The effects of potentials with point group symmetry on a single d-electron

Given a single d-electron, otherwise only influenced by a potential $V(r)$ with spherical symmetry, this set of calculations determines the effects that perturbations with symmetries belonging to different point groups would have on it. The total single-electron Hamiltonian being considered is

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(r) + V_{CF}(r,\theta,\phi). \tag{1}$$

This analysis is based on Clyde Morrison's work, specifically on *Angular Momentum Theory Applied to Interactions in Solids* (1988) and *Crystal Fields for Transition-Metal Ions in Laser Host Materials* (1992). In there the following expression is used for the crystal field potential

$$H_{CF} = \sum_{n,m} B^*_{n,m} C_{n,m}(\theta,\phi) \tag{2}$$

where $C_{k,q} = \sqrt{\frac{4\pi}{2k+1}} Y_{k,q}$, $n = 0, 2, 4$, $m = -n, -n+1, \ldots, n-1, n$, and the $B_{m,m}$ are accompanying coefficients which in principle could contain an arbitrary radial dependence, but whose influence in the perturbative effect is simply in providing a radial average over the appropriate wave-functions. The symmetries of each group limit the terms that may participate in this expansion. In what is shown below the corresponding algebraic expression is given for each the last 30 of the 32 crystallographic point groups. The super-index (either r or i) in the $B_{n,m}$ coefficients indicates whether this is the real or the imaginary part in the expression above for the potential.

After this expression is given, the matrix representation of this operator is given in the subspace appropriate to the d-electron. The next line, shows how an l=2 would split into different irreducible representation, from symmetry arguments alone. Following this, and with the purpose of clarifying how many free-parameters remained, a list of these is given.

Finally, if the eigenvalues and eigenvectors of the matrix can be found analytically, then the corresponding expressions are given. In each line the eigenvalue is first presented, followed by a list of vectors that span the subspace that corresponds to it (in $|l,m\rangle$ notation). These eigenvalues provide the corrections to the energy of the $l = 2$ state of this electron within the limitations of first-order perturbation theory.

For the purposes of further elaboration the results of these calculations are saved in a dictionary stored as a pickle in the file `crystal_splits.pkl` whose keys equal the indices of the crystallographic point groups and whose values are dictionaries which include the following keys: {'free_parameters', 'simple_free_parameters','matrices','eigen_system'}. The values being sympy expressions or iterables of them.

C_1 (1)

C_i (2)

C_2 (3)

$$V_{CF} = B_{1,0}C_{1,0} + B_{2,0}C_{2,0} + B_{3,0}C_{3,0} + B_{4,0}C_{4,0} + C_{2,-2}\left(iB^i_{2,2} + B^r_{2,2}\right) + C_{2,2}\left(-iB^i_{2,2} + B^r_{2,2}\right) + C_{3,-2}\left(iB^i_{3,2} + B^r_{3,2}\right) + C_{3,2}\left(-iB^i_{3,2} + B^r_{3,2}\right) + C_{4,-2}\left(iB^i_{4,2} + B^r_{4,2}\right) + C_{4,-4}\left(iB^i_{4,4} + B^r_{4,4}\right) + C_{4,2}\left(-iB^i_{4,2} + B^r_{4,2}\right) + C_{4,4}\left(-iB^i_{4,4} + B^r_{4,4}\right)$$

$$V^{l=2}_{CF} = \begin{bmatrix} -\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} & 0 & -\frac{2iB^i_{2,2}}{7} - \frac{2B^r_{2,2}}{7} + \frac{\sqrt{15}\left(iB^i_{4,2}+B^r_{4,2}\right)}{21} & 0 & \frac{\sqrt{70}\left(iB^i_{4,4}+B^r_{4,4}\right)}{21} \\ 0 & \frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} & 0 & -\frac{\sqrt{6}\left(iB^i_{2,2}+B^r_{2,2}\right)}{7} - \frac{2\sqrt{10}\left(iB^i_{4,2}+B^r_{4,2}\right)}{21} & 0 \\ \frac{2iB^i_{2,2}}{7} - \frac{2B^r_{2,2}}{7} + \frac{\sqrt{15}\left(-iB^i_{4,2}+B^r_{4,2}\right)}{21} & 0 & \frac{2B_{2,0}}{7} + \frac{2B_{4,0}}{7} & 0 & -\frac{2iB^i_{2,2}}{7} - \frac{2B^r_{2,2}}{7} + \frac{\sqrt{15}\left(iB^i_{4,2}+B^r_{4,2}\right)}{21} \\ 0 & -\frac{\sqrt{6}\left(-iB^i_{2,2}+B^r_{2,2}\right)}{7} - \frac{2\sqrt{10}\left(-iB^i_{4,2}+B^r_{4,2}\right)}{21} & 0 & \frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} & 0 \\ \frac{\sqrt{70}\left(-iB^i_{4,4}+B^r_{4,4}\right)}{21} & 0 & \frac{2iB^i_{2,2}}{7} - \frac{2B^r_{2,2}}{7} + \frac{\sqrt{15}\left(-iB^i_{4,2}+B^r_{4,2}\right)}{21} & 0 & -\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} \end{bmatrix}$$

$$3A \oplus 2B$$

Free-parameters for d-electrons: $\left\{B_{2,0}, B^i_{2,2}, B^r_{2,2}, B_{4,0}, B^i_{4,2}, B^r_{4,2}, B^i_{4,4}, B^r_{4,4}\right\}$

C_s (4)

$$V_{CF} = B_{2,0}C_{2,0} + B_{4,0}C_{4,0} + C_{1,-1}\left(-iB^i_{1,1} - B^r_{1,1}\right) + C_{1,1}\left(-iB^i_{1,1} + B^r_{1,1}\right) + C_{2,-2}\left(iB^i_{2,2} + B^r_{2,2}\right) + C_{2,2}\left(-iB^i_{2,2} + B^r_{2,2}\right) + C_{3,-1}\left(-iB^i_{3,1} - B^r_{3,1}\right) + C_{3,-3}\left(-iB^i_{3,3} - B^r_{3,3}\right) + C_{3,1}\left(-iB^i_{3,1} + B^r_{3,1}\right) + C_{3,3}\left(-iB^i_{3,3} + B^r_{3,3}\right) + C_{4,-2}\left(iB^i_{4,2} + B^r_{4,2}\right) + C_{4,-4}\left(iB^i_{4,4} + B^r_{4,4}\right) + C_{4,2}\left(-iB^i_{4,2} + B^r_{4,2}\right) + C_{4,4}\left(-iB^i_{4,4} + B^r_{4,4}\right)$$

$$V^{l=2}_{CF} = \begin{bmatrix} -\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} & 0 & -\frac{2iB^i_{2,2}}{7} - \frac{2B^r_{2,2}}{7} + \frac{\sqrt{15}\left(iB^i_{4,2}+B^r_{4,2}\right)}{21} & 0 & \frac{\sqrt{70}\left(iB^i_{4,4}+B^r_{4,4}\right)}{21} \\ 0 & \frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} & 0 & -\frac{\sqrt{6}\left(iB^i_{2,2}+B^r_{2,2}\right)}{7} - \frac{2\sqrt{10}\left(iB^i_{4,2}+B^r_{4,2}\right)}{21} & 0 \\ \frac{2iB^i_{2,2}}{7} - \frac{2B^r_{2,2}}{7} + \frac{\sqrt{15}\left(-iB^i_{4,2}+B^r_{4,2}\right)}{21} & 0 & \frac{2B_{2,0}}{7} + \frac{2B_{4,0}}{7} & 0 & -\frac{2iB^i_{2,2}}{7} - \frac{2B^r_{2,2}}{7} + \frac{\sqrt{15}\left(iB^i_{4,2}+B^r_{4,2}\right)}{21} \\ 0 & -\frac{\sqrt{6}\left(-iB^i_{2,2}+B^r_{2,2}\right)}{7} - \frac{2\sqrt{10}\left(-iB^i_{4,2}+B^r_{4,2}\right)}{21} & 0 & \frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} & 0 \\ \frac{\sqrt{70}\left(-iB^i_{4,4}+B^r_{4,4}\right)}{21} & 0 & \frac{2iB^i_{2,2}}{7} - \frac{2B^r_{2,2}}{7} + \frac{\sqrt{15}\left(-iB^i_{4,2}+B^r_{4,2}\right)}{21} & 0 & -\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} \end{bmatrix}$$

$$3A' \oplus 2A''$$

Free-parameters for d-electrons: $\left\{B_{2,0}, B^i_{2,2}, B^r_{2,2}, B_{4,0}, B^i_{4,2}, B^r_{4,2}, B^i_{4,4}, B^r_{4,4}\right\}$

C_{2h} (5)

$$V_{CF} = B_{2,0}C_{2,0} + B_{4,0}C_{4,0} + C_{2,-2}\left(iB^i_{2,2} + B^r_{2,2}\right) + C_{2,2}\left(-iB^i_{2,2} + B^r_{2,2}\right) + C_{4,-2}\left(iB^i_{4,2} + B^r_{4,2}\right) + C_{4,-4}\left(iB^i_{4,4} + B^r_{4,4}\right) + C_{4,2}\left(-iB^i_{4,2} + B^r_{4,2}\right) + C_{4,4}\left(-iB^i_{4,4} + B^r_{4,4}\right)$$

$$V^{l=2}_{CF} = \begin{bmatrix} -\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} & 0 & -\frac{2iB^i_{2,2}}{7} - \frac{2B^r_{2,2}}{7} + \frac{\sqrt{15}\left(iB^i_{4,2}+B^r_{4,2}\right)}{21} & 0 & \frac{\sqrt{70}\left(iB^i_{4,4}+B^r_{4,4}\right)}{21} \\ 0 & \frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} & 0 & -\frac{\sqrt{6}\left(iB^i_{2,2}+B^r_{2,2}\right)}{7} - \frac{2\sqrt{10}\left(iB^i_{4,2}+B^r_{4,2}\right)}{21} & 0 \\ \frac{2iB^i_{2,2}}{7} - \frac{2B^r_{2,2}}{7} + \frac{\sqrt{15}\left(-iB^i_{4,2}+B^r_{4,2}\right)}{21} & 0 & \frac{2B_{2,0}}{7} + \frac{2B_{4,0}}{7} & 0 & -\frac{2iB^i_{2,2}}{7} - \frac{2B^r_{2,2}}{7} + \frac{\sqrt{15}\left(iB^i_{4,2}+B^r_{4,2}\right)}{21} \\ 0 & -\frac{\sqrt{6}\left(-iB^i_{2,2}+B^r_{2,2}\right)}{7} - \frac{2\sqrt{10}\left(-iB^i_{4,2}+B^r_{4,2}\right)}{21} & 0 & \frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} & 0 \\ \frac{\sqrt{70}\left(-iB^i_{4,4}+B^r_{4,4}\right)}{21} & 0 & \frac{2iB^i_{2,2}}{7} - \frac{2B^r_{2,2}}{7} + \frac{\sqrt{15}\left(-iB^i_{4,2}+B^r_{4,2}\right)}{21} & 0 & -\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} \end{bmatrix}$$

$$3A_g \oplus 2B_g$$

Free-parameters for d-electrons: $\left\{B_{2,0}, B^i_{2,2}, B^r_{2,2}, B_{4,0}, B^i_{4,2}, B^r_{4,2}, B^i_{4,4}, B^r_{4,4}\right\}$

D_2 (6)

$$V_{CF} = B_{2,0}C_{2,0} + B_{2,2}C_{2,-2} + B_{2,2}C_{2,2} + iB_{3,2}C_{3,-2} - iB_{3,2}C_{3,2} + B_{4,0}C_{4,0} + B_{4,2}C_{4,-2} + B_{4,2}C_{4,2} + B_{4,4}C_{4,-4} + B_{4,4}C_{4,4}$$

$$V^{l=2}_{CF} = \begin{bmatrix} -\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} & 0 & -\frac{2B_{2,2}}{7} + \frac{\sqrt{15}B_{4,2}}{21} & 0 & \frac{\sqrt{70}B_{4,4}}{21} \\ 0 & \frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} & 0 & -\frac{\sqrt{6}B_{2,2}}{7} - \frac{2\sqrt{10}B_{4,2}}{21} & 0 \\ -\frac{2B_{2,2}}{7} + \frac{\sqrt{15}B_{4,2}}{21} & 0 & \frac{2B_{2,0}}{7} + \frac{2B_{4,0}}{7} & 0 & -\frac{2B_{2,2}}{7} + \frac{\sqrt{15}B_{4,2}}{21} \\ 0 & -\frac{\sqrt{6}B_{2,2}}{7} - \frac{2\sqrt{10}B_{4,2}}{21} & 0 & \frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} & 0 \\ \frac{\sqrt{70}B_{4,4}}{21} & 0 & -\frac{2B_{2,2}}{7} + \frac{\sqrt{15}B_{4,2}}{21} & 0 & -\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} \end{bmatrix}$$

$$2A_1 \oplus B_1 \oplus B_2 \oplus B_3$$

Free-parameters for d-electrons: $\{B_{2,0}, B_{2,2}, B_{4,0}, B_{4,2}, B_{4,4}\}$

C_{2v} (7)

$$V_{CF} = B_{1,0}C_{1,0} + B_{2,0}C_{2,0} + B_{2,2}C_{2,-2} + B_{2,2}C_{2,2} + B_{3,0}C_{3,0} + B_{3,2}C_{3,-2} + B_{3,2}C_{3,2} + B_{4,0}C_{4,0} + B_{4,2}C_{4,-2} + B_{4,2}C_{4,2} + B_{4,4}C_{4,-4} + B_{4,4}C_{4,4}$$

$$V^{l=2}_{CF} = \begin{bmatrix} -\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} & 0 & -\frac{2B_{2,2}}{7} + \frac{\sqrt{15}B_{4,2}}{21} & 0 & \frac{\sqrt{70}B_{4,4}}{21} \\ 0 & \frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} & 0 & -\frac{\sqrt{6}B_{2,2}}{7} - \frac{2\sqrt{10}B_{4,2}}{21} & 0 \\ -\frac{2B_{2,2}}{7} + \frac{\sqrt{15}B_{4,2}}{21} & 0 & \frac{2B_{2,0}}{7} + \frac{2B_{4,0}}{7} & 0 & -\frac{2B_{2,2}}{7} + \frac{\sqrt{15}B_{4,2}}{21} \\ 0 & -\frac{\sqrt{6}B_{2,2}}{7} - \frac{2\sqrt{10}B_{4,2}}{21} & 0 & \frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} & 0 \\ \frac{\sqrt{70}B_{4,4}}{21} & 0 & -\frac{2B_{2,2}}{7} + \frac{\sqrt{15}B_{4,2}}{21} & 0 & -\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} \end{bmatrix}$$

$$2A_1 \oplus A_2 \oplus B_1 \oplus B_2$$

Free-parameters for d-electrons: $\{B_{2,0}, B_{2,2}, B_{4,0}, B_{4,2}, B_{4,4}\}$

D_{2h} (8)

$$V_{CF} = B_{2,0}C_{2,0} + B_{2,2}C_{2,-2} + B_{2,2}C_{2,2} + B_{4,0}C_{4,0} + B_{4,2}C_{4,-2} + B_{4,2}C_{4,2} + B_{4,4}C_{4,-4} + B_{4,4}C_{4,4}$$

$$V^{l=2}_{CF} = \begin{bmatrix} -\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} & 0 & -\frac{2B_{2,2}}{7} + \frac{\sqrt{15}B_{4,2}}{21} & 0 & \frac{\sqrt{70}B_{4,4}}{21} \\ 0 & \frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} & 0 & -\frac{\sqrt{6}B_{2,2}}{7} - \frac{2\sqrt{10}B_{4,2}}{21} & 0 \\ -\frac{2B_{2,2}}{7} + \frac{\sqrt{15}B_{4,2}}{21} & 0 & \frac{2B_{2,0}}{7} + \frac{2B_{4,0}}{7} & 0 & -\frac{2B_{2,2}}{7} + \frac{\sqrt{15}B_{4,2}}{21} \\ 0 & -\frac{\sqrt{6}B_{2,2}}{7} - \frac{2\sqrt{10}B_{4,2}}{21} & 0 & \frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} & 0 \\ \frac{\sqrt{70}B_{4,4}}{21} & 0 & -\frac{2B_{2,2}}{7} + \frac{\sqrt{15}B_{4,2}}{21} & 0 & -\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} \end{bmatrix}$$

$$2A_{1g} \oplus B_{1g} \oplus B_{2g} \oplus B_{3g}$$

Free-parameters for d-electrons: $\{B_{2,0}, B_{2,2}, B_{4,0}, B_{4,2}, B_{4,4}\}$

C_4 (9)

$$V_{CF} = B_{1,0}C_{1,0} + B_{2,0}C_{2,0} + B_{3,0}C_{3,0} + B_{4,0}C_{4,0} + C_{4,-4}\left(iB^i_{4,4} + B^r_{4,4}\right) + C_{4,4}\left(-iB^i_{4,4} + B^r_{4,4}\right)$$

$$V^{l=2}_{CF} = \begin{bmatrix} -\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} & 0 & 0 & 0 & \frac{\sqrt{70}\left(iB^i_{4,4}+B^r_{4,4}\right)}{21} \\ 0 & \frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} & 0 & 0 & 0 \\ 0 & 0 & \frac{2B_{2,0}}{7} + \frac{2B_{4,0}}{7} & 0 & 0 \\ 0 & 0 & 0 & \frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} & 0 \\ \frac{\sqrt{70}\left(-iB^i_{4,4}+B^r_{4,4}\right)}{21} & 0 & 0 & 0 & -\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} \end{bmatrix}$$

$$A \oplus 2B \oplus E^1 \oplus E^2$$

Free-parameters for d-electrons: $\left\{B_{2,0}, B_{4,0}, B^i_{4,4}, B^r_{4,4}\right\}$

Eigenvalues and eigenvectors:

$$\frac{2B_{2,0}}{7} + \frac{2B_{4,0}}{7} : \{|2,0\rangle\}$$

$$\frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} : \{|2,-1\rangle, |2,1\rangle\}$$

$$-\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} - \frac{\sqrt{70}\sqrt{\left(B^i_{4,4}\right)^2 + \left(B^r_{4,4}\right)^2}}{21} : \{-\frac{|2,-2\rangle\left(iB^i_{4,4} + B^r_{4,4}\right)}{\sqrt{\left(B^i_{4,4}\right)^2 + \left(B^r_{4,4}\right)^2}} + |2,2\rangle\}$$

$$-\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} + \frac{\sqrt{70}\sqrt{\left(B^i_{4,4}\right)^2 + \left(B^r_{4,4}\right)^2}}{21} : \{-\frac{|2,-2\rangle\left(-iB^i_{4,4} - B^r_{4,4}\right)}{\sqrt{\left(B^i_{4,4}\right)^2 + \left(B^r_{4,4}\right)^2}} + |2,2\rangle\}$$

S_4 (10)

$$V_{CF} = B_{2,0}C_{2,0} + B_{4,0}C_{4,0} + C_{3,-2}\left(iB^i_{3,2} + B^r_{3,2}\right) + C_{3,2}\left(-iB^i_{3,2} + B^r_{3,2}\right) + C_{4,-4}\left(iB^i_{4,4} + B^r_{4,4}\right) + C_{4,4}\left(-iB^i_{4,4} + B^r_{4,4}\right)$$

$$V^{l=2}_{CF} = \begin{bmatrix} -\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} & 0 & 0 & 0 & \frac{\sqrt{70}\left(iB^i_{4,4}+B^r_{4,4}\right)}{21} \\ 0 & \frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} & 0 & 0 & 0 \\ 0 & 0 & \frac{2B_{2,0}}{7} + \frac{2B_{4,0}}{7} & 0 & 0 \\ 0 & 0 & 0 & \frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} & 0 \\ \frac{\sqrt{70}\left(-iB^i_{4,4}+B^r_{4,4}\right)}{21} & 0 & 0 & 0 & -\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} \end{bmatrix}$$

$$A \oplus 2B \oplus E^1 \oplus E^2$$

Free-parameters for d-electrons: $\left\{B_{2,0}, B_{4,0}, B^i_{4,4}, B^r_{4,4}\right\}$

Eigenvalues and eigenvectors:

$$\frac{2B_{2,0}}{7} + \frac{2B_{4,0}}{7} : \{|2,0\rangle\}$$

$$\frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} : \{|2,-1\rangle, |2,1\rangle\}$$

$$-\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} - \frac{\sqrt{70}\sqrt{\left(B^i_{4,4}\right)^2 + \left(B^r_{4,4}\right)^2}}{21} : \{-\frac{|2,-2\rangle\left(iB^i_{4,4} + B^r_{4,4}\right)}{\sqrt{\left(B^i_{4,4}\right)^2 + \left(B^r_{4,4}\right)^2}} + |2,2\rangle\}$$

$$-\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} + \frac{\sqrt{70}\sqrt{\left(B^i_{4,4}\right)^2 + \left(B^r_{4,4}\right)^2}}{21} : \{-\frac{|2,-2\rangle\left(-iB^i_{4,4} - B^r_{4,4}\right)}{\sqrt{\left(B^i_{4,4}\right)^2 + \left(B^r_{4,4}\right)^2}} + |2,2\rangle\}$$

C_{4h} (11)

$$V_{CF} = B_{2,0}C_{2,0} + B_{4,0}C_{4,0} + C_{4,-4}\left(iB^i_{4,4} + B^r_{4,4}\right) + C_{4,4}\left(-iB^i_{4,4} + B^r_{4,4}\right)$$

$$V^{l=2}_{CF} = \begin{bmatrix} -\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} & 0 & 0 & 0 & \frac{\sqrt{70}\left(iB^i_{4,4}+B^r_{4,4}\right)}{21} \\ 0 & \frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} & 0 & 0 & 0 \\ 0 & 0 & \frac{2B_{2,0}}{7} + \frac{2B_{4,0}}{7} & 0 & 0 \\ 0 & 0 & 0 & \frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} & 0 \\ \frac{\sqrt{70}\left(-iB^i_{4,4}+B^r_{4,4}\right)}{21} & 0 & 0 & 0 & -\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} \end{bmatrix}$$

$$\Gamma^1 \oplus \Gamma^6 \oplus \Gamma^7 \oplus 2\Gamma^8$$

Free-parameters for d-electrons: $\left\{B_{2,0}, B_{4,0}, B^i_{4,4}, B^r_{4,4}\right\}$

Eigenvalues and eigenvectors:

$$\frac{2B_{2,0}}{7} + \frac{2B_{4,0}}{7} : \{|2,0\rangle\}$$

$$\frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} : \{|2,-1\rangle, |2,1\rangle\}$$

$$-\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} - \frac{\sqrt{70}\sqrt{\left(B^i_{4,4}\right)^2 + \left(B^r_{4,4}\right)^2}}{21} : \{-\frac{|2,-2\rangle\left(iB^i_{4,4} + B^r_{4,4}\right)}{\sqrt{\left(B^i_{4,4}\right)^2 + \left(B^r_{4,4}\right)^2}} + |2,2\rangle\}$$

$$-\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} + \frac{\sqrt{70}\sqrt{\left(B^i_{4,4}\right)^2 + \left(B^r_{4,4}\right)^2}}{21} : \{-\frac{|2,-2\rangle\left(-iB^i_{4,4} - B^r_{4,4}\right)}{\sqrt{\left(B^i_{4,4}\right)^2 + \left(B^r_{4,4}\right)^2}} + |2,2\rangle\}$$

D_4 (12)

$$V_{CF} = B_{2,0}C_{2,0} + B_{4,0}C_{4,0} + B_{4,4}C_{4,-4} + B_{4,4}C_{4,4}$$

$$V^{l=2}_{CF} = \begin{bmatrix} -\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} & 0 & 0 & 0 & \frac{\sqrt{70}B_{4,4}}{21} \\ 0 & \frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} & 0 & 0 & 0 \\ 0 & 0 & \frac{2B_{2,0}}{7} + \frac{2B_{4,0}}{7} & 0 & 0 \\ 0 & 0 & 0 & \frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} & 0 \\ \frac{\sqrt{70}B_{4,4}}{21} & 0 & 0 & 0 & -\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} \end{bmatrix}$$

$$A_1 \oplus B_1 \oplus B_2 \oplus E$$

Free-parameters for d-electrons: $\{B_{2,0}, B_{4,0}, B_{4,4}\}$

Eigenvalues and eigenvectors:

$$\frac{2B_{2,0}}{7} + \frac{2B_{4,0}}{7} : \{|2,0\rangle\}$$

$$\frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} : \{|2,-1\rangle, |2,1\rangle\}$$

$$-\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} - \frac{\sqrt{70}B_{4,4}}{21} : \{-|2,-2\rangle + |2,2\rangle\}$$

$$-\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} + \frac{\sqrt{70}B_{4,4}}{21} : \{|2,-2\rangle + |2,2\rangle\}$$

C_{4v} (13)

$$V_{CF} = B_{1,0}C_{1,0} + B_{2,0}C_{2,0} + B_{3,0}C_{3,0} + B_{4,0}C_{4,0} + B_{4,4}C_{4,-4} + B_{4,4}C_{4,4}$$

$$V^{l=2}_{CF} = \begin{bmatrix} -\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} & 0 & 0 & 0 & \frac{\sqrt{70}B_{4,4}}{21} \\ 0 & \frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} & 0 & 0 & 0 \\ 0 & 0 & \frac{2B_{2,0}}{7} + \frac{2B_{4,0}}{7} & 0 & 0 \\ 0 & 0 & 0 & \frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} & 0 \\ \frac{\sqrt{70}B_{4,4}}{21} & 0 & 0 & 0 & -\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} \end{bmatrix}$$

$$A_1 \oplus B_1 \oplus B_2 \oplus E$$

Free-parameters for d-electrons: $\{B_{2,0}, B_{4,0}, B_{4,4}\}$

Eigenvalues and eigenvectors:

$$\frac{2B_{2,0}}{7} + \frac{2B_{4,0}}{7} : \{|2,0\rangle\}$$

$$\frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} : \{|2,-1\rangle, |2,1\rangle\}$$

$$-\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} - \frac{\sqrt{70}B_{4,4}}{21} : \{-|2,-2\rangle + |2,2\rangle\}$$

$$-\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} + \frac{\sqrt{70}B_{4,4}}{21} : \{|2,-2\rangle + |2,2\rangle\}$$

D_{2d} (14)

$$V_{CF} = B_{2,0}C_{2,0} + B_{3,2}C_{3,-2} + B_{3,2}C_{3,2} + B_{4,0}C_{4,0} + B_{4,4}C_{4,-4} + B_{4,4}C_{4,4}$$

$$V^{l=2}_{CF} = \begin{bmatrix} -\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} & 0 & 0 & 0 & \frac{\sqrt{70}B_{4,4}}{21} \\ 0 & \frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} & 0 & 0 & 0 \\ 0 & 0 & \frac{2B_{2,0}}{7} + \frac{2B_{4,0}}{7} & 0 & 0 \\ 0 & 0 & 0 & \frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} & 0 \\ \frac{\sqrt{70}B_{4,4}}{21} & 0 & 0 & 0 & -\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} \end{bmatrix}$$

$$A_1 \oplus B_1 \oplus B_2 \oplus E$$

Free-parameters for d-electrons: $\{B_{2,0}, B_{4,0}, B_{4,4}\}$

Eigenvalues and eigenvectors:

$$\frac{2B_{2,0}}{7} + \frac{2B_{4,0}}{7} : \{|2,0\rangle\}$$

$$\frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} : \{|2,-1\rangle, |2,1\rangle\}$$

$$-\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} - \frac{\sqrt{70}B_{4,4}}{21} : \{-|2,-2\rangle + |2,2\rangle\}$$

$$-\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} + \frac{\sqrt{70}B_{4,4}}{21} : \{|2,-2\rangle + |2,2\rangle\}$$

D_{4h} (15)

$$V_{CF} = B_{2,0}C_{2,0} + B_{4,0}C_{4,0} + B_{4,4}C_{4,-4} + B_{4,4}C_{4,4}$$

$$V^{l=2}_{CF} = \begin{bmatrix} -\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} & 0 & 0 & 0 & \frac{\sqrt{70}B_{4,4}}{21} \\ 0 & \frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} & 0 & 0 & 0 \\ 0 & 0 & \frac{2B_{2,0}}{7} + \frac{2B_{4,0}}{7} & 0 & 0 \\ 0 & 0 & 0 & \frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} & 0 \\ \frac{\sqrt{70}B_{4,4}}{21} & 0 & 0 & 0 & -\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} \end{bmatrix}$$

$$A_{1g} \oplus B_{1g} \oplus B_{2g} \oplus E_g$$

Free-parameters for d-electrons: $\{B_{2,0}, B_{4,0}, B_{4,4}\}$

Eigenvalues and eigenvectors:

$$\frac{2B_{2,0}}{7} + \frac{2B_{4,0}}{7} : \{|2,0\rangle\}$$

$$\frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} : \{|2,-1\rangle, |2,1\rangle\}$$

$$-\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} - \frac{\sqrt{70}B_{4,4}}{21} : \{-|2,-2\rangle + |2,2\rangle\}$$

$$-\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} + \frac{\sqrt{70}B_{4,4}}{21} : \{|2,-2\rangle + |2,2\rangle\}$$

C_3 (16)

$$V_{CF} = B_{1,0}C_{1,0} + B_{2,0}C_{2,0} + B_{3,0}C_{3,0} + B_{4,0}C_{4,0} + C_{3,-3}\left(-iB^i_{3,3} - B^r_{3,3}\right) + C_{3,3}\left(-iB^i_{3,3} + B^r_{3,3}\right) + C_{4,-3}\left(-iB^i_{4,3} - B^r_{4,3}\right) + C_{4,3}\left(-iB^i_{4,3} + B^r_{4,3}\right)$$

$$V^{l=2}_{CF} = \begin{bmatrix} -\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} & 0 & 0 & -\frac{\sqrt{35}\left(-iB^i_{4,3}-B^r_{4,3}\right)}{21} & 0 \\ 0 & \frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} & 0 & 0 & \frac{\sqrt{35}\left(-iB^i_{4,3}-B^r_{4,3}\right)}{21} \\ 0 & 0 & \frac{2B_{2,0}}{7} + \frac{2B_{4,0}}{7} & 0 & 0 \\ \frac{\sqrt{35}\left(-iB^i_{4,3}+B^r_{4,3}\right)}{21} & 0 & 0 & \frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} & 0 \\ 0 & -\frac{\sqrt{35}\left(-iB^i_{4,3}+B^r_{4,3}\right)}{21} & 0 & 0 & -\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} \end{bmatrix}$$

$$A \oplus 2E^1 \oplus 2E^2$$

Free-parameters for d-electrons: $\left\{B_{2,0}, B_{4,0}, B^i_{4,3}, B^r_{4,3}\right\}$

Eigenvalues and eigenvectors:

$$\frac{2B_{2,0}}{7} + \frac{2B_{4,0}}{7} : \{|2,0\rangle\}$$

$$-\frac{B_{2,0}}{14} - \frac{B_{4,0}}{14} - \frac{\sqrt{81B^2_{2,0} - 90B_{2,0}B_{4,0} + 25B^2_{4,0} + 140\left(B^i_{4,3}\right)^2 + 140\left(B^r_{4,3}\right)^2}}{42} : \{-\frac{|2,-2\rangle\left(2\sqrt{35}iB^i_{4,3} + 2\sqrt{35}B^r_{4,3}\right)}{-9B^r_{2,0} + 5B^r_{4,0} + \sqrt{81\left(B^r_{2,0}\right)^2 - 90B^r_{2,0}B^r_{4,0} + 25\left(B^r_{4,0}\right)^2 + 140\left(B^i_{4,3}\right)^2 + 140\left(B^r_{4,3}\right)^2}} + |2,1\rangle, -\frac{|2,-1\rangle\left(2\sqrt{35}iB^i_{4,3} + 2\sqrt{35}B^r_{4,3}\right)}{-9B^r_{2,0} + 5B^r_{4,0} - \sqrt{81\left(B^r_{2,0}\right)^2 - 90B^r_{2,0}B^r_{4,0} + 25\left(B^r_{4,0}\right)^2 + 140\left(B^i_{4,3}\right)^2 + 140\left(B^r_{4,3}\right)^2}} + |2,2\rangle\}$$

$$-\frac{B_{2,0}}{14} - \frac{B_{4,0}}{14} + \frac{\sqrt{81B^2_{2,0} - 90B_{2,0}B_{4,0} + 25B^2_{4,0} + 140\left(B^i_{4,3}\right)^2 + 140\left(B^r_{4,3}\right)^2}}{42} : \{-\frac{|2,-2\rangle\left(2\sqrt{35}iB^i_{4,3} + 2\sqrt{35}B^r_{4,3}\right)}{-9B^r_{2,0} + 5B^r_{4,0} - \sqrt{81\left(B^r_{2,0}\right)^2 - 90B^r_{2,0}B^r_{4,0} + 25\left(B^r_{4,0}\right)^2 + 140\left(B^i_{4,3}\right)^2 + 140\left(B^r_{4,3}\right)^2}} + |2,1\rangle, -\frac{|2,-1\rangle\left(2\sqrt{35}iB^i_{4,3} + 2\sqrt{35}B^r_{4,3}\right)}{-9B^r_{2,0} + 5B^r_{4,0} + \sqrt{81\left(B^r_{2,0}\right)^2 - 90B^r_{2,0}B^r_{4,0} + 25\left(B^r_{4,0}\right)^2 + 140\left(B^i_{4,3}\right)^2 + 140\left(B^r_{4,3}\right)^2}} + |2,2\rangle\}$$

S_6 (17)

$$V_{CF} = B_{2,0}C_{2,0} + B_{4,0}C_{4,0} + C_{4,-3}\left(-iB^i_{4,3} - B^r_{4,3}\right) + C_{4,3}\left(-iB^i_{4,3} + B^r_{4,3}\right)$$

$$V^{l=2}_{CF} = \begin{bmatrix} -\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} & 0 & 0 & -\frac{\sqrt{35}\left(-iB^i_{4,3}-B^r_{4,3}\right)}{21} & 0 \\ 0 & \frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} & 0 & 0 & \frac{\sqrt{35}\left(-iB^i_{4,3}-B^r_{4,3}\right)}{21} \\ 0 & 0 & \frac{2B_{2,0}}{7} + \frac{2B_{4,0}}{7} & 0 & 0 \\ \frac{\sqrt{35}\left(-iB^i_{4,3}+B^r_{4,3}\right)}{21} & 0 & 0 & \frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} & 0 \\ 0 & -\frac{\sqrt{35}\left(-iB^i_{4,3}+B^r_{4,3}\right)}{21} & 0 & 0 & -\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} \end{bmatrix}$$

$$A_g \oplus 2E^1_g \oplus 2E^2_g$$

Free-parameters for d-electrons: $\left\{B_{2,0}, B_{4,0}, B^i_{4,3}, B^r_{4,3}\right\}$

Eigenvalues and eigenvectors:

$$\frac{2B_{2,0}}{7} + \frac{2B_{4,0}}{7} : \{|2,0\rangle\}$$

$$-\frac{B_{2,0}}{14} - \frac{B_{4,0}}{14} - \frac{\sqrt{81B^2_{2,0} - 90B_{2,0}B_{4,0} + 25B^2_{4,0} + 140\left(B^i_{4,3}\right)^2 + 140\left(B^r_{4,3}\right)^2}}{42} : \{-\frac{|2,-2\rangle\left(2\sqrt{35}iB^i_{4,3} + 2\sqrt{35}B^r_{4,3}\right)}{-9B^r_{2,0} + 5B^r_{4,0} + \sqrt{81\left(B^r_{2,0}\right)^2 - 90B^r_{2,0}B^r_{4,0} + 25\left(B^r_{4,0}\right)^2 + 140\left(B^i_{4,3}\right)^2 + 140\left(B^r_{4,3}\right)^2}} + |2,1\rangle, -\frac{|2,-1\rangle\left(2\sqrt{35}iB^i_{4,3} + 2\sqrt{35}B^r_{4,3}\right)}{-9B^r_{2,0} + 5B^r_{4,0} - \sqrt{81\left(B^r_{2,0}\right)^2 - 90B^r_{2,0}B^r_{4,0} + 25\left(B^r_{4,0}\right)^2 + 140\left(B^i_{4,3}\right)^2 + 140\left(B^r_{4,3}\right)^2}} + |2,2\rangle\}$$

$$-\frac{B_{2,0}}{14} - \frac{B_{4,0}}{14} + \frac{\sqrt{81B^2_{2,0} - 90B_{2,0}B_{4,0} + 25B^2_{4,0} + 140\left(B^i_{4,3}\right)^2 + 140\left(B^r_{4,3}\right)^2}}{42} : \{-\frac{|2,-2\rangle\left(2\sqrt{35}iB^i_{4,3} + 2\sqrt{35}B^r_{4,3}\right)}{-9B^r_{2,0} + 5B^r_{4,0} - \sqrt{81\left(B^r_{2,0}\right)^2 - 90B^r_{2,0}B^r_{4,0} + 25\left(B^r_{4,0}\right)^2 + 140\left(B^i_{4,3}\right)^2 + 140\left(B^r_{4,3}\right)^2}} + |2,1\rangle, -\frac{|2,-1\rangle\left(2\sqrt{35}iB^i_{4,3} + 2\sqrt{35}B^r_{4,3}\right)}{-9B^r_{2,0} + 5B^r_{4,0} + \sqrt{81\left(B^r_{2,0}\right)^2 - 90B^r_{2,0}B^r_{4,0} + 25\left(B^r_{4,0}\right)^2 + 140\left(B^i_{4,3}\right)^2 + 140\left(B^r_{4,3}\right)^2}} + |2,2\rangle\}$$

D_3 (18)

$$V_{CF} = B_{2,0}C_{2,0} - iB_{3,3}C_{3,-3} - iB_{3,3}C_{3,3} + B_{4,0}C_{4,0} - B_{4,3}C_{4,-3} + B_{4,3}C_{4,3}$$

$$V_{CF}^{l=2} = \begin{bmatrix} -\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} & 0 & 0 & \frac{\sqrt{35}B_{4,3}}{21} & 0 \\ 0 & \frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} & 0 & 0 & -\frac{\sqrt{35}B_{4,3}}{21} \\ 0 & 0 & \frac{2B_{2,0}}{7} + \frac{2B_{4,0}}{7} & 0 & 0 \\ \frac{\sqrt{35}B_{4,3}}{21} & 0 & 0 & \frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} & 0 \\ 0 & -\frac{\sqrt{35}B_{4,3}}{21} & 0 & 0 & -\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} \end{bmatrix}$$

$$A_1 \oplus 2E$$

Free-parameters for d-electrons: $\{B_{2,0}, B_{4,0}, B_{4,3}\}$

Eigenvalues and eigenvectors:

$$\frac{2B_{2,0}}{7} + \frac{2B_{4,0}}{7} : \{|2,0\rangle\}$$

$$-\frac{B_{2,0}}{14} - \frac{B_{4,0}}{14} - \frac{\sqrt{81B_{2,0}^2 - 90B_{2,0}B_{4,0} + 25B_{4,0}^2 + 140B_{4,3}^2}}{42} : \{\frac{2\sqrt{35}B_{4,3}^r|2,-2\rangle}{9B_{2,0}^r - 5B_{4,0}^r - \sqrt{81\left(B_{2,0}^r\right)^2 - 90B_{2,0}^rB_{4,0}^r + 25\left(B_{4,0}^r\right)^2 + 140\left(B_{4,3}^r\right)^2}} + |2,1\rangle, \frac{2\sqrt{35}B_{4,3}^r|2,-1\rangle}{9B_{2,0}^r - 5B_{4,0}^r + \sqrt{81\left(B_{2,0}^r\right)^2 - 90B_{2,0}^rB_{4,0}^r + 25\left(B_{4,0}^r\right)^2 + 140\left(B_{4,3}^r\right)^2}} + |2,2\rangle\}$$

$$-\frac{B_{2,0}}{14} - \frac{B_{4,0}}{14} + \frac{\sqrt{81B_{2,0}^2 - 90B_{2,0}B_{4,0} + 25B_{4,0}^2 + 140B_{4,3}^2}}{42} : \{\frac{2\sqrt{35}B_{4,3}^r|2,-2\rangle}{9B_{2,0}^r - 5B_{4,0}^r + \sqrt{81\left(B_{2,0}^r\right)^2 - 90B_{2,0}^rB_{4,0}^r + 25\left(B_{4,0}^r\right)^2 + 140\left(B_{4,3}^r\right)^2}} + |2,1\rangle, \frac{2\sqrt{35}B_{4,3}^r|2,-1\rangle}{9B_{2,0}^r - 5B_{4,0}^r - \sqrt{81\left(B_{2,0}^r\right)^2 - 90B_{2,0}^rB_{4,0}^r + 25\left(B_{4,0}^r\right)^2 + 140\left(B_{4,3}^r\right)^2}} + |2,2\rangle\}$$

C_{3v} (19)

$$V_{CF} = B_{1,0}C_{1,0} + B_{2,0}C_{2,0} + B_{3,0}C_{3,0} - B_{3,3}C_{3,-3} + B_{3,3}C_{3,3} + B_{4,0}C_{4,0} - B_{4,3}C_{4,-3} + B_{4,3}C_{4,3}$$

$$V_{CF}^{l=2} = \begin{bmatrix} -\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} & 0 & 0 & \frac{\sqrt{35}B_{4,3}}{21} & 0 \\ 0 & \frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} & 0 & 0 & -\frac{\sqrt{35}B_{4,3}}{21} \\ 0 & 0 & \frac{2B_{2,0}}{7} + \frac{2B_{4,0}}{7} & 0 & 0 \\ \frac{\sqrt{35}B_{4,3}}{21} & 0 & 0 & \frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} & 0 \\ 0 & -\frac{\sqrt{35}B_{4,3}}{21} & 0 & 0 & -\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} \end{bmatrix}$$

$$A_1 \oplus 2E$$

Free-parameters for d-electrons: $\{B_{2,0}, B_{4,0}, B_{4,3}\}$

Eigenvalues and eigenvectors:

$$\frac{2B_{2,0}}{7} + \frac{2B_{4,0}}{7} : \{|2,0\rangle\}$$

$$-\frac{B_{2,0}}{14} - \frac{B_{4,0}}{14} - \frac{\sqrt{81B_{2,0}^2 - 90B_{2,0}B_{4,0} + 25B_{4,0}^2 + 140B_{4,3}^2}}{42} : \{\frac{2\sqrt{35}B_{4,3}^r|2,-2\rangle}{9B_{2,0}^r - 5B_{4,0}^r - \sqrt{81\left(B_{2,0}^r\right)^2 - 90B_{2,0}^rB_{4,0}^r + 25\left(B_{4,0}^r\right)^2 + 140\left(B_{4,3}^r\right)^2}} + |2,1\rangle, \frac{2\sqrt{35}B_{4,3}^r|2,-1\rangle}{9B_{2,0}^r - 5B_{4,0}^r + \sqrt{81\left(B_{2,0}^r\right)^2 - 90B_{2,0}^rB_{4,0}^r + 25\left(B_{4,0}^r\right)^2 + 140\left(B_{4,3}^r\right)^2}} + |2,2\rangle\}$$

$$-\frac{B_{2,0}}{14} - \frac{B_{4,0}}{14} + \frac{\sqrt{81B_{2,0}^2 - 90B_{2,0}B_{4,0} + 25B_{4,0}^2 + 140B_{4,3}^2}}{42} : \{\frac{2\sqrt{35}B_{4,3}^r|2,-2\rangle}{9B_{2,0}^r - 5B_{4,0}^r + \sqrt{81\left(B_{2,0}^r\right)^2 - 90B_{2,0}^rB_{4,0}^r + 25\left(B_{4,0}^r\right)^2 + 140\left(B_{4,3}^r\right)^2}} + |2,1\rangle, \frac{2\sqrt{35}B_{4,3}^r|2,-1\rangle}{9B_{2,0}^r - 5B_{4,0}^r - \sqrt{81\left(B_{2,0}^r\right)^2 - 90B_{2,0}^rB_{4,0}^r + 25\left(B_{4,0}^r\right)^2 + 140\left(B_{4,3}^r\right)^2}} + |2,2\rangle\}$$

D_{3d} (20)

$$V_{CF} = B_{2,0}C_{2,0} + B_{4,0}C_{4,0} - B_{4,3}C_{4,-3} + B_{4,3}C_{4,3}$$

$$V_{CF}^{l=2} = \begin{bmatrix} -\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} & 0 & 0 & \frac{\sqrt{35}B_{4,3}}{21} & 0 \\ 0 & \frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} & 0 & 0 & -\frac{\sqrt{35}B_{4,3}}{21} \\ 0 & 0 & \frac{2B_{2,0}}{7} + \frac{2B_{4,0}}{7} & 0 & 0 \\ \frac{\sqrt{35}B_{4,3}}{21} & 0 & 0 & \frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} & 0 \\ 0 & -\frac{\sqrt{35}B_{4,3}}{21} & 0 & 0 & -\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} \end{bmatrix}$$

$$A_{1g} \oplus 2E_g$$

Free-parameters for d-electrons: $\{B_{2,0}, B_{4,0}, B_{4,3}\}$

Eigenvalues and eigenvectors:

$$\frac{2B_{2,0}}{7} + \frac{2B_{4,0}}{7} : \{|2,0\rangle\}$$

$$-\frac{B_{2,0}}{14} - \frac{B_{4,0}}{14} - \frac{\sqrt{81B_{2,0}^2 - 90B_{2,0}B_{4,0} + 25B_{4,0}^2 + 140B_{4,3}^2}}{42} : \{\frac{2\sqrt{35}B_{4,3}^r|2,-2\rangle}{9B_{2,0}^r - 5B_{4,0}^r - \sqrt{81\left(B_{2,0}^r\right)^2 - 90B_{2,0}^rB_{4,0}^r + 25\left(B_{4,0}^r\right)^2 + 140\left(B_{4,3}^r\right)^2}} + |2,1\rangle, \frac{2\sqrt{35}B_{4,3}^r|2,-1\rangle}{9B_{2,0}^r - 5B_{4,0}^r + \sqrt{81\left(B_{2,0}^r\right)^2 - 90B_{2,0}^rB_{4,0}^r + 25\left(B_{4,0}^r\right)^2 + 140\left(B_{4,3}^r\right)^2}} + |2,2\rangle\}$$

$$-\frac{B_{2,0}}{14} - \frac{B_{4,0}}{14} + \frac{\sqrt{81B_{2,0}^2 - 90B_{2,0}B_{4,0} + 25B_{4,0}^2 + 140B_{4,3}^2}}{42} : \{\frac{2\sqrt{35}B_{4,3}^r|2,-2\rangle}{9B_{2,0}^r - 5B_{4,0}^r + \sqrt{81\left(B_{2,0}^r\right)^2 - 90B_{2,0}^rB_{4,0}^r + 25\left(B_{4,0}^r\right)^2 + 140\left(B_{4,3}^r\right)^2}} + |2,1\rangle, \frac{2\sqrt{35}B_{4,3}^r|2,-1\rangle}{9B_{2,0}^r - 5B_{4,0}^r - \sqrt{81\left(B_{2,0}^r\right)^2 - 90B_{2,0}^rB_{4,0}^r + 25\left(B_{4,0}^r\right)^2 + 140\left(B_{4,3}^r\right)^2}} + |2,2\rangle\}$$

C_6 (21)

$$V_{CF} = B_{1,0}C_{1,0} + B_{2,0}C_{2,0} + B_{3,0}C_{3,0} + B_{4,0}C_{4,0}$$

$$V_{CF}^{l=2} = \begin{bmatrix} -\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} & 0 & 0 & 0 & 0 \\ 0 & \frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} & 0 & 0 & 0 \\ 0 & 0 & \frac{2B_{2,0}}{7} + \frac{2B_{4,0}}{7} & 0 & 0 \\ 0 & 0 & 0 & \frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} & 0 \\ 0 & 0 & 0 & 0 & -\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} \end{bmatrix}$$

$$A \oplus E''^1 \oplus E''^2 \oplus E'^1 \oplus E'^2$$

Free-parameters for d-electrons: $\{B_{2,0}, B_{4,0}\}$

Eigenvalues and eigenvectors:

$$-\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} : \{|2,-2\rangle, |2,2\rangle\}$$

$$\frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} : \{|2,-1\rangle, |2,1\rangle\}$$

$$\frac{2B_{2,0}}{7} + \frac{2B_{4,0}}{7} : \{|2,0\rangle\}$$

C_{3h} (22)

$$V_{CF} = B_{2,0}C_{2,0} + B_{3,0}C_{3,0} - B_{3,3}C_{3,-3} + B_{3,3}C_{3,3} + B_{4,0}C_{4,0}$$

$$V_{CF}^{l=2} = \begin{bmatrix} -\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} & 0 & 0 & 0 & 0 \\ 0 & \frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} & 0 & 0 & 0 \\ 0 & 0 & \frac{2B_{2,0}}{7} + \frac{2B_{4,0}}{7} & 0 & 0 \\ 0 & 0 & 0 & \frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} & 0 \\ 0 & 0 & 0 & 0 & -\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} \end{bmatrix}$$

$$A' \oplus E''^1 \oplus E''^2 \oplus E'^1 \oplus E'^2$$

Free-parameters for d-electrons: $\{B_{2,0}, B_{4,0}\}$

Eigenvalues and eigenvectors:

$$-\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} : \{|2,-2\rangle, |2,2\rangle\}$$

$$\frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} : \{|2,-1\rangle, |2,1\rangle\}$$

$$\frac{2B_{2,0}}{7} + \frac{2B_{4,0}}{7} : \{|2,0\rangle\}$$

C_{6h} (23)

$$V_{CF} = B_{2,0}C_{2,0} + B_{4,0}C_{4,0}$$

$$V_{CF}^{l=2} = \begin{bmatrix} -\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} & 0 & 0 & 0 & 0 \\ 0 & \frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} & 0 & 0 & 0 \\ 0 & 0 & \frac{2B_{2,0}}{7} + \frac{2B_{4,0}}{7} & 0 & 0 \\ 0 & 0 & 0 & \frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} & 0 \\ 0 & 0 & 0 & 0 & -\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} \end{bmatrix}$$

$$\Gamma^1 \oplus \Gamma^9 \oplus \Gamma^{10} \oplus \Gamma^{11} \oplus \Gamma^{12}$$

Free-parameters for d-electrons: $\{B_{2,0}, B_{4,0}\}$

Eigenvalues and eigenvectors:

$$-\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} : \{|2,-2\rangle, |2,2\rangle\}$$

$$\frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} : \{|2,-1\rangle, |2,1\rangle\}$$

$$\frac{2B_{2,0}}{7} + \frac{2B_{4,0}}{7} : \{|2,0\rangle\}$$

D_6 (24)

$$V_{CF} = B_{2,0}C_{2,0} + B_{4,0}C_{4,0}$$

$$V_{CF}^{l=2} = \begin{bmatrix} -\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} & 0 & 0 & 0 & 0 \\ 0 & \frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} & 0 & 0 & 0 \\ 0 & 0 & \frac{2B_{2,0}}{7} + \frac{2B_{4,0}}{7} & 0 & 0 \\ 0 & 0 & 0 & \frac{B_{2,0}}{7} - \frac{4B_{4,0}}{21} & 0 \\ 0 & 0 & 0 & 0 & -\frac{2B_{2,0}}{7} + \frac{B_{4,0}}{21} \end{bmatrix}$$

$$A_1 \oplus E_1 \oplus E_2$$

Free-parameters for d-electrons: $\{B_{2,0}, B_{4,0}\}$

Eigenvalues and eigenvectors:

$$-\frac{2B_{2,0}}{7}+\frac{B_{4,0}}{21} : \{|2,-2\rangle, |2,2\rangle\}$$

$$\frac{B_{2,0}}{7}-\frac{4B_{4,0}}{21} : \{|2,-1\rangle, |2,1\rangle\}$$

$$\frac{2B_{2,0}}{7}+\frac{2B_{4,0}}{7} : \{|2,0\rangle\}$$

C_{6v} (25)

$$V_{CF} = B_{1,0}C_{1,0} + B_{2,0}C_{2,0} + B_{3,0}C_{3,0} + B_{4,0}C_{4,0}$$

$$V_{CF}^{l=2} = \begin{bmatrix} -\frac{2B_{2,0}}{7}+\frac{B_{4,0}}{21} & 0 & 0 & 0 & 0 \\ 0 & \frac{B_{2,0}}{7}-\frac{4B_{4,0}}{21} & 0 & 0 & 0 \\ 0 & 0 & \frac{2B_{2,0}}{7}+\frac{2B_{4,0}}{7} & 0 & 0 \\ 0 & 0 & 0 & \frac{B_{2,0}}{7}-\frac{4B_{4,0}}{21} & 0 \\ 0 & 0 & 0 & 0 & -\frac{2B_{2,0}}{7}+\frac{B_{4,0}}{21} \end{bmatrix}$$

$$A_1 \oplus E_1 \oplus E_2$$

Free-parameters for d-electrons: $\{B_{2,0}, B_{4,0}\}$

Eigenvalues and eigenvectors:

$$-\frac{2B_{2,0}}{7}+\frac{B_{4,0}}{21} : \{|2,-2\rangle, |2,2\rangle\}$$

$$\frac{B_{2,0}}{7}-\frac{4B_{4,0}}{21} : \{|2,-1\rangle, |2,1\rangle\}$$

$$\frac{2B_{2,0}}{7}+\frac{2B_{4,0}}{7} : \{|2,0\rangle\}$$

D_{3h} (26)

$$V_{CF} = B_{2,0}C_{2,0} + B_{3,0}C_{3,0} + B_{4,0}C_{4,0}$$

$$V_{CF}^{l=2} = \begin{bmatrix} -\frac{2B_{2,0}}{7}+\frac{B_{4,0}}{21} & 0 & 0 & 0 & 0 \\ 0 & \frac{B_{2,0}}{7}-\frac{4B_{4,0}}{21} & 0 & 0 & 0 \\ 0 & 0 & \frac{2B_{2,0}}{7}+\frac{2B_{4,0}}{7} & 0 & 0 \\ 0 & 0 & 0 & \frac{B_{2,0}}{7}-\frac{4B_{4,0}}{21} & 0 \\ 0 & 0 & 0 & 0 & -\frac{2B_{2,0}}{7}+\frac{B_{4,0}}{21} \end{bmatrix}$$

$$A_1^{'} \oplus E^{'} \oplus E^{''}$$

Free-parameters for d-electrons: $\{B_{2,0}, B_{4,0}\}$

Eigenvalues and eigenvectors:

$$-\frac{2B_{2,0}}{7}+\frac{B_{4,0}}{21} : \{|2,-2\rangle, |2,2\rangle\}$$

$$\frac{B_{2,0}}{7}-\frac{4B_{4,0}}{21} : \{|2,-1\rangle, |2,1\rangle\}$$

$$\frac{2B_{2,0}}{7}+\frac{2B_{4,0}}{7} : \{|2,0\rangle\}$$

D_{6h} (27)

$$V_{CF} = B_{2,0}C_{2,0} + B_{4,0}C_{4,0}$$

$$V_{CF}^{l=2} = \begin{bmatrix} -\frac{2B_{2,0}}{7}+\frac{B_{4,0}}{21} & 0 & 0 & 0 & 0 \\ 0 & \frac{B_{2,0}}{7}-\frac{4B_{4,0}}{21} & 0 & 0 & 0 \\ 0 & 0 & \frac{2B_{2,0}}{7}+\frac{2B_{4,0}}{7} & 0 & 0 \\ 0 & 0 & 0 & \frac{B_{2,0}}{7}-\frac{4B_{4,0}}{21} & 0 \\ 0 & 0 & 0 & 0 & -\frac{2B_{2,0}}{7}+\frac{B_{4,0}}{21} \end{bmatrix}$$

$$A_{1g} \oplus E_{1g} \oplus E_{2g}$$

Free-parameters for d-electrons: $\{B_{2,0}, B_{4,0}\}$

Eigenvalues and eigenvectors:

$$-\frac{2B_{2,0}}{7}+\frac{B_{4,0}}{21} : \{|2,-2\rangle, |2,2\rangle\}$$

$$\frac{B_{2,0}}{7}-\frac{4B_{4,0}}{21} : \{|2,-1\rangle, |2,1\rangle\}$$

$$\frac{2B_{2,0}}{7}+\frac{2B_{4,0}}{7} : \{|2,0\rangle\}$$

T (28)

$$V_{CF} = B_{3,2}C_{3,-2} + B_{3,2}C_{3,2} + \frac{\sqrt{70}B_{4,0}C_{4,-4}}{14} + B_{4,0}C_{4,0} + \frac{\sqrt{70}B_{4,0}C_{4,4}}{14} - \frac{\sqrt{14}B_{6,0}C_{6,-4}}{2} + B_{6,0}C_{6,0} - \frac{\sqrt{14}B_{6,0}C_{6,4}}{2}$$

$$V_{CF}^{l=2} = \begin{bmatrix} \frac{B_{4,0}}{21} & 0 & 0 & 0 & \frac{5B_{4,0}}{21} \\ 0 & -\frac{4B_{4,0}}{21} & 0 & 0 & 0 \\ 0 & 0 & \frac{2B_{4,0}}{7} & 0 & 0 \\ 0 & 0 & 0 & -\frac{4B_{4,0}}{21} & 0 \\ \frac{5B_{4,0}}{21} & 0 & 0 & 0 & \frac{B_{4,0}}{21} \end{bmatrix}$$

$$E^1 \oplus E^2 \oplus T$$

Free-parameters for d-electrons: $\{B_{4,0}\}$

Eigenvalues and eigenvectors:

$$-\frac{4B_{4,0}}{21} : \{|2,-1\rangle, |2,1\rangle, -|2,-2\rangle + |2,2\rangle\}$$

$$\frac{2B_{4,0}}{7} : \{|2,0\rangle, |2,-2\rangle + |2,2\rangle\}$$

$$V_{CF} = -\frac{\sqrt{70}B_{4,0}C_{4,-4}}{14} + B_{4,0}C_{4,0} - \frac{\sqrt{70}B_{4,0}C_{4,4}}{14} + \frac{\sqrt{14}B_{6,0}C_{6,-4}}{2} + B_{6,0}C_{6,0} + \frac{\sqrt{14}B_{6,0}C_{6,4}}{2}$$

$$V_{CF}^{l=2} = \begin{bmatrix} \frac{B_{4,0}}{21} & 0 & 0 & 0 & -\frac{5B_{4,0}}{21} \\ 0 & -\frac{4B_{4,0}}{21} & 0 & 0 & 0 \\ 0 & 0 & \frac{2B_{4,0}}{7} & 0 & 0 \\ 0 & 0 & 0 & -\frac{4B_{4,0}}{21} & 0 \\ -\frac{5B_{4,0}}{21} & 0 & 0 & 0 & \frac{B_{4,0}}{21} \end{bmatrix}$$

$$E^1 \oplus E^2 \oplus T$$

Free-parameters for d-electrons: $\{B_{4,0}\}$

Eigenvalues and eigenvectors:

$$-\frac{4B_{4,0}}{21} : \{|2,-1\rangle, |2,1\rangle, |2,-2\rangle + |2,2\rangle\}$$

$$\frac{2B_{4,0}}{7} : \{|2,0\rangle, -|2,-2\rangle + |2,2\rangle\}$$

T_h (29)

$$V_{CF} = \frac{\sqrt{70}B_{4,0}C_{4,-4}}{14} + B_{4,0}C_{4,0} + \frac{\sqrt{70}B_{4,0}C_{4,4}}{14} - \frac{\sqrt{14}B_{6,0}C_{6,-4}}{2} + B_{6,0}C_{6,0} - \frac{\sqrt{14}B_{6,0}C_{6,4}}{2}$$

$$V_{CF}^{l=2} = \begin{bmatrix} \frac{B_{4,0}}{21} & 0 & 0 & 0 & \frac{5B_{4,0}}{21} \\ 0 & -\frac{4B_{4,0}}{21} & 0 & 0 & 0 \\ 0 & 0 & \frac{2B_{4,0}}{7} & 0 & 0 \\ 0 & 0 & 0 & -\frac{4B_{4,0}}{21} & 0 \\ \frac{5B_{4,0}}{21} & 0 & 0 & 0 & \frac{B_{4,0}}{21} \end{bmatrix}$$

$$E_g^1 \oplus E_g^2 \oplus T_g$$

Free-parameters for d-electrons: $\{B_{4,0}\}$

Eigenvalues and eigenvectors:

$$-\frac{4B_{4,0}}{21} : \{|2,-1\rangle, |2,1\rangle, -|2,-2\rangle + |2,2\rangle\}$$

$$\frac{2B_{4,0}}{7} : \{|2,0\rangle, |2,-2\rangle + |2,2\rangle\}$$

$$V_{CF} = -\frac{\sqrt{70}B_{4,0}C_{4,-4}}{14} + B_{4,0}C_{4,0} - \frac{\sqrt{70}B_{4,0}C_{4,4}}{14} + \frac{\sqrt{14}B_{6,0}C_{6,-4}}{2} + B_{6,0}C_{6,0} + \frac{\sqrt{14}B_{6,0}C_{6,4}}{2}$$

$$V_{CF}^{l=2} = \begin{bmatrix} \frac{B_{4,0}}{21} & 0 & 0 & 0 & -\frac{5B_{4,0}}{21} \\ 0 & -\frac{4B_{4,0}}{21} & 0 & 0 & 0 \\ 0 & 0 & \frac{2B_{4,0}}{7} & 0 & 0 \\ 0 & 0 & 0 & -\frac{4B_{4,0}}{21} & 0 \\ -\frac{5B_{4,0}}{21} & 0 & 0 & 0 & \frac{B_{4,0}}{21} \end{bmatrix}$$

$$E_g^1 \oplus E_g^2 \oplus T_g$$

Free-parameters for d-electrons: $\{B_{4,0}\}$

Eigenvalues and eigenvectors:

$$-\frac{4B_{4,0}}{21} : \{|2,-1\rangle, |2,1\rangle, -|2,-2\rangle + |2,2\rangle\}$$

$$\frac{2B_{4,0}}{7} : \{|2,0\rangle, -|2,-2\rangle + |2,2\rangle\}$$

O (30)

$$V_{CF} = \frac{\sqrt{70}B_{4,0}C_{4,-4}}{14} + B_{4,0}C_{4,0} + \frac{\sqrt{70}B_{4,0}C_{4,4}}{14} - \frac{\sqrt{14}B_{6,0}C_{6,-4}}{2} + B_{6,0}C_{6,0} - \frac{\sqrt{14}B_{6,0}C_{6,4}}{2}$$

$$V_{CF}^{l=2} = \begin{bmatrix} \frac{B_{4,0}}{21} & 0 & 0 & 0 & \frac{5B_{4,0}}{21} \\ 0 & -\frac{4B_{4,0}}{21} & 0 & 0 & 0 \\ 0 & 0 & \frac{2B_{4,0}}{7} & 0 & 0 \\ 0 & 0 & 0 & -\frac{4B_{4,0}}{21} & 0 \\ \frac{5B_{4,0}}{21} & 0 & 0 & 0 & \frac{B_{4,0}}{21} \end{bmatrix}$$

$$E \oplus T_2$$

Free-parameters for d-electrons: $\{B_{4,0}\}$

Eigenvalues and eigenvectors:

$$-\frac{4B_{4,0}}{21} : \{|2,-1\rangle, |2,1\rangle, -|2,-2\rangle + |2,2\rangle\}$$

$$\frac{2B_{4,0}}{7} : \{|2,0\rangle, |2,-2\rangle + |2,2\rangle\}$$

$$V_{CF} = -\frac{\sqrt{70}B_{4,0}C_{4,-4}}{14} + B_{4,0}C_{4,0} - \frac{\sqrt{70}B_{4,0}C_{4,4}}{14} + \frac{\sqrt{14}B_{6,0}C_{6,-4}}{2} + B_{6,0}C_{6,0} + \frac{\sqrt{14}B_{6,0}C_{6,4}}{2}$$

$$V_{CF}^{l=2} = \begin{bmatrix} \frac{B_{4,0}}{21} & 0 & 0 & 0 & -\frac{5B_{4,0}}{21} \\ 0 & -\frac{4B_{4,0}}{21} & 0 & 0 & 0 \\ 0 & 0 & \frac{2B_{4,0}}{7} & 0 & 0 \\ 0 & 0 & 0 & -\frac{4B_{4,0}}{21} & 0 \\ -\frac{5B_{4,0}}{21} & 0 & 0 & 0 & \frac{B_{4,0}}{21} \end{bmatrix}$$

$$E \oplus T_2$$

Free-parameters for d-electrons: $\{B_{4,0}\}$

Eigenvalues and eigenvectors:

$$-\frac{4B_{4,0}}{21} : \{|2,-1\rangle, |2,1\rangle, |2,-2\rangle + |2,2\rangle\}$$

$$\frac{2B_{4,0}}{7} : \{|2,0\rangle, -|2,-2\rangle + |2,2\rangle\}$$

T_d (31)

$$V_{CF} = B_{3,2}C_{3,-2} + B_{3,2}C_{3,2} + \frac{\sqrt{70}B_{4,0}C_{4,-4}}{14} + B_{4,0}C_{4,0} + \frac{\sqrt{70}B_{4,0}C_{4,4}}{14} - \frac{\sqrt{14}B_{6,0}C_{6,-4}}{2} + B_{6,0}C_{6,0} - \frac{\sqrt{14}B_{6,0}C_{6,4}}{2}$$

$$V_{CF}^{l=2} = \begin{bmatrix} \frac{B_{4,0}}{21} & 0 & 0 & 0 & \frac{5B_{4,0}}{21} \\ 0 & -\frac{4B_{4,0}}{21} & 0 & 0 & 0 \\ 0 & 0 & \frac{2B_{4,0}}{7} & 0 & 0 \\ 0 & 0 & 0 & -\frac{4B_{4,0}}{21} & 0 \\ \frac{5B_{4,0}}{21} & 0 & 0 & 0 & \frac{B_{4,0}}{21} \end{bmatrix}$$

$$E \oplus T_2$$

Free-parameters for d-electrons: $\{B_{4,0}\}$

Eigenvalues and eigenvectors:

$$-\frac{4B_{4,0}}{21} : \{|2,-1\rangle, |2,1\rangle, -|2,-2\rangle + |2,2\rangle\}$$

$$\frac{2B_{4,0}}{7} : \{|2,0\rangle, |2,-2\rangle + |2,2\rangle\}$$

$$V_{CF} = B_{3,2}C_{3,-2} + B_{3,2}C_{3,2} - \frac{\sqrt{70}B_{4,0}C_{4,-4}}{14} + B_{4,0}C_{4,0} - \frac{\sqrt{70}B_{4,0}C_{4,4}}{14} + \frac{\sqrt{14}B_{6,0}C_{6,-4}}{2} + B_{6,0}C_{6,0} + \frac{\sqrt{14}B_{6,0}C_{6,4}}{2}$$

$$V_{CF}^{l=2} = \begin{bmatrix} \frac{B_{4,0}}{21} & 0 & 0 & 0 & -\frac{5B_{4,0}}{21} \\ 0 & -\frac{4B_{4,0}}{21} & 0 & 0 & 0 \\ 0 & 0 & \frac{2B_{4,0}}{7} & 0 & 0 \\ 0 & 0 & 0 & -\frac{4B_{4,0}}{21} & 0 \\ -\frac{5B_{4,0}}{21} & 0 & 0 & 0 & \frac{B_{4,0}}{21} \end{bmatrix}$$

$$E \oplus T_2$$

Free-parameters for d-electrons: $\{B_{4,0}\}$

Eigenvalues and eigenvectors:

$$-\frac{4B_{4,0}}{21} : \{|2,-1\rangle, |2,1\rangle, |2,-2\rangle + |2,2\rangle\}$$

$$\frac{2B_{4,0}}{7} : \{|2,0\rangle, -|2,-2\rangle + |2,2\rangle\}$$

O_h (32)

$$V_{CF} = \frac{\sqrt{70}B_{4,0}C_{4,-4}}{14} + B_{4,0}C_{4,0} + \frac{\sqrt{70}B_{4,0}C_{4,4}}{14} - \frac{\sqrt{14}B_{6,0}C_{6,-4}}{2} + B_{6,0}C_{6,0} - \frac{\sqrt{14}B_{6,0}C_{6,4}}{2}$$

$$V_{CF}^{l=2} = \begin{bmatrix} \frac{B_{4,0}}{21} & 0 & 0 & 0 & \frac{5B_{4,0}}{21} \\ 0 & -\frac{4B_{4,0}}{21} & 0 & 0 & 0 \\ 0 & 0 & \frac{2B_{4,0}}{7} & 0 & 0 \\ 0 & 0 & 0 & -\frac{4B_{4,0}}{21} & 0 \\ \frac{5B_{4,0}}{21} & 0 & 0 & 0 & \frac{B_{4,0}}{21} \end{bmatrix}$$

$$E_g \oplus T_{2g}$$

Free-parameters for d-electrons: $\{B_{4,0}\}$

Eigenvalues and eigenvectors:

$$-\frac{4B_{4,0}}{21} : \{|2,-1\rangle, |2,1\rangle, -|2,-2\rangle + |2,2\rangle\}$$

$$\frac{2B_{4,0}}{7} : \{|2,0\rangle, |2,-2\rangle + |2,2\rangle\}$$

$$V_{CF} = -\frac{\sqrt{70}B_{4,0}C_{4,-4}}{14} + B_{4,0}C_{4,0} - \frac{\sqrt{70}B_{4,0}C_{4,4}}{14} + \frac{\sqrt{14}B_{6,0}C_{6,-4}}{2} + B_{6,0}C_{6,0} + \frac{\sqrt{14}B_{6,0}C_{6,4}}{2}$$

$$V_{CF}^{l=2} = \begin{bmatrix} \frac{B_{4,0}}{21} & 0 & 0 & 0 & -\frac{5B_{4,0}}{21} \\ 0 & -\frac{4B_{4,0}}{21} & 0 & 0 & 0 \\ 0 & 0 & \frac{2B_{4,0}}{7} & 0 & 0 \\ 0 & 0 & 0 & -\frac{4B_{4,0}}{21} & 0 \\ -\frac{5B_{4,0}}{21} & 0 & 0 & 0 & \frac{B_{4,0}}{21} \end{bmatrix}$$

$$E_g \oplus T_{2g}$$

Free-parameters for d-electrons: $\{B_{4,0}\}$

Eigenvalues and eigenvectors:

$$-\frac{4B_{4,0}}{21} : \{|2,-1\rangle, |2,1\rangle, |2,-2\rangle + |2,2\rangle\}$$

$$\frac{2B_{4,0}}{7} : \{|2,0\rangle, -|2,-2\rangle + |2,2\rangle\}$$