2(T_2)\!:\!E\theta\rangle = \frac{1}{\sqrt{6}}(-|\lambda_l\nu_l\kappa_u\mu_u| + |\kappa_l\lambda_l\kappa_u\lambda_u| - |\kappa_l\lambda_l\mu_u\nu_u| - |\mu_l\nu_l\kappa_u\lambda_u|$$
$$+|\mu_l\nu_l\mu_u\nu_u| - |\kappa_l\mu_l\lambda_u\nu_u|)$$

$$|\gamma_{8l}^2(T_2)\gamma_{8u}^2(T_2)\!:\!T_1 1\rangle = \tfrac{1}{2}(|\lambda_l\nu_l\kappa_u\lambda_u| - |\lambda_l\nu_l\mu_u\nu_u| - |\kappa_l\lambda_l\lambda_u\nu_u| + |\mu_l\nu_l\lambda_u\nu_u|)$$

$$|\gamma_{8l}^2(T_2)\gamma_{8u}^2(T_2)\!:\!T_2 1\rangle = \tfrac{1}{2}(-|\kappa_l\lambda_l\kappa_u\mu_u| + |\mu_l\nu_l\kappa_u\mu_u| - |\kappa_l\mu_l\kappa_u\lambda_u| + |\kappa_l\mu_l\mu_u\nu_u|)$$

$$|\gamma_{8l}^2(E)\gamma_{8u}^2(E)\!:\!A_1a_1\rangle = \frac{1}{2\sqrt{2}}(|\kappa_l\nu_l\kappa_u\nu_u| + |\kappa_l\nu_l\lambda_u\mu_u| + |\lambda_l\mu_l\kappa_u\nu_u| + |\lambda_l\mu_l\lambda_u\mu_u|$$

$$+|\kappa_l\lambda_l\kappa_u\lambda_u| + |\kappa_l\lambda_l\mu_u\nu_u| + |\mu_l\nu_l\kappa_u\lambda_u| + |\mu_l\nu_l\mu_u\nu_u|)$$

$$|\gamma_{8l}^2(E)\gamma_{8u}^2(E):A_2a_2\rangle = \frac{1}{2\sqrt{2}}(|\kappa_l\nu_l\kappa_u\lambda_u| + |\kappa_l\nu_l\mu_u\nu_u| + |\lambda_l\mu_l\kappa_u\lambda_u| + |\lambda_l\mu_l\mu_u\nu_u|$$

$$-|\kappa_l\lambda_l\kappa_u\nu_u| - |\kappa_l\lambda_l\lambda_u\mu_u| - |\mu_l\nu_l\kappa_u\nu_u| - |\mu_l\nu_l\lambda_u\mu_u|)$$

$$|\gamma_{8l}^2(E)\gamma_{8u}^2(E):E\theta\rangle = \frac{1}{2\sqrt{2}}(-|\kappa_l\nu_l\kappa_u\nu_u| - |\kappa_l\nu_l\lambda_u\mu_u| - |\lambda_l\mu_l\kappa_u\nu_u| - |\lambda_l\mu_l\lambda_u\mu_u|$$

$$+|\kappa_l\lambda_l\kappa_u\lambda_u| + |\kappa_l\lambda_l\mu_u\nu_u| + |\mu_l\nu_l\kappa_u\lambda_u| + |\mu_l\nu_l\mu_u\nu_u|)$$

$$|\gamma_{8l}^2(E)\gamma_{8u}^2(T_2):T_11\rangle = \frac{1}{2\sqrt{2}}(-\sqrt{3}|\kappa_l\nu_l\kappa_u\mu_u| - \sqrt{3}|\lambda_l\mu_l\kappa_u\mu_u| - |\kappa_l\lambda_l\lambda_u\nu_u| - |\mu_l\nu_l\lambda_u\nu_u|)$$

$$|\gamma_{8l}^2(E)\gamma_{8u}^2(T_2):T_21\rangle = \frac{1}{2\sqrt{2}}(-|\kappa_l\nu_l\lambda_u\nu_u| - |\lambda_l\mu_l\lambda_u\nu_u| + \sqrt{3}|\kappa_l\lambda_l\kappa_u\mu_u| + \sqrt{3}|\mu_l\nu_l\kappa_u\mu_u|)$$

$$|\gamma_{8l}^2(T_2)\gamma_{8u}^2(A_1):T_21\rangle = \frac{1}{\sqrt{2}}(|\lambda_l\nu_l\kappa_u\nu_u| - |\lambda_l\nu_l\lambda_u\mu_u|)$$

Configuration $\gamma_{8p}^3\gamma_7$ $(p=l$ or $p=u)$

$$|\gamma_{8p}^3\gamma_7:E\theta\rangle = -\frac{1}{\sqrt{2}}(|\kappa_p\lambda_p\mu_p\alpha''| + |\lambda_p\mu_p\nu_p\beta''|)$$

$$|\gamma_{8p}^3\gamma_7:T_11\rangle = -\tfrac{1}{2}|\lambda_p\mu_p\nu_p\alpha''| - \frac{\sqrt{3}}{2}|\kappa_p\mu_p\nu_p\beta''|$$

$$|\gamma_{8p}^3\gamma_7:T_21\rangle = \tfrac{1}{2}|\kappa_p\lambda_p\nu_p\alpha''| - \frac{\sqrt{3}}{2}|\kappa_p\lambda_p\mu_p\beta''|$$

Configuration $\gamma_{8p}^2\gamma_7^2$ $(p=l$ or $p=\mu)$

$$|\gamma_{8p}^2(A_1)\gamma_7^2:A_1a_1\rangle = \frac{1}{\sqrt{2}}(|\kappa_p\nu_p\alpha''\beta''| - |\lambda_p\mu_p\alpha''\beta''|)$$

$$|\gamma_{8p}^2(E)\gamma_7^2:E\theta\rangle = \frac{1}{\sqrt{2}}(|\kappa_p\nu_p\alpha''\beta''| + |\lambda_p\mu_p\alpha''\beta''|)$$

$$|\gamma_{8p}^2(T_2)\gamma_7^2:T_21\rangle = |\lambda_p\nu_p\alpha''\beta''|$$

Configuration $\gamma_{8p}^2\gamma_{8q}\gamma_7$ $(p=l,q=u$ or $p=u,q=l)$

$$|\underline{\gamma_{8p}^2}(A_1)\underline{\gamma_7\gamma_{8q}}(T_1):T_11\rangle = \frac{1}{2\sqrt{2}}(|\kappa_p\nu_p\nu_q\alpha''| + \sqrt{3}|\kappa_p\nu_p\mu_q\beta''| - |\lambda_p\mu_p\nu_q\alpha''| - \sqrt{3}|\lambda_p\mu_p\mu_q\beta''|)$$

$$|\underline{\gamma_{8p}^2}(A_1)\underline{\gamma_7\gamma_{8q}}(T_2):T_21\rangle = \frac{1}{2\sqrt{2}}(-|\kappa_p\nu_p\lambda_q\alpha''| + \sqrt{3}|\kappa_p\nu_p\kappa_q\beta''| + |\lambda_p\mu_p\lambda_q\alpha''| - \sqrt{3}|\lambda_p\mu_p\kappa_q\beta''|)$$

$$|\underline{\gamma_{8p}^2}(E)\underline{\gamma_7\gamma_{8q}}(E):A_1a_1\rangle = \frac{1}{2\sqrt{2}}(|\kappa_p\nu_p\kappa_q\alpha''| + |\kappa_p\nu_p\nu_q\beta''| + |\lambda_p\mu_p\kappa_q\alpha''| + |\lambda_p\mu_p\nu_q\beta''|$$

$$-|\kappa_p\lambda_p\mu_q\alpha''| - |\kappa_p\lambda_p\lambda_q\beta''| - |\mu_p\nu_p\mu_q\alpha''| - |\mu_p\nu_p\lambda_q\beta''|)$$

$$|\underline{\gamma_{8p}^2}(E)\underline{\gamma_7\gamma_{8q}}(E):A_2a_2\rangle=\frac{1}{2\sqrt{2}}(-|\kappa_p\nu_p\mu_q\alpha''|-|\kappa_p\nu_p\lambda_q\beta''|-|\lambda_p\mu_p\mu_q\alpha''|-|\lambda_p\mu_p\lambda_q\beta''|$$
$$-|\kappa_p\lambda_p\kappa_q\alpha''|-|\kappa_p\lambda_p\nu_q\beta''|-|\mu_p\nu_p\kappa_q\alpha''|-|\mu_p\nu_p\nu_q\beta''|)$$

$$|\underline{\gamma_{8p}^2}(E)\underline{\gamma_7\gamma_{8q}}(E):E\theta\rangle=\frac{1}{2\sqrt{2}}(-|\kappa_p\nu_p\kappa_q\alpha''|-|\kappa_p\nu_p\nu_q\beta''|-|\lambda_p\mu_p\kappa_q\alpha''|-|\lambda_p\mu_p\nu_q\beta''|$$
$$-|\kappa_p\lambda_p\mu_q\alpha''|-|\kappa_p\lambda_p\lambda_q\beta''|-|\mu_p\nu_p\mu_q\alpha''|-|\mu_p\nu_p\lambda_q\beta''|)$$

$$|\underline{\gamma_{8p}^2}(E)\underline{\gamma_7\gamma_{8q}}(T_1):T_11\rangle=\frac{1}{4\sqrt{2}}(-|\kappa_p\nu_p\nu_q\alpha''|-\sqrt{3}|\kappa_p\nu_p\mu_q\beta''|-|\lambda_p\mu_p\nu_q\alpha''|-\sqrt{3}|\lambda_p\mu_p\mu_q\beta''|$$
$$+3|\kappa_p\lambda_p\lambda_q\alpha''|+\sqrt{3}|\kappa_p\lambda_p\kappa_q\beta''|+3|\mu_p\nu_p\lambda_q\alpha''|+\sqrt{3}|\mu_p\nu_p\kappa_q\beta''|)$$

$$|\underline{\gamma_{8p}^2}(E)\underline{\gamma_7\gamma_{8q}}(T_1):T_21\rangle=\frac{1}{4\sqrt{2}}(-3|\kappa_p\nu_p\lambda_q\alpha''|-\sqrt{3}|\kappa_p\nu_p\kappa_q\beta''|-3|\lambda_p\mu_p\lambda_q\alpha''|-\sqrt{3}|\lambda_p\mu_p\kappa_q\beta''|$$
$$-|\kappa_p\lambda_p\nu_q\alpha''|-\sqrt{3}|\kappa_p\lambda_p\mu_q\beta''|-|\mu_p\nu_p\nu_q\alpha''|-\sqrt{3}|\mu_p\nu_p\mu_q\beta''|)$$

$$|\underline{\gamma_{8p}^2}(E)\underline{\gamma_7\gamma_{8q}}(T_2):T_11\rangle=\frac{1}{4\sqrt{2}}(-3|\kappa_p\nu_p\nu_q\alpha''|+\sqrt{3}|\kappa_p\nu_p\mu_q\beta''|-3|\lambda_p\mu_p\nu_q\alpha''|+\sqrt{3}|\lambda_p\mu_p\mu_q\beta''|$$
$$+|\kappa_p\lambda_p\lambda_q\alpha''|-\sqrt{3}|\kappa_p\lambda_p\kappa_q\beta''|+|\mu_p\nu_p\lambda_q\alpha''|-\sqrt{3}|\mu_p\nu_p\kappa_q\beta''|)$$

$$|\underline{\gamma_{8p}^2}(E)\underline{\gamma_7\gamma_{8q}}(T_2):T_21\rangle=\frac{1}{4\sqrt{2}}(|\kappa_p\nu_p\lambda_q\alpha''|-\sqrt{3}|\kappa_p\nu_p\kappa_q\beta''|+|\lambda_p\mu_p\lambda_q\alpha''|-\sqrt{3}|\lambda_p\mu_p\kappa_q\beta''|$$
$$+3|\kappa_p\lambda_p\nu_q\alpha''|-\sqrt{3}|\kappa_p\lambda_p\mu_q\beta''|+3|\mu_p\nu_p\nu_q\alpha''|-\sqrt{3}|\mu_p\nu_p\mu_q\beta''|)$$

$$|\underline{\gamma_{8p}^2}(T_2)\underline{\gamma_7\gamma_{8q}}(E):T_11\rangle=\frac{1}{2\sqrt{2}}(-\sqrt{3}|\kappa_p\mu_p\kappa_q\alpha''|-\sqrt{3}|\kappa_p\mu_p\nu_q\beta''|+|\lambda_p\nu_p\mu_q\alpha''|+|\lambda_p\nu_p\lambda_q\beta''|)$$

$$|\underline{\gamma_{8p}^2}(T_2)\underline{\gamma_7\gamma_{8q}}(E):T_21\rangle=\frac{1}{2\sqrt{2}}(-|\lambda_p\nu_p\kappa_q\alpha''|-|\lambda_p\nu_p\nu_q\beta''|-\sqrt{3}|\kappa_p\mu_p\mu_q\alpha''|-\sqrt{3}|\kappa_p\mu_p\lambda_q\beta''|)$$

$$|\underline{\gamma_{8p}^2}(T_2)\underline{\gamma_7\gamma_{8q}}(T_1):A_2a_2\rangle=\frac{1}{2\sqrt{3}}(-|\kappa_p\mu_p\nu_q\alpha''|-\sqrt{3}|\kappa_p\mu_p\mu_q\beta''|-|\kappa_p\lambda_p\kappa_q\alpha''|+|\kappa_p\lambda_p\nu_q\beta''|$$
$$+|\mu_p\nu_p\kappa_q\alpha''|-|\mu_p\nu_p\nu_q\beta''|-\sqrt{3}|\lambda_p\nu_p\lambda_q\alpha''|-|\lambda_p\nu_p\kappa_q\beta''|)$$

$$|\underline{\gamma_{8p}^2}(T_2)\underline{\gamma_7\gamma_{8q}}(T_1):E\theta\rangle=\frac{1}{2\sqrt{2}}(|\lambda_p\nu_p\nu_q\alpha''|+\sqrt{3}|\lambda_p\nu_p\mu_q\beta''|+\sqrt{3}|\kappa_p\mu_p\lambda_q\alpha''|+|\kappa_p\mu_p\kappa_q\beta''|)$$

$$|\underline{\gamma_{8p}^2}(T_2)\underline{\gamma_7\gamma_{8q}}(T_1):T_11\rangle=\tfrac{1}{4}(-2|\kappa_p\mu_p\kappa_q\alpha''|+2|\kappa_p\mu_p\nu_q\beta''|-\sqrt{3}|\kappa_p\lambda_p\lambda_q\alpha''|-|\kappa_p\lambda_p\kappa_q\beta''|$$
$$+\sqrt{3}|\mu_p\nu_p\lambda_q\alpha''|+|\mu_p\nu_p\kappa_q\beta''|)$$

$$|\underline{\gamma_{8p}^2}(T_2)\underline{\gamma_7\gamma_{8q}}(T_1):T_21\rangle=\tfrac{1}{4}(|\kappa_p\lambda_p\nu_q\alpha''|+\sqrt{3}|\kappa_p\lambda_p\mu_q\beta''|-|\mu_p\nu_p\nu_q\alpha''|-\sqrt{3}|\mu_p\nu_p\mu_q\beta''|$$
$$-2|\lambda_p\nu_p\kappa_q\alpha''|+2|\lambda_p\nu_p\nu_q\beta''|)$$

$$|\underline{\gamma_{8p}^2}(T_2)\underline{\gamma_7\gamma_{8q}}(T_2):A_1a_1\rangle=\frac{1}{2\sqrt{3}}(-\sqrt{3}|\lambda_p\nu_p\nu_q\alpha''|+|\lambda_p\nu_p\mu_q\beta''|+|\kappa_p\lambda_p\mu_q\alpha''|-|\kappa_p\lambda_p\lambda_q\beta''|$$
$$-|\mu_p\nu_p\mu_q\alpha''|+|\mu_p\nu_p\lambda_q\beta''|+|\kappa_p\mu_p\lambda_q\alpha''|-\sqrt{3}|\kappa_p\mu_p\kappa_q\beta''|)$$

$$|\underline{\gamma_{8p}^2}(T_2)\underline{\gamma_7\gamma_{8q}}(T_2):E\theta\rangle=\frac{1}{2\sqrt{6}}(-\sqrt{3}|\lambda_p\nu_p\nu_q\alpha''|+|\lambda_p\nu_p\mu_q\beta''|-2|\kappa_p\lambda_p\mu_q\alpha''|+2|\kappa_p\lambda_p\lambda_q\beta''|$$

$$+2\,|\,\mu_p\nu_p\mu_q\alpha''\,|\,-2\,|\,\mu_p\nu_p\lambda_q\beta''\,|\,+\,|\,\kappa_p\mu_p\lambda_q\alpha''\,|\,-\sqrt{3}\,|\,\kappa_p\mu_p\kappa_q\beta''\,|\,)$$

$$|\,\underline{\gamma_{8p}^2}(T_2)\underline{\gamma_7\gamma_{8q}}(T_2){:}T_1 1\,\rangle=\tfrac{1}{4}(-2\,|\,\lambda_p\nu_p\mu_q\alpha''\,|\,+2\,|\,\lambda_p\nu_p\lambda_q\beta''\,|\,+\,|\,\kappa_p\lambda_p\lambda_q\alpha''\,|\,-\sqrt{3}\,|\,\kappa_p\lambda_p\kappa_q\beta''\,|$$
$$-\,|\,\mu_p\nu_p\lambda_q\alpha''\,|\,+\sqrt{3}\,|\,\mu_p\nu_p\kappa_q\beta''\,|\,)$$

$$|\,\underline{\gamma_{8p}^2}(T_2)\underline{\gamma_7\gamma_{8q}}(T_2){:}T_2 1\,\rangle=\tfrac{1}{4}(-\sqrt{3}\,|\,\kappa_p\lambda_p\nu_q\alpha''\,|\,+\,|\,\kappa_p\lambda_p\mu_q\beta''\,|\,+\sqrt{3}\,|\,\mu_p\nu_p\nu_q\alpha''\,|\,-\,|\,\mu_p\nu_p\mu_q\beta''\,|$$
$$+2\,|\,\kappa_p\mu_p\mu_q\alpha''\,|\,-2\,|\,\kappa_p\mu_p\lambda_q\beta''\,|\,)$$

Configuration $\gamma_{8l}\gamma_{8u}\gamma_7^2$

$$|\,\gamma_{8l}\gamma_{8u}\gamma_7^2{:}A_1a_1\,\rangle=\tfrac{1}{2}(\,|\,\kappa_l\nu_u\alpha''\beta''\,|\,-\,|\,\nu_l\kappa_u\alpha''\beta''\,|\,-\,|\,\lambda_l\mu_u\alpha''\beta''\,|\,+\,|\,\mu_l\lambda_u\alpha''\beta''\,|\,)$$
$$|\,\gamma_{8l}\gamma_{8u}\gamma_7^2{:}A_2a_2\,\rangle=\tfrac{1}{2}(\,|\,\kappa_l\lambda_u\alpha''\beta''\,|\,+\,|\,\lambda_l\kappa_u\alpha''\beta''\,|\,-\,|\,\mu_l\nu_u\alpha''\beta''\,|\,-\,|\,\nu_l\mu_u\alpha''\beta''\,|\,)$$
$$|\,\gamma_{8l}\gamma_{8u}\gamma_7^2{:}E\theta\,\rangle=\tfrac{1}{2}(\,|\,\kappa_l\nu_u\alpha''\beta''\,|\,-\,|\,\nu_l\kappa_u\alpha''\beta''\,|\,+\,|\,\lambda_l\mu_u\alpha''\beta''\,|\,-\,|\,\mu_l\lambda_u\alpha''\beta''\,|\,)$$
$$|\,\gamma_{8l}\gamma_{8u}\gamma_7^2{:}3{:}T_1 1\,\rangle=\frac{1}{2\sqrt{10}}(-\sqrt{3}\,|\,\kappa_l\mu_u\alpha''\beta''\,|\,-\sqrt{3}\,|\,\mu_l\kappa_u\alpha''\beta''\,|\,-3\,|\,\lambda_l\lambda_u\alpha''\beta''\,|\,-5\,|\,\nu_l\nu_u\alpha''\beta''\,|\,)$$
$$|\,\gamma_{8l}\gamma_{8u}\gamma_7^2{:}3{:}T_2 1\,\rangle=\frac{1}{2\sqrt{2}}(-\sqrt{3}\,|\,\kappa_l\kappa_u\alpha''\beta''\,|\,+\,|\,\lambda_l\nu_u\alpha''\beta''\,|\,+\,|\,\nu_l\lambda_u\alpha''\beta''\,|\,+\sqrt{3}\,|\,\mu_l\mu_u\alpha''\beta''\,|\,)$$
$$|\,\gamma_{8l}\gamma_{8u}\gamma_7^2{:}2{:}T_2 1\,\rangle=\frac{1}{\sqrt{2}}(\,|\,\lambda_l\nu_u\alpha''\beta''\,|\,-\,|\,\nu_l\lambda_u\alpha''\beta''\,|\,)$$
$$|\,\gamma_{8l}\gamma_{8u}\gamma_7^2{:}1{:}T_1 1\,\rangle=\frac{1}{\sqrt{10}}(\sqrt{3}\,|\,\kappa_l\mu_u\alpha''\beta''\,|\,+\sqrt{3}\,|\,\mu_l\kappa_u\alpha''\beta''\,|\,-2\,|\,\lambda_l\lambda_u\alpha''\beta''\,|\,)$$

4. d^5 system

The wave function for the first component of each irreducible representation has been given. Other wave functions can be similarly constructed by combining those of the d', d^2, and d^3 systems through proper coupling coefficients.

Configuration $\gamma_{8p}^4\gamma_{8q}$ $(p=l,q=u$ or $p=u,q=l)$

$$|\,\gamma_{8p}^4\gamma_{8q}{:}\Gamma_8\kappa\,\rangle=-\,|\,\kappa_p\lambda_p\mu_p\nu_p\kappa_q\,|$$

Configuration $\gamma_{8p}^3\gamma_{8q}^2$ $(p=l,q=u$ or $p=u,q=l)$

$$|\,\gamma_{8p}^3\underline{\gamma_{8q}^2}(A_1){:}\Gamma_8\kappa\,\rangle=\frac{1}{\sqrt{2}}(\,|\,\kappa_p\lambda_p\mu_p\lambda_q\mu_q\,|\,-\,|\,\kappa_p\lambda_p\mu_p\kappa_q\nu_q\,|\,)$$
$$|\,\gamma_{8p}^3\underline{\gamma_{8q}^2}(E){:}\Gamma_6\alpha'\,\rangle=-\tfrac{1}{2}(\,|\,\kappa_p\lambda_p\nu_p\kappa_q\nu_q\,|\,+\,|\,\kappa_p\lambda_p\nu_p\lambda_q\mu_q\,|\,+\,|\,\lambda_p\mu_p\nu_p\kappa_q\lambda_q\,|\,+\,|\,\lambda_p\mu_p\nu_p\mu_q\nu_q\,|\,)$$
$$|\,\gamma_{8p}^3\underline{\gamma_{8q}^2}(E){:}\Gamma_7\alpha''\,\rangle=\tfrac{1}{2}(\,|\,\lambda_p\mu_p\nu_p\kappa_q\nu_q\,|\,+\,|\,\lambda_p\mu_p\nu_p\lambda_q\mu_q\,|\,-\,|\,\kappa_p\lambda_p\nu_p\kappa_q\lambda_q\,|\,-\,|\,\kappa_p\lambda_p\nu_p\mu_q\nu_q\,|\,)$$
$$|\,\gamma_{8p}^3\underline{\gamma_{8q}^2}(E){:}\Gamma_8\kappa\,\rangle=-\tfrac{1}{2}(\,|\,\kappa_p\lambda_p\mu_p\kappa_q\nu_q\,|\,+\,|\,\kappa_p\lambda_p\mu_p\lambda_q\mu_q\,|\,+\,|\,\kappa_p\mu_p\nu_p\kappa_q\lambda_q\,|\,+\,|\,\kappa_p\mu_p\nu_p\mu_q\nu_q\,|\,)$$

$$|\gamma_{8p}^3\underline{\gamma_{8q}^2}(T_2){:}\Gamma_6\alpha'\rangle=\frac{1}{\sqrt{6}}(-|\kappa_p\lambda_p\mu_p\lambda_q\nu_q|-\sqrt{3}|\kappa_p\mu_p\nu_p\kappa_q\mu_q|+|\lambda_p\mu_p\nu_p\kappa_q\lambda_q|-|\lambda_p\mu_p\nu_p\mu_q\nu_q|)$$

$$|\gamma_{8p}^3\underline{\gamma_{8q}^2}(T_2){:}\Gamma_7\alpha''\rangle=\frac{1}{\sqrt{6}}(\sqrt{3}|\kappa_p\lambda_p\mu_p\kappa_q\mu_q|+|\kappa_p\lambda_p\nu_p\kappa_q\lambda_q|-|\kappa_p\lambda_p\nu_p\mu_q\nu_q|-|\kappa_p\mu_p\nu_p\lambda_q\nu_q|)$$

$$|\gamma_{8p}^3\underline{\gamma_{8q}^2}(T_2){:}\tfrac{3}{2}\Gamma_8\kappa\rangle=\frac{1}{\sqrt{30}}(-4|\kappa_p\lambda_p\nu_p\kappa_q\mu_q|-|\kappa_p\mu_p\nu_p\kappa_q\lambda_q|+|\kappa_p\mu_p\nu_p\mu_q\nu_q|-2\sqrt{3}|\lambda_p\mu_p\nu_p\lambda_q\nu_q|)$$

$$|\gamma_{8p}^3\underline{\gamma_{8q}^2}(T_2){:}\tfrac{5}{2}\Gamma_8\kappa\rangle=\frac{1}{\sqrt{10}}(\sqrt{3}|\kappa_p\lambda_p\nu_p\kappa_q\mu_q|-\sqrt{3}|\kappa_p\mu_p\nu_p\kappa_q\lambda_q|+\sqrt{3}|\kappa_p\mu_p\nu_p\mu_q\nu_q|-|\lambda_p\mu_p\nu_p\lambda_q\nu_q|)$$

Configuration $\gamma_{8p}^2\gamma_{8q}\gamma_7^2$ $(p=l,q=u$ or $p=u,q=l)$

$$|\gamma_{8p}^2(E)\gamma_{8q}\gamma_7^2{:}\Gamma_6\alpha'\rangle=\tfrac{1}{2}(|\kappa_p\nu_p\lambda_q\alpha''\beta''|+|\lambda_p\mu_p\lambda_q\alpha''\beta''|+|\kappa_p\lambda_p\nu_q\alpha''\beta''|+|\mu_p\nu_p\nu_q\alpha''\beta''|)$$

$$|\gamma_{8p}^2(E)\gamma_{8q}\gamma_7^2{:}\Gamma_7\alpha''\rangle=\tfrac{1}{2}(-|\kappa_p\nu_p\nu_q\alpha''\beta''|-|\lambda_p\mu_p\nu_q\alpha''\beta''|+|\kappa_p\lambda_p\lambda_q\alpha''\beta''|+|\mu_p\nu_p\lambda_q\alpha''\beta''|)$$

$$|\gamma_{8p}^2(E)\gamma_{8q}\gamma_7^2{:}\Gamma_8\kappa\rangle=\tfrac{1}{2}(|\kappa_p\nu_p\kappa_q\alpha''\beta''|+|\lambda_p\mu_p\kappa_q\alpha''\beta''|+|\kappa_p\lambda_p\mu_q\alpha''\beta''|+|\mu_p\nu_p\mu_q\alpha''\beta''|)$$

$$|\gamma_{8p}^2(A_1)\gamma_{8q}\gamma_7^2{:}\Gamma_8\kappa\rangle=\frac{1}{\sqrt{2}}(|\kappa_p\nu_p\kappa_q\alpha''\beta''|-|\lambda_p\mu_p\kappa_q\alpha''\beta''|)$$

$$|\gamma_{8p}^2(T_2)\gamma_{8q}\gamma_7^2{:}\Gamma_6\alpha'\rangle=\frac{1}{\sqrt{6}}(|\lambda_p\nu_p\kappa_q\alpha''\beta''|+\sqrt{3}|\kappa_p\mu_p\mu_q\alpha''\beta''|-|\kappa_p\lambda_p\nu_q\alpha''\beta''|+|\mu_p\nu_p\nu_q\alpha''\beta''|)$$

$$|\gamma_{8p}^2(T_2)\gamma_{8q}\gamma_7^2{:}\Gamma_7\alpha''\rangle=\frac{1}{\sqrt{6}}(-\sqrt{3}|\kappa_p\mu_p\kappa_q\alpha''\beta''|-|\kappa_p\lambda_p\lambda_q\alpha''\beta''|+|\mu_p\nu_p\lambda_q\alpha''\beta''|+|\lambda_p\nu_p\mu_q\alpha''\beta''|)$$

$$|\gamma_{8p}^2(T_2)\gamma_{8q}\gamma_7^2{:}\tfrac{3}{2}\Gamma_8\kappa\rangle=\frac{1}{\sqrt{30}}(4|\kappa_p\mu_p\lambda_q\alpha''\beta''|+|\kappa_p\lambda_p\mu_q\alpha''\beta''|$$
$$-|\mu_p\nu_p\mu_q\alpha''\beta''|+2\sqrt{3}|\lambda_p\nu_p\nu_q\alpha''\beta''|)$$

$$|\gamma_{8p}^2(T_2)\gamma_{8q}\gamma_7^2{:}\tfrac{5}{2}\Gamma_8\kappa\rangle=\frac{1}{\sqrt{10}}(-\sqrt{3}|\kappa_p\mu_p\lambda_q\alpha''\beta''|+\sqrt{3}|\kappa_p\lambda_p\mu_q\alpha''\beta''|-\sqrt{3}|\mu_p\nu_p\mu_q\alpha''\beta''|$$
$$+|\lambda_p\nu_p\nu_q\alpha''\beta''|)$$

Configuration $\gamma_{8p}^3\gamma_7^2$ $(p=l$ or $p=u)$

$$|\gamma_{8p}^3\gamma_7^2{:}\Gamma_8\kappa\rangle=-|\kappa_p\lambda_p\mu_p\alpha''\beta''|$$

Configuration $\gamma_{8p}^4\gamma_7$ $(p=l$ or $p=u)$

$$|\gamma_{8p}^4\gamma_7{:}\Gamma_7\alpha''\rangle=-|\kappa_p\lambda_p\mu_p\nu_p\alpha''|$$

Configuration $\gamma_{8p}^3\gamma_{8q}\gamma_7$ $(p=l,q=u$ or $p=u,q=l)$

$$|\gamma_{8p}^3\underline{\gamma_7\gamma_{8q}}(E){:}\Gamma_6\alpha'\rangle=\tfrac{1}{2}(|\kappa_p\lambda_p\nu_p\kappa_q\alpha''|+|\kappa_p\lambda_p\nu_p\nu_q\beta''|-|\lambda_p\mu_p\nu_p\mu_q\alpha''|-|\lambda_p\mu_p\nu_p\lambda_q\beta''|)$$

$$|\gamma_{8p}^3\underline{\gamma_7\gamma_{8q}}(E){:}\Gamma_7\alpha''\rangle=\tfrac{1}{2}(-|\lambda_p\mu_p\nu_p\kappa_q\alpha''|-|\lambda_p\mu_p\nu_p\nu_q\beta''|-|\kappa_p\lambda_p\nu_p\mu_q\alpha''|-|\kappa_p\lambda_p\nu_p\lambda_q\beta''|)$$

$$|\gamma_{8p}^3\underline{\gamma_7\gamma_{8q}}(E):\Gamma_8\kappa\rangle=\tfrac{1}{2}(\,|\kappa_p\lambda_p\mu_p\kappa_q\alpha''|+|\kappa_p\lambda_p\mu_p\nu_q\beta''|-|\kappa_p\mu_p\nu_p\mu_q\alpha''|-|\kappa_p\mu_p\nu_p\lambda_q\beta''|\,)$$

$$|\gamma_{8p}^3\underline{\gamma_7\gamma_{8q}}(T_1):\Gamma_6\alpha'\rangle=\frac{1}{2\sqrt{6}}(-3|\kappa_p\lambda_p\mu_p\lambda_q\alpha''|-\sqrt{3}|\kappa_p\lambda_p\mu_p\kappa_q\beta''|-2|\kappa_p\lambda_p\nu_p\kappa_q\alpha''|$$
$$+2|\kappa_p\lambda_p\nu_p\nu_q\beta''|+|\kappa_p\mu_p\nu_p\nu_q\alpha''|+\sqrt{3}|\kappa_p\mu_p\nu_p\mu_q\beta''|\,)$$

$$|\gamma_{8p}^3\underline{\gamma_7\gamma_{8q}}(T_1):\Gamma_7\alpha''\rangle=\frac{1}{2\sqrt{6}}(\,|\kappa_p\lambda_p\mu_p\nu_q\alpha''|+\sqrt{3}|\kappa_p\lambda_p\mu_p\mu_q\beta''|+3|\kappa_p\mu_p\nu_p\lambda_q\alpha''|$$
$$+\sqrt{3}|\kappa_p\mu_p\nu_p\kappa_q\beta''|-2|\lambda_p\mu_p\nu_p\kappa_q\alpha''|+2|\lambda_p\mu_p\nu_p\nu_q\beta''|\,)$$

$$|\gamma_{8p}^3\underline{\gamma_7\gamma_{8q}}(T_1):\tfrac{3}{2}\Gamma_8\kappa\rangle=\frac{1}{\sqrt{10}}(\,\sqrt{3}|\kappa_p\lambda_p\mu_p\kappa_q\alpha''|-\sqrt{3}|\kappa_p\lambda_p\mu_p\nu_q\beta''|-|\kappa_p\lambda_p\nu_p\nu_q\alpha''|$$
$$-\sqrt{3}|\kappa_p\lambda_p\nu_p\mu_q\beta''|\,)$$

$$|\gamma_{8p}^3\underline{\gamma_7\gamma_{8q}}(T_1):\tfrac{5}{2}\Gamma_8\kappa\rangle=\frac{1}{2\sqrt{30}}(-2|\kappa_p\lambda_p\mu_p\kappa_q\alpha''|+2|\kappa_p\lambda_p\mu_p\nu_q\beta''|-\sqrt{3}|\kappa_p\lambda_p\nu_p\nu_q\alpha''|$$
$$-3|\kappa_p\lambda_p\nu_p\mu_q\beta''|+5\sqrt{3}|\lambda_p\mu_p\nu_p\lambda_q\alpha''|+5|\lambda_p\mu_p\nu_p\kappa_q\beta''|\,)$$

$$|\gamma_{8p}^3\underline{\gamma_7\gamma_{8q}}(T_2):\Gamma_6\alpha'\rangle=\frac{1}{2\sqrt{6}}(\,-|\kappa_p\lambda_p\mu_p\lambda_q\alpha''|+\sqrt{3}|\kappa_p\lambda_p\mu_p\kappa_q\beta''|+3|\kappa_p\mu_p\nu_p\nu_q\alpha''|$$
$$-\sqrt{3}|\kappa_p\mu_p\nu_p\mu_q\beta''|+2|\lambda_p\mu_p\nu_p\mu_q\alpha''|-2|\lambda_p\mu_p\nu_p\lambda_q\beta''|\,)$$

$$|\gamma_{8p}^3\underline{\gamma_7\gamma_{8q}}(T_2):\Gamma_7\alpha''\rangle=\frac{1}{2\sqrt{6}}(-3|\kappa_p\lambda_p\mu_p\nu_q\alpha''|+\sqrt{3}|\kappa_p\lambda_p\mu_p\mu_q\beta''|+2|\kappa_p\lambda_p\nu_p\mu_q\alpha''|$$
$$-2|\kappa_p\lambda_p\nu_p\lambda_q\beta''|-|\kappa_p\mu_p\nu_p\lambda_q\alpha''|+\sqrt{3}|\kappa_p\mu_p\nu_p\kappa_q\beta''|\,)$$

$$|\gamma_{8p}^3\underline{\gamma_7\gamma_{8q}}(T_2):\tfrac{3}{2}\Gamma_8\kappa\rangle=\frac{1}{\sqrt{30}}(\,2\sqrt{3}|\kappa_p\lambda_p\nu_p\nu_q\alpha''|-2|\kappa_p\lambda_p\nu_p\mu_q\beta''|-|\kappa_p\mu_p\nu_p\mu_q\alpha''|$$
$$+|\kappa_p\mu_p\nu_p\lambda_q\beta''|-\sqrt{3}|\lambda_p\mu_p\nu_p\lambda_q\alpha''|+3|\lambda_p\mu_p\nu_p\kappa_q\beta''|\,)$$

$$|\gamma_{8p}^3\underline{\gamma_7\gamma_{8q}}(T_2):\tfrac{5}{2}\Gamma_8\kappa\rangle=\frac{1}{2\sqrt{10}}(-3|\kappa_p\lambda_p\nu_p\nu_q\alpha''|+\sqrt{3}|\kappa_p\lambda_p\nu_p\mu_q\beta''|-2\sqrt{3}|\kappa_p\mu_p\nu_p\mu_q\alpha''|$$
$$+2\sqrt{3}|\kappa_p\mu_p\nu_p\lambda_q\beta''|-|\lambda_p\mu_p\nu_p\lambda_q\alpha''|+\sqrt{3}|\lambda_p\mu_p\nu_p\kappa_q\beta''|\,)$$

Configuration $\gamma_{8l}^2\gamma_{8u}^2\gamma_7$

$$|\underline{\gamma_{8l}^2}(A_1)\gamma_7\gamma_{8u}^2(A_1):\Gamma_7\alpha''\rangle=\tfrac{1}{2}(\,|\kappa_l\nu_l\kappa_u\nu_u\alpha''|-|\kappa_l\nu_l\lambda_u\mu_u\alpha''|-|\lambda_l\mu_l\kappa_u\nu_u\alpha''|+|\lambda_l\mu_l\lambda_u\mu_u\alpha''|\,)$$

$$|\underline{\gamma_{8l}^2(E)\gamma_7}((\Gamma_8))\underline{\gamma_{8u}^2}(A_1):\Gamma_8\kappa\rangle=\tfrac{1}{2}(\,|\kappa_l\nu_l\kappa_u\nu_u\beta''|-|\kappa_l\nu_l\lambda_u\mu_u\beta''|+|\lambda_l\mu_l\kappa_u\nu_u\beta''|-|\lambda_l\mu_l\lambda_u\mu_u\beta''|\,)$$

$$|\underline{\gamma_{8l}^2(T_2)\gamma_7}((\Gamma_6))\underline{\gamma_{8u}^2}(A_1):\Gamma_6\alpha'\rangle=\frac{1}{2\sqrt{3}}(\,|\kappa_l\lambda_l\kappa_u\nu_u\alpha''|-|\mu_l\nu_l\kappa_u\nu_u\alpha''|-2|\lambda_l\nu_l\kappa_u\nu_u\beta''|$$
$$-|\kappa_l\lambda_l\lambda_u\mu_u\alpha''|+|\mu_l\nu_l\lambda_u\mu_u\alpha''|+2|\lambda_l\nu_l\lambda_u\mu_u\beta''|\,)$$

$$|\underline{\gamma_{8l}^2(T_2)\gamma_7}((\Gamma_8))\underline{\gamma_{8u}^2}(A_1):\Gamma_8\kappa\rangle=\frac{1}{\sqrt{2}}(\,|\lambda_l\nu_l\kappa_u\nu_u\alpha''|-|\lambda_l\nu_l\lambda_u\mu_u\alpha''|\,)$$

$$|\underline{\gamma_{8l}^2(A_1)}\gamma_7\gamma_{8u}^2(E):\Gamma_8\kappa\rangle=\tfrac{1}{2}(\,|\kappa_l\nu_l\kappa_u\nu_u\beta''|+|\kappa_l\nu_l\lambda_u\mu_u\beta''|-|\lambda_l\mu_l\kappa_u\nu_u\beta''|-|\lambda_l\mu_l\lambda_u\mu_u\beta''|\,)$$

$$\begin{aligned}|\underline{\gamma_{8l}^2(E)\gamma_7}((\Gamma_8))\underline{\gamma_{8u}^2}(E):\Gamma_6\alpha'\rangle=\frac{1}{2\sqrt{2}}(\,&|\kappa_l\lambda_l\kappa_u\nu_u\alpha''|+|\kappa_l\lambda_l\lambda_u\mu_u\alpha''|+|\mu_l\nu_l\kappa_u\nu_u\alpha''|\\&+|\mu_l\nu_l\lambda_u\mu_u\alpha''|-|\kappa_l\nu_l\kappa_u\lambda_u\alpha''|-|\kappa_l\nu_l\mu_u\nu_u\alpha''|\\&-|\lambda_l\mu_l\kappa_u\lambda_u\alpha''|-|\lambda_l\mu_l\mu_u\nu_u\alpha''|\,)\end{aligned}$$

$$\begin{aligned}|\underline{\gamma_{8l}^2(E)\gamma_7}((\Gamma_8))\underline{\gamma_{8u}^2}(E):\Gamma_7\alpha''\rangle=\frac{1}{2\sqrt{2}}(\,&|\kappa_l\nu_l\kappa_u\nu_u\alpha''|+|\kappa_l\nu_l\lambda_u\mu_u\alpha''|+|\lambda_l\mu_l\kappa_u\nu_u\alpha''|\\&+|\lambda_l\mu_l\lambda_u\mu_u\alpha''|+|\kappa_l\lambda_l\kappa_u\lambda_u\alpha''|+|\kappa_l\lambda_l\mu_u\nu_u\alpha''|\\&+|\mu_l\nu_l\kappa_u\lambda_u\alpha''|+|\mu_l\nu_l\mu_u\nu_u\alpha''|\,)\end{aligned}$$

$$\begin{aligned}|\underline{\gamma_{8l}^2(E)\gamma_7}((\Gamma_8))\underline{\gamma_{8u}^2}(E):\Gamma_8\kappa\rangle=\frac{1}{2\sqrt{2}}(\,&|\kappa_l\nu_l\kappa_u\nu_u\beta''|+|\kappa_l\nu_l\lambda_u\mu_u\beta''|+|\lambda_l\mu_l\kappa_u\nu_u\beta''|\\&+|\lambda_l\mu_l\lambda_u\mu_u\beta''|-|\kappa_l\lambda_l\kappa_u\lambda_u\beta''|-|\kappa_l\lambda_l\mu_u\nu_u\beta''|\\&-|\mu_l\nu_l\kappa_u\lambda_u\beta''|-|\mu_l\nu_l\mu_u\nu_u\beta''|\,)\end{aligned}$$

$$\begin{aligned}|\underline{\gamma_{8l}^2(T_2)\gamma_7}((\Gamma_6))\underline{\gamma_{8u}^2}(E):\Gamma_8\kappa\rangle=\frac{1}{2\sqrt{3}}(&-2\,|\kappa_l\mu_l\kappa_u\lambda_u\alpha''|-|\kappa_l\lambda_l\kappa_u\lambda_u\beta''|+|\mu_l\nu_l\kappa_u\lambda_u\beta''|\\&-2\,|\kappa_l\mu_l\mu_u\nu_u\alpha''|-|\kappa_l\lambda_l\mu_u\nu_u\beta''|+|\mu_l\nu_l\mu_u\nu_u\beta''|\,)\end{aligned}$$

$$\begin{aligned}|\underline{\gamma_{8l}^2(T_2)\gamma_7}((\Gamma_8))\underline{\gamma_{8u}^2}(E):\Gamma_6\alpha'\rangle=\frac{1}{2\sqrt{3}}(\,&|\kappa_l\lambda_l\kappa_u\nu_u\alpha''|-|\mu_l\nu_l\kappa_u\nu_u\alpha''|+|\lambda_l\nu_l\kappa_u\nu_u\beta''|\\&+|\kappa_l\lambda_l\lambda_u\mu_u\alpha''|-|\mu_l\nu_l\lambda_u\mu_u\alpha''|+|\lambda_l\nu_l\lambda_u\mu_u\beta''|\\&-\sqrt{3}\,|\kappa_l\mu_l\kappa_u\lambda_u\beta''|-\sqrt{3}\,|\kappa_l\mu_l\mu_u\nu_u\beta''|\,)\end{aligned}$$

$$\begin{aligned}|\underline{\gamma_{8l}^2(T_2)\gamma_7}((\Gamma_8))\underline{\gamma_{8u}^2}(E):\Gamma_7\alpha''\rangle=\frac{1}{2\sqrt{3}}(\,&\sqrt{3}\,|\kappa_l\mu_l\kappa_u\nu_u\beta''|+\sqrt{3}\,|\kappa_l\mu_l\lambda_u\mu_u\beta''|+|\kappa_l\lambda_l\kappa_u\lambda_u\alpha''|\\&-|\mu_l\nu_l\kappa_u\lambda_u\alpha''|+|\lambda_l\nu_l\kappa_u\lambda_u\beta''|+|\kappa_l\lambda_l\mu_u\nu_u\alpha''|\\&-|\mu_l\nu_l\mu_u\nu_u\alpha''|+|\lambda_l\nu_l\mu_u\nu_u\beta''|\,)\end{aligned}$$

$$\begin{aligned}|\underline{\gamma_{8l}^2(T_2)\gamma_7}((\Gamma_8))\underline{\gamma_{8u}^2}(E):\Gamma_8\kappa\rangle=\frac{1}{2\sqrt{3}}(\,&\sqrt{3}\,|\lambda_l\nu_l\kappa_u\nu_u\alpha''|+\sqrt{3}\,|\lambda_l\nu_l\lambda_u\mu_u\alpha''|-|\kappa_l\mu_l\kappa_u\lambda_u\alpha''|\\&+|\kappa_l\lambda_l\kappa_u\lambda_u\beta''|-|\mu_l\nu_l\kappa_u\lambda_u\beta''|-|\kappa_l\mu_l\mu_u\nu_u\alpha''|\\&+|\kappa_l\lambda_l\mu_u\nu_u\beta''|-|\mu_l\nu_l\mu_u\nu_u\beta''|\,)\end{aligned}$$

TABLE I. The ^2E electrostatic matrix block in the strong-field coupling scheme for the d^3 system.

^2E	t_2^3	$t_2^2(^1A_1)e$	$t_2^2(^1E)e$	e^3
t_2^3	$3A_0-6B_0+3C_0$	$-6\sqrt{2}B_1$	$3\sqrt{2}B_1$	0
$t_2^2(^1A_1)e$		$2A_2+A_0$ $-2B_2+10B_0$ $+C_2+5C_0$	$-10B_2$	$\sqrt{3}(2B_2+C_2)$
$t_2^2(^1E)e$			$2A_2+A_0$ $-2B_2+B_0$ $+C_2+2C_0$	$-2\sqrt{3}B_2$
e^3				$3A_4-8B_4+4C_4$

$$|\underline{\gamma_{8l}^2(A_1)\gamma_7}\gamma_{8u}^2(T_2):\Gamma_6\alpha'\rangle=\frac{1}{2\sqrt{3}}(\,|\kappa_l\nu_l\kappa_u\lambda_u\alpha''|-|\kappa_l\nu_l\mu_u\nu_u\alpha''|-|\lambda_l\mu_l\kappa_u\lambda_u\alpha''|$$
$$+|\lambda_l\mu_l\mu_u\nu_u\alpha''|-2|\kappa_l\nu_l\lambda_u\nu_u\beta''|+2|\lambda_l\mu_l\lambda_u\nu_u\beta''|\,)$$

$$|\underline{\gamma_{8l}^2(A_1)\gamma_7}\gamma_{8u}^2(T_2):\Gamma_8\kappa\rangle=\frac{1}{\sqrt{2}}(\,|\kappa_l\nu_l\lambda_u\nu_u\alpha''|-|\lambda_l\mu_l\lambda_u\nu_u\alpha''|\,)$$

$$|\underline{\gamma_{8l}^2(E)\gamma_7}((\Gamma_8))\underline{\gamma_{8u}^2}(T_2):\Gamma_6\alpha'\rangle=\frac{1}{2\sqrt{3}}(\,|\kappa_l\nu_l\lambda_u\nu_u\beta''|+|\lambda_l\mu_l\lambda_u\nu_u\beta''|-\sqrt{3}|\kappa_l\lambda_l\kappa_u\mu_u\beta''|$$
$$-\sqrt{3}|\mu_l\nu_l\kappa_u\mu_u\beta''|+|\kappa_l\nu_l\kappa_u\lambda_u\alpha''|-|\kappa_l\nu_l\mu_u\nu_u\alpha''|$$
$$+|\lambda_l\mu_l\kappa_u\lambda_u\alpha''|-|\lambda_l\mu_l\mu_u\nu_u\alpha''|\,)$$

$$|\underline{\gamma_{8l}^2(E)\gamma_7}((\Gamma_8))\underline{\gamma_{8u}^2}(T_2):\Gamma_7\alpha''\rangle=\frac{1}{2\sqrt{3}}(-|\kappa_l\lambda_l\kappa_u\lambda_u\alpha''|+|\kappa_l\lambda_l\mu_u\nu_u\alpha''|-|\mu_l\nu_l\kappa_u\lambda_u\alpha''|$$
$$+|\mu_l\nu_l\mu_u\nu_u\alpha''|-\sqrt{3}|\kappa_l\nu_l\kappa_u\mu_u\beta''|-\sqrt{3}|\lambda_l\mu_l\kappa_u\mu_u\beta''|$$
$$-|\kappa_l\lambda_l\lambda_u\nu_u\beta''|-|\mu_l\nu_l\lambda_u\nu_u\beta''|\,)$$

TABLE II. The $^2T_1$ electrostatic matrix block in the strong-field coupling scheme for the d^3 system.

$^2T_1$	t_2^3	$t^2(^3T_1)e$	$t_2^2(^1T_2)e$	$t_2e^2(^3A_2)$	$t_2e^2(^1E)$
t_2^3	$3A_0-6B_0+3C_0$	$3B_1$	$-3B_1$	0	$-2\sqrt{3}B_2$
$t_2^2(^3T_1)e$		$2A_2+A_0$ $+5B_2-5B_0+3C_2$	$-3B_2$	$3B_1$	$-3\sqrt{3}B_1$
$t_2^2(^1T_2)e$			$2A_2+A_0$ $-7B_2+B_0$ $+C_2+2C_0$	$-3B_1$	$\sqrt{3}B_1$
$t_2e^2(^3A_2)$				A_4+2A_2 $-8B_4+2B_2+3C_2$	$-2\sqrt{3}B_2$
$t_2e^2(^1E)$					A_4+2A_2 $-2B_2+2C_4+C_2$

TABLE III. The $^2T_2$ electrostatic matrix block in the strong-field coupling scheme for the d^3 system.

$^2T_2$	t_2^3	$t_2^2(^3T_1)e$	$t_2^2(^1T_2)e$	$t_2e^2(^1A_1)$	$t_2e^2(^1E)$
t_2^3	$3A_0+5C_0$	$-3\sqrt{3}B_1$	$5\sqrt{3}B_1$	$4B_2+2C_2$	$2B_2$
$t^2(^3T_1)e$		$2A_2+A_0$ $-B_2-5B_0+3C_2$	$-3B_2$	$-3\sqrt{3}B_1$	$-3\sqrt{3}B_1$
$t_2^2(^1T_2)e$			$2A_2+A_0$ $+3B_2+B_0$ $+C_2+2C_0$	$\sqrt{3}B_1$	$-\sqrt{3}B_1$
$t_2e^2(^1A_1)$				A_4+2A_2 $+8B_4-2B_2$ $+4C_4+C_2$	$10B_2$
$t_2e^2(^1E)$					A_4+2A_2 $-2B_2+2C_4+C_2$

$$
\begin{aligned}
|\underline{\gamma_{8l}^2(E)\gamma_7}((\Gamma_8))\underline{\gamma_{8u}^2}(T_2):\tfrac{3}{2}\Gamma_8\kappa\rangle = \frac{1}{2\sqrt{15}}(&4\,|\kappa_l\lambda_l\kappa_u\mu_u\alpha''|+4\,|\mu_l\nu_l\kappa_u\mu_u\alpha''|-|\kappa_l\lambda_l\kappa_u\lambda_u\beta''|\\
&+|\kappa_l\lambda_l\mu_u\nu_u\beta''|-|\mu_l\nu_l\kappa_u\lambda_u\beta''|+|\mu_l\nu_l\mu_u\nu_u\beta''|\\
&-2\sqrt{3}\,|\kappa_l\nu_l\lambda_u\nu_u\alpha''|-2\sqrt{3}\,|\lambda_l\mu_l\lambda_u\nu_u\alpha''|)
\end{aligned}
$$

$$
\begin{aligned}
|\underline{\gamma_{8l}^2(E)\gamma_7}((\Gamma_8))\underline{\gamma_{8u}^2}(T_2):\tfrac{5}{2}\Gamma_8\kappa\rangle = \frac{1}{2\sqrt{5}}(&-\sqrt{3}\,|\kappa_l\lambda_l\kappa_u\mu_u\alpha''|-\sqrt{3}\,|\mu_l\nu_l\kappa_u\mu_u\alpha''|-\sqrt{3}\,|\kappa_l\lambda_l\kappa_u\lambda_u\beta''|\\
&+\sqrt{3}\,|\kappa_l\lambda_l\mu_u\nu_u\beta''|-\sqrt{3}\,|\mu_l\nu_l\kappa_u\lambda_u\beta''|+\sqrt{3}\,|\mu_l\nu_l\mu_u\nu_u\beta''|\\
&-|\kappa_l\nu_l\lambda_u\nu_u\alpha''|-|\lambda_l\mu_l\lambda_u\nu_u\alpha''|)
\end{aligned}
$$

$$
\begin{aligned}
|\underline{\gamma_{8l}^2(T_2)\gamma_7}((\Gamma_6))\underline{\gamma_{8u}^2}(T_2):\Gamma_7\alpha''\rangle = \tfrac{1}{6}(&|\kappa_l\lambda_l\kappa_u\lambda_u\alpha''|-|\kappa_l\lambda_l\mu_u\nu_u\alpha''|-|\mu_l\nu_l\kappa_u\lambda_u\alpha''|\\
&+|\mu_l\nu_l\mu_u\nu_u\alpha''|+2\,|\lambda_l\nu_l\mu_u\nu_u\beta''|-2\,|\lambda_l\nu_l\kappa_u\lambda_u\beta''|\\
&+4\,|\kappa_l\mu_l\lambda_u\nu_u\alpha''|+2\,|\kappa_l\lambda_l\lambda_u\nu_u\beta''|-2\,|\mu_l\nu_l\lambda_u\nu_u\beta''|)
\end{aligned}
$$

$$
\begin{aligned}
|\underline{\gamma_{8l}^2(T_2)\gamma_7}((\Gamma_6))\underline{\gamma_{8u}^2}(T_2):\Gamma_8\kappa\rangle = \frac{1}{3\sqrt{2}}(&|\kappa_l\lambda_l\kappa_u\mu_u\alpha''|-|\mu_l\nu_l\kappa_u\mu_u\alpha''|-2\,|\lambda_l\nu_l\kappa_u\mu_u\beta''|\\
&+2\,|\kappa_l\mu_l\kappa_u\lambda_u\alpha''|-|2\kappa_l\mu_l\mu_u\nu_u\alpha''|+|\kappa_l\lambda_l\kappa_u\lambda_u\beta''|\\
&-|\kappa_l\lambda_l\mu_u\nu_u\beta''|-|\mu_l\nu_l\kappa_u\lambda_u\beta''|+|\mu_l\nu_l\mu_u\nu_u\beta''|)
\end{aligned}
$$

TABLE IV. The $^4T_1$ electrostatic matrix block in the strong-field coupling scheme for the d^3 system.

$^4T_1$	$t_2^2(^3T_1)e$	$t_2e^2(^3A_2)$
$t_2^2(^3T_1)e$	$2A_2+A_0$ $+2B_2-5B_0$	$6B_1$
$t_2e^2(^3A_2)$		A_4+2A_2 $-8B_4-4B_2$

TABLE V. The $^2A_1$ electrostatic matrix block (element) in the strong-field coupling scheme for the d^3 system.

$^2A_1$	$t_2^2(^1E)e$
$t_2^2(^1E)e$	$2A_2+A_0-12B_2+B_0+C_2+2C_0$

TABLE VI. The $^2A_2$ electrostatic matrix block (element) in the strong-field coupling scheme for the d^3 system.

$^2A_2$	$t_2^2(^1E)e$
$t_2^2(^1E)e$	$2A_2+A_0+8B_2+B_0+C_2+2C_0$

TABLE VII. The $^4A_2$ electrostatic matrix block (element) in the strong-field coupling scheme for the d^3 system.

$^4A_2$	t_2^3
t_2^3	$3A_0-15B_0$

$$|\underline{\gamma_{8l}^2(T_2)\gamma_7}((\Gamma_8))\underline{\gamma_{8u}^2}(T_2):\Gamma_6\alpha'\rangle=\frac{1}{\sqrt{6}}(\,|\lambda_l\nu_l\lambda_u\nu_u\alpha''|-|\kappa_l\mu_l\kappa_u\mu_u\alpha''|+|\kappa_l\lambda_l\kappa_u\mu_u\beta''|$$
$$-|\mu_l\nu_l\kappa_u\mu_u\beta''|+|\kappa_l\mu_l\kappa_u\lambda_u\beta''|-|\kappa_l\mu_l\mu_u\nu_u|\,)$$

$$|\underline{\gamma_{8l}^2(T_2)\gamma_7}((\Gamma_8))\underline{\gamma_{8u}^2}(T_2):\Gamma_7\alpha''\rangle=\frac{1}{3\sqrt{2}}(-3|\lambda_l\nu_l\kappa_u\mu_u\alpha''|-|\kappa_l\lambda_l\kappa_u\lambda_u\alpha''|+|\kappa_l\lambda_l\mu_u\nu_u\alpha''|$$
$$+|\mu_l\nu_l\kappa_u\lambda_u\alpha''|-|\mu_l\nu_l\mu_u\nu_u\alpha''|-|\lambda_l\nu_l\kappa_u\lambda_u\beta''|$$
$$+|\lambda_l\nu_l\mu_u\nu_u\beta''|-|\kappa_l\mu_l\lambda_u\nu_u\alpha''|+|\kappa_l\lambda_l\lambda_u\nu_u\beta''|$$
$$-|\mu_l\nu_l\lambda_u\nu_u\beta''|\,)$$

$$|\underline{\gamma_{8l}^2(T_2)\gamma_7}((\Gamma_8))\underline{\gamma_{8u}^2}(T_2):\tfrac{3}{2}\Gamma_8\kappa\rangle=\frac{1}{3\sqrt{10}}(4|\kappa_l\lambda_l\kappa_u\mu_u\alpha''|-4|\mu_l\nu_l\kappa_u\mu_u\alpha''|+4|\lambda_l\nu_l\kappa_u\mu_u\beta''|$$
$$-|\kappa_l\mu_l\kappa_u\lambda_u\alpha''|+|\kappa_l\mu_l\mu_u\nu_u\alpha''|+|\kappa_l\lambda_l\kappa_u\lambda_u\beta''|$$
$$-|\kappa_l\lambda_l\mu_u\nu_u\beta''|-|\mu_l\nu_l\kappa_u\lambda_u\beta''|+|\mu_l\nu_l\mu_u\nu_u\beta''|$$
$$-6|\kappa_l\mu_l\lambda_u\nu_u\beta''|\,)$$

$$|\underline{\gamma_{8l}^2(T_2)\gamma_7}((\Gamma_8))\underline{\gamma_{8u}^2}(T_2):\tfrac{5}{2}\Gamma_8\kappa\rangle=\frac{1}{\sqrt{10}}(-|\kappa_l\lambda_l\kappa_u\mu_u\alpha''|+|\mu_l\nu_l\kappa_u\mu_u\alpha''|-|\lambda_l\nu_l\kappa_u\mu_u\beta''|$$
$$-|\kappa_l\mu_l\kappa_u\lambda_u\alpha''|+|\kappa_l\mu_l\mu_u\nu_u\alpha''|+|\kappa_l\lambda_l\kappa_u\lambda_u\beta''|$$
$$-|\kappa_l\lambda_l\mu_u\nu_u\beta''|-|\mu_l\nu_l\kappa_u\lambda_u\beta''|+|\mu_l\nu_l\mu_u\nu_u\beta''|$$
$$-|\kappa_l\mu_l\lambda_u\nu_u\beta''|\,)$$

APPENDIX B

The transformation matrices between the $\gamma_{8l}^{n_1}\gamma_{8u}^{n_2}\gamma_7^{n_3}$ and $\gamma_{8t_2}^{n_1}\gamma_{8e}^{n_2}\gamma_7^{n_3}$ (wave functions are given in Appendix A) and those between the $\gamma_{8t_2}^{n_1}\gamma_{8e}^{n_2}\gamma_7^{n_3}$ and $t_2^{m_1}e^{m_2}$ wave functions are given in Ref. 27.

TABLE VIII. The $^4T_2$ electrostatic matrix block (element) in the strong-field coupling scheme for the d^3 system.

$^4T_2$	$t_2^2(^3T_1)e$
$t_2^2(^3T_1)e$	$2A_2+A_0-10B_2-5B_0$

APPENDIX C

The electrostatic matrices for the d^3 system in the strong-field coupling scheme are given in Tables I–VIII.

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