1. (a)

\[ \chi^{as}_{(tot)} = A_{1g} + B_{1g} + B_{2u} + B_{3u} + A_{1g} + B_{3u} \]

\[ \text{H} \]

\[ \text{C} \]

\[ = 2A_{1g} + B_{1g} + B_{2u} + 2B_{3u} \]

The symmetries of vibrational modes are obtained by

\[ \chi^{as}_{(tot)} \otimes \chi^{vector} = \chi^{translation} - \chi^{rotation} \]

From the character table,

\[ \chi^{translation} = B_{1u} + B_{2u} + B_{3u} \]

\[ \chi^{rotation} = B_{1g} + B_{2g} + B_{3g} \]

\[ \chi^{as}_{vibration} = (2A_{1g} + B_{1g} + B_{2u} + 2B_{3u}) \otimes (B_{1u} + B_{2u} + B_{3u}) \]

\[ - B_{1g} + B_{2g} + B_{3g} - B_{1u} - B_{3u} - B_{3u} \]

\[ = 2B_{1u} + 2B_{2g} + B_{3g} + A_{1u} \]

\[ + 2B_{2u} + 2A_{1g} + B_{1g} + B_{3u} \]

\[ + 2B_{3u} + 2B_{1g} + A_{1g} + B_{3u} \]

\[ - B_{1u} - B_{2u} - B_{3u} - B_{1g} - B_{2g} - B_{3g} \]

\[ = 3A_{1g} + 2B_{1g} + B_{2g} \]

\[ \text{even} \]

\[ + B_{1u} + 2B_{2u} + 2B_{3u} + A_{1u} \]

\[ \text{odd} \]
(b) $3A_{1g}$

$A_{1u}$

$2B_{2u}$

$B_{1u}$

$B_{2g}$

$2B_{1g}$

(Up (+) & down (-) thru plane of paper.)
(c)

For infrared active vibration modes, they must have symmetry $B_{1u}$ or $B_{2u}$ or $B_{3u}$.

Since $B_{1u} + 2B_{2u} + 2B_{3u}$ are infrared active, the vibration modes in $B_{1u} + 2B_{2u} + 2B_{3u}$ are infrared active.

For Raman active modes, they must transform like $x^2$, $y^2$, $z^2$, $xz$, $yz$, $xy$. That is, they must have symmetry $A_{1g}$ or $B_{1g}$ or $B_{3g}$ or $B_{3g}$.

All the even modes $3A_{1g} + 2B_{1g} + B_{3g}$ are Raman active. Since $x^2 + y^2 + z^2$ transforms like $A_{1g}$, the three $A_{1g}$ modes will have diagonal components ($\tilde{E}_i \parallel \tilde{E}_s$).

$B_{1g}, B_{3g}$ transform like $xy$ and $yz$, i.e. The two $B_{1g}$ modes have off-diagonal components ($\tilde{E}_i \perp \tilde{E}_s$) and $\tilde{E}_i, \tilde{E}_s$ are all in the $x-y$ plane.

The $B_{3g}$ mode has off-diagonal component ($\tilde{E}_i \perp \tilde{E}_s$) and one of them ($\tilde{E}_i$ or $\tilde{E}_s$) must be perpendicular to the plane. $A_{1u}$ is silent mode.
2(a) Point Groups for CO$_2$ and N$_2$O:
CO$_2$ : D$_{nah}$
N$_2$O : C$_{ov}$

(b) For CO$_2$:

<table>
<thead>
<tr>
<th></th>
<th>E</th>
<th>2C$_{j}$</th>
<th>C$_{2j}$</th>
<th>i</th>
<th>2iC$_{j}$</th>
<th>iC$_{2j}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\chi_{\text{as.}}$</td>
<td>3</td>
<td>3</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
</tbody>
</table>

\[ \chi_{\text{as.}} = 2A_{1g} + A_{2u} \]

\[ \chi_{\text{m.o.}} = \chi_{\text{as.}} \otimes \chi_{\text{vector}} - \chi_{\text{translation}} - \chi_{\text{rotation}} \]

\[ = (2A_{1g} + A_{1u}) \otimes (A_{2u} + E_{1u}) - (A_{2u} + E_{1u}) - (E_{1g}) \]

\[ = 2A_{2u} + 2E_{1u} + A_{1g} + E_{1g} \]

\[ = A_{1g} + A_{2u} + E_{1u} \]

For N$_2$O:

<table>
<thead>
<tr>
<th></th>
<th>E</th>
<th>2C$_{j}$</th>
<th>C$_{v}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\chi_{\text{as.}}$</td>
<td>3</td>
<td>3</td>
<td>3</td>
</tr>
</tbody>
</table>

\[ \chi_{\text{as.}} = 3A_{1} \]

\[ \chi_{\text{m.o.}} = \chi_{\text{as.}} \otimes \chi_{\text{vector}} - \chi_{\text{trans}} - \chi_{\text{rot}} \]

\[ = 3A_{1} \otimes (A_{i} + E_{i}) - (A_{i} + E_{i}) - E_{i} = 2A_{i} + E_{i} \]
(c) \( \text{CO}_2 \)

\[
\begin{align*}
\text{A}_{1g} & \quad \rightarrow \quad \leftarrow \\
\text{E}_{1u} & \quad \rightarrow \\
\text{A}_{1u} & \quad \rightarrow \\
\end{align*}
\]

\( \text{N}_2\text{O} \)

\[
\begin{align*}
\text{A}_{1g}^1 & \quad \rightarrow \quad \leftarrow \\
\text{E}_1 & \quad \uparrow \\
\text{A}_{1g}^2 & \quad \rightarrow \\
\end{align*}
\]

(d) IR active modes

\[
\begin{align*}
\text{CO}_2: \quad \Gamma_{IR} &= \Gamma_{\text{vector}} \otimes \Gamma_{\text{Ag}} = \text{A}_{2u} + \text{E}_{1u} \\
\text{N}_2\text{O}: \quad \Gamma_{IR} &= \Gamma_{\text{vector}} \otimes \Gamma_{\text{A}_1} = \text{A}_1 + \text{E}_1
\end{align*}
\]

\(
\Rightarrow \text{In IR Spectra, there are 2 modes (peaks) for CO}_2 \text{ 3 modes (peaks) for N}_2\text{O}
\)

Raman Active modes

\[
\begin{align*}
\text{CO}_2: \quad \Gamma_{R} &= (\Gamma_{\text{vector}} \otimes \Gamma_{\text{vector}}) \otimes \Gamma_{\text{Ag}} \\
&= 2\text{A}_{1g} + \text{A}_{2g} + 2\text{E}_{1g} + \text{E}_{2g}
\end{align*}
\]

compared with X-ray, only A_{1g} is Raman active.
\( N_2O \quad \Gamma_R = (\Gamma_{\text{vector}} \otimes \Gamma_{\text{vector}}) \otimes \Gamma_{\text{A}} \)
\[ = 2A_1 + A_2 + 2E_1 + E_2 \]

Compared with \( \chi_{u.v.} \) all the modes are Raman active \((2A_1 + E_1)\)

\( \Rightarrow \) difference in Raman spectra:
Three modes for \( N_2O \), while only one mode for \( CO_2 \).

\( f) \) Since \( N_2O \) has permanent dipole moment while \( CO_2 \) doesn't, the rotational modes for \( N_2O \) molecule can be excited by infrared or Raman spectroscopy.

\( e) \) For a linear molecule, the equation for the rotation energy spectra can be expressed as
\[ E_j = \hbar^2 j (j+1)/2I \]

where \( I \) is principal moment of inertia for the molecule.

This equation suggests that \( CO_2 \) and \( N_2O \) molecules have different spacing in the rotation energy spectra.
Use the decomposition rule,
\[ \chi^{as}_{(tot)} = 2 \Gamma_{1u} + F_{1u} + F_{2u} + H_g \]

(b) \[ \chi^{as} \otimes \chi_{vector} = (2 \Gamma_{1u} + F_{1u} + F_{2u} + H_g) \otimes F_{1u} \]
\[ = 2 \Gamma_{1u} + F_{1u} \otimes F_{1u} + F_{1u} \otimes F_{2u} + F_{1u} \otimes H_g \]

\[
\begin{array}{cccccccccccc}
E & 12C_5 & 12C^2_5 & 20C_3 & 15C_2 & i & 12S^3_{10} & 12S_{10} & 20S_3 & 15S_1 & 15O \\
F_{1u} \otimes F_{1u} & 9 & \Gamma_{1u} & 2-\Gamma & 0 & 1 & 9 & \Gamma_{1u} & 2-\Gamma & 0 & 1 \\
F_{1u} \otimes F_{2u} & 9 & -1 & -1 & 0 & 1 & 9 & -1 & -1 & 0 & 1 \\
F_{1u} \otimes F_{3u} & 15 & 0 & 0 & 0 & -1 & -15 & 0 & 0 & 0 & 1 \\
\end{array}
\]

\[ F_{1u} \otimes F_{1u} = A_{1g} + F_{1g} + H_g \]
\[ F_{1u} \otimes F_{2u} = H_g + G_g \]
\[ F_{1u} \otimes H_g = F_{1u} + F_{2u} + G_u + H_u \]
\[ \chi_{vibration} = 2 \Gamma_{1u} + A_{1g} + F_{1g} + 2H_g + G_g + F_{1u} + F_{2u} + G_u + H_u \]
\[ - F_{1g} - F_{1u} \]
\[ = A_{1g} + G_g + 2H_g + 2F_{1u} + F_{2u} + G_u + H_u \]
Among these normal modes,

IR active : $2 \Gamma_{1u}$

Raman active : $A_{1g} + 2H_g$

(c) For the three normal modes in each $\Gamma_{1u}$ symmetry, the one that transforms like the $x$ partner can only be excited by the $x$-polarized light. Similarly, the ones that correspond to the $y, z$ partners can be excited by $y$-polarized and $z$-polarized light respectively.

For Raman active modes : $A_{1g}$ and $2H_g$

From the character table we see that $A_{1g}$ has only diagonal elements ($\vec{E}_i \parallel \vec{E}_s$) while $H_g$ can have both diagonal ($\vec{E}_i \parallel \vec{E}_s$) and off-diagonal elements.
(a) 
\[ P_i P_j = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 \\ 5 & 2 & 4 & 1 & 3 \end{pmatrix} \]
\[ P_j P_i = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 \\ 4 & 2 & 5 & 3 & 1 \end{pmatrix} \]

To check whether the results are consistent with the character table, note that both \( P_i P_j \) and \( P_j P_i \) are in the class \((4,1)\), while \( P_i \) is in class \((2,1)\) and \( P_j \) is in class \((2^2,1)\).

Now, look at the 1 dimensional representations \( \Gamma_i^s \) and \( \Gamma_i^a \). The characters are also the representations.

We check that:
\[ \Gamma_i^s(P_i) \Gamma_i^s(P_j) = 1 \cdot 1 = 1 = \Gamma_i^s(P_i P_j) \]
\[ \Gamma_i^a(P_i) \Gamma_i^a(P_j) = -1 \cdot 1 = -1 = \Gamma_i^a(P_i P_j) \]

Similarly we check that:
\[ \Gamma_i^s(P_j) \Gamma_i^s(P_i) = \Gamma_i^s(P_i P_j) \]
\[ \Gamma_i^a(P_j) \Gamma_i^a(P_i) = \Gamma_i^a(P_i P_j) \]

The results are consistent!!
4(b) Using eq. (10.9)

\[
\frac{9!}{1^3 \lambda_1! \cdot 2^2 \lambda_2! \cdot \ldots \cdot \Gamma^\lambda \lambda_t!}
\]

We get for the class \((2, 1^3)\), there are

\[
\frac{5!}{1^3 \lambda_1! \cdot 2^1 \lambda_2!} = 10
\]
elements, while for the class \((3, 2)\), there are

\[
\frac{5!}{2^1 \lambda_1! \cdot 3^2 \lambda_2!} = 20
\]
elements.

(c) If we consider \(5^p\) state as an hole in the \(p\) orbit, the spin of the allowed state must be \(S = \Delta = \frac{1}{2}\) and the total angular momentum is \(L = \ell = 1\), because there is only one hole.

The allowed state is \(2^p\), which is exactly same as the result in Table 10.6.

(d) The irreducible representation for \((\uparrow \uparrow \downarrow \downarrow \downarrow)\) is \(X_{\text{perm}}(4, 4, 4, 4, 4)\)

By decomposing (see part (f))

\[
X_{\text{perm}}(4, 4, 4, 4, 4) = \Gamma_1^S + \Gamma_4 + \Gamma_5
\]
According to Table 10.6, $\Gamma_i^s$ corresponds to $s = 5/2$, $\Gamma_4$ corresponds to $s = 3/2$ and $\Gamma_5$ corresponds to $s = 1/2$.

(e) Hund's rule

\[ \Rightarrow \quad d^5 \quad \begin{array}{cccccc} \uparrow & \uparrow & \uparrow & \uparrow & \uparrow \end{array} \]

\[ m_s: -2 \quad -1 \quad 0 \quad 1 \quad 2 \]

\[ \Rightarrow \quad \text{Total angular momentum} \quad L = 0 \]

\[ \Rightarrow \quad \text{Total spin} \quad S = 5/2 \]

\[ \Rightarrow \quad 6S \text{ state} \]

From Table 10.6, we find

\[ \chi_{L=0} = \Gamma_1^a + \Gamma_4 + \Gamma_5 + \Gamma_6 \]

\[ \chi_{S=5/2} = \Gamma_1^3 \]

We can check whether this is an allowed state by taking the direct product.

\[ \chi_{L=0} \otimes \chi_{S=5/2} = (\Gamma_1^a + \Gamma_4 + \Gamma_5 + \Gamma_6) \otimes \Gamma_1^s \]

\[ = \Gamma_1^a + \Gamma_4 + \Gamma_5 + \Gamma_6 \]

We can see that this is an allowed state since the direct product contains $\Gamma_1^a$. 

To make life easier, we first work out the irreducible representations contained in each $\chi_{\text{perm}}$.

The results are:

$\chi_{\text{perm}}(V_i V_i V_i V_i V_i) = \Gamma_1^s$

$\chi_{\text{perm}}(V_i V_i V_i V_i V_2) = \Gamma_1^s + \Gamma_4$

$\chi_{\text{perm}}(V_i V_i V_i V_2 V_3) = \Gamma_1^s + \Gamma_4 + \Gamma_5$

$\chi_{\text{perm}}(V_i V_i V_2 V_3 V_3) = \Gamma_1^s + 2\Gamma_4 + \Gamma_5 + \Gamma_6$

$\chi_{\text{perm}}(V_i V_2 V_3 V_4 V_4) = \Gamma_1^s + 3\Gamma_4 + \Gamma_4' + 3\Gamma_5' + 2\Gamma_5' + 3\Gamma_6$

$\chi_{\text{perm}}(V_i V_2 V_3 V_4 V_5) = \Gamma_1^s + \Gamma_1^a + 4\Gamma_4 + 4\Gamma_4' + 5\Gamma_5 + 5\Gamma_5' + 6\Gamma_6$
The character for the equivalence transformation for a (3, 2) state have been listed in the extended character table:

\[
\begin{array}{c|ccccc}
\text{Xperm}(4; 4; 4; 4; 4) & 10 & 4 & 2 & 1 & \vdots \\
\text{Xperm}(4; 4; 4; 4; 4) & 10 & 4 & 2 & 1 & \vdots \\
\end{array}
\]

To get these, one observes that there are \( \binom{5}{3} = 10 \) possible ways to form a (3, 2) state, therefore \((4, 4, 4, 4, 4)\) transforms as a 10-dimensional reducible representation of the group \( P(5) \) with 10 partners for this state. So we get \( \text{Xperm}(15) = 10 \).

Each of the permutation operations \([10 (2, 1^3)]\) leaves 4 partners invariant:

10 partners for (3, 2) state

\[
\begin{align*}
(1 & 2)(3 & 4 & 5) \\
(1 & 3)(2 & 4 & 5) \\
(1 & 4)(2 & 3 & 5) \\
(1 & 5)(2 & 3 & 4) \\
(2 & 3)(1 & 4 & 5) \\
(2 & 4)(1 & 3 & 5) \\
(2 & 5)(1 & 3 & 4) \\
(3 & 4)(1 & 2 & 5) \\
(3 & 5)(1 & 2 & 4) \\
(4 & 5)(1 & 2 & 3)
\end{align*}
\]

One of these operations corresponds to:

\[
\begin{align*}
(1 & 2)(3 & 4 & 5) \\
(3 & 4)(1 & 2 & 5) \\
(3 & 5)(1 & 2 & 4) \\
(4 & 5)(1 & 2 & 3)
\end{align*}
\]

are the 4 invariant partners.
Therefore, $X_{perm}(2, 1^3) = 4$. Similarly, $X_{perm}(2^2, 1) = 2$, $X_{perm}(3, 1^2) = X_{perm}(3, 2) = 1$, $X_{perm}(4, 1) = X_{perm}(5) = 0$

Clearly, $X_{perm}(4, 4, 4, 4, 2, 4, 2) \Rightarrow \Gamma_1^S + \Gamma_4 + \Gamma_5$
(f) For p states we have \( p^+, p^0, p^- \), and for d states there are \( d^2, d', d^0, d^-, d^{-2} \) states. The character of 
\( p^3d^2 \) depends on the which three p states and which two 
d states are occupied.

(i) \((\Psi_1 \Psi_2 \Psi_3 \Psi_4 \Psi_5)\) type:
\[
\begin{align*}
p^+p^+p^+d^2d^2, & \quad p^0p^0p^0d^2d^2, \quad p^-p^-p^-d^2d^2, \\
p^+p^+p^+d'd', & \quad p^0p^0p^0d'd', \quad p^-p^-p^-d'd' \\
p^+p^+p^+d'd^2, & \quad p^0p^0p^0d'd^2, \quad p^-p^-p^-d'd^2 \\
p^+p^+p^+d^2d^2, & \quad p^0p^0p^0d^2d^2, \quad p^-p^-p^-d^2d^2 \\
\end{align*}
\]
Totally 15 configurations.

For this type of configuration,
\[
\chi = \chi_{\text{perm}}(\Psi_1 \Psi_2 \Psi_3 \Psi_4 \Psi_5) = \Gamma_1^5 + \Gamma_4 + \Gamma_5
\]

(ii) \((\Psi_1 \Psi_2 \Psi_3 \Psi_4 \Psi_5)\) type:

For this type, three electrons are in the same p state
while the 2 d electrons are in different d orbitals.
For example, \( p^+p^+p^+d^2d' \), \( p^+p^+p^+d^0d^0 \),

\[
\rightarrow \text{There are } 3 \times C_2^5 = 30 \text{ configurations in this type of configuration.}
\]
\[
\chi = \chi_{\text{perm}}(\Psi_1 \Psi_2 \Psi_3 \Psi_4 \Psi_5) = \Gamma_1^5 + 2\Gamma_4 + \Gamma_5 + \Gamma_6
\]

(iii) \((\Psi_1 \Psi_2 \Psi_3 \Psi_4 \Psi_5)\) type:

For this case, 2 electrons are in the same p state and
one in a different p state. The two d electrons are
in the same d state. For example, \( p^+p^+p^-d^2d^2 \),

\[
\rightarrow \text{There are } C_2^3 \times C_2^5 \times C_1^5 = 30 \text{ configurations.}
\]
\[
\chi = \chi_{\text{perm}}(\Psi_1 \Psi_2 \Psi_3 \Psi_4 \Psi_5) = \Gamma_1^{5} + 2\Gamma_4 + 2\Gamma_5 + \Gamma_5' + \Gamma_6
\]
(iv) \((\Psi_1, \Psi_2, \Psi_3, \Psi_4)\) type:

For this type, we can have

(1) all \(p\) electrons are in different states and \(d\) electrons are in the same state.

(2) two \(p\) electrons are in the same state, the rest three electrons are all in different states.

The number of configurations is \(1 \times C_1^5 + C_1^3 \times C_1^2 \times C_4^2 = 35\)

\[\chi = \chi_{\text{perm.}} (\Psi_1, \Psi_2, \Psi_3, \Psi_4) = \Gamma_1^5 + 2 \Gamma_4^1 + 2 \Gamma_5^1 + \Gamma_5^1 + \Gamma_6^1\]

(v) \((\Psi_1, \Psi_2, \Psi_3, \Psi_4, \Psi_5)\) type:

all electrons are in different \(p\) or \(d\) states.

For example, \(p^1 p^1 p^0 d^0 d^2\).

The number of configurations is \(1 \times C_5^5 = 10\)

\[\chi = \chi_{\text{perm.}} (\Psi_1, \Psi_2, \Psi_3, \Psi_4, \Psi_5)\]

\[= \Gamma_1^5 + \Gamma_1^4 + 4 \Gamma_4^1 + 4 \Gamma_4^1 + 5 \Gamma_5^1 + 5 \Gamma_5^1 + 6 \Gamma_6^1\]
<table>
<thead>
<tr>
<th>Configuration</th>
<th>State</th>
<th>Irreducible Representation</th>
<th>Allowed State</th>
</tr>
</thead>
<tbody>
<tr>
<td>(↑↑↑↓↓)</td>
<td>$S = 1/2$</td>
<td>$\Gamma_5^*$</td>
<td></td>
</tr>
<tr>
<td>(↑↑↑↑↓)</td>
<td>$S = 3/2$</td>
<td>$\Gamma_4$</td>
<td></td>
</tr>
<tr>
<td>(↑↑↑↑↑)</td>
<td>$S = 5/2$</td>
<td>$\Gamma_1^*$</td>
<td></td>
</tr>
<tr>
<td>$s^5$</td>
<td>$L = 0$</td>
<td>$\Gamma_1^*$</td>
<td></td>
</tr>
<tr>
<td>$1s^42s$</td>
<td>$L = 0$</td>
<td>$\Gamma_1^* + \Gamma_4$</td>
<td></td>
</tr>
<tr>
<td>$1s^22s^23s$</td>
<td>$L = 0$</td>
<td>$\Gamma_1^* + 2\Gamma_4 + 2\Gamma_5 + \Gamma_5' + \Gamma_6$</td>
<td>$2S$</td>
</tr>
<tr>
<td>$p^5$</td>
<td>$L = 0$</td>
<td>$\Gamma_6$</td>
<td></td>
</tr>
<tr>
<td>$p^5$</td>
<td>$L = 1$</td>
<td>$\Gamma_1^* + \Gamma_4 + \Gamma_5 + \Gamma_5'$</td>
<td>$2P$</td>
</tr>
<tr>
<td>$p^5$</td>
<td>$L = 2$</td>
<td>$\Gamma_4 + \Gamma_5 + \Gamma_6$</td>
<td></td>
</tr>
<tr>
<td>$p^5$</td>
<td>$L = 3$</td>
<td>$\Gamma_1^* + \Gamma_4 + \Gamma_5$</td>
<td></td>
</tr>
<tr>
<td>$p^5$</td>
<td>$L = 4$</td>
<td>$\Gamma_4$</td>
<td></td>
</tr>
<tr>
<td>$p^5$</td>
<td>$L = 5$</td>
<td>$\Gamma_1^*$</td>
<td></td>
</tr>
<tr>
<td>$d^5$</td>
<td>$L = 0$</td>
<td>$\Gamma_1^* + \Gamma_4 + \Gamma_5 + \Gamma_6$</td>
<td>$2S, 6S$</td>
</tr>
<tr>
<td>$d^5$</td>
<td>$L = 1$</td>
<td>$\Gamma_1^* + 2\Gamma_4 + \Gamma_5 + 3\Gamma_5 + \Gamma_5' + 2\Gamma_6$</td>
<td>$2P, 4P$</td>
</tr>
<tr>
<td>$d^5$</td>
<td>$L = 2$</td>
<td>$2\Gamma_1^* + 3\Gamma_4 + \Gamma_5 + 4\Gamma_5 + 3\Gamma_5' + 2\Gamma_6$</td>
<td>$2D, 2D, 2D, 4D$</td>
</tr>
<tr>
<td>$d^5$</td>
<td>$L = 3$</td>
<td>$\Gamma_1^* + 4\Gamma_4 + \Gamma_5 + 3\Gamma_5 + 2\Gamma_5' + 4\Gamma_6$</td>
<td>$2F, 2F, 4F$</td>
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<tr>
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<td>$2\Gamma_1^* + 4\Gamma_4 - \Gamma_5 + 4\Gamma_5 + 2\Gamma_5' + 2\Gamma_6$</td>
<td>$2G, 2G, 4G$</td>
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<tr>
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<td>$L = 5$</td>
<td>$\Gamma_1^* + 3\Gamma_4 + 3\Gamma_5 + \Gamma_5' + 3\Gamma_6$</td>
<td>$2H$</td>
</tr>
<tr>
<td>$d^5$</td>
<td>$L = 6$</td>
<td>$2\Gamma_1^* + 3\Gamma_4 - 2\Gamma_5 + \Gamma_5' + \Gamma_6$</td>
<td>$2I$</td>
</tr>
<tr>
<td>$d^5$</td>
<td>$L = 7$</td>
<td>$\Gamma_1^* + 2\Gamma_4 + \Gamma_5 + \Gamma_6$</td>
<td></td>
</tr>
<tr>
<td>$d^5$</td>
<td>$L = 8$</td>
<td>$\Gamma_1^* + \Gamma_4 + \Gamma_5$</td>
<td></td>
</tr>
<tr>
<td>$d^5$</td>
<td>$L = 9$</td>
<td>$\Gamma_4$</td>
<td></td>
</tr>
<tr>
<td>$d^5$</td>
<td>$L = 10$</td>
<td>$\Gamma_1^*$</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$S_5$</th>
<th>Irreducible representations</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\chi_{\text{perm.}}(\psi_1 \psi_1 \psi_1 \psi_1 \psi_1)$</td>
<td>$\Rightarrow \Gamma_1^*$</td>
</tr>
<tr>
<td>$\chi_{\text{perm.}}(\psi_1 \psi_1 \psi_1 \psi_1 \psi_2)$</td>
<td>$\Rightarrow \Gamma_1^* + \Gamma_4$</td>
</tr>
<tr>
<td>$\chi_{\text{perm.}}(\psi_1 \psi_1 \psi_1 \psi_2 \psi_2)$</td>
<td>$\Rightarrow \Gamma_1^* + \Gamma_4 + \Gamma_5$</td>
</tr>
<tr>
<td>$\chi_{\text{perm.}}(\psi_1 \psi_1 \psi_1 \psi_2 \psi_3)$</td>
<td>$\Rightarrow \Gamma_1^* + 2\Gamma_4 + \Gamma_5 + \Gamma_6$</td>
</tr>
<tr>
<td>$\chi_{\text{perm.}}(\psi_1 \psi_1 \psi_2 \psi_2 \psi_2)$</td>
<td>$\Rightarrow \Gamma_1^* + 2\Gamma_4 + 2\Gamma_5 + \Gamma_5' + \Gamma_6$</td>
</tr>
<tr>
<td>$\chi_{\text{perm.}}(\psi_1 \psi_1 \psi_2 \psi_3 \psi_4)$</td>
<td>$\Rightarrow \Gamma_1^* + 3\Gamma_4 + \Gamma_5' + 3\Gamma_5 + 2\Gamma_5' + 3\Gamma_6$</td>
</tr>
<tr>
<td>$\chi_{\text{perm.}}(\psi_1 \psi_2 \psi_3 \psi_4 \psi_5)$</td>
<td>$\Rightarrow \Gamma_1^* + \Gamma_4 + 4\Gamma_4 + 4\Gamma_4' - 5\Gamma_5 + 5\Gamma_5' + 6\Gamma_6$</td>
</tr>
</tbody>
</table>
(3) For \( p^3 d^2 \), the total orbital angular momentum can be
\[ L = 1 + 1 + 2 + 2 = 7 \] to \( L = 0 \)

(1) \( L = 7 \), the configuration can only be \( p^* p^* p^* d^2 d^2 \) to
make \( M_L = 7 \).
\[ \chi_{L=7} = \chi_{\text{perm.}} (\Psi_1 \Psi_2 \Psi_2 \Psi_2) \]
\[ = \Gamma_1^S + \Gamma_4 + \Gamma_5 \]

(2) \( L = 6 \); to make \( M_L = 6 \), we can use \( p_0 p^* p^* d^2 d^2 \) only.
\[ \chi_{M_L=6} = \chi_{\text{perm.}} (\Psi_1 \Psi_1 \Psi_2 \Psi_2 \Psi_3) \]
\[ = \Gamma_1^S + 2 \Gamma_4 + 2 \Gamma_5 + \Gamma_5' + \Gamma_6 \]
We have to subtract the representations that go to \( L = 7 \).
\[ \chi_{L=6} = \Gamma_1^S + 2 \Gamma_4 + 2 \Gamma_5 + \Gamma_5' + \Gamma_6 - (\Gamma_1^S + \Gamma_4 + \Gamma_5) \]
\[ = \Gamma_4 + \Gamma_5 + \Gamma_5' + \Gamma_6 \]

(3) \( L = 5 \), the \( M_L = 5 \) state can be constructed from
\( p_0 p^* p^* d^2 d^2 \), \( p^0 p^0 p^* d^2 d^2 \), \( p^0 p^* p^* d^2 d^2 \), \( p^* p^* p^* d^2 d^2 \)
\[ \chi_{M_L=5} = 2 \chi_{\text{perm.}} (\Psi_1 \Psi_1 \Psi_2 \Psi_2 \Psi_3) + \chi_{\text{perm.}} (\Psi_1 \Psi_1 \Psi_2 \Psi_3 \Psi_4) + \chi_{\text{perm.}} (\Psi_1 \Psi_1 \Psi_1 \Psi_1 \Psi_5) \]
\[ = 2 (\Gamma_1^S + 2 \Gamma_4 + 2 \Gamma_5 + \Gamma_5' + \Gamma_6) + (\Gamma_1^S + 3 \Gamma_4 + \Gamma_4' + 3 \Gamma_5 + 2 \Gamma_5' + \Gamma_6) \]
\[ + (\Gamma_1^S + 2 \Gamma_4 + \Gamma_5 + \Gamma_6) \]
\[ = 4 \Gamma_1^S + 9 \Gamma_4 + \Gamma_4' + 8 \Gamma_5 + 4 \Gamma_5' + 6 \Gamma_6 \]
\[ \chi_{L=5} = \chi_{M_L=5} - \chi_{L=7} - \chi_{L=6} \]
\[ = 3 \Gamma_1^S + 7 \Gamma_4 + \Gamma_4' + 6 \Gamma_5 + 3 \Gamma_5' + 5 \Gamma_6 \]
We stop here and check if there are allowed states for \( L=7 \) or \( 6 \) or \( 5 \).

From Table 10.6, \( \chi_{S=1/2} = \Gamma_5 \), \( \chi_{S=3/2} = \Gamma_4 \), \( \chi_{S=5/2} = \Gamma_1^s \).

For \( L=7 \),
\[
\chi_{L=7} \otimes \chi_{S=1/2} = (\Gamma_1^s + \Gamma_4 + \Gamma_5) \otimes \Gamma_5
\]
\[
= \Gamma_5 + (\Gamma_4^' + \Gamma_5 + \Gamma_5^' + \Gamma_6) + (\Gamma_1^s + \Gamma_4 + \Gamma_5^' + \Gamma_6)
\]
\[
\chi_{L=7} \otimes \chi_{S=3/2} = (\Gamma_1^s + \Gamma_4 + \Gamma_5) \otimes \Gamma_4
\]
\[
= \Gamma_4 + (\Gamma_1^s + \Gamma_4 + \Gamma_5^' + \Gamma_6) + (\Gamma_4^' + \Gamma_5 + \Gamma_5^' + \Gamma_6)
\]
\[
\chi_{L=7} \otimes \chi_{S=5/2} = (\Gamma_1^s + \Gamma_4 + \Gamma_5) \otimes \Gamma_1^s
\]
\[
= (\Gamma_4 + \Gamma_5 + \Gamma_6)
\]

There is no allowed states for \( L=7 \) since no \( \Gamma_1^a \) appears in the representations.

For \( L=6 \),
\[
\chi_{L=6} \otimes \chi_{S=1/2} = (\Gamma_4 + \Gamma_5 + \Gamma_5^' + \Gamma_6) \otimes \Gamma_5
\]
\[
\chi_{L=6} \otimes \chi_{S=3/2} = (\Gamma_4 + \Gamma_5 + \Gamma_5^' + \Gamma_6) \otimes \Gamma_4
\]
\[
\chi_{L=6} \otimes \chi_{S=5/2} = (\Gamma_4 + \Gamma_5 + \Gamma_5^' + \Gamma_6) \otimes \Gamma_1^s
\]

We only have to look at \( \Gamma_5 \otimes \Gamma_5 \), \( \Gamma_5 \otimes \Gamma_6 \), \( \Gamma_5 \otimes \Gamma_4 \), \( \Gamma_6 \otimes \Gamma_4 \) since the others are already known.

\[
\Gamma_5 \otimes \Gamma_5 = \Gamma_1^a + \Gamma_4 + \Gamma_4^' + \Gamma_5 + \Gamma_5^' + \Gamma_6
\]
\[
\Gamma_5 \otimes \Gamma_6 = \Gamma_4 + \Gamma_4^' + \Gamma_5 + \Gamma_5^' + 2\Gamma_6
\]
\[
\Gamma_5 \otimes \Gamma_4 = \Gamma_4 + \Gamma_5 + \Gamma_5^' + \Gamma_6
\]
\[
\Gamma_6 \otimes \Gamma_4 = \Gamma_4 + \Gamma_4^' + \Gamma_5 + \Gamma_5^' + \Gamma_6
\]
So, we see $\Gamma_a$ is contained in $\chi_{L=6} \otimes \chi_{S=\frac{1}{2}}$!

The Pauli allowed state with the largest $L$ is $L=6, S=\frac{1}{2}$, that is, $\frac{2}{I}$

(h)

Let's determine the spin states first.

Obviously, $(\uparrow \uparrow \uparrow \uparrow \uparrow) \rightarrow \chi_{\text{perm}}(4,4,4,4) = \Gamma_S$

$S = \frac{3}{2}$ $(\uparrow \uparrow \uparrow \uparrow \uparrow) \rightarrow \chi_{\text{perm}}(4,4,4,4) = \Gamma_S$

$A_{\Gamma_S} = \frac{1}{120} \left( 5 + 10 \times 3 + 15 + 20 \times 2 + 30 \right) = 1$

$A_{\Gamma_4} = \frac{1}{120} \left( 20 + 60 + 40 \right) = 1$

$\Rightarrow \chi_{\text{perm}}(4,4,4,4) = \Gamma_S$

$M = \frac{3}{2}$ $S = \frac{3}{2}$

for $S = \frac{3}{2}$

$S = \frac{1}{2}$ $(\uparrow \uparrow \uparrow \uparrow \uparrow) \rightarrow \chi_{\text{perm}}(4,4,4,4,4)$

$A_{\Gamma_S} = \frac{1}{120} \left( 10 + 40 + 30 + 20 + 20 \right) = 1$

$A_{\Gamma_4} = \frac{1}{120} \left( 10 - 40 + 30 + 20 - 20 \right) = 0$
\[ A_{\text{r}}^t = \frac{1}{120} (40 + 80 + 20 + (-20)) = 1. \]

\[ A_{\text{f,5}}^t = \frac{1}{120} (50 + 40 + 30 - 20 + 20) = 1. \]

\[ \chi_{\text{perm}}(\psi_1\psi_2\psi_3\psi_4) = \Gamma^s + \Gamma_4 + \Gamma_5 \]

\[ M_s = \frac{1}{2} \quad M_5 = \frac{1}{2} \quad S = \frac{1}{2}. \]

For \( S = \frac{5}{2} \) for \( S = \frac{3}{2} \)

Therefore, I get

\[ (\uparrow \uparrow \uparrow \uparrow \uparrow) = \Gamma^s \quad (S = \frac{5}{2}) \]

\[ (\uparrow \uparrow \uparrow \uparrow \downarrow) = \Gamma_4 \quad (S = \frac{3}{2}) \]

\[ (\uparrow \uparrow \uparrow \downarrow \downarrow) = \Gamma_5 \quad (S = \frac{1}{2}) \]

For orbital states, consider

\[ M_L = 10 \quad d^{2+}d^{2+}d^{2+}d^{2+}d^{2+} \]

\[ \Rightarrow \chi_{\text{perm}}(\psi_1\psi_1\psi_1\psi_3\psi_1) = \Gamma^i \]

\[ \Gamma^i \otimes (\Gamma^i + \Gamma_4 + \Gamma_5) \Rightarrow \text{No } \Gamma^i \text{ contained } \Rightarrow \text{not allowed.} \]

\[ l = 10 \]

\[ L = 9 \quad d^{2+}d^{2+}d^{2+}d^{2+}d^+ \]

\[ \Rightarrow \chi_{\text{perm}}(\psi_1\psi_1\psi_1\psi_1\psi_1) = \Gamma_4 + \Gamma^i \]

\[ \Rightarrow \Gamma_4 \otimes (\Gamma^i + \Gamma_4 + \Gamma_5) \Rightarrow \text{No } \Gamma^i \Rightarrow \text{not allowed.} \]

\[ L = 8 \quad d^{2+}d^{2+}d^{2+}d^{2+}d^0 \quad \text{and } d^{2+}d^{2+}d^{2+}d^+d^+ \]

\[ \Rightarrow \chi_{\text{perm}}(\psi_1\psi_1\psi_1\psi_1\psi_1) \quad \text{and} \quad \chi_{\text{perm}}(\psi_1\psi_1\psi_1\psi_2\psi_2) \]
\[ L = 7 \quad d^{2+}d^{2+}d^{2+}d^+d^+ \quad d^{2+}d^{2+}d^+d^+d^+ \]

\[ \chi_{\text{perm}}(4, 4, 4, 4, 4) \quad \chi_{\text{perm}}(4, 4, 4, 4, 4) \]

\[ d^{2+}d^{2+}d^{2+}d^+d^- \Rightarrow \chi_{\text{perm}}(4, 4, 4, 4, 4) = \Gamma_4^5 + \Gamma_4 \]

\[ \chi_{\text{perm}}(4, 4, 4, 4, 4) = \Gamma_4^5 + 2\Gamma_4^5 + \Gamma_5 + \Gamma_6 \]

\[ a\Gamma_4^5 = \frac{1}{120}(20 + 60 + 40) = 1 \]

\[ a\Gamma_4^a = \frac{1}{120}(20 - 60 + 40) = 0 \]

\[ a\Gamma_4^b = \frac{1}{120}(80 + 120 + 40) = 2 \]

\[ a\Gamma_4^c = \frac{1}{120}(80 - 120 + 40) = 0 \]

\[ a\Gamma_5^5 = \frac{1}{120}(100 + 60 - 40) = 1 \]

\[ a\Gamma_5^5 = \frac{1}{120}(100 - 60 - 40) = 0 \]

\[ a\Gamma_6 = \frac{1}{120}(120) = 1 \]
\[
L = 10 \quad L = 9
\]
\[
\Downarrow \quad \Downarrow
\]
\[
L = 7 \quad (\Gamma_1^s + 2\Gamma_4 + \Gamma_5 + \Gamma_6) + (\Gamma_1^s + \Gamma_4 + \Gamma_5)
\]
\[
+ \Gamma_1^s + \Gamma_4
\]
\[
\Rightarrow \Gamma_1^s + 2\Gamma_4 + \Gamma_5 + \Gamma_6
\]
\[
(\Gamma_1^s + 2\Gamma_4 + \Gamma_5 + \Gamma_6) \otimes (\Gamma_1^s + \Gamma_4 + \Gamma_5)
\]
\[
\Rightarrow \text{No } \Gamma_1^a \text{ contained} \quad \Rightarrow \text{no allowed state.}
\]

\[
L = 6
\]
\[
d^2 d^2 d^2 d^0 d^0 \quad x_{perm} (4_i 4_i 4_i 4_i 4_i) = \Gamma_1^s + \Gamma_4 + \Gamma_5
\]
\[
d^2 d^2 d^2 d^0 d^0 \quad x_{perm} (4_i 4_i 4_i 4_i 4_i) = \Gamma_1^s + 2\Gamma_4 + 2\Gamma_5 + \Gamma_5' + \Gamma_6
\]
\[
d^2 d^2 d^2 d^0 d^0 \quad x_{perm} (4_i 4_i 4_i 4_i 4_i) = \Gamma_1^s + \Gamma_4
\]
\[
d^2 d^2 d^2 d^2 d^0 \quad x_{perm} (4_i 4_i 4_i 4_i 4_i) = \Gamma_1^s + 2\Gamma_4 + \Gamma_5 + \Gamma_6
\]
\[
d^2 d^2 d^2 d^2 d^2 \quad x_{perm} (4_i 4_i 4_i 4_i 4_i) = \Gamma_1^s + \Gamma_4
\]

\[
L = 8
\]
\[
\Rightarrow \begin{cases}
\Gamma_1^s + \Gamma_4 + \Gamma_5 + \Gamma_6
\end{cases}
\]
\[
\Rightarrow \begin{cases}
\Gamma_1^s + \Gamma_4 + \Gamma_5 + \Gamma_6
\end{cases}
\]
\[
\Rightarrow \Gamma_1^s + 2\Gamma_4 + \Gamma_5 + \Gamma_6
\]
\[
(2\Gamma_1^s + 3\Gamma_4 + 2\Gamma_5 + \Gamma_5' + \Gamma_6) \otimes (\Gamma_1^s + \Gamma_4 + \Gamma_5)
\]

contains
\[
\Gamma_5 \otimes \Gamma_5 = \Gamma_1^a + \Gamma_4 + \Gamma_4' + \Gamma_5 + \Gamma_5' + \Gamma_6
\]

\[
\Rightarrow \text{There is one allowed state.} \quad \overline{2}I
\]
\[ L = 5 \]
\[ d^{2t} d^{2+} d^{10} d^0 \]
\[ \chi_{\text{perm}}(4, 4, 4, 4, 4) = \Gamma_1^s + 2 \Gamma_4 + 2 \Gamma_5 + \Gamma_5^r + \Gamma_6 \]
\[ d^{2t} d^{2+} d^0 d^0 \]
\[ \chi_{\text{perm}}(4, 4, 4, 4, 4) = \Gamma_1^s + 2 \Gamma_4 + \Gamma_5 + \Gamma_6 \]
\[ d^{2t} d^+ d^+ d^0 \]
\[ \chi_{\text{perm}}(4, 4, 4, 4, 4) = \Gamma_1^s \]
\[ d^{2t} d^{2+} d^t d^0 \]
\[ \chi_{\text{perm}}(4, 4, 4, 4, 4) = \Gamma_1^s \]
\[ d^{2t} d^{2+} d^t d^0 \]
\[ \chi_{\text{perm}}(4, 4, 4, 4, 4) = \Gamma_1^s + 2 \Gamma_4 + \Gamma_5 + \Gamma_6 \]
\[ d^{2t} d^t d^t d^t \]
\[ \chi_{\text{perm}}(4, 4, 4, 4, 4) = \Gamma_1^s + 2 \Gamma_4 + 2 \Gamma_5 + \Gamma_6 \]
\[ \Rightarrow 2 \chi_{\text{perm}}(4, 4, 4, 4, 4) + 3 \chi_{\text{perm}}(4, 4, 4, 4, 4) + \chi_{\text{perm}}(4, 4, 4, 4, 4) \]
\[ = 2(\Gamma_1^s + 2 \Gamma_4 + 2 \Gamma_5 + \Gamma_5^r + \Gamma_6) + 3(\Gamma_1^s + 2 \Gamma_4 + \Gamma_5 + \Gamma_6) + \Gamma_1^g \]
\[ = 6 \Gamma_1^s + 10 \Gamma_4 + 7 \Gamma_5 + 2 \Gamma_5^r + 5 \Gamma_6 \]
\[ L = 10 \sim L = 6 \Rightarrow 5 \Gamma_1^s + 7 \Gamma_4 + 4 \Gamma_5 + \Gamma_5^r + 2 \Gamma_6 \]

For \( L = 5 \):
\[ \Rightarrow (\Gamma_1^s + 3 \Gamma_4 + 3 \Gamma_5 + \Gamma_5^r + 3 \Gamma_6) \otimes (\Gamma_1^s + \Gamma_5 + \Gamma_6) \]

Contains one \( \Gamma_5^r \otimes \Gamma_5^r \)

\[ \Rightarrow \text{allowed state } 2H \]

\[ L = 4 \]
\[ d^{2t} d^{2+} d^{10} d^0 \]
\[ \chi_{\text{perm}}(4, 4, 4, 4, 4) = \Gamma_1^s + \Gamma_4 + \Gamma_5 \]
\[ d^{2t} d^{2+} d^+ d^0 \]
\[ \chi_{\text{perm}}(4, 4, 4, 4, 4) = \Gamma_1^s + 3 \Gamma_4 + \Gamma_5 + 3 \Gamma_5^r + 2 \Gamma_5^r + 3 \Gamma_6 \]
\[ d^{2t} d^+ d^+ d^0 \]
\[ \chi_{\text{perm}}(4, 4, 4, 4, 4) = \Gamma_1^s + 2 \Gamma_4 + 2 \Gamma_5 + \Gamma_5^r + \Gamma_6 \]
\[ d^{2t} d^+ d^+ d^0 \]
\[ \chi_{\text{perm}}(4, 4, 4, 4, 4) = \Gamma_1^s + 2 \Gamma_4 + \Gamma_5 + \Gamma_6 \]
\[ d^{2t} d^+ d^+ d^0 \]
\[ \chi_{\text{perm}}(4, 4, 4, 4, 4) = \Gamma_1^s + \Gamma_4 + \Gamma_5 \]
\[ d^{2t} d^+ d^+ d^0 \]
\[ \chi_{\text{perm}}(4, 4, 4, 4, 4) = \Gamma_1^s + 2 \Gamma_4 + 2 \Gamma_5 + \Gamma_5^r + \Gamma_6 \]
\[ d^{2t} d^+ d^+ d^0 \]
\[ \chi_{\text{perm}}(4, 4, 4, 4, 4) = \Gamma_1^s + 2 \Gamma_4 + \Gamma_5 + \Gamma_6 \]
\[ d^{2+} d^+ d^+ d^0 \]
\[ \chi_{\text{perm}}(4, 4, 4, 4, 4) = \Gamma_1^s + \Gamma_4 \]
\[ \chi_{\text{perm}}(4, 4, 4, 4, 4) = \Gamma_1^S + 3 \Gamma_4 + \Gamma_4' + 3 \Gamma_5 + 2 \Gamma_5' + 3 \Gamma_6 \]

\[ A_{\Gamma_1} = \frac{1}{120} \left( 60 + 60 \right) = 1 \]

\[ A_{\Gamma_4} = \frac{1}{120} \left( 240 + 120 \right) = 3 \]

\[ A_{\Gamma_4'} = \frac{1}{120} \left( 240 - 120 \right) = 1 \]

\[ A_{\Gamma_5} = \frac{1}{120} \left( 300 + 60 \right) = 3 \]

\[ A_{\Gamma_5'} = \frac{1}{120} \left( 300 - 60 \right) = 2 \]

\[ A_{\Gamma_6} = \frac{1}{120} \left( 360 \right) = 3 \]

\[ \Rightarrow 8 \Gamma_1^S + 4 \Gamma_4 + 4 \Gamma_4' + 11 \Gamma_5 + 4 \Gamma_5' + 5 \Gamma_6 \]

\[ - \left( 5 \Gamma_1^S + 10 \Gamma_4 + 7 \Gamma_5 + 2 \Gamma_5' + 5 \Gamma_6 \right) \]

\[ = 2 \Gamma_1^S + 4 \Gamma_4 + 4 \Gamma_4' + 4 \Gamma_5 + 2 \Gamma_5' \]

\[ = \left( 2 \Gamma_1^S + 4 \Gamma_4 + 4 \Gamma_4' + 4 \Gamma_5 + 2 \Gamma_5' \right) \otimes \left( \Gamma_1^S + \Gamma_4 + \Gamma_5 \right) \]

Contains one \( \Gamma_4' \otimes \Gamma_4 = \Gamma_1^S + \Gamma_4 + \Gamma_5 + \Gamma_6 \)

and two \( \Gamma_5 \otimes \Gamma_5 = \Gamma_1^S + \Gamma_4 + \Gamma_4' + \Gamma_5 + \Gamma_5' + \Gamma_6 \)

\[ \Rightarrow \text{There are three allowed states. } 4 \Gamma, \, 2 \Gamma, \, 0 \Gamma \]

\[ L = 3 \]

\[ d^2d^2d^1d^1d^1 \]

\[ \chi_{\text{perm}}(4, 4, 4, 4, 4) = \Gamma_1^S + 2 \Gamma_4 + \Gamma_5 + \Gamma_6 \]

\[ \chi_{\text{perm}}(4, 4, 4, 4, 4) = \Gamma_1^S + 3 \Gamma_4 + \Gamma_4' + 3 \Gamma_5 + 2 \Gamma_5' + 3 \Gamma_6 \]

\[ \chi_{\text{perm}}(4, 4, 4, 4, 4) = \Gamma_1^S + 3 \Gamma_4 + \Gamma_4' + \Gamma_5 + \Gamma_5' + \Gamma_6 \]

\[ \chi_{\text{perm}}(4, 4, 4, 4, 4) = \Gamma_1^S + 2 \Gamma_4 + 2 \Gamma_5 + \Gamma_5' + \Gamma_6 \]

\[ \chi_{\text{perm}}(4, 4, 4, 4, 4) = \Gamma_1^S + 2 \Gamma_4 + \Gamma_5 + \Gamma_6 \]

\[ \chi_{\text{perm}}(4, 4, 4, 4, 4) = \Gamma_1^S + 3 \Gamma_4 + \Gamma_4' + \Gamma_5 + 2 \Gamma_5' + 3 \Gamma_6 \]

\[ \chi_{\text{perm}}(4, 4, 4, 4, 4) = \Gamma_1^S + 2 \Gamma_4 + \Gamma_5 + \Gamma_6 \]

\[ \chi_{\text{perm}}(4, 4, 4, 4, 4) = \Gamma_1^S + \Gamma_4 + \Gamma_4' + \Gamma_5 + \Gamma_6 + \Gamma_5' + \Gamma_6 \]
\[ d^+ d^+ d^0 d^0 \quad \chi_{\text{perm}}(4,4,4,4,4) = \Gamma_1^s + \Gamma_4^s + \Gamma_5^s \]

\[ 9 \Gamma_1^s + 18 \Gamma_4^s + 2 \Gamma_4^r + 14 \Gamma_5^r + 6 \Gamma_5^r + 11 \Gamma_6^r \]

\[- (8 \Gamma_1^s + 14 \Gamma_4^s + \Gamma_4^r + 11 \Gamma_5^r + 4 \Gamma_5^r + 5 \Gamma_6) \]

\[ = \Gamma_1^s + 4 \Gamma_4^s + \Gamma_4^r + 3 \Gamma_5^r + 2 \Gamma_5^r + 6 \Gamma_6^r \]

\[ (\Gamma_1^s + 4 \Gamma_4^s + \Gamma_4^r + 3 \Gamma_5^r + 2 \Gamma_5^r + 6 \Gamma_6^r) \otimes (\Gamma_1^s + \Gamma_4^s + \Gamma_5^r + \Gamma_6) \]

Contains one \( \Gamma_4^r \otimes \Gamma_4^s = \Gamma_1^s + \Gamma_4^s + \Gamma_5^r + \Gamma_6^r \)

two \( \Gamma_5^r \otimes \Gamma_5^s = \Gamma_1^s + \Gamma_4^s + \Gamma_4^r + \Gamma_5^r + \Gamma_5^r + \Gamma_6^r \)

\[ \Rightarrow \text{There are three allowed states} \quad 4^F, \ 2F', \ 3F' \]

\[ L = 2 \]

\[ d^2+ d^2+ d^2- d^2- \quad \chi_{\text{perm}}(4,4,4,4,4) = \Gamma_1^s + \Gamma_4^s + \Gamma_5^s \]

\[ d^2+ d^2+ d^1+ d^1- \quad \chi_{\text{perm}}(4,4,4,4,4) = \Gamma_1^s + 3 \Gamma_4^s + \Gamma_4^r + 3 \Gamma_5^r + 2 \Gamma_5^r + 3 \Gamma_6^r \]

\[ d^2+ d^2+ d^0+ d^0- \quad \chi_{\text{perm}}(4,4,4,4,4) = \Gamma_1^s + 2 \Gamma_4^s + 2 \Gamma_5^r + \Gamma_5^r + \Gamma_6^r \]

\[ d^2+ d^2+ d^0- d^0- \quad \chi_{\text{perm}}(4,4,4,4,4) = \Gamma_1^s + 2 \Gamma_4^s + 2 \Gamma_5^r + \Gamma_5^r + \Gamma_6^r \]

\[ d^2+ d^1+ d^1- d^1- \quad \chi_{\text{perm}}(4,4,4,4,4) = \Gamma_1^s + 3 \Gamma_4^s + \Gamma_4^r + 3 \Gamma_5^r + 2 \Gamma_5^r + 3 \Gamma_6^r \]

\[ d^2+ d^1+ d^0+ d^0- \quad \chi_{\text{perm}}(4,4,4,4,4) = \Gamma_1^s + 2 \Gamma_4^s + 2 \Gamma_5^r + \Gamma_5^r + \Gamma_6^r \]

\[ d^2+ d^1+ d^0- d^0- \quad \chi_{\text{perm}}(4,4,4,4,4) = \Gamma_1^s + 3 \Gamma_4^s + \Gamma_4^r + 3 \Gamma_5^r + 2 \Gamma_5^r + 3 \Gamma_6^r \]

\[ d^2+ d^2+ d^2- d^2- \quad \chi_{\text{perm}}(4,4,4,4,4) = \Gamma_1^s + \Gamma_4^s \]

\[ d^2+ d^2+ d^1+ d^1- \quad \chi_{\text{perm}}(4,4,4,4,4) = \Gamma_1^s + 2 \Gamma_4^s + \Gamma_5^r + \Gamma_6^r \]

\[ d^2+ d^1+ d^0+ d^0- \quad \chi_{\text{perm}}(4,4,4,4,4) = \Gamma_1^s + \Gamma_4^s + \Gamma_5^r \]

\[ d^2+ d^1+ d^0- d^0- \quad \chi_{\text{perm}}(4,4,4,4,4) = \Gamma_1^s + 2 \Gamma_4^s + \Gamma_5^r + \Gamma_6^r \]

\[ \Rightarrow \ 10 \Gamma_1^s + 20 \Gamma_4^s + 3 \Gamma_4^r + 18 \Gamma_5^r + 9 \Gamma_5^r + 13 \Gamma_6 \]

\[- (9 \Gamma_1^s + 18 \Gamma_4^s + 2 \Gamma_4^r + 14 \Gamma_5^r + 6 \Gamma_5^r + 11 \Gamma_6) \]
\[
\Rightarrow (\Gamma_1^S + 2\Gamma_4 + \Gamma_4^c + 4\Gamma_5 + 3\Gamma_5^c + 2\Gamma_6) \otimes (\Gamma_1^S + \Gamma_4 + \Gamma_5)
\]

contains

one \( \Gamma_4 \otimes \Gamma_4 = \Gamma_{1^c} + \Gamma_4 + \Gamma_5 + \Gamma_6 \)

three \( \Gamma_5 \otimes \Gamma_5 = \Gamma_{1^c} + \Gamma_4 + \Gamma_5 + \Gamma_5^c + \Gamma_6 \)

\[
\Rightarrow 4D, \quad 2D, \quad 2D, \quad 2D
\]

\[
L = 1
\]

\[
\begin{align*}
\Gamma_1^S + 2\Gamma_4 + \Gamma_4^c + 4\Gamma_5 + 3\Gamma_5^c + 2\Gamma_6 & \ \longmapsto \ \chi_{\text{perm}}(4,4,4^c,4;4) \quad \Gamma_1^S + 2\Gamma_4 + 2\Gamma_5 + \Gamma_5^c + \Gamma_6 \\
\Gamma_4 \otimes \Gamma_4 & = \Gamma_{1^c} + \Gamma_4 + \Gamma_5 + \Gamma_6 \\
\Gamma_5 \otimes \Gamma_5 & = \Gamma_{1^c} + \Gamma_4 + \Gamma_5 + \Gamma_5^c + \Gamma_6 \\
\Gamma_1^S + 3\Gamma_4 + \Gamma_4^c + 3\Gamma_5 + 2\Gamma_5^c + 3\Gamma_6 & \ \longmapsto \ \chi_{\text{perm}}(4,4,4^c,4;4)
\end{align*}
\]

\[
\begin{align*}
\Gamma_2^S + 2\Gamma_4 + \Gamma_4^c + 4\Gamma_5 + 3\Gamma_5^c + 2\Gamma_6 & \ \longmapsto \ \chi_{\text{perm}}(4,4,4^c,4;4) \quad \Gamma_1^S + 2\Gamma_4 + \Gamma_5 + \Gamma_6 \\
\chi_{\text{perm}}(4,4,4^c,4;4) & = \Gamma_{1^c} + \Gamma_4 + \Gamma_5 \\
\Gamma_5^c + \Gamma_5 & \ \longmapsto \ \chi_{\text{perm}}(4,4,4^c,4;4) \\
\Gamma_1^S + 2\Gamma_4 + 2\Gamma_5 + \Gamma_5^c + \Gamma_6 & \ \longmapsto \ \chi_{\text{perm}}(4,4,4^c,4;4) \\
\chi_{\text{perm}}(4,4,4^c,4;4) & = \Gamma_1^S + \Gamma_4
\end{align*}
\]

\[
\Rightarrow (10\Gamma_1^S + (2+12+4+4)\Gamma_4 + 4\Gamma_4^c + (2+12+2+3)\Gamma_5
\]

\[
\quad + 10\Gamma_5^c + (1+12+2+1)\Gamma_6)
\]

\[
\Rightarrow 10\Gamma_1^S + 22\Gamma_4 + 4\Gamma_4^c + 19\Gamma_5 + 10\Gamma_5^c + 16\Gamma_6
\]

\[
\Rightarrow [(10\Gamma_1^S + 20\Gamma_4 + 3\Gamma_4^c + 18\Gamma_5 + 9\Gamma_5^c + 13\Gamma_6)
\]

\[
\Rightarrow 2\Gamma_4 + \Gamma_4^c + \Gamma_5 + \Gamma_5^c + 3\Gamma_6
\]

\[
\Rightarrow (2\Gamma_4 + \Gamma_4^c + \Gamma_5 + \Gamma_5^c + 3\Gamma_6) \otimes (\Gamma_1^S + \Gamma_4 + \Gamma_5)
\]
Contains one $\Gamma_4 \otimes \Gamma_4$

one $\Gamma_5 \otimes \Gamma_5$

$\Rightarrow$ There are two allowed states $^4P, \ 2P$

$L = 0$

\[
\begin{align*}
\Gamma_{1s}^s + 2\Gamma_{4s}^s + 2\Gamma_{5s}^s + \Gamma_{6s}^s & \quad \text{A} \\
\Gamma_{1s}^s + \Gamma_{4s}^s + 4\Gamma_{4s}^s + 4\Gamma_{5s}^s + 5\Gamma_{5s}^s + 5\Gamma_{5s}^s + 6\Gamma_{6s}^s & \\
\Gamma_{1s}^s + 2\Gamma_{4s}^s + \Gamma_{5s}^s + \Gamma_{6s}^s & \quad \text{B} \\
\Gamma_{1s}^s + 2\Gamma_{4s}^s + 2\Gamma_{5s}^s + \Gamma_{5s}^s + \Gamma_{6s}^s & \quad \text{A} \\
\Gamma_{1s}^s + 2\Gamma_{4s}^s + \Gamma_{5s}^s + \Gamma_{6s}^s & \quad \text{B} \\
\Gamma_{1s}^s & \\
\Gamma_{1s}^s + 2\Gamma_{4s}^s + \Gamma_{5s}^s + \Gamma_{6s}^s & \quad \text{A} \\
\Gamma_{1s}^s + \Gamma_{4s}^s + \Gamma_{6s}^s & \\
\Gamma_{1s}^s + \Gamma_{4s}^s + \Gamma_{5s}^s & \quad \text{B} \\
\Gamma_{1s}^s & \\
\Gamma_{1s}^s & \\
\Rightarrow 6\times A + 4\times B + \chi_{perm}(\psi_{1s}^2 \psi_{2s}^2 \psi_{4s}^2) + \Gamma_{1s}^s
\end{align*}
\]

\[
= 6 \times (\Gamma_{1s}^s + 2\Gamma_{4s}^s + 2\Gamma_{5s}^s + \Gamma_{6s}^s) + 4 \times (\Gamma_{1s}^s + 2\Gamma_{4s}^s + \Gamma_{5s}^s + \Gamma_{6s}^s) + \\
\Gamma_{1s}^s + \Gamma_{4s}^s + 4\Gamma_{4s}^s + 4\Gamma_{5s}^s + 5\Gamma_{5s}^s + 5\Gamma_{5s}^s + 6\Gamma_{6s}^s + \Gamma_{6s}^s
\]

\[
= 12\Gamma_{1s}^s + \Gamma_{4s}^s + (12 + 8 + 4)\Gamma_{4s}^s + 4\Gamma_{4s}^s + (12 + 4 + 5)\Gamma_{5s}^s + \\
(6 + 5)\Gamma_{5s}^s + (6 + 4 + 6)\Gamma_{6s}^s
\]
\[
2\Gamma_1^s + \Gamma_1^a + 24\Gamma_4 + 4\Gamma_4' + 21\Gamma_5 + 11\Gamma_5' + 16\Gamma_6
- (10\Gamma_1^s + 22\Gamma_4 + 4\Gamma_4' + 19\Gamma_5 + 10\Gamma_5' + 16\Gamma_6)
= 2\Gamma_1^s + \Gamma_1^a + 2\Gamma_4 + 2\Gamma_5 + \Gamma_5'
\]

\[(2\Gamma_1^s + \Gamma_1^a + 2\Gamma_4 + 2\Gamma_5 + \Gamma_5') \otimes (\Gamma_1^s + \Gamma_4 + \Gamma_5')\]
contains one \(\Gamma_1^a\)
and one \(\Gamma_5 \otimes \Gamma_5\)

\[
\Rightarrow \text{there are two allowed states } {}^6S, {}^2S
\]

To summarize the result, I get the following:

<table>
<thead>
<tr>
<th>(L)</th>
<th>(d^5)</th>
<th>Irreducible rep.</th>
<th>Allowed State</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>(L=0)</td>
<td>(2\Gamma_1^s + \Gamma_1^a + 2\Gamma_4 + 2\Gamma_5 + \Gamma_5')</td>
<td>({}^6S, {}^2S)</td>
</tr>
<tr>
<td>1</td>
<td>(L=1)</td>
<td>(2\Gamma_4 + \Gamma_4' + \Gamma_5 + \Gamma_5' + 3\Gamma_6)</td>
<td>(4\Gamma, {}^2P)</td>
</tr>
<tr>
<td>2</td>
<td>(L=2)</td>
<td>(\Gamma_1^s + 2\Gamma_4 + \Gamma_4' + 4\Gamma_5 + 3\Gamma_5' + 2\Gamma_6)</td>
<td>(4\Gamma, {}^2D, {}^3D, {}^2D)</td>
</tr>
<tr>
<td>3</td>
<td>(L=3)</td>
<td>(\Gamma_1^s + 4\Gamma_4 + \Gamma_4' + 3\Gamma_5 + 2\Gamma_5' + 6\Gamma_6)</td>
<td>(4\Gamma, {}^2F, {}^2F)</td>
</tr>
<tr>
<td>4</td>
<td>(L=4)</td>
<td>(2\Gamma_1^s + 4\Gamma_4 + \Gamma_4' + 4\Gamma_5 + 2\Gamma_5')</td>
<td>(4\Gamma, {}^2G, {}^2G)</td>
</tr>
<tr>
<td>5</td>
<td>(L=5)</td>
<td>(\Gamma_1^s + 3\Gamma_4 + 3\Gamma_5 + \Gamma_5' + 3\Gamma_6)</td>
<td>(2\Gamma, {}^2H)</td>
</tr>
<tr>
<td>6</td>
<td>(L=6)</td>
<td>(2\Gamma_1^s + 3\Gamma_4 + 2\Gamma_5 + \Gamma_5' + \Gamma_6)</td>
<td>(2\Gamma)</td>
</tr>
<tr>
<td>7</td>
<td>(L=7)</td>
<td>(\Gamma_1^s + 2\Gamma_4 + \Gamma_5 + \Gamma_6)</td>
<td>(\longrightarrow)</td>
</tr>
<tr>
<td>8</td>
<td>(L=8)</td>
<td>(\Gamma_1^s + \Gamma_4 + \Gamma_5)</td>
<td>(\longrightarrow)</td>
</tr>
<tr>
<td>9</td>
<td>(L=9)</td>
<td>(\Gamma_4)</td>
<td>(\longrightarrow)</td>
</tr>
<tr>
<td>10</td>
<td>(L=10)</td>
<td>(\Gamma_1^s)</td>
<td>(\longrightarrow)</td>
</tr>
</tbody>
</table>
Hund's rule \[ \rightarrow S = \frac{5}{2}. \]

Ground state is \[ ^6S \]

Since the problem may be asking to do the above calculation taking into account the crystal field splitting in the cubic symmetry, I tried that from the next page.
In cubic symmetry, $\Gamma_{l=2}$ orbitals split according to

$$\Gamma_{l=2} = \text{E}_{g} + \text{T}_{2g}$$

Let the partners for $\text{E}_{g}$ and $\text{T}_{2g}$ be $e_1, e_2$ and $t_1, t_2, t_3$, respectively.

Since we have total 5 electrons, we can assign these electrons in the following way

<table>
<thead>
<tr>
<th></th>
<th>$\text{E}_{g}$</th>
<th>$\text{T}_{2g}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>5</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>4</td>
<td>1</td>
</tr>
<tr>
<td>3</td>
<td>3</td>
<td>2</td>
</tr>
<tr>
<td>4</td>
<td>2</td>
<td>3</td>
</tr>
<tr>
<td>5</td>
<td>1</td>
<td>4</td>
</tr>
<tr>
<td>6</td>
<td>0</td>
<td>5</td>
</tr>
</tbody>
</table>

Let's look at each case separately

1. 5 electrons are in $\text{E}_{g}$

   **Spin state**
   
   \[ S = \frac{1}{2} \quad \Gamma_5 \]
   \[ S = \frac{3}{2} \quad \Gamma_4, \Gamma_5 \]
   \[ S = \frac{5}{2} \quad \Gamma_1 \]

   **Orbital state**
   
   $e_1, e_1, e_1, e_1, e_1 = \chi_{\text{perm}}(1 1 1 1 1) = \Gamma_5$
   
   $e_1, e_1, e_1, e_2 = \chi_{\text{perm}}(1 1 1 1 2) = \Gamma_5 + \Gamma_4$
\[ e_1 e_2 e_3 e_4 = \text{perm}(11122) = \Gamma_1^5 + \Gamma_4 + \Gamma_5 \]
\[ e_1 e_2 e_3 e_4 = \text{perm}(11112) = \Gamma_1^5 + \Gamma_4 \]
\[ e_2 e_3 e_4 e_1 = \text{perm}(11111) = \Gamma_1^5 \]

\[ \Rightarrow \text{no allowed state} \]

(2) 4 electrons are in \( E_g \), one electron in \( T_{2g} \)

Spin State
\[ S = \frac{1}{2} \quad \Gamma_5 \]
\[ S = \frac{3}{2} \quad \Gamma_4 \]
\[ S = \frac{5}{2} \quad \Gamma_1^5 \]

Orbital State \[ \big( \big( i = 1, 2, 3 \big) \big) e_i \leftrightarrow e_2 \]
\[ e_1 e_2 e_3 e_4 = 3 \times (\Gamma_1^5 + \Gamma_4) \times 2 \]
\[ e_1 e_2 e_3 e_4 = 3 \times (\Gamma_1^5 + 2\Gamma_4 + \Gamma_5 + \Gamma_6) \times 2 \]
\[ e_1 e_2 e_3 e_4 = 3 \times (\Gamma_1^5 + 2\Gamma_4 + 2\Gamma_5 + \Gamma_5^r + \Gamma_6) \]

\[ \Rightarrow \text{Three allowed states} \quad 3 \times \Gamma_5 \otimes \Gamma_5 \]

\[ \Rightarrow S = \frac{1}{2} \]
\[ \big( 1E_g + 2T_{2g} \big) \times 3 \]

(3) 3 electrons are in \( E_g \), two electrons in \( T_{2g} \)

\[ \big( e_1 \leftrightarrow e_2 \big) \times \big( i = 1, 2, 3 \big) \]
\[ e_1 e_2 e_1 t_i t_i = 6 \times (\Gamma_1^5 + \Gamma_4 + \Gamma_5) \]
\[ e_1 e_2 e_1 t_i t_i = 6 \times (\Gamma_1^5 + 2\Gamma_4 + 2\Gamma_5 + \Gamma_5^r + \Gamma_6) \]
\[ e_1 e_2 e_1 t_i t_j = 6 \times (\Gamma_1^5 + 2\Gamma_4 + \Gamma_5 + \Gamma_6) \]
\[ e_1 e_2 e_1 t_i t_j = 6 \times (\Gamma_1^5 + 3\Gamma_4 + \Gamma_5^r + 3\Gamma_5 + 2\Gamma_5^r + 3\Gamma_6) \]
\( \Rightarrow \text{allowed states} \) 

\[
\begin{align*}
6 \Gamma_5 \otimes \Gamma_5 & \quad (s = \frac{1}{2}) \quad 6 \left( ^{2}E_g + \frac{1}{2} \right) \\
6 \Gamma_4 \otimes \Gamma_4 & \quad (s = \frac{3}{2}) \quad 6 \ q = \frac{3}{2} \text{ state} \\
12 \Gamma_5 \otimes \Gamma_5 & \quad (s = \frac{1}{2}) \quad 12 \ q = \frac{1}{2} \text{ state} 
\end{align*}
\]

4 Two electrons in \( E_g \) three in \( T_{2g} \)

\[
e_{ij} t_1 t_i t_i (j=1,2, i=1,2,3) = 6 \times (\Gamma_1^s + \Gamma_4 + \Gamma_5)
\]

\[
e_{ij} t_1 t_i t_i t_i (j=1,2, i,k) \times (1,2), (1,3), (2,1), (2,3), (3,1), (3,2) = 12 \times (\Gamma_1^s + 2 \Gamma_4 + 2 \Gamma_5 + \Gamma_5^r + \Gamma_6)
\]

\[
e_{ij} t_1 t_2 t_3 \times (j=1,2) = 2 \times (\Gamma_1^s + 3 \Gamma_4 + \Gamma_4^r + 3 \Gamma_5 + 2 \Gamma_5^r + 3 \Gamma_6)
\]

\[
e_{12} t_1 t_i t_i (i=1,1,3) = 3 \times (\Gamma_1^s + 2 \Gamma_4 + \Gamma_5 + \Gamma_6)
\]

\[
e_{12} t_1 t_i t_i t_j (i,j) = (1,2), (1,3), (2,1), (2,3), (3,1) (3,2)
\]

\[
e_{12} t_1 t_2 t_3 = \Gamma_1^s + 4 \Gamma_4 + 4 \Gamma_4^r + 5 \Gamma_5 + 5 \Gamma_5^r + 6 \Gamma_6
\]

Allowed states

\[
e_{ij} t_1 t_i t_i t_k 
\]

\[
e_{ij} t_1 t_i t_i t_3 
\]

\[
e_{12} t_1 t_i t_i t_j 
\]

\[
e_{12} t_1 t_2 t_3 
\]
one electron in $E_g$ and 4 electrons in $T_{2g}$

$e_i t_j t_j t_j (i,j=1,2, j=1,2,3) = 6 \times (\Gamma^s_1 + \Gamma^s_4)$

$e_i t_j t_j t_k (i=1,2, (j,k)=(1,2), (1,3), (2,1), (2,3), (3,1), (3,2))$

$= 12 \times (\Gamma^s_1 + 2\Gamma^s_4 + \Gamma^s_5 + \Gamma^s_6)$

$e_i t_j t_j t_k t_l (i=1,2, (j,k,l)=(1,2), (1,3), (2,3))$

$= 6 \times (\Gamma^s_1 + 2\Gamma^s_4 + 2\Gamma^s_5 + \Gamma^s_6 + \Gamma^s_5)$

$e_i t_j t_j t_k t_l t_m (i=1,2, (j,k,l,m)=(1,2,3), (2,1,3), (3,1,2))$

$= 6 \times (\Gamma^s_1 + 3\Gamma^s_4 + 3\Gamma^s_5 + 2\Gamma^s_6 + 3\Gamma^s_5)$

Allowed states

$e_i t_j t_j t_k t_k \quad 6 \times \Gamma^s_3 \otimes \Gamma^s_5 \quad (s=\frac{1}{2}) \quad 6 \times (2E_g + 1T_{2g})$

$e_i t_j t_j t_k t_l \quad 6 \times \Gamma^s_4 \otimes \Gamma^s_4 \quad (s=\frac{3}{2}) \quad 6 \times \frac{3}{2} \quad \text{states}$

$12 \times \Gamma^s_5 \otimes \Gamma^s_5 \quad (s=\frac{1}{2}) \quad 12 \times \frac{1}{2} \quad \text{states}$

5 electrons in $T_{2g}$

$tititi (i=1,2,3) = 3 \times \Gamma^s_1$

$tititi t_j (i,k,j)=(1,2),(1,3),(2,1),(2,3),(3,1),(3,2)$

$= 6 \times (\Gamma^s_1 + \Gamma^s_4)$

$tititi t_j t_j (II) = 6 \times (\Gamma^s_1 + \Gamma^s_4 + \Gamma^s_5)$

$tititi t_j t_k (i=1,2,3) = 3 \times (\Gamma^s_1 + 2\Gamma^s_4 + \Gamma^s_5 + \Gamma^s_6)$

$tititi t_j t_k t_k (k=1,2,3) = 3 \times (\Gamma^s_1 + 2\Gamma^s_4 + 2\Gamma^s_5 + \Gamma^s_6 + \Gamma^s_6)$

Allowed states

$tititi t_j t_k \quad 3 \times \Gamma^s_5 \otimes \Gamma^s_5 \quad (s=\frac{1}{2}) \quad 3 \times (1E_g + 2T_{2g})$
The ground state by Hund's rule is

\[(E_g)^2 (T_{2g})^3 \quad S = \frac{5}{2}\] state.

(i)

First I will try to find \(3d^4 4p\) allowed states.

<table>
<thead>
<tr>
<th>3d</th>
<th>4p</th>
</tr>
</thead>
<tbody>
<tr>
<td>(E_g)</td>
<td>(T_{2g})</td>
</tr>
<tr>
<td>4</td>
<td>0</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>1</td>
<td>3</td>
</tr>
<tr>
<td>0</td>
<td>4</td>
</tr>
</tbody>
</table>

\# of electrons in each level

1. \((E_g)^4 (T_{2g})^0 (T_{1u})^1\)

\[e;e;e;e; p_j \quad (i=1,2, j=x,y,z) = 6 \times (\Gamma_1^5 + \Gamma_4)\]

\[e;e;e;e; p_j \quad (i\neq k, \quad \text{""}) = 6 \times (\Gamma_1^5 + 2\Gamma_4 + \Gamma_5 + \Gamma_6)\]

\[e;e;e;e; p_j \quad (j=x,y,z) = 3 \times (\Gamma_1^5 + 2\Gamma_4 + 2\Gamma_5 + \Gamma_5' + \Gamma_6)\]

\(\Rightarrow 3 \quad \Gamma_5 \otimes \Gamma_5\) states \((S = \frac{1}{2})\)

2. \((E_g)^3 (T_{2g})^1 (T_{1u})^0\)

\[e;e;e; t_j p_k \quad (i=1,2, j=1,2,3, k=x,y,z) = 18 \times (\Gamma_1^5 + 2\Gamma_4 + \Gamma_5 + \Gamma_6)\]

\[e;e;e; t_j p_k \quad (i\neq l, \quad \text{""}) = 18 \times (\Gamma_1^5 + 3\Gamma_4 + \Gamma_5 + 3\Gamma_5 + 2\Gamma_5' + 3\Gamma_6)\]

\(\Rightarrow 18 \quad \Gamma_4 \otimes \Gamma_4\) \((S = \frac{3}{2})\) states

36 \quad \Gamma_5 \otimes \Gamma_5\) \((S = \frac{1}{2})\) states.
\((E_g)^2 (T_{2g})^2 (T_{1u})\)

\[ e_1 e_i t_j t_j P_k \quad (i=1,2, j=1,2,3, k=x,y,z) = 18 \left( \Gamma_1^3 + 2 \Gamma_4 + 2 \Gamma_5 + \Gamma_5 + \Gamma_6 \right) \]

\[ e_1 e_i t_j t_j P_k \quad (i=1,2, j=1,2,3, k=x,y,z) = 18 \times \left( \Gamma_1^3 + 3 \Gamma_4 + \Gamma_4 + 3 \Gamma_5 + 2 \Gamma_5 + 3 \Gamma_6 \right) \]

\[ e_1 e_2 t_j t_j P_k \quad (j=1,2,3, k=x,y,z) = 9 \times \left( \Gamma_1^3 + 3 \Gamma_4 + \Gamma_4 + 3 \Gamma_5 + 2 \Gamma_5 + 3 \Gamma_6 \right) \]

\[ e_1 e_2 t_j t_j P_k \quad (j=1,2,3, k=x,y,z) = 9 \times \left( \Gamma_1^3 + \Gamma_4 + 4 \Gamma_4 + 4 \Gamma_4 + 5 \Gamma_5 + 5 \Gamma_5 + 6 \Gamma_6 \right) \]

\[ \Rightarrow \quad 18 \quad \Gamma_1^3 \quad (S = \frac{1}{2}) \quad \text{States} \]

\[ 18 \quad \Gamma_1^3 \quad (S = \frac{3}{2}) \quad \text{States} \]

\[ 36 \quad \Gamma_1^3 \quad (S = 1) \quad \text{States} \]

\[ 9 \quad \Gamma_4 \quad (S = \frac{3}{2}) \quad \text{States} \]

\[ 18 \quad \Gamma_5 \quad (S = 1) \quad \text{States} \]

\[ 9 \quad S = \frac{5}{2} \quad \text{States} \]

\[ 36 \quad S = \frac{3}{2} \quad \text{States} \]

\[ 45 \quad S = \frac{1}{2} \quad \text{States} \]

\[ \text{Total States} = 144 \]

\((E_g)^3 (T_{2g})^3 (T_{1u})\)

\[ e_1 e_2 e_3 t_j t_j t_j P_k \Rightarrow 18 \times \left( \Gamma_1^3 + 2 \Gamma_4 + \Gamma_5 + \Gamma_6 \right) \]

\[ e_1 e_2 e_3 t_j t_j t_j P_k \Rightarrow 36 \times \left( \Gamma_1^3 + 3 \Gamma_4 + \Gamma_4 + 3 \Gamma_5 + 2 \Gamma_5 + 3 \Gamma_6 \right) \]

\[ e_1 e_2 e_3 t_j t_j t_j P_k \Rightarrow 6 \times \left( \Gamma_1^3 + \Gamma_4 + 4 \Gamma_4 + 4 \Gamma_4 + 5 \Gamma_5 + 5 \Gamma_5 + 6 \Gamma_6 \right) \]

\[ \text{allowed States} \]

\[ \Rightarrow \quad 36 \quad S = \frac{3}{2} \quad \text{States} \]

\[ 72 \quad S = \frac{1}{2} \quad \text{States} \]

\[ 6 \quad S = \frac{5}{2} \quad \text{States} \]

\[ 24 \quad S = \frac{3}{2} \quad \text{States} \]

\[ 30 \quad S = \frac{1}{2} \quad \text{States} \]
\[ (E_g)^{2} (T_{2g})^{3} (T_{1u})^{1} \]

\[ t; t; i; t; i; \rho_{k} (i=1, 2, 3, k=x, y, z) = 9 \times (\Gamma_1^{5} + \Gamma_4) \]

\[ t; t; i; t; j; \rho_{k} (i=1, 2, 3, j=i \neq i) = (8 \times (\Gamma_1^{5} + 2 \Gamma_4 + \Gamma_5 + \Gamma_6) \]

\[ t; t; i; t; j; \rho_{k} \left( (i, j) = \left\{ \frac{1}{3}, \frac{2}{3} \right\} \right) = 9 \times (\Gamma_1^{5} + 2 \Gamma_4 + 2 \Gamma_5 + \Gamma_6) \]

\[ t; t; i; t; j; \rho_{k} (i=1, 2, 3) \neq i) = 9 \times (\Gamma_1^{5} + 3 \Gamma_4 + 3 \Gamma_5 + 2 \Gamma_6) \]

\[ \Rightarrow \]

\[ 9 \text{ S = 1/2 states} \]

\[ 9 \text{ S = 3/2 states} \]

\[ 18 \text{ S = 1/2 states} \]

Since a dipole doesn't couple spin states, spin state has to be conserved.

So the possible transitions are,

\[ (E_g)^{2} (T_{2g})^{3} (S = 5/2) \rightarrow 9 (E_g)^{2} (T_{2g})^{2} (T_{1u})^{1} (S = 5/2) \]

and \( (E_g)^{2} (T_{2g})^{3} (S = 5/2) \rightarrow 6 (E_g)^{1} (T_{2g})^{3} (T_{1u})^{1} (S = 5/2) \)

Actually both are allowed transitions, since

\[ \text{Eg} \otimes T_{1u} = T_{1u} + T_{2u} \]

\[ \text{ initial state } \]

\[ \text{dipole (vector) } \]

\[ \text{final state } \]

\[ T_{2g} \otimes T_{1u} = A_{2g} + E_{u} + T_{1u} + T_{2u} \]
Using the method described in lecture notes, we get the Pauli allowed states for 3d\(^5\) configuration. Various allowed states are listed in the table next page. The decomposition of the reducible equivalence representation are also listed, which is reformulated in part (b).

The three Hund rules determine the ground state of an atom whose configuration is given. These rules dictate that to find the ground state:

1. Choose the maximum value of \(S\) consistent with the Pauli principle.
2. Choose the maximum value of \(L\) consistent with the Pauli principle and rule 1.
3a. If the shell is less than half full, choose \(J = J_{\text{min}} = |L - S|\).
3b. If the shell is more than half full, choose \(J = J_{\text{max}} = L + S\).

By Hund's rule, we see that \(6S_{5/2}\) state is the ground state. In this case, \(L = 0, \quad S = \frac{5}{2}\), therefore \(J = \frac{5}{2}\). So the ground state is \(6S_{5/2}\).

For electric dipole transitions, according to the following selection rules:

1. Transitions can occur only between configurations which differ in the \(n\) and \(l\) quantum numbers of a single electron. This means that two or more electrons cannot simultaneously make transitions between subshells.
2. Transitions can occur only between configurations in which the change in the \(l\) quantum number of that electron satisfies the same restriction that applies to one-electron atoms. (8-37)

\[\Delta l = \pm 1\]

3. Transitions can occur only between states in these configurations for which the changes in the \(s', l', j'\) quantum numbers satisfy the restrictions

\[\Delta s' = 0\]
\[\Delta l' = 0, \pm 1\]
\[\Delta j' = 0, \pm 1\] (but not \(j' = 0\) to \(j' = 0\))

the allowed transitions are:

\[6S_{5/2} \rightarrow 6P_{7/2}\]

\[6P_{3/2} \rightarrow 6S_{5/2}\]

\[6P_{3/2} \rightarrow 6P_{3/2}\]