

Group Theory in Quantum Mechanics

Lecture 22 (4.18.13)

Octahedral $O_h \supset O \supset D_4 \supset C_4$ eigensolution in coset spaces II

(Int.J.Mol.Sci, 14, 714(2013) p.755-774 , QTCA Unit 5 Ch. 15)
(PSDS - Ch. 4)

Review Coset factored splitting of $O \supset D_4 \supset C_4$ projectors and levels

Irreducible idempotent projectors $\mathbf{P}^{\mu}_{m,m}$ of $O \supset C_4 \sim T_d \supset C_{4i}$

Calculating \mathbf{P}^E_{0404} \mathbf{P}^E_{2424} $\mathbf{P}^{T_1}_{0404}$ $\mathbf{P}^{T_1}_{1414}$ $\mathbf{P}^{T_2}_{2424}$

Factoring out $O \supset C_4$ subgroup cosets:

Factoring \mathbf{P}^E_{0404} \mathbf{P}^E_{2424} $\mathbf{P}^{T_1}_{0404}$ $\mathbf{P}^{T_1}_{1414}$ $\mathbf{P}^{T_2}_{2424}$

Irreducible nilpotent projectors $\mathbf{P}^{\mu}_{m,n}$

Fundamental $\mathbf{P}^{\mu}_{m,n}$ definitions:

Review of $D_3 \supset C_2 \sim C_{3v} \supset C_v$

Calculating and Factoring $\mathbf{P}^{T_1}_{1404}$

Structure and applications of various subgroup chain ireps

$O_h \supset D_{4h} \supset C_{4v}$

$O_h \supset D_{3h} \supset C_{3v}$

$O_h \supset C_{2v}$

➔ Review Coset factored splitting of $O \supset D_4 \supset C_4$ projectors and levels

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$O_h \supset D_{4h} \supset C_{4v}$

$O_h \supset D_{3h} \supset C_{3v}$

$O_h \supset C_{2v}$

Calculating \mathbf{P}^E_{2424}

$O \supset C_4$	0_4	1_4	2_4	3_4
$A_1 \downarrow C_4$	1	.	.	.
$A_2 \downarrow C_4$.	.	1	.
$E \downarrow C_4$	1	.	1	.
$T_1 \downarrow C_4$	1	1	.	1
$T_2 \downarrow C_4$.	1	1	1

$O: \chi_g^\mu$	$g=1$	\mathbf{r}_{1-4} $\tilde{\mathbf{r}}_{1-4}$	ρ_{xyz}	\mathbf{R}_{xyz} $\tilde{\mathbf{R}}_{xyz}$	\mathbf{i}_{1-6}
$\mu=A_1$	1	1	1	1	1
A_2	1	1	1	-1	-1
E	2	-1	2	0	0
T_1	3	0	-1	1	-1
T_2	3	0	-1	-1	1

$$\mathbf{p}_{m_4} = \sum_{p=0}^3 \frac{e^{2\pi i m \cdot p/4}}{4} \mathbf{R}_z^p = \begin{cases} \mathbf{p}_{0_4} = (1 + \mathbf{R}_z + \rho_z + \tilde{\mathbf{R}}_z)/4 \\ \mathbf{p}_{1_4} = (1 + i\mathbf{R}_z - \rho_z - i\tilde{\mathbf{R}}_z)/4 \\ \mathbf{p}_{2_4} = (1 - \mathbf{R}_z + \rho_z - \tilde{\mathbf{R}}_z)/4 \\ \mathbf{p}_{3_4} = (1 - i\mathbf{R}_z - \rho_z + i\tilde{\mathbf{R}}_z)/4 \end{cases}$$

$$\mathbf{P}^E_{2424} = \mathbf{p}_{2_4} \mathbf{P}^E = \mathbf{P}^E \mathbf{p}_{2_4}$$

$$= \sum_g \frac{\ell^E}{\circ O} (\chi_g^E) \cdot \mathbf{g} \cdot (\mathbf{p}_{2_4}) = \sum_g \frac{2}{96} (\chi_g^E) \cdot \mathbf{g} \cdot (1 \cdot \mathbf{1} + 1 \cdot \rho_z - 1 \cdot \mathbf{R}_z - 1 \cdot \tilde{\mathbf{R}}_z)$$

$$1C_4 = \mathbf{1} \{ \mathbf{1}, \rho_z, \mathbf{R}_z, \tilde{\mathbf{R}}_z \} \quad \rho_x C_4 = \{ \rho_x, \rho_y, \mathbf{i}_4, \mathbf{i}_3 \} \quad \mathbf{r}_1 C_4 = \{ \mathbf{r}_1, \mathbf{r}_4, \mathbf{i}_1, \mathbf{R}_y \} \quad \mathbf{r}_2 C_4 = \{ \mathbf{r}_2, \mathbf{r}_3, \mathbf{i}_2, \tilde{\mathbf{R}}_y \} \quad \tilde{\mathbf{r}}_1 C_4 = \{ \tilde{\mathbf{r}}_1, \tilde{\mathbf{r}}_3, \tilde{\mathbf{R}}_x, \mathbf{i}_6 \} \quad \tilde{\mathbf{r}}_2 C_4 = \{ \tilde{\mathbf{r}}_2, \tilde{\mathbf{r}}_4, \mathbf{R}_x, \mathbf{i}_5 \}$$

$$= \frac{1}{48} \chi_1^E(1, d_{\rho_z}^{24}, d_{\mathbf{R}_z}^{24}, d_{\tilde{\mathbf{R}}_z}^{24}) + \frac{1}{48} \chi_{\rho_x}^E(1, d_{\rho_z}^{24}, d_{\mathbf{R}_z}^{24}, d_{\tilde{\mathbf{R}}_z}^{24}) + \frac{1}{48} \chi_{\mathbf{r}_1}^E(1, d_{\rho_z}^{24}, d_{\mathbf{R}_z}^{24}, d_{\tilde{\mathbf{R}}_z}^{24}) + \frac{1}{48} \chi_{\mathbf{r}_2}^E(1, d_{\rho_z}^{24}, d_{\mathbf{R}_z}^{24}, d_{\tilde{\mathbf{R}}_z}^{24}) + \frac{1}{48} \chi_{\tilde{\mathbf{r}}_1}^E(1, d_{\rho_z}^{24}, d_{\mathbf{R}_z}^{24}, d_{\tilde{\mathbf{R}}_z}^{24}) + \frac{1}{48} \chi_{\tilde{\mathbf{r}}_2}^E(1, d_{\rho_z}^{24}, d_{\mathbf{R}_z}^{24}, d_{\tilde{\mathbf{R}}_z}^{24})$$

$$+ \frac{1}{48} \chi_{\rho_z}^E(d_{\rho_z}^{24}, 1, d_{\tilde{\mathbf{R}}_z}^{24}, d_{\mathbf{R}_z}^{24}) + \frac{1}{48} \chi_{\rho_y}^E(d_{\rho_z}^{24}, 1, d_{\tilde{\mathbf{R}}_z}^{24}, d_{\mathbf{R}_z}^{24}) + \frac{1}{48} \chi_{\mathbf{r}_4}^E(d_{\rho_z}^{24}, 1, d_{\tilde{\mathbf{R}}_z}^{24}, d_{\mathbf{R}_z}^{24}) + \frac{1}{48} \chi_{\mathbf{r}_3}^E(d_{\rho_z}^{24}, 1, d_{\tilde{\mathbf{R}}_z}^{24}, d_{\mathbf{R}_z}^{24}) + \frac{1}{48} \chi_{\tilde{\mathbf{r}}_3}^E(d_{\rho_z}^{24}, 1, d_{\tilde{\mathbf{R}}_z}^{24}, d_{\mathbf{R}_z}^{24}) + \frac{1}{48} \chi_{\tilde{\mathbf{r}}_4}^E(d_{\rho_z}^{24}, 1, d_{\tilde{\mathbf{R}}_z}^{24}, d_{\mathbf{R}_z}^{24})$$

$$+ \frac{1}{48} \chi_{\mathbf{R}_z}^E(d_{\tilde{\mathbf{R}}_z}^{24}, d_{\mathbf{R}_z}^{24}, 1, d_{\rho_z}^{24}) + \frac{1}{48} \chi_{\mathbf{i}_4}^E(d_{\tilde{\mathbf{R}}_z}^{24}, d_{\mathbf{R}_z}^{24}, 1, d_{\rho_z}^{24}) + \frac{1}{48} \chi_{\mathbf{i}_1}^E(d_{\tilde{\mathbf{R}}_z}^{24}, d_{\mathbf{R}_z}^{24}, 1, d_{\rho_z}^{24}) + \frac{1}{48} \chi_{\mathbf{i}_2}^E(d_{\tilde{\mathbf{R}}_z}^{24}, d_{\mathbf{R}_z}^{24}, 1, d_{\rho_z}^{24}) + \frac{1}{48} \chi_{\tilde{\mathbf{R}}_x}^E(d_{\tilde{\mathbf{R}}_z}^{24}, d_{\mathbf{R}_z}^{24}, 1, d_{\rho_z}^{24}) + \frac{1}{48} \chi_{\mathbf{R}_x}^E(d_{\tilde{\mathbf{R}}_z}^{24}, d_{\mathbf{R}_z}^{24}, 1, d_{\rho_z}^{24})$$

$$+ \frac{1}{48} \chi_{\tilde{\mathbf{R}}_z}^E(d_{\mathbf{R}_z}^{24}, d_{\tilde{\mathbf{R}}_z}^{24}, d_{\rho_z}^{24}, 1) + \frac{1}{48} \chi_{\mathbf{i}_3}^E(d_{\mathbf{R}_z}^{24}, d_{\tilde{\mathbf{R}}_z}^{24}, d_{\rho_z}^{24}, 1) + \frac{1}{48} \chi_{\mathbf{R}_y}^E(d_{\mathbf{R}_z}^{24}, d_{\tilde{\mathbf{R}}_z}^{24}, d_{\rho_z}^{24}, 1) + \frac{1}{48} \chi_{\tilde{\mathbf{R}}_y}^E(d_{\mathbf{R}_z}^{24}, d_{\tilde{\mathbf{R}}_z}^{24}, d_{\rho_z}^{24}, 1) + \frac{1}{48} \chi_{\mathbf{i}_6}^E(d_{\mathbf{R}_z}^{24}, d_{\tilde{\mathbf{R}}_z}^{24}, d_{\rho_z}^{24}, 1) + \frac{1}{48} \chi_{\mathbf{i}_5}^E(d_{\mathbf{R}_z}^{24}, d_{\tilde{\mathbf{R}}_z}^{24}, d_{\rho_z}^{24}, 1)$$

$$= \frac{1}{48} (+2)(1, +1, -1, -1) = \frac{1}{48} (+2)(1, +1, -1, -1) + \frac{1}{48} (-1)(1, +1, -1, -1) + \frac{1}{48} (-1)(1, +1, -1, -1) + \frac{1}{48} (-1)(1, +1, -1, -1) + \frac{1}{48} (-1)(1, +1, -1, -1) + \frac{1}{48} (-1)(1, +1, -1, -1)$$

$$+ \frac{1}{48} (+2)(+1, 1, -1, -1) + \frac{1}{48} (+2)(+1, 1, -1, -1) + \frac{1}{48} (-1)(+1, 1, -1, -1) + \frac{1}{48} (-1)(+1, 1, -1, -1) + \frac{1}{48} (-1)(+1, 1, -1, -1) + \frac{1}{48} (-1)(+1, 1, -1, -1)$$

$$+ \frac{1}{48} (0)(-1, -1, 1, +1) + \frac{1}{48} (0)(-1, -1, 1, +1) + \frac{1}{48} (0)(-1, -1, 1, +1) + \frac{1}{48} (0)(-1, -1, 1, +1) + \frac{1}{48} (0)(-1, -1, 1, +1) + \frac{1}{48} (0)(-1, -1, 1, +1)$$

$$+ \frac{1}{48} (0)(-1, -1, +1, 1) + \frac{1}{48} (0)(-1, -1, +1, 1) + \frac{1}{48} (0)(-1, -1, +1, 1) + \frac{1}{48} (0)(-1, -1, +1, 1) + \frac{1}{48} (0)(-1, -1, +1, 1) + \frac{1}{48} (0)(-1, -1, +1, 1)$$

$$\frac{1}{12} (\underline{11} + \underline{1\rho_z} - \underline{1\mathbf{R}_z} - \underline{1\tilde{\mathbf{R}}_z} + \underline{1\rho_x} + \underline{1\rho_y} - \underline{1\mathbf{i}_4} - \underline{1\mathbf{i}_3} \quad \underline{-\frac{1}{2}\mathbf{r}_1} \underline{-\frac{1}{2}\mathbf{r}_4} + \underline{\frac{1}{2}\mathbf{i}_1} + \underline{\frac{1}{2}\mathbf{R}_y} \quad \underline{-\frac{1}{2}\mathbf{r}_2} \underline{-\frac{1}{2}\mathbf{r}_3} + \underline{\frac{1}{2}\mathbf{i}_2} + \underline{\frac{1}{2}\tilde{\mathbf{R}}_y} \quad \underline{-\frac{1}{2}\tilde{\mathbf{r}}_1} \underline{-\frac{1}{2}\tilde{\mathbf{r}}_3} + \underline{\frac{1}{2}\tilde{\mathbf{R}}_x} + \underline{\frac{1}{2}\mathbf{i}_6} \quad \underline{-\frac{1}{2}\tilde{\mathbf{r}}_2} \underline{-\frac{1}{2}\tilde{\mathbf{r}}_4} + \underline{\frac{1}{2}\mathbf{R}_x} + \underline{\frac{1}{2}\mathbf{i}_5})$$

$$\mathbf{P}^E_{2424} = \frac{1}{12} (\underline{11} \underline{-\frac{1}{2}\mathbf{r}_1} \underline{-\frac{1}{2}\mathbf{r}_2} \underline{-\frac{1}{2}\mathbf{r}_3} \underline{-\frac{1}{2}\mathbf{r}_4} \quad \underline{-\frac{1}{2}\tilde{\mathbf{r}}_1} \underline{-\frac{1}{2}\tilde{\mathbf{r}}_2} \underline{-\frac{1}{2}\tilde{\mathbf{r}}_3} \underline{-\frac{1}{2}\tilde{\mathbf{r}}_4} \quad + \underline{1\rho_x} + \underline{1\rho_y} + \underline{1\rho_z} \quad \underline{+\frac{1}{2}\mathbf{R}_x} + \underline{\frac{1}{2}\mathbf{R}_y} - \underline{1\mathbf{R}_z} \quad \underline{+\frac{1}{2}\tilde{\mathbf{R}}_x} + \underline{\frac{1}{2}\tilde{\mathbf{R}}_y} - \underline{1\tilde{\mathbf{R}}_z} \quad \underline{+\frac{1}{2}\mathbf{i}_1} + \underline{\frac{1}{2}\mathbf{i}_2} - \underline{1\mathbf{i}_3} - \underline{1\mathbf{i}_4} + \underline{\frac{1}{2}\mathbf{i}_5} + \underline{\frac{1}{2}\mathbf{i}_6})$$

Calculating $\mathbf{P}^{T_1}_{0_4 0_4}$

$O \supset C_4$	0_4	1_4	2_4	3_4
$A_1 \downarrow C_4$	1	.	.	.
$A_2 \downarrow C_4$.	.	1	.
$E \downarrow C_4$	1	.	1	.
$T_1 \downarrow C_4$	1	1	.	1
$T_2 \downarrow C_4$.	1	1	1

$O: \chi_g^\mu$	$g=1$	\mathbf{r}_{1-4} $\tilde{\mathbf{r}}_{1-4}$	ρ_{xyz}	\mathbf{R}_{xyz} $\tilde{\mathbf{R}}_{xyz}$	\mathbf{i}_{1-6}
$\mu=A_1$	1	1	1	1	1
A_2	1	1	1	-1	-1
E	2	-1	2	0	0
T_1	3	0	-1	1	-1
T_2	3	0	-1	-1	1

$$\mathbf{p}_{m_4} = \sum_{p=0}^3 \frac{e^{2\pi i m \cdot p/4}}{4} \mathbf{R}_z^p =$$

$$\left\{ \begin{array}{l} \mathbf{p}_{0_4} = (1 + \mathbf{R}_z + \rho_z + \tilde{\mathbf{R}}_z)/4 \\ \mathbf{p}_{1_4} = (1 + i\mathbf{R}_z - \rho_z - i\tilde{\mathbf{R}}_z)/4 \\ \mathbf{p}_{2_4} = (1 - \mathbf{R}_z + \rho_z - \tilde{\mathbf{R}}_z)/4 \\ \mathbf{p}_{3_4} = (1 - i\mathbf{R}_z - \rho_z + i\tilde{\mathbf{R}}_z)/4 \end{array} \right.$$

$$\mathbf{P}_{0_4 0_4}^{T_1} = \mathbf{p}_{0_4} \mathbf{P}^{T_1} = \mathbf{P}^{T_1} \mathbf{p}_{0_4}$$

$$= \sum_g \frac{\ell^{T_1}}{\circ O} (\chi_g^{T_1}) \cdot \mathbf{g} \cdot (\mathbf{p}_{0_4}) = \sum_g \frac{3}{96} (\chi_g^{T_1}) \cdot \mathbf{g} \cdot (1 \cdot \mathbf{1} + 1 \cdot \rho_z + 1 \cdot \mathbf{R}_z + 1 \cdot \tilde{\mathbf{R}}_z)$$

$$\mathbf{1}C_4 = \mathbf{1} \{ \mathbf{1}, \rho_z, \mathbf{R}_z, \tilde{\mathbf{R}}_z \} \quad \rho_x C_4 = \{ \rho_x, \rho_y, \mathbf{i}_4, \mathbf{i}_3 \} \quad \mathbf{r}_1 C_4 = \{ \mathbf{r}_1, \mathbf{r}_4, \mathbf{i}_1, \mathbf{R}_y \} \quad \mathbf{r}_2 C_4 = \{ \mathbf{r}_2, \mathbf{r}_3, \mathbf{i}_2, \tilde{\mathbf{R}}_y \} \quad \tilde{\mathbf{r}}_1 C_4 = \{ \tilde{\mathbf{r}}_1, \tilde{\mathbf{r}}_3, \tilde{\mathbf{R}}_x, \mathbf{i}_6 \} \quad \tilde{\mathbf{r}}_2 C_4 = \{ \tilde{\mathbf{r}}_2, \tilde{\mathbf{r}}_4, \mathbf{R}_x, \mathbf{i}_5 \}$$

$$\begin{aligned} &= \frac{1}{32} \chi_{\mathbf{1}}^{T_1} (1, d_{\rho_z}^{0_4}, d_{\mathbf{R}_z}^{0_4}, d_{\tilde{\mathbf{R}}_z}^{0_4}) + \frac{1}{32} \chi_{\rho_x}^{T_1} (1, d_{\rho_z}^{0_4}, d_{\mathbf{R}_z}^{0_4}, d_{\tilde{\mathbf{R}}_z}^{0_4}) + \frac{1}{32} \chi_{\mathbf{r}_1}^{T_1} (1, d_{\rho_z}^{0_4}, d_{\mathbf{R}_z}^{0_4}, d_{\tilde{\mathbf{R}}_z}^{0_4}) + \frac{1}{32} \chi_{\mathbf{r}_2}^{T_1} (1, d_{\rho_z}^{0_4}, d_{\mathbf{R}_z}^{0_4}, d_{\tilde{\mathbf{R}}_z}^{0_4}) + \frac{1}{32} \chi_{\tilde{\mathbf{r}}_1}^{T_1} (1, d_{\rho_z}^{0_4}, d_{\mathbf{R}_z}^{0_4}, d_{\tilde{\mathbf{R}}_z}^{0_4}) + \frac{1}{32} \chi_{\tilde{\mathbf{r}}_2}^{T_1} (1, d_{\rho_z}^{0_4}, d_{\mathbf{R}_z}^{0_4}, d_{\tilde{\mathbf{R}}_z}^{0_4}) \\ &+ \frac{1}{32} \chi_{\rho_z}^{T_1} (d_{\rho_z}^{0_4}, 1, d_{\tilde{\mathbf{R}}_z}^{0_4}, d_{\mathbf{R}_z}^{0_4}) + \frac{1}{32} \chi_{\rho_y}^{T_1} (d_{\rho_z}^{0_4}, 1, d_{\tilde{\mathbf{R}}_z}^{0_4}, d_{\mathbf{R}_z}^{0_4}) + \frac{1}{32} \chi_{\mathbf{r}_4}^{T_1} (d_{\rho_z}^{0_4}, 1, d_{\tilde{\mathbf{R}}_z}^{0_4}, d_{\mathbf{R}_z}^{0_4}) + \frac{1}{32} \chi_{\mathbf{r}_3}^{T_1} (d_{\rho_z}^{0_4}, 1, d_{\tilde{\mathbf{R}}_z}^{0_4}, d_{\mathbf{R}_z}^{0_4}) + \frac{1}{32} \chi_{\tilde{\mathbf{r}}_3}^{T_1} (d_{\rho_z}^{0_4}, 1, d_{\tilde{\mathbf{R}}_z}^{0_4}, d_{\mathbf{R}_z}^{0_4}) + \frac{1}{32} \chi_{\tilde{\mathbf{r}}_4}^{T_1} (d_{\rho_z}^{0_4}, 1, d_{\tilde{\mathbf{R}}_z}^{0_4}, d_{\mathbf{R}_z}^{0_4}) \\ &+ \frac{1}{32} \chi_{\mathbf{R}_z}^{T_1} (d_{\tilde{\mathbf{R}}_z}^{0_4}, d_{\mathbf{R}_z}^{0_4}, 1, d_{\rho_z}^{0_4}) + \frac{1}{32} \chi_{\mathbf{i}_4}^{T_1} (d_{\tilde{\mathbf{R}}_z}^{0_4}, d_{\mathbf{R}_z}^{0_4}, 1, d_{\rho_z}^{0_4}) + \frac{1}{32} \chi_{\mathbf{i}_1}^{T_1} (d_{\tilde{\mathbf{R}}_z}^{0_4}, d_{\mathbf{R}_z}^{0_4}, 1, d_{\rho_z}^{0_4}) + \frac{1}{32} \chi_{\mathbf{i}_2}^{T_1} (d_{\tilde{\mathbf{R}}_z}^{0_4}, d_{\mathbf{R}_z}^{0_4}, 1, d_{\rho_z}^{0_4}) + \frac{1}{32} \chi_{\tilde{\mathbf{R}}_x}^{T_1} (d_{\tilde{\mathbf{R}}_z}^{0_4}, d_{\mathbf{R}_z}^{0_4}, 1, d_{\rho_z}^{0_4}) + \frac{1}{32} \chi_{\mathbf{R}_x}^{T_1} (d_{\tilde{\mathbf{R}}_z}^{0_4}, d_{\mathbf{R}_z}^{0_4}, 1, d_{\rho_z}^{0_4}) \\ &+ \frac{1}{32} \chi_{\tilde{\mathbf{R}}_z}^{T_1} (d_{\mathbf{R}_z}^{0_4}, d_{\tilde{\mathbf{R}}_z}^{0_4}, d_{\rho_z}^{0_4}, 1) + \frac{1}{32} \chi_{\mathbf{i}_3}^{T_1} (d_{\mathbf{R}_z}^{0_4}, d_{\tilde{\mathbf{R}}_z}^{0_4}, d_{\rho_z}^{0_4}, 1) + \frac{1}{32} \chi_{\mathbf{R}_y}^{T_1} (d_{\mathbf{R}_z}^{0_4}, d_{\tilde{\mathbf{R}}_z}^{0_4}, d_{\rho_z}^{0_4}, 1) + \frac{1}{32} \chi_{\tilde{\mathbf{R}}_y}^{T_1} (d_{\mathbf{R}_z}^{0_4}, d_{\tilde{\mathbf{R}}_z}^{0_4}, d_{\rho_z}^{0_4}, 1) + \frac{1}{32} \chi_{\mathbf{i}_6}^{T_1} (d_{\mathbf{R}_z}^{0_4}, d_{\tilde{\mathbf{R}}_z}^{0_4}, d_{\rho_z}^{0_4}, 1) + \frac{1}{32} \chi_{\mathbf{i}_5}^{T_1} (d_{\mathbf{R}_z}^{0_4}, d_{\tilde{\mathbf{R}}_z}^{0_4}, d_{\rho_z}^{0_4}, 1) \end{aligned}$$

$$\begin{aligned} &= \frac{1}{32} (+3) (1, +1, +1, +1) + \frac{1}{32} (-1) (1, +1, +1, +1) + \frac{1}{32} (0) (1, +1, +1, +1) + \frac{1}{32} (0) (1, +1, +1, +1) + \frac{1}{32} (0) (1, +1, +1, +1) + \frac{1}{32} (0) (1, +1, +1, +1) \\ &+ \frac{1}{32} (-1) (+1, 1, +1, +1) + \frac{1}{32} (-1) (+1, 1, +1, +1) + \frac{1}{32} (0) (+1, 1, +1, +1) + \frac{1}{32} (0) (+1, 1, +1, +1) + \frac{1}{32} (0) (+1, 1, +1, +1) + \frac{1}{32} (0) (+1, 1, +1, +1) \\ &+ \frac{1}{32} (+1) (+1, +1, 1, +1) + \frac{1}{32} (-1) (+1, +1, 1, +1) + \frac{1}{32} (-1) (+1, +1, 1, +1) + \frac{1}{32} (-1) (+1, +1, 1, +1) + \frac{1}{32} (+1) (+1, +1, 1, +1) + \frac{1}{32} (+1) (+1, +1, 1, +1) \\ &+ \frac{1}{32} (+1) (+1, +1, +1, 1) + \frac{1}{32} (-1) (+1, +1, +1, 1) + \frac{1}{32} (+1) (+1, +1, +1, 1) + \frac{1}{32} (+1) (+1, +1, +1, 1) + \frac{1}{32} (-1) (+1, +1, +1, 1) + \frac{1}{32} (-1) (+1, +1, +1, 1) \end{aligned}$$

$$\underline{4, 4, 0, 0}, \quad \underline{-4, -4, -4, -4}, \quad \underline{0, 0, 0, 0}, \quad \underline{0, 0, 0, 0}, \quad \underline{0, 0, 0, 0}, \quad \underline{0, 0, 0, 0}$$

$$\frac{1}{8} (\underline{11+1\rho_z+1\mathbf{R}_z+1\tilde{\mathbf{R}}_z} \quad \underline{-1\rho_x-1\rho_y-1\mathbf{i}_4-1\mathbf{i}_3} \quad + \underline{0\mathbf{r}_1+0\mathbf{r}_4+0\mathbf{i}_1+0\mathbf{R}_y} \quad + \underline{0\mathbf{r}_2+0\mathbf{r}_3+0\mathbf{i}_2+0\tilde{\mathbf{R}}_y} \quad + \underline{0\tilde{\mathbf{r}}_1+0\tilde{\mathbf{r}}_3+0\tilde{\mathbf{R}}_x+0\mathbf{i}_6} \quad + \underline{0\tilde{\mathbf{r}}_2+0\tilde{\mathbf{r}}_4+0\mathbf{R}_x+0\mathbf{i}_5})$$

$$\mathbf{P}_{0_4 0_4}^{T_1} = \frac{1}{8} (\underline{11} \quad + \underline{1\rho_z} \quad \underline{-1\rho_x-1\rho_y} \quad + \underline{1\mathbf{R}_z+1\tilde{\mathbf{R}}_z} \quad \underline{-1\mathbf{i}_4-1\mathbf{i}_3})$$

Calculating $\mathbf{P}^{T_1}_{1414}$

$O \supset C_4$	0_4	1_4	2_4	3_4
$A_1 \downarrow C_4$	1	.	.	.
$A_2 \downarrow C_4$.	.	1	.
$E \downarrow C_4$	1	.	1	.
$T_1 \downarrow C_4$	1	1	.	1
$T_2 \downarrow C_4$.	1	1	1

$O: \chi_g^\mu$	$g=1$	\mathbf{r}_{1-4} $\tilde{\mathbf{r}}_{1-4}$	ρ_{xyz}	\mathbf{R}_{xyz} $\tilde{\mathbf{R}}_{xyz}$	\mathbf{i}_{1-6}
$\mu=A_1$	1	1	1	1	1
A_2	1	1	1	-1	-1
E	2	-1	2	0	0
T_1	3	0	-1	1	-1
T_2	3	0	-1	-1	1

$$\mathbf{p}_{m_4} = \sum_{p=0}^3 \frac{e^{2\pi i m \cdot p/4}}{4} \mathbf{R}_z^p =$$

$$\begin{cases} \mathbf{p}_{0_4} = (\mathbf{1} + \mathbf{R}_z + \rho_z + \tilde{\mathbf{R}}_z)/4 \\ \mathbf{p}_{1_4} = (\mathbf{1} + i\mathbf{R}_z - \rho_z - i\tilde{\mathbf{R}}_z)/4 \\ \mathbf{p}_{2_4} = (\mathbf{1} - \mathbf{R}_z + \rho_z - \tilde{\mathbf{R}}_z)/4 \\ \mathbf{p}_{3_4} = (\mathbf{1} - i\mathbf{R}_z - \rho_z + i\tilde{\mathbf{R}}_z)/4 \end{cases}$$

$$\mathbf{P}^{T_1}_{1414} = \mathbf{p}_{1_4} \mathbf{P}^{T_1} = \mathbf{P}^{T_1} \mathbf{p}_{1_4}$$

$$= \sum_g \frac{\ell^{T_1}}{\circ O} (\chi_g^{T_1}) \cdot \mathbf{g} \cdot (\mathbf{p}_{1_4}) = \sum_g \frac{3}{96} (\chi_g^{T_1}) \cdot \mathbf{g} \cdot (\mathbf{1} \cdot \mathbf{1} - \mathbf{1} \cdot \rho_z + i \cdot \mathbf{R}_z - i \cdot \tilde{\mathbf{R}}_z)$$

$$\mathbf{1}C_4 = \mathbf{1} \{ \mathbf{1}, \rho_z, \mathbf{R}_z, \tilde{\mathbf{R}}_z \} \quad \rho_x C_4 = \{ \rho_x, \rho_y, \mathbf{i}_4, \mathbf{i}_3 \} \quad \mathbf{r}_1 C_4 = \{ \mathbf{r}_1, \mathbf{r}_4, \mathbf{i}_1, \mathbf{R}_y \} \quad \mathbf{r}_2 C_4 = \{ \mathbf{r}_2, \mathbf{r}_3, \mathbf{i}_2, \tilde{\mathbf{R}}_y \} \quad \tilde{\mathbf{r}}_1 C_4 = \{ \tilde{\mathbf{r}}_1, \tilde{\mathbf{r}}_3, \tilde{\mathbf{R}}_x, \mathbf{i}_6 \} \quad \tilde{\mathbf{r}}_2 C_4 = \{ \tilde{\mathbf{r}}_2, \tilde{\mathbf{r}}_4, \mathbf{R}_x, \mathbf{i}_5 \}$$

$$\begin{aligned} &= \frac{1}{32} \chi_{\mathbf{1}}^{T_1} (1, d_{\rho_z}^{14}, d_{R_z}^{14}, d_{\tilde{R}_z}^{14}) + \frac{1}{32} \chi_{\rho_x}^{T_1} (1, d_{\rho_z}^{14}, d_{R_z}^{14}, d_{\tilde{R}_z}^{14}) + \frac{1}{32} \chi_{\mathbf{r}_1}^{T_1} (1, d_{\rho_z}^{14}, d_{R_z}^{14}, d_{\tilde{R}_z}^{14}) + \frac{1}{32} \chi_{\mathbf{r}_2}^{T_1} (1, d_{\rho_z}^{14}, d_{R_z}^{14}, d_{\tilde{R}_z}^{14}) + \frac{1}{32} \chi_{\tilde{\mathbf{r}}_1}^{T_1} (1, d_{\rho_z}^{14}, d_{R_z}^{14}, d_{\tilde{R}_z}^{14}) + \frac{1}{32} \chi_{\tilde{\mathbf{r}}_2}^{T_1} (1, d_{\rho_z}^{14}, d_{R_z}^{14}, d_{\tilde{R}_z}^{14}) \\ &+ \frac{1}{32} \chi_{\rho_z}^{T_1} (d_{\rho_z}^{14}, 1, d_{\tilde{R}_z}^{14}, d_{R_z}^{14}) + \frac{1}{32} \chi_{\rho_y}^{T_1} (d_{\rho_z}^{14}, 1, d_{\tilde{R}_z}^{14}, d_{R_z}^{14}) + \frac{1}{32} \chi_{\mathbf{r}_4}^{T_1} (d_{\rho_z}^{14}, 1, d_{\tilde{R}_z}^{14}, d_{R_z}^{14}) + \frac{1}{32} \chi_{\mathbf{r}_3}^{T_1} (d_{\rho_z}^{14}, 1, d_{\tilde{R}_z}^{14}, d_{R_z}^{14}) + \frac{1}{32} \chi_{\tilde{\mathbf{r}}_3}^{T_1} (d_{\rho_z}^{14}, 1, d_{\tilde{R}_z}^{14}, d_{R_z}^{14}) + \frac{1}{32} \chi_{\tilde{\mathbf{r}}_4}^{T_1} (d_{\rho_z}^{14}, 1, d_{\tilde{R}_z}^{14}, d_{R_z}^{14}) \\ &+ \frac{1}{32} \chi_{\mathbf{R}_z}^{T_1} (d_{\tilde{R}_z}^{14}, d_{R_z}^{14}, 1, d_{\rho_z}^{14}) + \frac{1}{32} \chi_{\mathbf{i}_4}^{T_1} (d_{\tilde{R}_z}^{14}, d_{R_z}^{14}, 1, d_{\rho_z}^{14}) + \frac{1}{32} \chi_{\mathbf{i}_1}^{T_1} (d_{\tilde{R}_z}^{14}, d_{R_z}^{14}, 1, d_{\rho_z}^{14}) + \frac{1}{32} \chi_{\mathbf{i}_2}^{T_1} (d_{\tilde{R}_z}^{14}, d_{R_z}^{14}, 1, d_{\rho_z}^{14}) + \frac{1}{32} \chi_{\tilde{\mathbf{R}}_x}^{T_1} (d_{\tilde{R}_z}^{14}, d_{R_z}^{14}, 1, d_{\rho_z}^{14}) + \frac{1}{32} \chi_{\mathbf{R}_x}^{T_1} (d_{\tilde{R}_z}^{14}, d_{R_z}^{14}, 1, d_{\rho_z}^{14}) \\ &+ \frac{1}{32} \chi_{\tilde{\mathbf{R}}_z}^{T_1} (d_{R_z}^{14}, d_{\tilde{R}_z}^{14}, d_{\rho_z}^{14}, 1) + \frac{1}{32} \chi_{\mathbf{i}_3}^{T_1} (d_{R_z}^{14}, d_{\tilde{R}_z}^{14}, d_{\rho_z}^{14}, 1) + \frac{1}{32} \chi_{\mathbf{R}_y}^{T_1} (d_{R_z}^{14}, d_{\tilde{R}_z}^{14}, d_{\rho_z}^{14}, 1) + \frac{1}{32} \chi_{\tilde{\mathbf{R}}_y}^{T_1} (d_{R_z}^{14}, d_{\tilde{R}_z}^{14}, d_{\rho_z}^{14}, 1) + \frac{1}{32} \chi_{\mathbf{i}_6}^{T_1} (d_{R_z}^{14}, d_{\tilde{R}_z}^{14}, d_{\rho_z}^{14}, 1) + \frac{1}{32} \chi_{\mathbf{i}_5}^{T_1} (d_{R_z}^{14}, d_{\tilde{R}_z}^{14}, d_{\rho_z}^{14}, 1) \end{aligned}$$

$$\begin{aligned} &= \frac{1}{32} (+3)(1, -1, +i, -i) + \frac{1}{32} (-1)(1, -1, +i, -i) + \frac{1}{32} (0)(1, -1, +i, -i) + \frac{1}{32} (0)(1, -1, +i, -i) + \frac{1}{32} (0)(1, -1, +i, -i) + \frac{1}{32} (0)(1, -1, +i, -i) \\ &+ \frac{1}{32} (-1)(-1, 1, -i, +i) + \frac{1}{32} (-1)(-1, 1, -i, +i) + \frac{1}{32} (0)(-1, 1, -i, +i) + \frac{1}{32} (0)(-1, 1, -i, +i) + \frac{1}{32} (0)(-1, 1, -i, +i) + \frac{1}{32} (0)(-1, 1, -i, +i) \\ &+ \frac{1}{32} (+1)(-i, +i, 1, -1) + \frac{1}{32} (-1)(-i, +i, 1, -1) + \frac{1}{32} (-1)(-i, +i, 1, -1) + \frac{1}{32} (-1)(-i, +i, 1, -1) + \frac{1}{32} (+1)(-i, +i, 1, -1) + \frac{1}{32} (+1)(-i, +i, 1, -1) \\ &+ \frac{1}{32} (+1)(+i, -i, -1, 1) + \frac{1}{32} (-1)(+i, -i, -1, 1) + \frac{1}{32} (+1)(+i, -i, -1, 1) + \frac{1}{32} (+1)(+i, -i, -1, 1) + \frac{1}{32} (-1)(+i, -i, -1, 1) + \frac{1}{32} (-1)(+i, -i, -1, 1) \\ &\underline{+4, -4, 4i, -4i, \quad 0, \quad 0, \quad 0, \quad 0, \quad +2i, -2i, -2, +2, \quad +2i, -2i, -2, +2, \quad -2i, +2i, +2, -2 \quad -2i, +2i, +2, -2.} \\ &\frac{1}{8} (\underline{\mathbf{11}} - \underline{\mathbf{1}} \rho_z + i \underline{\mathbf{R}}_z - i \underline{\tilde{\mathbf{R}}}_z \quad + \underline{\mathbf{0}} \rho_x + \underline{\mathbf{0}} \rho_y + \underline{\mathbf{0}} \mathbf{i}_4 + \underline{\mathbf{0}} \mathbf{i}_3 \quad + \frac{i}{2} \underline{\mathbf{r}}_1 - \frac{i}{2} \underline{\mathbf{r}}_4 - \frac{1}{2} \underline{\mathbf{i}}_1 + \frac{1}{2} \underline{\mathbf{R}}_y \quad + \frac{i}{2} \underline{\mathbf{r}}_2 - \frac{i}{2} \underline{\mathbf{r}}_3 - \frac{1}{2} \underline{\mathbf{i}}_2 + \frac{1}{2} \underline{\tilde{\mathbf{R}}}_y \quad - \frac{i}{2} \underline{\tilde{\mathbf{r}}}_1 + \frac{i}{2} \underline{\tilde{\mathbf{r}}}_3 + \frac{1}{2} \underline{\tilde{\mathbf{R}}}_x - \frac{1}{2} \underline{\mathbf{i}}_6 \quad - \frac{i}{2} \underline{\tilde{\mathbf{r}}}_2 + \frac{i}{2} \underline{\tilde{\mathbf{r}}}_4 + \frac{1}{2} \underline{\mathbf{R}}_x - \frac{1}{2} \underline{\mathbf{i}}_5) \end{aligned}$$

$$\mathbf{P}^{T_1}_{1414} = \frac{1}{8} (\underline{\mathbf{11}} + \underline{\mathbf{0}} \rho_x + \underline{\mathbf{0}} \rho_y - \underline{\mathbf{1}} \rho_z \quad + \frac{i}{2} \underline{\mathbf{r}}_1 + \frac{i}{2} \underline{\mathbf{r}}_2 \quad - \frac{i}{2} \underline{\mathbf{r}}_3 - \frac{i}{2} \underline{\mathbf{r}}_4 \quad - \frac{i}{2} \underline{\tilde{\mathbf{r}}}_1 - \frac{i}{2} \underline{\tilde{\mathbf{r}}}_2 \quad + \frac{i}{2} \underline{\tilde{\mathbf{r}}}_3 + \frac{i}{2} \underline{\tilde{\mathbf{r}}}_4 \quad + \frac{1}{2} \underline{\mathbf{R}}_x + \frac{1}{2} \underline{\mathbf{R}}_y + i \underline{\mathbf{R}}_z + \frac{1}{2} \underline{\tilde{\mathbf{R}}}_x + \frac{1}{2} \underline{\tilde{\mathbf{R}}}_y - i \underline{\tilde{\mathbf{R}}}_z \quad - \frac{1}{2} \underline{\mathbf{i}}_1 - \frac{1}{2} \underline{\mathbf{i}}_2 + \underline{\mathbf{0}} \underline{\mathbf{i}}_3 + \underline{\mathbf{0}} \underline{\mathbf{i}}_4 \quad - \frac{1}{2} \underline{\mathbf{i}}_5 \quad - \frac{1}{2} \underline{\mathbf{i}}_6)$$

Calculating $\mathbf{P}^{T_2}_{2_4 2_4}$

$O \supset C_4$	0_4	1_4	2_4	3_4
$A_1 \downarrow C_4$	1	.	.	.
$A_2 \downarrow C_4$.	.	1	.
$E \downarrow C_4$	1	.	1	.
$T_1 \downarrow C_4$	1	1	.	1
$T_2 \downarrow C_4$.	1	1	1

$O: \chi_g^\mu$	$g=1$	r_{1-4} \tilde{r}_{1-4}	ρ_{xyz}	R_{xyz} \tilde{R}_{xyz}	i_{1-6}
$\mu=A_1$	1	1	1	1	1
A_2	1	1	1	-1	-1
E	2	-1	2	0	0
T_1	3	0	-1	1	-1
T_2	3	0	-1	-1	1

$$\mathbf{p}_{m_4} = \sum_{p=0}^3 \frac{e^{2\pi i m \cdot p/4}}{4} \mathbf{R}_z^p = \begin{cases} \mathbf{p}_{0_4} = (1 + \mathbf{R}_z + \rho_z + \tilde{\mathbf{R}}_z)/4 \\ \mathbf{p}_{1_4} = (1 + i\mathbf{R}_z - \rho_z - i\tilde{\mathbf{R}}_z)/4 \\ \mathbf{p}_{2_4} = (1 - \mathbf{R}_z + \rho_z - \tilde{\mathbf{R}}_z)/4 \\ \mathbf{p}_{3_4} = (1 - i\mathbf{R}_z - \rho_z + i\tilde{\mathbf{R}}_z)/4 \end{cases}$$

$$\mathbf{P}_{2_4 2_4}^{T_2} = \mathbf{p}_{2_4} \mathbf{P}^{T_2} = \mathbf{P}^{T_2} \mathbf{p}_{2_4} = \sum_g \frac{\ell^{T_2}}{\circ O} (\chi_g^{T_2}) \cdot \mathbf{g} \cdot (\mathbf{p}_{2_4}) = \sum_g \frac{3}{96} (\chi_g^{T_2}) \cdot \mathbf{g} \cdot (1 \cdot \mathbf{1} + 1 \cdot \rho_z - 1 \cdot \mathbf{R}_z - 1 \cdot \tilde{\mathbf{R}}_z)$$

$$1C_4 = \mathbf{1} \{ \mathbf{1}, \rho_z, \mathbf{R}_z, \tilde{\mathbf{R}}_z \} \quad \rho_x C_4 = \{ \rho_x, \rho_y, \mathbf{i}_4, \mathbf{i}_3 \} \quad \mathbf{r}_1 C_4 = \{ \mathbf{r}_1, \mathbf{r}_4, \mathbf{i}_1, \mathbf{R}_y \} \quad \mathbf{r}_2 C_4 = \{ \mathbf{r}_2, \mathbf{r}_3, \mathbf{i}_2, \tilde{\mathbf{R}}_y \} \quad \tilde{\mathbf{r}}_1 C_4 = \{ \tilde{\mathbf{r}}_1, \tilde{\mathbf{r}}_3, \tilde{\mathbf{R}}_x, \mathbf{i}_6 \} \quad \tilde{\mathbf{r}}_2 C_4 = \{ \tilde{\mathbf{r}}_2, \tilde{\mathbf{r}}_4, \mathbf{R}_x, \mathbf{i}_5 \}$$

$$= \frac{1}{32} \chi_1^{T_2} (1, d_{\rho_z}^{24}, d_{R_z}^{24}, d_{\tilde{R}_z}^{24}) + \frac{1}{32} \chi_{\rho_x}^{T_2} (1, d_{\rho_z}^{24}, d_{R_z}^{24}, d_{\tilde{R}_z}^{24}) + \frac{1}{32} \chi_{r_1}^{T_2} (1, d_{\rho_z}^{24}, d_{R_z}^{24}, d_{\tilde{R}_z}^{24}) + \frac{1}{32} \chi_{r_2}^{T_2} (1, d_{\rho_z}^{24}, d_{R_z}^{24}, d_{\tilde{R}_z}^{24}) + \frac{1}{32} \chi_{\tilde{r}_1}^{T_2} (1, d_{\rho_z}^{24}, d_{R_z}^{24}, d_{\tilde{R}_z}^{24}) + \frac{1}{32} \chi_{\tilde{r}_2}^{T_2} (1, d_{\rho_z}^{24}, d_{R_z}^{24}, d_{\tilde{R}_z}^{24})$$

$$+ \frac{1}{32} \chi_{\rho_z}^{T_2} (d_{\rho_z}^{24}, 1, d_{\tilde{R}_z}^{24}, d_{R_z}^{24}) + \frac{1}{32} \chi_{\rho_y}^{T_2} (d_{\rho_z}^{24}, 1, d_{\tilde{R}_z}^{24}, d_{R_z}^{24}) + \frac{1}{32} \chi_{r_4}^{T_2} (d_{\rho_z}^{24}, 1, d_{\tilde{R}_z}^{24}, d_{R_z}^{24}) + \frac{1}{32} \chi_{r_3}^{T_2} (d_{\rho_z}^{24}, 1, d_{\tilde{R}_z}^{24}, d_{R_z}^{24}) + \frac{1}{32} \chi_{\tilde{r}_3}^{T_2} (d_{\rho_z}^{24}, 1, d_{\tilde{R}_z}^{24}, d_{R_z}^{24}) + \frac{1}{32} \chi_{\tilde{r}_4}^{T_2} (d_{\rho_z}^{24}, 1, d_{\tilde{R}_z}^{24}, d_{R_z}^{24})$$

$$+ \frac{1}{32} \chi_{R_z}^{T_2} (d_{\tilde{R}_z}^{24}, d_{R_z}^{24}, 1, d_{\rho_z}^{24}) + \frac{1}{32} \chi_{i_4}^{T_2} (d_{\tilde{R}_z}^{24}, d_{R_z}^{24}, 1, d_{\rho_z}^{24}) + \frac{1}{32} \chi_{i_1}^{T_2} (d_{\tilde{R}_z}^{24}, d_{R_z}^{24}, 1, d_{\rho_z}^{24}) + \frac{1}{32} \chi_{i_2}^{T_2} (d_{\tilde{R}_z}^{24}, d_{R_z}^{24}, 1, d_{\rho_z}^{24}) + \frac{1}{32} \chi_{\tilde{R}_x}^{T_2} (d_{\tilde{R}_z}^{24}, d_{R_z}^{24}, 1, d_{\rho_z}^{24}) + \frac{1}{32} \chi_{R_x}^{T_2} (d_{\tilde{R}_z}^{24}, d_{R_z}^{24}, 1, d_{\rho_z}^{24})$$

$$+ \frac{1}{32} \chi_{\tilde{R}_z}^{T_2} (d_{R_z}^{24}, d_{\tilde{R}_z}^{24}, d_{\rho_z}^{24}, 1) + \frac{1}{32} \chi_{i_3}^{T_2} (d_{R_z}^{24}, d_{\tilde{R}_z}^{24}, d_{\rho_z}^{24}, 1) + \frac{1}{32} \chi_{R_y}^{T_2} (d_{R_z}^{24}, d_{\tilde{R}_z}^{24}, d_{\rho_z}^{24}, 1) + \frac{1}{32} \chi_{\tilde{R}_y}^{T_2} (d_{R_z}^{24}, d_{\tilde{R}_z}^{24}, d_{\rho_z}^{24}, 1) + \frac{1}{32} \chi_{i_6}^{T_2} (d_{R_z}^{24}, d_{\tilde{R}_z}^{24}, d_{\rho_z}^{24}, 1) + \frac{1}{32} \chi_{i_5}^{T_2} (d_{R_z}^{24}, d_{\tilde{R}_z}^{24}, d_{\rho_z}^{24}, 1)$$

$$= \frac{1}{32} (+3)(1, +1, -1, -1) + \frac{1}{32} (-1)(1, +1, -1, -1) + \frac{1}{32} (0)(1, +1, -1, -1) + \frac{1}{32} (0)(1, +1, -1, -1) + \frac{1}{32} (0)(1, +1, -1, -1) + \frac{1}{32} (0)(1, +1, -1, -1)$$

$$+ \frac{1}{32} (-1)(+1, 1, -1, -1) + \frac{1}{32} (-1)(+1, 1, -1, -1) + \frac{1}{32} (0)(+1, 1, -1, -1) + \frac{1}{32} (0)(+1, 1, -1, -1) + \frac{1}{32} (0)(+1, 1, -1, -1) + \frac{1}{32} (0)(+1, 1, -1, -1)$$

$$+ \frac{1}{32} (-1)(-1, -1, 1, +1) + \frac{1}{32} (+1)(-1, -1, 1, +1) + \frac{1}{32} (+1)(-1, -1, 1, +1) + \frac{1}{32} (+1)(-1, -1, 1, +1) + \frac{1}{32} (-1)(-1, -1, 1, +1) + \frac{1}{32} (-1)(-1, -1, 1, +1)$$

$$+ \frac{1}{32} (-1)(-1, -1, +1, 1) + \frac{1}{32} (+1)(-1, -1, +1, 1) + \frac{1}{32} (-1)(-1, -1, +1, 1) + \frac{1}{32} (-1)(-1, -1, +1, 1) + \frac{1}{32} (+1)(-1, -1, +1, 1) + \frac{1}{32} (+1)(-1, -1, +1, 1)$$

$$\frac{1}{8} (\underline{11} + \underline{1\rho_z} - \underline{1R_z} - \underline{1\tilde{R}_z} \quad -\underline{1\rho_x} - \underline{1\rho_y} + \underline{1i_4} + \underline{1i_3} \quad + \underline{0r_1} + \underline{0r_4} + \underline{0i_1} + \underline{0R_y} \quad + \underline{0r_2} + \underline{0r_3} + \underline{0i_2} + \underline{0\tilde{R}_y} \quad + \underline{0\tilde{r}_1} + \underline{0\tilde{r}_3} + \underline{0\tilde{R}_x} + \underline{0i_6} \quad + \underline{0\tilde{r}_2} + \underline{0\tilde{r}_4} + \underline{0R_x} + \underline{0i_5})$$

$$\mathbf{P}_{2_4 2_4}^{T_2} = \frac{1}{8} (\underline{11} \quad + \underline{1\rho_z} - \underline{1\rho_x} - \underline{1\rho_y} \quad - \underline{1R_z} - \underline{1\tilde{R}_z} \quad + \underline{1i_4} + \underline{1i_3} \quad)$$

Calculating $\mathbf{P}^{T_2}_{1414}$

$O \supset C_4$	0_4	1_4	2_4	3_4
$A_1 \downarrow C_4$	1	.	.	.
$A_2 \downarrow C_4$.	.	1	.
$E \downarrow C_4$	1	.	1	.
$T_1 \downarrow C_4$	1	1	.	1
$T_2 \downarrow C_4$.	1	1	1

O: χ_g^μ	$g=1$	\mathbf{r}_{1-4} $\tilde{\mathbf{r}}_{1-4}$	ρ_{xyz}	\mathbf{R}_{xyz} $\tilde{\mathbf{R}}_{xyz}$	\mathbf{i}_{1-6}
$\mu=A_1$	1	1	1	1	1
A_2	1	1	1	-1	-1
E	2	-1	2	0	0
T_1	3	0	-1	1	-1
T_2	3	0	-1	-1	1

$$\mathbf{p}_{m_4} = \sum_{p=0}^3 \frac{e^{2\pi i m \cdot p/4}}{4} \mathbf{R}_z^p = \begin{cases} \mathbf{p}_{0_4} = (1 + \mathbf{R}_z + \rho_z + \tilde{\mathbf{R}}_z)/4 \\ \mathbf{p}_{1_4} = (1 + i\mathbf{R}_z - \rho_z - i\tilde{\mathbf{R}}_z)/4 \\ \mathbf{p}_{2_4} = (1 - \mathbf{R}_z + \rho_z - \tilde{\mathbf{R}}_z)/4 \\ \mathbf{p}_{3_4} = (1 - i\mathbf{R}_z - \rho_z + i\tilde{\mathbf{R}}_z)/4 \end{cases}$$

$$\mathbf{P}_{1414}^{T_2} = \mathbf{p}_{14} \mathbf{P}^{T_2} = \mathbf{P}^{T_2} \mathbf{p}_{14} = \sum_g \frac{\ell^{T_2}}{\circ O} (\chi_g^{T_2}) \cdot \mathbf{g} \cdot (\mathbf{p}_{14}) = \sum_g \frac{3}{96} (\chi_g^{T_2}) \cdot \mathbf{g} \cdot (1 \cdot 1 - 1 \cdot \rho_z + i \cdot \mathbf{R}_z - i \cdot \tilde{\mathbf{R}}_z)$$

$$1C_4 = 1 \{1, \rho_z, \mathbf{R}_z, \tilde{\mathbf{R}}_z\} \quad \rho_x C_4 = \{\rho_x, \rho_y, \mathbf{i}_4, \mathbf{i}_3\} \quad \mathbf{r}_1 C_4 = \{\mathbf{r}_1, \mathbf{r}_4, \mathbf{i}_1, \mathbf{R}_y\} \quad \mathbf{r}_2 C_4 = \{\mathbf{r}_2, \mathbf{r}_3, \mathbf{i}_2, \tilde{\mathbf{R}}_y\} \quad \tilde{\mathbf{r}}_1 C_4 = \{\tilde{\mathbf{r}}_1, \tilde{\mathbf{r}}_3, \tilde{\mathbf{R}}_x, \mathbf{i}_6\} \quad \tilde{\mathbf{r}}_2 C_4 = \{\tilde{\mathbf{r}}_2, \tilde{\mathbf{r}}_4, \mathbf{R}_x, \mathbf{i}_5\}$$

$$= \frac{1}{32} \chi_1^{T_2}(1, d_{\rho_z}^{14}, d_{R_z}^{14}, d_{\tilde{R}_z}^{14}) + \frac{1}{32} \chi_{\rho_x}^{T_2}(1, d_{\rho_z}^{14}, d_{R_z}^{14}, d_{\tilde{R}_z}^{14}) + \frac{1}{32} \chi_{\mathbf{r}_1}^{T_2}(1, d_{\rho_z}^{14}, d_{R_z}^{14}, d_{\tilde{R}_z}^{14}) + \frac{1}{32} \chi_{\mathbf{r}_2}^{T_2}(1, d_{\rho_z}^{14}, d_{R_z}^{14}, d_{\tilde{R}_z}^{14}) + \frac{1}{32} \chi_{\tilde{\mathbf{r}}_1}^{T_2}(1, d_{\rho_z}^{14}, d_{R_z}^{14}, d_{\tilde{R}_z}^{14}) + \frac{1}{32} \chi_{\tilde{\mathbf{r}}_2}^{T_2}(1, d_{\rho_z}^{14}, d_{R_z}^{14}, d_{\tilde{R}_z}^{14})$$

$$+ \frac{1}{32} \chi_{\rho_z}^{T_2}(d_{\rho_z}^{14}, 1, d_{\tilde{R}_z}^{14}, d_{R_z}^{14}) + \frac{1}{32} \chi_{\rho_y}^{T_2}(d_{\rho_z}^{14}, 1, d_{\tilde{R}_z}^{14}, d_{R_z}^{14}) + \frac{1}{32} \chi_{\mathbf{r}_4}^{T_2}(d_{\rho_z}^{14}, 1, d_{\tilde{R}_z}^{14}, d_{R_z}^{14}) + \frac{1}{32} \chi_{\mathbf{r}_3}^{T_2}(d_{\rho_z}^{14}, 1, d_{\tilde{R}_z}^{14}, d_{R_z}^{14}) + \frac{1}{32} \chi_{\tilde{\mathbf{r}}_3}^{T_2}(d_{\rho_z}^{14}, 1, d_{\tilde{R}_z}^{14}, d_{R_z}^{14}) + \frac{1}{32} \chi_{\tilde{\mathbf{r}}_4}^{T_2}(d_{\rho_z}^{14}, 1, d_{\tilde{R}_z}^{14}, d_{R_z}^{14})$$

$$+ \frac{1}{32} \chi_{\mathbf{R}_z}^{T_2}(d_{\tilde{R}_z}^{14}, d_{R_z}^{14}, 1, d_{\rho_z}^{14}) + \frac{1}{32} \chi_{\mathbf{i}_4}^{T_2}(d_{\tilde{R}_z}^{14}, d_{R_z}^{14}, 1, d_{\rho_z}^{14}) + \frac{1}{32} \chi_{\mathbf{i}_1}^{T_2}(d_{\tilde{R}_z}^{14}, d_{R_z}^{14}, 1, d_{\rho_z}^{14}) + \frac{1}{32} \chi_{\mathbf{i}_2}^{T_2}(d_{\tilde{R}_z}^{14}, d_{R_z}^{14}, 1, d_{\rho_z}^{14}) + \frac{1}{32} \chi_{\tilde{\mathbf{R}}_x}^{T_2}(d_{\tilde{R}_z}^{14}, d_{R_z}^{14}, 1, d_{\rho_z}^{14}) + \frac{1}{32} \chi_{\mathbf{R}_x}^{T_2}(d_{\tilde{R}_z}^{14}, d_{R_z}^{14}, 1, d_{\rho_z}^{14})$$

$$+ \frac{1}{32} \chi_{\tilde{\mathbf{R}}_z}^{T_2}(d_{R_z}^{14}, d_{\tilde{R}_z}^{14}, d_{\rho_z}^{14}, 1) + \frac{1}{32} \chi_{\mathbf{i}_3}^{T_2}(d_{R_z}^{14}, d_{\tilde{R}_z}^{14}, d_{\rho_z}^{14}, 1) + \frac{1}{32} \chi_{\mathbf{R}_y}^{T_2}(d_{R_z}^{14}, d_{\tilde{R}_z}^{14}, d_{\rho_z}^{14}, 1) + \frac{1}{32} \chi_{\tilde{\mathbf{R}}_y}^{T_2}(d_{R_z}^{14}, d_{\tilde{R}_z}^{14}, d_{\rho_z}^{14}, 1) + \frac{1}{32} \chi_{\mathbf{i}_6}^{T_2}(d_{R_z}^{14}, d_{\tilde{R}_z}^{14}, d_{\rho_z}^{14}, 1) + \frac{1}{32} \chi_{\mathbf{i}_5}^{T_2}(d_{R_z}^{14}, d_{\tilde{R}_z}^{14}, d_{\rho_z}^{14}, 1)$$

$$= \frac{1}{32} (+3)(1, -1, +i, -i) + \frac{1}{32} (-1)(1, -1, +i, -i) + \frac{1}{32} (0)(1, -1, +i, -i) + \frac{1}{32} (0)(1, -1, +i, -i) + \frac{1}{32} (0)(1, -1, +i, -i) + \frac{1}{32} (0)(1, -1, +i, -i)$$

$$+ \frac{1}{32} (-1)(-1, 1, -i, +i) + \frac{1}{32} (-1)(-1, 1, -i, +i) + \frac{1}{32} (0)(-1, 1, -i, +i) + \frac{1}{32} (0)(-1, 1, -i, +i) + \frac{1}{32} (0)(-1, 1, -i, +i) + \frac{1}{32} (0)(-1, 1, -i, +i)$$

$$+ \frac{1}{32} (-1)(-i, +i, 1, -1) + \frac{1}{32} (+1)(-i, +i, 1, -1) + \frac{1}{32} (+1)(-i, +i, 1, -1) + \frac{1}{32} (+1)(-i, +i, 1, -1) + \frac{1}{32} (-1)(-i, +i, 1, -1) + \frac{1}{32} (-1)(-i, +i, 1, -1)$$

$$+ \frac{1}{32} (-1)(+i, -i, -1, 1) + \frac{1}{32} (+1)(+i, -i, -1, 1) + \frac{1}{32} (-1)(+i, -i, -1, 1) + \frac{1}{32} (-1)(+i, -i, -1, 1) + \frac{1}{32} (+1)(+i, -i, -1, 1) + \frac{1}{32} (+1)(+i, -i, -1, 1)$$

$$\underline{+4, -4, 4i, -4i} \quad \underline{0, 0, 0, 0} \quad \underline{-2i, 2i, 2, -2} \quad \underline{-2i, 2i, 2, -2} \quad \underline{2i, -2i, -2, 2} \quad \underline{2i, -2i, -2, 2}$$

$$\frac{1}{8} (\underline{11} - \underline{1}\rho_z + \underline{i}\mathbf{R}_z - \underline{i}\tilde{\mathbf{R}}_z \quad + \underline{0}\rho_x + \underline{0}\rho_y + \underline{0}\mathbf{i}_4 + \underline{0}\mathbf{i}_3 \quad - \frac{i}{2}\mathbf{r}_1 + \frac{i}{2}\mathbf{r}_4 + \frac{1}{2}\mathbf{i}_1 - \frac{1}{2}\mathbf{R}_y \quad - \frac{i}{2}\mathbf{r}_2 + \frac{i}{2}\mathbf{r}_3 + \frac{1}{2}\mathbf{i}_2 - \frac{1}{2}\tilde{\mathbf{R}}_y \quad + \frac{i}{2}\tilde{\mathbf{r}}_1 - \frac{i}{2}\tilde{\mathbf{r}}_3 - \frac{1}{2}\tilde{\mathbf{R}}_x + \frac{1}{2}\mathbf{i}_6 \quad + \frac{i}{2}\tilde{\mathbf{r}}_2 - \frac{i}{2}\tilde{\mathbf{r}}_4 - \frac{1}{2}\mathbf{R}_x + \frac{1}{2}\mathbf{i}_5)$$

$$\mathbf{P}_{1414}^{T_2} = \frac{1}{8} (\underline{11} \quad + \underline{0}\rho_x + \underline{0}\rho_y - \underline{1}\rho_z \quad - \frac{i}{2}\mathbf{r}_1 - \frac{i}{2}\mathbf{r}_2 \quad + \frac{i}{2}\mathbf{r}_3 + \frac{i}{2}\mathbf{r}_4 \quad + \frac{i}{2}\tilde{\mathbf{r}}_1 + \frac{i}{2}\tilde{\mathbf{r}}_2 \quad - \frac{i}{2}\tilde{\mathbf{r}}_3 - \frac{i}{2}\tilde{\mathbf{r}}_4 \quad - \frac{1}{2}\mathbf{R}_x - \frac{1}{2}\mathbf{R}_y + \underline{i}\mathbf{R}_z \quad - \frac{1}{2}\tilde{\mathbf{R}}_x - \frac{1}{2}\tilde{\mathbf{R}}_y - \underline{i}\tilde{\mathbf{R}}_z \quad + \frac{1}{2}\mathbf{i}_1 + \frac{1}{2}\mathbf{i}_2 \quad + \underline{0}\mathbf{i}_3 \underline{0}\mathbf{i}_4 \quad + \frac{1}{2}\mathbf{i}_5 + \frac{1}{2}\mathbf{i}_6)$$

Review Coset factored splitting of $O \supset D_4 \supset C_4$ projectors and levels

Irreducible idempotent projectors $P^{\mu}_{m,m}$ of $O \supset C_4 \sim T_d \supset C_{4i}$

Calculating $P^{E_{0404}}$ $P^{E_{2424}}$ $P^{T_1_{0404}}$ $P^{T_1_{1414}}$ $P^{T_2_{2424}}$

Factoring out $O \supset C_4$ subgroup cosets:

Factoring $P^{E_{0404}}$ $P^{E_{2424}}$ $P^{T_1_{0404}}$ $P^{T_1_{1414}}$ $P^{T_2_{2424}}$

Irreducible nilpotent projectors $P^{\mu}_{m,n}$

Fundamental $P^{\mu}_{m,n}$ definitions:

Review of $D_3 \supset C_2 \sim C_{3v} \supset C_v$

Calculating and Factoring $P^{T_1_{1404}}$

Structure and applications of various subgroup chain ireps

$O_h \supset D_{4h} \supset C_{4v}$

$O_h \supset D_{3h} \supset C_{3v}$

$O_h \supset C_{2v}$

Irreducible idempotent projectors $\mathbf{P}^\mu_{m,m}$ of $O \supset C_4 \sim T_d \supset C_{4i}$

Broken-class-ordered A_1 -sum:

$$\mathbf{P}_{0_4 0_4}^{A_1} = \frac{1}{24} (\mathbf{1} \cdot \mathbf{1} \quad +\mathbf{1r}_1+\mathbf{1r}_2+\mathbf{1r}_3+\mathbf{1r}_4+\mathbf{1\tilde{r}}_1+\mathbf{1\tilde{r}}_2 \quad +\mathbf{1\tilde{r}}_3+\mathbf{1\tilde{r}}_4 \quad +\mathbf{1\rho}_x+\mathbf{1\rho}_y+\mathbf{1\rho}_z \quad +\mathbf{1R}_x+\mathbf{1R}_y \quad +\mathbf{1R}_z \quad +\mathbf{1\tilde{R}}_x+\mathbf{1\tilde{R}}_y \quad +\mathbf{1\tilde{R}}_z \quad +\mathbf{1i}_1+\mathbf{1i}_2 \quad +\mathbf{1i}_3+\mathbf{1i}_4 \quad +\mathbf{1i}_5+\mathbf{1i}_6)$$

Broken-class-ordered A_2 -sum:

$$\mathbf{P}_{2_4 2_4}^{A_2} = \frac{1}{24} (\mathbf{1} \cdot \mathbf{1} \quad +\mathbf{1r}_1+\mathbf{1r}_2+\mathbf{1r}_3+\mathbf{1r}_4+\mathbf{1\tilde{r}}_1+\mathbf{1\tilde{r}}_2 \quad +\mathbf{1\tilde{r}}_3+\mathbf{1\tilde{r}}_4 \quad +\mathbf{1\rho}_x+\mathbf{1\rho}_y+\mathbf{1\rho}_z \quad -\mathbf{1R}_x-\mathbf{1R}_y \quad -\mathbf{1R}_z \quad -\mathbf{1\tilde{R}}_x-\mathbf{1\tilde{R}}_y \quad -\mathbf{1\tilde{R}}_z \quad -\mathbf{1i}_1-\mathbf{1i}_2 \quad -\mathbf{1i}_3-\mathbf{1i}_4 \quad -\mathbf{1i}_5-\mathbf{1i}_6)$$

Broken-class-ordered E -sum:

$$\mathbf{P}_{0_4 0_4}^E = \frac{1}{12} (\mathbf{1} \cdot \mathbf{1} \quad -\frac{1}{2}\mathbf{r}_1-\frac{1}{2}\mathbf{r}_2 \quad -\frac{1}{2}\mathbf{r}_3-\frac{1}{2}\mathbf{r}_4 \quad -\frac{1}{2}\mathbf{\tilde{r}}_1-\frac{1}{2}\mathbf{\tilde{r}}_2 \quad -\frac{1}{2}\mathbf{\tilde{r}}_3-\frac{1}{2}\mathbf{\tilde{r}}_4 \quad +\mathbf{1\rho}_x+\mathbf{1\rho}_y+\mathbf{1\rho}_z \quad -\frac{1}{2}\mathbf{R}_x-\frac{1}{2}\mathbf{R}_y \quad +\mathbf{1R}_z \quad -\frac{1}{2}\mathbf{\tilde{R}}_x-\frac{1}{2}\mathbf{\tilde{R}}_y \quad +\mathbf{1\tilde{R}}_z \quad -\frac{1}{2}\mathbf{i}_1-\frac{1}{2}\mathbf{i}_2 \quad +\mathbf{1i}_3+\mathbf{1i}_4 \quad -\frac{1}{2}\mathbf{i}_5-\frac{1}{2}\mathbf{i}_6)$$

$$\mathbf{P}_{2_4 2_4}^E = \frac{1}{12} (\mathbf{1} \cdot \mathbf{1} \quad -\frac{1}{2}\mathbf{r}_1-\frac{1}{2}\mathbf{r}_2 \quad -\frac{1}{2}\mathbf{r}_3-\frac{1}{2}\mathbf{r}_4 \quad -\frac{1}{2}\mathbf{\tilde{r}}_1-\frac{1}{2}\mathbf{\tilde{r}}_2 \quad -\frac{1}{2}\mathbf{\tilde{r}}_3-\frac{1}{2}\mathbf{\tilde{r}}_4 \quad +\mathbf{1\rho}_x+\mathbf{1\rho}_y+\mathbf{1\rho}_z \quad +\frac{1}{2}\mathbf{R}_x+\frac{1}{2}\mathbf{R}_y \quad -\mathbf{1R}_z \quad +\frac{1}{2}\mathbf{\tilde{R}}_x+\frac{1}{2}\mathbf{\tilde{R}}_y \quad -\mathbf{1\tilde{R}}_z \quad +\frac{1}{2}\mathbf{i}_1+\frac{1}{2}\mathbf{i}_2 \quad -\mathbf{1i}_3-\mathbf{1i}_4 \quad +\frac{1}{2}\mathbf{i}_5+\frac{1}{2}\mathbf{i}_6)$$

Broken-class-ordered T_1 -sum:

$$\mathbf{P}_{1_4 1_4}^{T_1} = \frac{1}{8} (\mathbf{1} \cdot \mathbf{1} \quad +\frac{i}{2}\mathbf{r}_1+\frac{i}{2}\mathbf{r}_2 \quad -\frac{i}{2}\mathbf{r}_3-\frac{i}{2}\mathbf{r}_4 \quad -\frac{i}{2}\mathbf{\tilde{r}}_1-\frac{i}{2}\mathbf{\tilde{r}}_2 \quad +\frac{i}{2}\mathbf{\tilde{r}}_3+\frac{i}{2}\mathbf{\tilde{r}}_4 \quad +\mathbf{0\rho}_x+\mathbf{0\rho}_y \quad -\mathbf{1\rho}_z \quad +\frac{1}{2}\mathbf{R}_x+\frac{1}{2}\mathbf{R}_y \quad +i\mathbf{R}_z \quad +\frac{1}{2}\mathbf{\tilde{R}}_x+\frac{1}{2}\mathbf{\tilde{R}}_y \quad -i\mathbf{\tilde{R}}_z \quad -\frac{1}{2}\mathbf{i}_1-\frac{1}{2}\mathbf{i}_2 \quad +\mathbf{0i}_3+\mathbf{0i}_4 \quad -\frac{1}{2}\mathbf{i}_5 \quad -\frac{1}{2}\mathbf{i}_6)$$

$$\mathbf{P}_{3_4 3_4}^{T_1} = \frac{1}{8} (\mathbf{1} \cdot \mathbf{1} \quad -\frac{i}{2}\mathbf{r}_1 \quad -\frac{i}{2}\mathbf{r}_2 \quad +\frac{i}{2}\mathbf{r}_3+\frac{i}{2}\mathbf{r}_4 \quad +\frac{i}{2}\mathbf{\tilde{r}}_1+\frac{i}{2}\mathbf{\tilde{r}}_2 \quad -\frac{i}{2}\mathbf{\tilde{r}}_3 \quad -\frac{i}{2}\mathbf{\tilde{r}}_4 \quad +\mathbf{0\rho}_x+\mathbf{0\rho}_y \quad -\mathbf{1\rho}_z \quad +\frac{1}{2}\mathbf{R}_x+\frac{1}{2}\mathbf{R}_y \quad -i\mathbf{R}_z \quad +\frac{1}{2}\mathbf{\tilde{R}}_x+\frac{1}{2}\mathbf{\tilde{R}}_y \quad +i\mathbf{\tilde{R}}_z \quad -\frac{1}{2}\mathbf{i}_1-\frac{1}{2}\mathbf{i}_2 \quad +\mathbf{0i}_3+\mathbf{0i}_4 \quad -\frac{1}{2}\mathbf{i}_5 \quad -\frac{1}{2}\mathbf{i}_6)$$

$$\mathbf{P}_{0_4 0_4}^{T_1} = \frac{1}{8} (\mathbf{1} \cdot \mathbf{1} \quad +\mathbf{0}+\mathbf{0} \quad +\mathbf{0}+\mathbf{0} \quad +\mathbf{0}+\mathbf{0} \quad +\mathbf{0}+\mathbf{0} \quad -\mathbf{1\rho}_x-\mathbf{1\rho}_y \quad +\mathbf{1\rho}_z \quad +\mathbf{0} \quad +\mathbf{0} \quad +\mathbf{1R}_z \quad +\mathbf{0} \quad +\mathbf{0} \quad +\mathbf{1\tilde{R}}_z \quad +\mathbf{0}+\mathbf{0} \quad -\mathbf{1i}_3 \quad -\mathbf{1i}_4 \quad +\mathbf{0}+\mathbf{0})$$

Broken-class-ordered T_2 -sum:

$$\mathbf{P}_{1_4 1_4}^{T_2} = \frac{1}{8} (\mathbf{1} \cdot \mathbf{1} \quad -\frac{i}{2}\mathbf{r}_1-\frac{i}{2}\mathbf{r}_2 \quad +\frac{i}{2}\mathbf{r}_3+\frac{i}{2}\mathbf{r}_4 \quad +\frac{i}{2}\mathbf{\tilde{r}}_1+\frac{i}{2}\mathbf{\tilde{r}}_2 \quad -\frac{i}{2}\mathbf{\tilde{r}}_3-\frac{i}{2}\mathbf{\tilde{r}}_4 \quad +\mathbf{0\rho}_x+\mathbf{0\rho}_y \quad -\mathbf{1\rho}_z \quad -\frac{1}{2}\mathbf{R}_x-\frac{1}{2}\mathbf{R}_y \quad +i\mathbf{R}_z \quad -\frac{1}{2}\mathbf{\tilde{R}}_x-\frac{1}{2}\mathbf{\tilde{R}}_y \quad -i\mathbf{\tilde{R}}_z \quad +\frac{1}{2}\mathbf{i}_1+\frac{1}{2}\mathbf{i}_2 \quad +\mathbf{0i}_3+\mathbf{0i}_4 \quad +\frac{1}{2}\mathbf{i}_5 \quad +\frac{1}{2}\mathbf{i}_6)$$

$$\mathbf{P}_{3_4 3_4}^{T_2} = \frac{1}{8} (\mathbf{1} \cdot \mathbf{1} \quad +\frac{i}{2}\mathbf{r}_1+\frac{i}{2}\mathbf{r}_2 \quad -\frac{i}{2}\mathbf{r}_3-\frac{i}{2}\mathbf{r}_4 \quad -\frac{i}{2}\mathbf{\tilde{r}}_1-\frac{i}{2}\mathbf{\tilde{r}}_2 \quad +\frac{i}{2}\mathbf{\tilde{r}}_3+\frac{i}{2}\mathbf{\tilde{r}}_4 \quad +\mathbf{0\rho}_x+\mathbf{0\rho}_y \quad -\mathbf{1\rho}_z \quad -\frac{1}{2}\mathbf{R}_x-\frac{1}{2}\mathbf{R}_y \quad -i\mathbf{R}_z \quad -\frac{1}{2}\mathbf{\tilde{R}}_x-\frac{1}{2}\mathbf{\tilde{R}}_y \quad +i\mathbf{\tilde{R}}_z \quad +\frac{1}{2}\mathbf{i}_1+\frac{1}{2}\mathbf{i}_2 \quad +\mathbf{0i}_3+\mathbf{0i}_4 \quad +\frac{1}{2}\mathbf{i}_5 \quad +\frac{1}{2}\mathbf{i}_6)$$

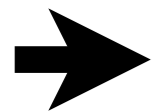
$$\mathbf{P}_{2_4 2_4}^{T_2} = \frac{1}{8} (\mathbf{1} \cdot \mathbf{1} \quad +\mathbf{0}+\mathbf{0} \quad +\mathbf{0}+\mathbf{0} \quad +\mathbf{0}+\mathbf{0} \quad +\mathbf{0}+\mathbf{0} \quad -\mathbf{1\rho}_x-\mathbf{1\rho}_y \quad +\mathbf{1\rho}_z \quad +\mathbf{0}+\mathbf{0} \quad -\mathbf{1R}_z \quad +\mathbf{0}+\mathbf{0} \quad -\mathbf{1\tilde{R}}_z \quad +\mathbf{0}+\mathbf{0} \quad +\mathbf{1i}_4+\mathbf{1i}_3 \quad +\mathbf{0}+\mathbf{0})$$

$O: \chi_g^\mu$	$g=1$	\mathbf{r}_{1-4} $\mathbf{\tilde{r}}_{1-4}$	ρ_{xyz}	\mathbf{R}_{xyz} $\mathbf{\tilde{R}}_{xyz}$	\mathbf{i}_{1-6}
$\mu=A_1$	1	1	1	1	1
A_2	1	1	1	-1	-1
E	2	-1	2	0	0
T_1	3	0	-1	1	-1
T_2	3	0	-1	-1	1

Review Coset factored splitting of $O \supset D_4 \supset C_4$ projectors and levels

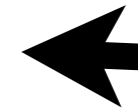
Irreducible idempotent projectors $P^{\mu}_{m,m}$ of $O \supset C_4 \sim T_d \supset C_{4i}$

Calculating $P^{E_{0404}}$ $P^{E_{2424}}$ $P^{T_1_{0404}}$ $P^{T_1_{1414}}$ $P^{T_2_{2424}}$



Factoring out $O \supset C_4$ subgroup cosets:

Factoring $P^{E_{0404}}$ $P^{E_{2424}}$ $P^{T_1_{0404}}$ $P^{T_1_{1414}}$ $P^{T_2_{2424}}$



Irreducible nilpotent projectors $P^{\mu}_{m,n}$

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$O_h \supset D_{4h} \supset C_{4v}$

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$O_h \supset C_{2v}$

Irreducible idempotent projectors $\mathbf{P}^\mu_{m,m}$ of $O \supset C_4 \sim T_d \supset C_{4i}$

Factoring out $O \supset C_4$ subgroup cosets:

$$1C_4 = \mathbf{1}\{\mathbf{1}, \rho_z, \mathbf{R}_z, \tilde{\mathbf{R}}_z\} \quad \rho_x C_4 = \{\rho_x, \rho_y, \mathbf{i}_4, \mathbf{i}_3\} \quad \mathbf{r}_1 C_4 = \{\mathbf{r}_1, \mathbf{r}_4, \mathbf{i}_1, \mathbf{R}_y\} \quad \mathbf{r}_2 C_4 = \{\mathbf{r}_2, \mathbf{r}_3, \mathbf{i}_2, \tilde{\mathbf{R}}_y\} \quad \tilde{\mathbf{r}}_1 C_4 = \{\tilde{\mathbf{r}}_1, \tilde{\mathbf{r}}_3, \tilde{\mathbf{R}}_x, \mathbf{i}_6\} \quad \tilde{\mathbf{r}}_2 C_4 = \{\tilde{\mathbf{r}}_2, \tilde{\mathbf{r}}_4, \mathbf{R}_x, \mathbf{i}_5\}$$

Coset-factored A_1 -sum:

$$\mathbf{P}_{0_4 0_4}^{A_1} = \frac{1}{12} [(1) \cdot \mathbf{1} \mathbf{p}_{0_4} + (1) \cdot \rho_x \mathbf{p}_{0_4} + (1) \cdot \mathbf{r}_1 \mathbf{p}_{0_4} + (1) \cdot \mathbf{r}_2 \mathbf{p}_{0_4} + (1) \cdot \tilde{\mathbf{r}}_1 \mathbf{p}_{0_4} + (1) \cdot \tilde{\mathbf{r}}_2 \mathbf{p}_{0_4}]$$

Coset-factored A_2 -sum:

$$\mathbf{P}_{2_4 2_4}^{A_2} = \frac{1}{12} [(1) \cdot \mathbf{1} \mathbf{p}_{2_4} + (1) \cdot \rho_x \mathbf{p}_{2_4} + (1) \cdot \mathbf{r}_1 \mathbf{p}_{2_4} + (1) \cdot \mathbf{r}_2 \mathbf{p}_{2_4} + (1) \cdot \tilde{\mathbf{r}}_1 \mathbf{p}_{2_4} + (1) \cdot \tilde{\mathbf{r}}_2 \mathbf{p}_{2_4}]$$

Coset-factored E -sum:

$$\mathbf{P}_{0_4 0_4}^E = \frac{1}{12} [(1) \cdot \mathbf{1} \mathbf{p}_{0_4} + (1) \cdot \rho_x \mathbf{p}_{0_4} + (-\frac{1}{2}) \cdot \mathbf{r}_1 \mathbf{p}_{0_4} + (-\frac{1}{2}) \cdot \mathbf{r}_2 \mathbf{p}_{0_4} + (-\frac{1}{2}) \cdot \tilde{\mathbf{r}}_1 \mathbf{p}_{0_4} + (-\frac{1}{2}) \cdot \tilde{\mathbf{r}}_2 \mathbf{p}_{0_4}]$$

$$\mathbf{P}_{2_4 2_4}^E = \frac{1}{12} [(1) \cdot \mathbf{1} \mathbf{p}_{2_4} + (1) \cdot \rho_x \mathbf{p}_{2_4} + (-\frac{1}{2}) \cdot \mathbf{r}_1 \mathbf{p}_{2_4} + (-\frac{1}{2}) \cdot \mathbf{r}_2 \mathbf{p}_{2_4} + (-\frac{1}{2}) \cdot \tilde{\mathbf{r}}_1 \mathbf{p}_{2_4} + (-\frac{1}{2}) \cdot \tilde{\mathbf{r}}_2 \mathbf{p}_{2_4}]$$

Coset-factored T_1 -sum:

$$\mathbf{P}_{1_4 1_4}^{T_1} = \frac{1}{8} [(1) \cdot \mathbf{1} \mathbf{p}_{1_4} + (0) \cdot \rho_x \mathbf{p}_{1_4} + (+\frac{i}{2}) \cdot \mathbf{r}_1 \mathbf{p}_{1_4} + (+\frac{i}{2}) \cdot \mathbf{r}_2 \mathbf{p}_{1_4} + (-\frac{i}{2}) \cdot \tilde{\mathbf{r}}_1 \mathbf{p}_{1_4} + (-\frac{i}{2}) \cdot \tilde{\mathbf{r}}_2 \mathbf{p}_{1_4}]$$

$$\mathbf{P}_{3_4 3_4}^{T_1} = \frac{1}{8} [(1) \cdot \mathbf{1} \mathbf{p}_{3_4} + (0) \cdot \rho_x \mathbf{p}_{3_4} + (-\frac{i}{2}) \cdot \mathbf{r}_1 \mathbf{p}_{3_4} + (-\frac{i}{2}) \cdot \mathbf{r}_2 \mathbf{p}_{3_4} + (+\frac{i}{2}) \cdot \tilde{\mathbf{r}}_1 \mathbf{p}_{3_4} + (+\frac{i}{2}) \cdot \tilde{\mathbf{r}}_2 \mathbf{p}_{3_4}]$$

$$\mathbf{P}_{0_4 0_4}^{T_1} = \frac{1}{8} [(1) \cdot \mathbf{1} \mathbf{p}_{0_4} + (-1) \cdot \rho_x \mathbf{p}_{0_4} + (0) \cdot \mathbf{r}_1 \mathbf{p}_{0_4} + (0) \cdot \mathbf{r}_2 \mathbf{p}_{0_4} + (0) \cdot \tilde{\mathbf{r}}_1 \mathbf{p}_{0_4} + (0) \cdot \tilde{\mathbf{r}}_2 \mathbf{p}_{0_4}]$$

Coset-factored T_2 -sum:

$$\mathbf{P}_{1_4 1_4}^{T_2} = \frac{1}{8} [(1) \cdot \mathbf{1} \mathbf{p}_{1_4} + (0) \cdot \rho_x \mathbf{p}_{1_4} + (-\frac{i}{2}) \cdot \mathbf{r}_1 \mathbf{p}_{1_4} + (-\frac{i}{2}) \cdot \mathbf{r}_2 \mathbf{p}_{1_4} + (-\frac{i}{2}) \cdot \tilde{\mathbf{r}}_1 \mathbf{p}_{1_4} + (-\frac{i}{2}) \cdot \tilde{\mathbf{r}}_2 \mathbf{p}_{1_4}]$$

$$\mathbf{P}_{3_4 3_4}^{T_2} = \frac{1}{8} [(1) \cdot \mathbf{1} \mathbf{p}_{3_4} + (0) \cdot \rho_x \mathbf{p}_{3_4} + (+\frac{i}{2}) \cdot \mathbf{r}_1 \mathbf{p}_{3_4} + (+\frac{i}{2}) \cdot \mathbf{r}_2 \mathbf{p}_{3_4} + (+\frac{i}{2}) \cdot \tilde{\mathbf{r}}_1 \mathbf{p}_{3_4} + (+\frac{i}{2}) \cdot \tilde{\mathbf{r}}_2 \mathbf{p}_{3_4}]$$

$$\mathbf{P}_{2_4 2_4}^{T_2} = \frac{1}{8} [(1) \cdot \mathbf{1} \mathbf{p}_{2_4} + (1) \cdot \rho_x \mathbf{p}_{2_4} + (0) \cdot \mathbf{r}_1 \mathbf{p}_{2_4} + (0) \cdot \mathbf{r}_2 \mathbf{p}_{2_4} + (0) \cdot \tilde{\mathbf{r}}_1 \mathbf{p}_{2_4} + (0) \cdot \tilde{\mathbf{r}}_2 \mathbf{p}_{2_4}]$$

$$\mathbf{p}_{m_4} = \sum_{p=0}^3 \frac{e^{2\pi i m \cdot p/4}}{4} \mathbf{R}_z^p =$$

$$\left\{ \begin{array}{l} \mathbf{p}_{0_4} = (\mathbf{1} + \mathbf{R}_z + \rho_z + \tilde{\mathbf{R}}_z)/4 \\ \mathbf{p}_{1_4} = (\mathbf{1} + i\mathbf{R}_z - \rho_z - i\tilde{\mathbf{R}}_z)/4 \\ \mathbf{p}_{2_4} = (\mathbf{1} - \mathbf{R}_z + \rho_z - \tilde{\mathbf{R}}_z)/4 \\ \mathbf{p}_{3_4} = (\mathbf{1} - i\mathbf{R}_z - \rho_z + i\tilde{\mathbf{R}}_z)/4 \end{array} \right.$$

$C_4: \chi_g^\mu$	$\mathbf{g}=\mathbf{1}$	\mathbf{R}_z	ρ_z	$\tilde{\mathbf{R}}_z$
$\mu=0_4$	1	1	1	1
1_4	1	$-i$	-1	i
2_4	1	-1	1	-1
3_4	1	$-i$	-1	$-i$

C_4 subgroup correlation to O

$O \supset C_4 \quad (0)_4 \quad (1)_4 \quad (2)_4 \quad (3)_4 = (-1)_4$

A_1	1	•	•	•
A_2	•	•	1	•
E	1	•	1	•
T_1	1	1	•	1
T_2	•	1	1	1

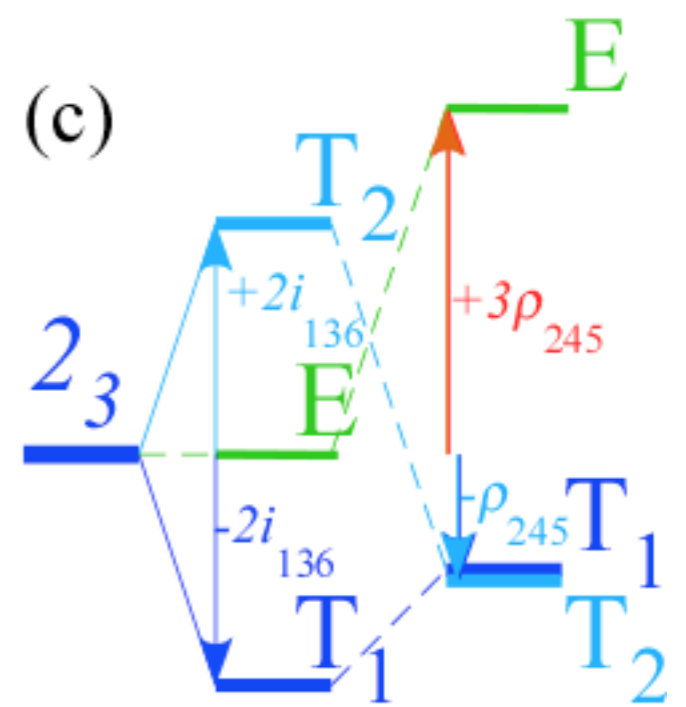
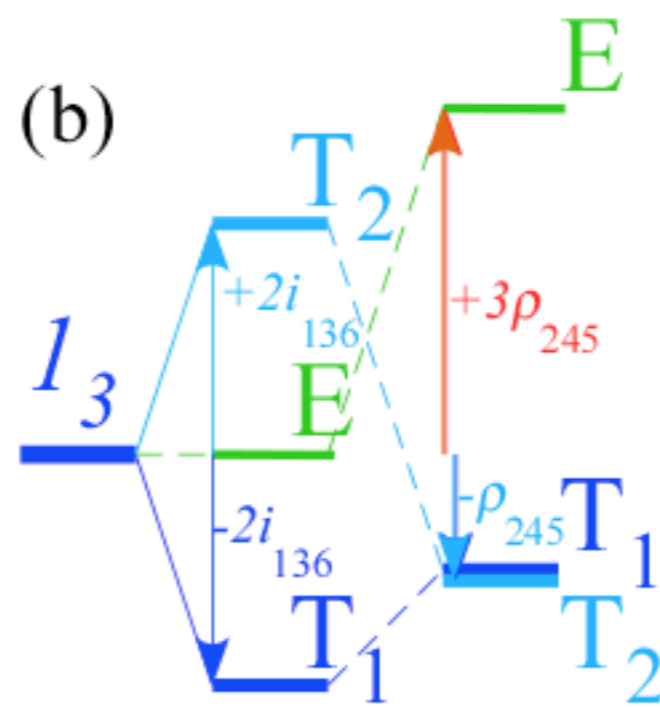
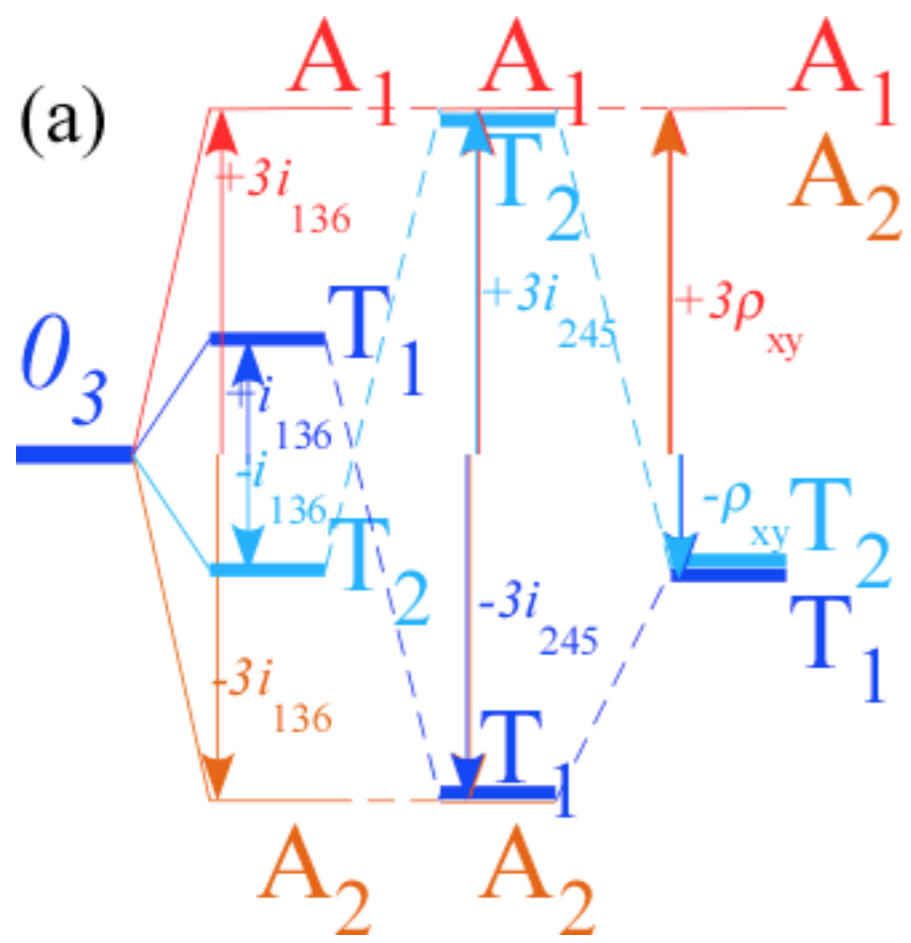
C_4 Projectors to split octahedral P^α

$$P_{m_4} = \sum_{p=0}^3 \frac{e^{2\pi i m \cdot p/4}}{4} R_z^p = \begin{cases} P_{0_4} = (1 + R_z + \rho_z + \tilde{R}_z)/4 \\ P_{1_4} = (1 + iR_z - \rho_z - i\tilde{R}_z)/4 \\ P_{2_4} = (1 - R_z + \rho_z - \tilde{R}_z)/4 \\ P_{3_4} = (1 - iR_z - \rho_z + i\tilde{R}_z)/4 \end{cases}$$

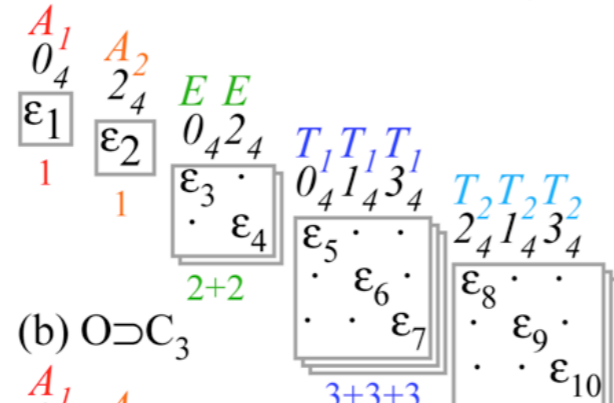
$1 \cdot P^\alpha =$	$(P_{0_4} + P_{1_4} + P_{2_4} + P_{3_4}) \cdot P^\alpha$
$1 \cdot P^{A_1} =$	$P_{0_4}^{A_1} + 0 + 0 + 0$
$1 \cdot P^{A_2} =$	$0 + 0 + P_{2_4}^{A_2} + 0$
$1 \cdot P^E =$	$P_{0_4}^E + 0 + P_{2_4}^E + 0$
$1 \cdot P^{T_1} =$	$P_{0_4}^{T_1} + P_{1_4}^{T_1} + 0 + P_{3_4}^{T_1}$
$1 \cdot P^{T_2} =$	$0 + P_{1_4}^{T_2} + P_{2_4}^{T_2} + P_{3_4}^{T_2}$

10 split $O \supset C_4$ octahedral P^α related to 10 split sub-classes

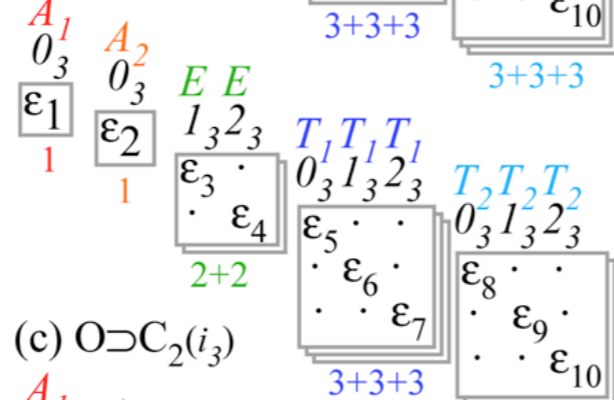
$P_{n_4 n_4}^{(\alpha)} (O \supset C_4)$	1	$r_1 r_2 \tilde{r}_3 \tilde{r}_4$	$\tilde{r}_1 \tilde{r}_2 r_3 r_4$	$\rho_x \rho_y$	ρ_z	$R_x \tilde{R}_x R_y \tilde{R}_y$	R_z	\tilde{R}_z	$i_1 i_2 i_5 i_6$	$i_3 i_4$
$24 \cdot P_{0_4 0_4}^{A_1}$	1	1	1	1	1	1	1	1	1	1
$24 \cdot P_{2_4 2_4}^{A_2}$	1	1	1	1	1	-1	-1	-1	-1	-1
$12 \cdot P_{0_4 0_4}^E$	1	$-\frac{1}{2}$	$-\frac{1}{2}$	1	1	$-\frac{1}{2}$	1	1	$-\frac{1}{2}$	1
$12 \cdot P_{2_4 2_4}^E$	1	$-\frac{1}{2}$	$-\frac{1}{2}$	1	1	$+\frac{1}{2}$	-1	-1	$+\frac{1}{2}$	-1
$8 \cdot P_{1_4 1_4}^{T_1}$	1	$-\frac{i}{2}$	$+\frac{i}{2}$	0	-1	$+\frac{1}{2}$	-i	+i	$-\frac{1}{2}$	0
$8 \cdot P_{3_4 3_4}^{T_1}$	1	$+\frac{i}{2}$	$-\frac{i}{2}$	0	-1	$+\frac{1}{2}$	+i	-i	$-\frac{1}{2}$	0
$8 \cdot P_{0_4 0_4}^{T_1}$	1	0	0	-1	1	0	1	1	0	-1
$8 \cdot P_{1_4 1_4}^{T_2}$	1	$+\frac{i}{2}$	$-\frac{i}{2}$	0	-1	$-\frac{1}{2}$	-i	+i	$+\frac{1}{2}$	0
$8 \cdot P_{3_4 3_4}^{T_2}$	1	$-\frac{i}{2}$	$+\frac{i}{2}$	0	-1	$-\frac{1}{2}$	+i	-i	$+\frac{1}{2}$	0
$8 \cdot P_{2_4 2_4}^{T_2}$	1	0	0	-1	1	0	-1	-1	0	1



$$(a) O^{global} * O^{local} \supset O^{global} * C_4^{local}$$



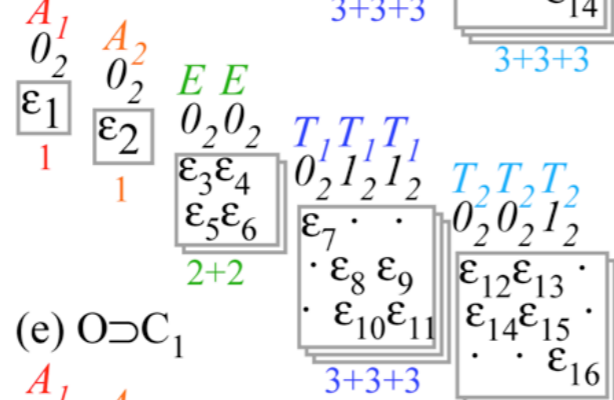
$$(b) O \supset C_3$$



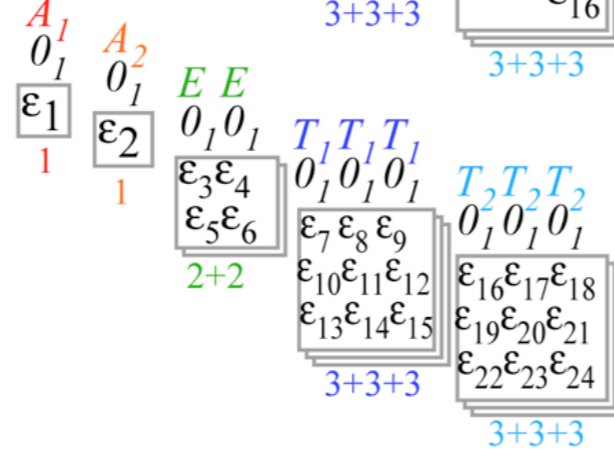
$$(c) O \supset C_2(i_3)$$



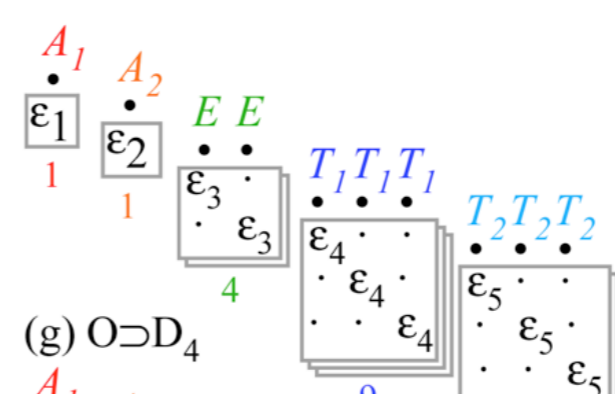
$$(d) O \supset C_2(\rho_z)$$



$$(e) O \supset C_1$$



$$(f) O^{global} * O^{local}$$



$$(g) O \supset D_4$$



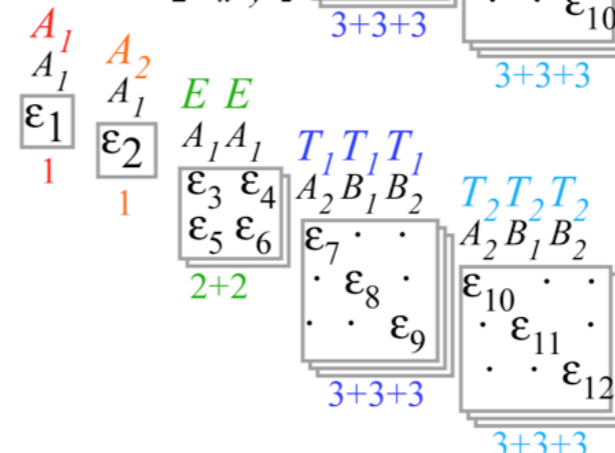
$$(h) O \supset D_3$$



$$(i) O \supset D_2(i_3, i_4, \rho_z)$$



$$(j) O \supset D_2(\rho_x, \rho_y, \rho_z)$$



Effects of broken or transition local symmetry for i -class

$$D_{0_4 0_4}^{A_1}(i_k \mathbf{i}_k) = i_1 + i_2 + i_3 + i_4 + i_5 + i_6$$

$$D_{2_4 2_4}^{A_2}(i_k \mathbf{i}_k) = -(i_1 + i_2 + i_3 + i_4 + i_5 + i_6)$$

$$D^E(i_k \mathbf{i}_k) = \begin{array}{c|cc} & 0_4 & 2_4 \\ \hline 0_4 & -\frac{1}{2}(i_1 + i_2 + i_5 + i_6) + i_3 + i_4 & \frac{\sqrt{3}}{2}(i_1 + i_2 - i_5 - i_6) \\ 2_4 & h.c. & \frac{1}{2}(i_1 + i_2 + i_5 + i_6) - i_3 - i_4 \end{array}$$

$$D^{T_1^*}(i_k \mathbf{i}_k) = \begin{array}{c|ccc} & 1_4 & 3_4 & 0_4 \\ \hline 1_4 & -\frac{1}{2}(i_1 + i_2 + i_5 + i_6) & -\frac{1}{2}(i_1 + i_2 - i_5 - i_6) - i(i_3 - i_4) & -\frac{1}{\sqrt{2}}(i_1 - i_2) + \frac{i}{\sqrt{2}}(i_5 - i_6) \\ 3_4 & h.c. & -\frac{1}{2}(i_1 + i_2 + i_5 + i_6) & +\frac{1}{\sqrt{2}}(i_1 - i_2) + \frac{i}{\sqrt{2}}(i_5 - i_6) \\ 0_4 & h.c. & h.c. & -(i_3 + i_4) \end{array}$$

$$D^{T_2^*}(i_k \mathbf{i}_k) = \begin{array}{c|ccc} & 1_4 & 3_4 & 2_4 \\ \hline 1_4 & +\frac{1}{2}(i_1 + i_2 + i_5 + i_6) & +\frac{1}{2}(i_1 + i_2 - i_5 - i_6) - i(i_3 - i_4) & +\frac{1}{\sqrt{2}}(i_1 - i_2) + \frac{i}{\sqrt{2}}(i_5 - i_6) \\ 3_4 & h.c. & +\frac{1}{2}(i_1 + i_2 + i_5 + i_6) & -\frac{1}{\sqrt{2}}(i_1 - i_2) + \frac{i}{\sqrt{2}}(i_5 - i_6) \\ 0_4 & h.c. & h.c. & +(i_3 + i_4) \end{array}$$

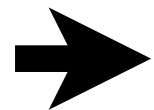
Review Coset factored splitting of $O \supset D_4 \supset C_4$ projectors and levels

Irreducible idempotent projectors $\mathbf{P}^\mu_{m,m}$ of $O \supset C_4 \sim T_d \supset C_{4i}$

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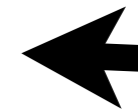


Irreducible nilpotent projectors $\mathbf{P}^\mu_{m,n}$

Fundamental $\mathbf{P}^\mu_{m,n}$ definitions:

Review of $D_3 \supset C_2 \sim C_{3v} \supset C_v$

Calculating and Factoring $\mathbf{P}^{T_1}_{1404}$



Structure and applications of various subgroup chain ireps

$O_h \supset D_{4h} \supset C_{4v}$

$O_h \supset D_{3h} \supset C_{3v}$

$O_h \supset C_{2v}$

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$$(1) \mathbf{P}^{\mu}_{mm} \mathbf{g} \mathbf{P}^{\mu}_{nn} = D^{\mu}_{mn}(\mathbf{g}) \mathbf{P}^{\mu}_{mn} \quad (2) \mathbf{g} = \sum_{\mu} \sum_{m,n}^{\ell^{\mu}} D^{\mu}_{mn}(\mathbf{g}) \mathbf{P}^{\mu}_{mn} \quad (3) \mathbf{P}^{\mu}_{mn} = \frac{\ell^{\mu}}{\circ G} \sum_{\mathbf{g}}^{\circ G} D^{\mu*}_{mn}(\mathbf{g}) \mathbf{g}$$

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Problem: (1)-(3) all require $\mathbf{P}^{\mu}_{m,n}$ and $D^{\mu}_{m,n}(\mathbf{g})$ from the get-go.

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$$\mathbf{P}^\mu_{mm} \mathbf{g} \mathbf{P}^\mu_{nn} = (?) \cdot \mathbf{P}^\mu_{mn}$$

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$$\mathbf{g} |\mathbf{P}^\mu_{mn}\rangle = \sum_k^{\ell^\mu} D^\mu_{km}(\mathbf{g}) |\mathbf{P}^\mu_{kn}\rangle$$

or by direct (k,m) -matrix elements for any (n) that gives nonzero value: $\langle \mathbf{P}^\mu_{kn} | \mathbf{g} | \mathbf{P}^\mu_{mn} \rangle = D^\mu_{km}(\mathbf{g})$

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Hint: Sub-group chain factoring helps. Since \mathbf{P}^μ is all-commuting: $\mathbf{p}_{m_4} \mathbf{P}^\mu = \mathbf{P}^\mu_{m_4 m_4} = \mathbf{P}^\mu \mathbf{p}_{m_4}$

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This reduces to a smaller object $\mathbf{p}_{m_4} \mathbf{g} \mathbf{p}_{n_4}$ to calculate: $\mathbf{P}^\mu_{m_4 m_4} \mathbf{g} \mathbf{P}^\mu_{n_4 n_4} = \mathbf{P}^\mu \mathbf{p}_{m_4} \mathbf{g} \mathbf{p}_{n_4}$

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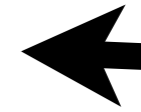
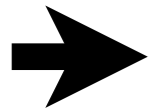
Calculating and Factoring $\mathbf{P}^{T_1}_{1404}$

Structure and applications of various subgroup chain ireps

$O_h \supset D_{4h} \supset C_{4v}$

$O_h \supset D_{3h} \supset C_{3v}$

$O_h \supset C_{2v}$



Irreducible nilpotent projectors $\mathbf{P}^{\mu}_{m,n}$

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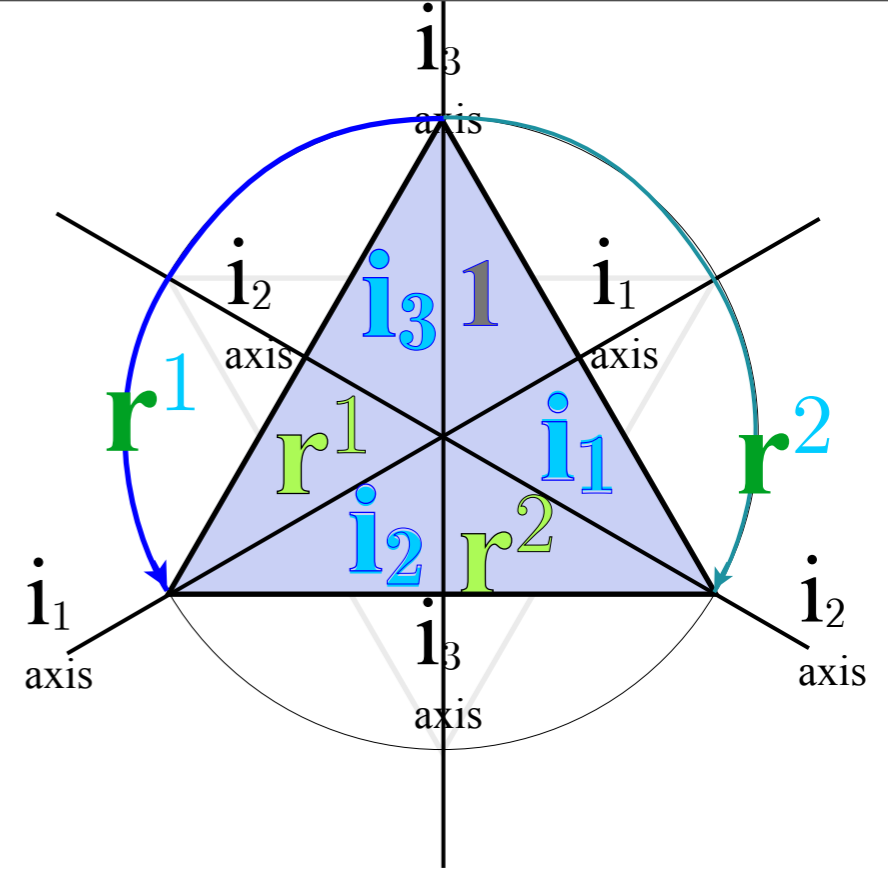
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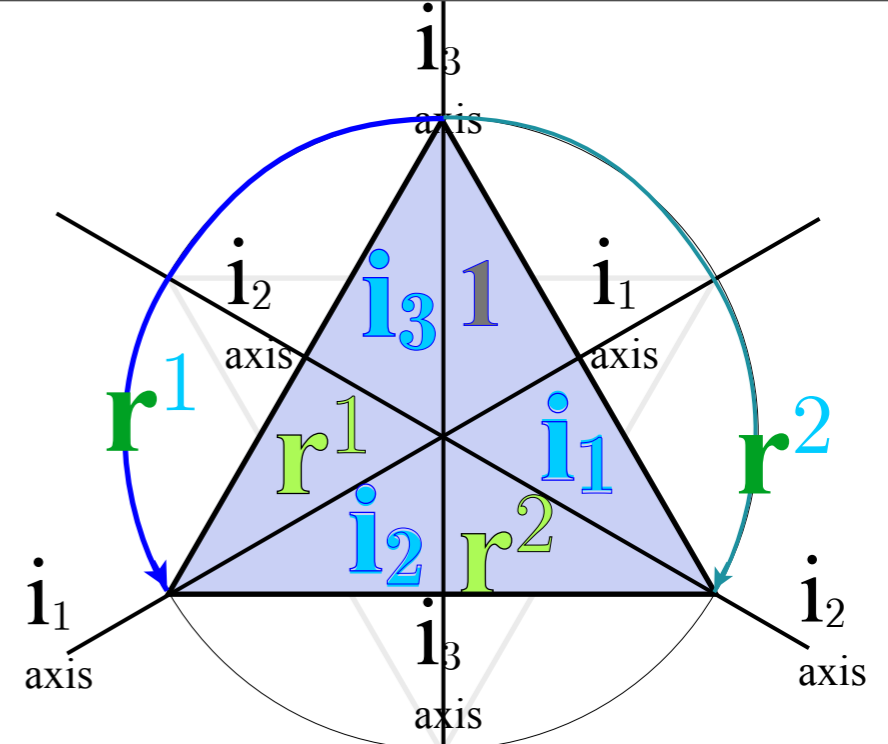
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	\mathbf{r}	$+\mathbf{r}\mathbf{i}_3$
$\mathbf{1}$	\mathbf{r}	$+\mathbf{r}\mathbf{i}_3$
$-\mathbf{i}_3$	$-\mathbf{i}_3\mathbf{r}$	$-\mathbf{i}_3\mathbf{r}\mathbf{i}_3$



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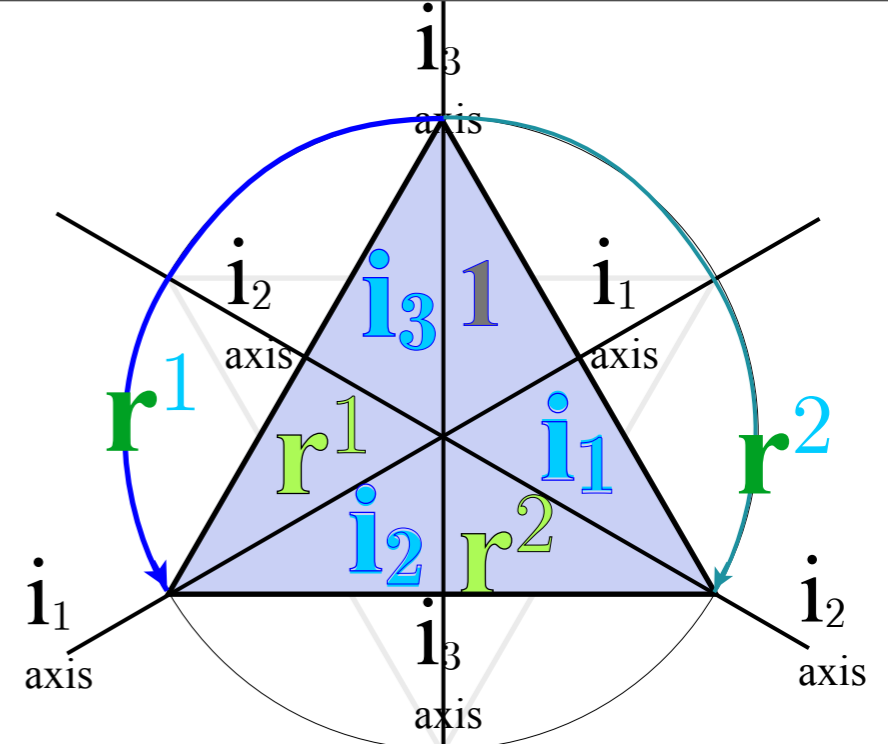
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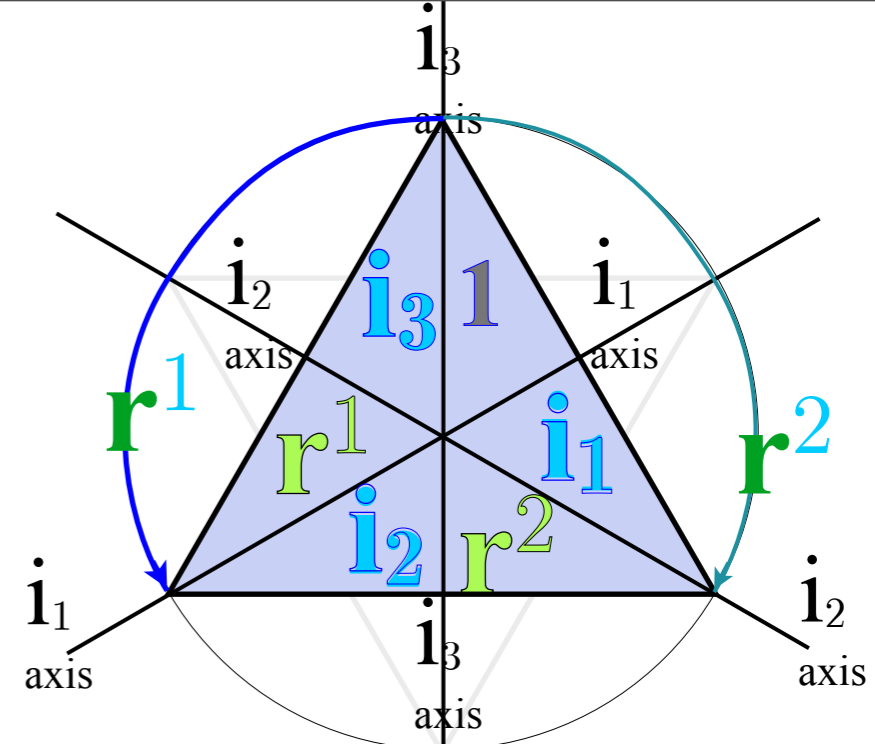
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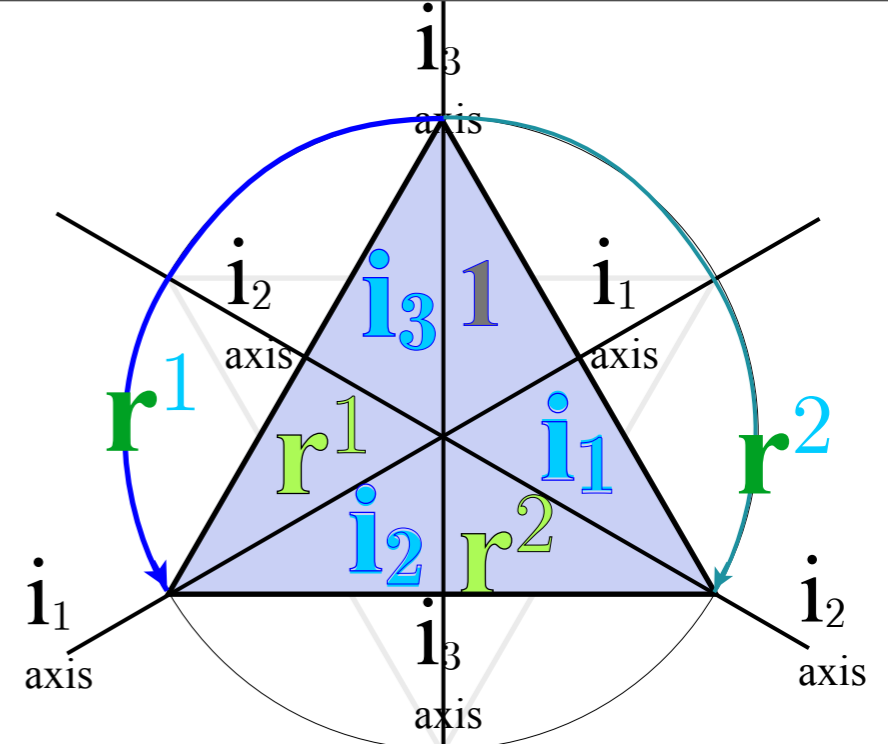
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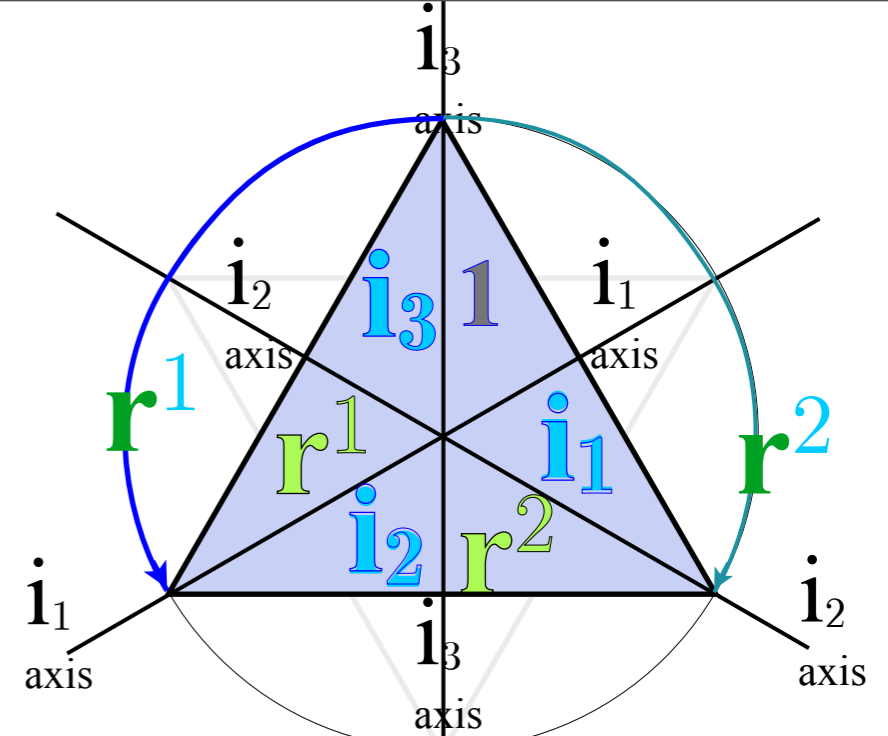
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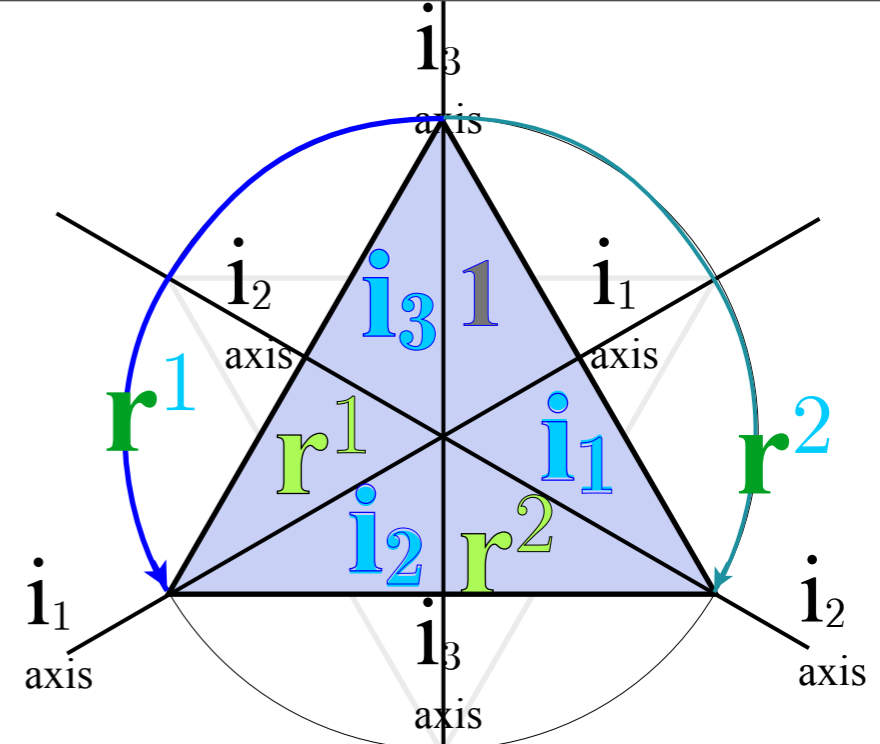
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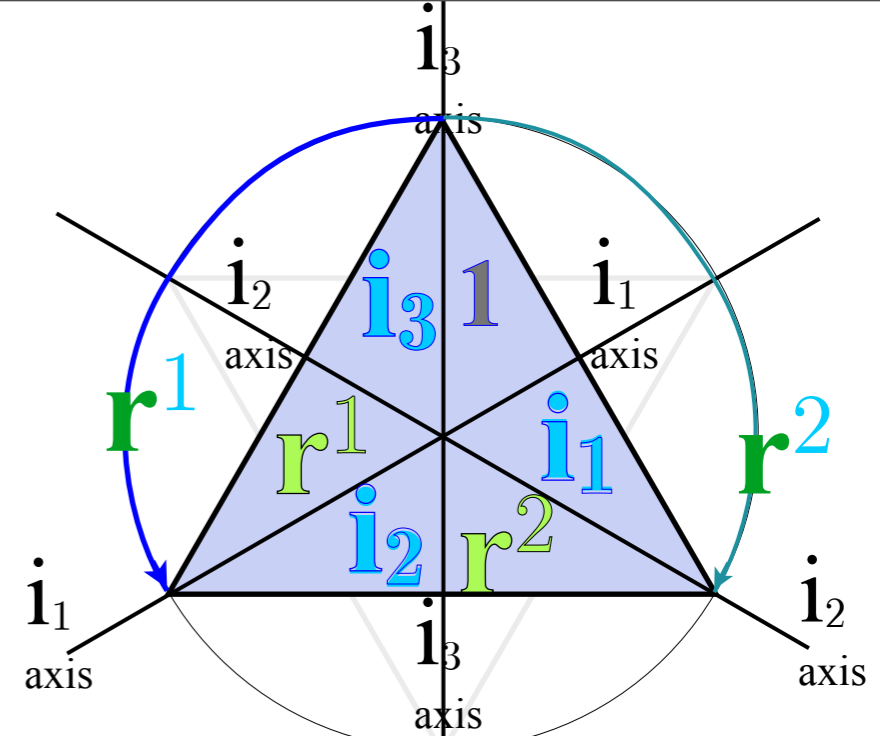
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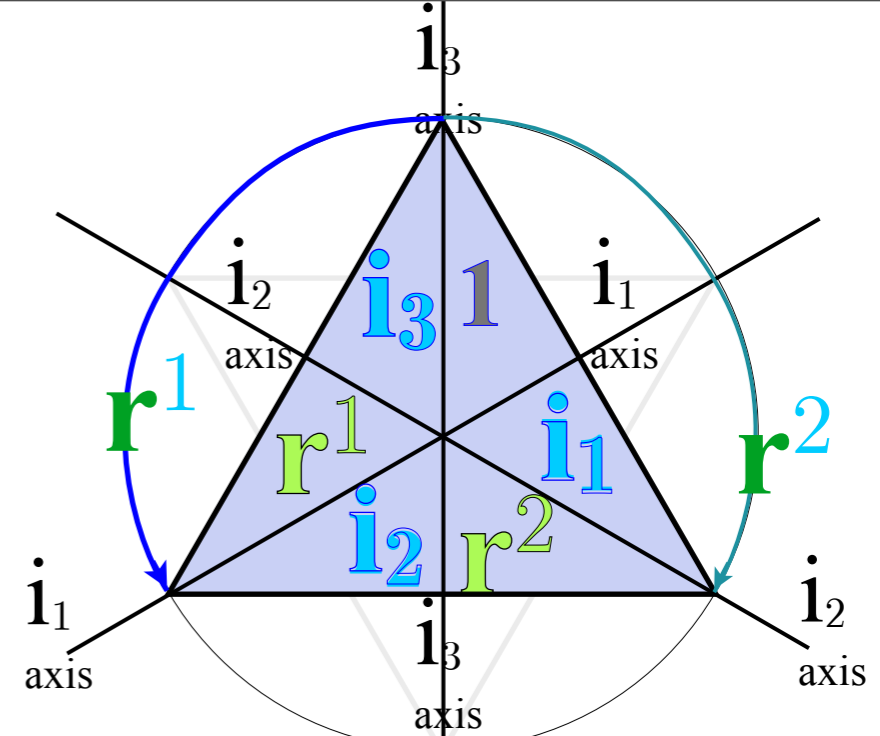
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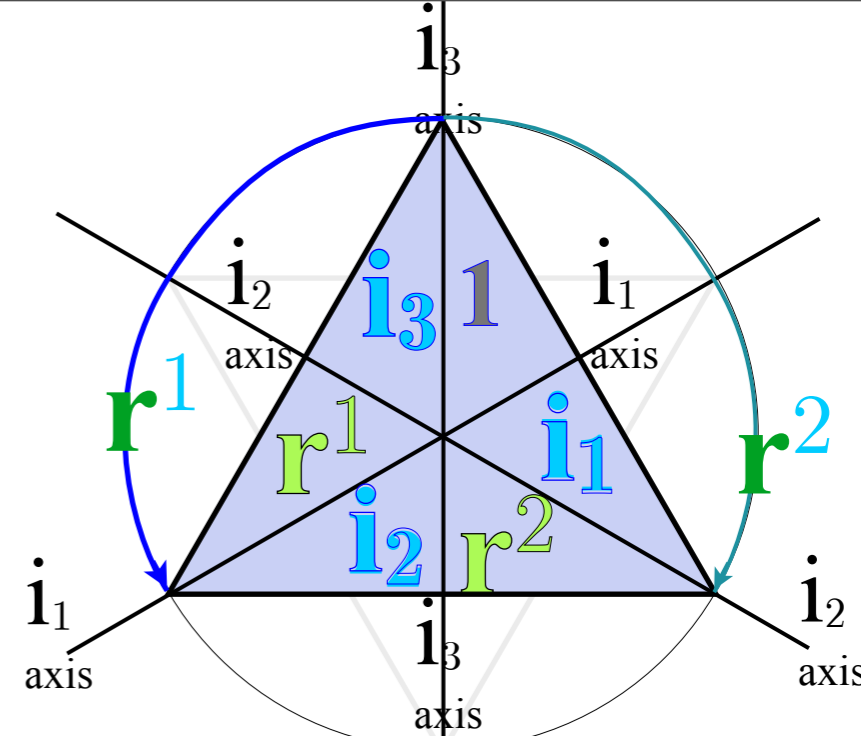
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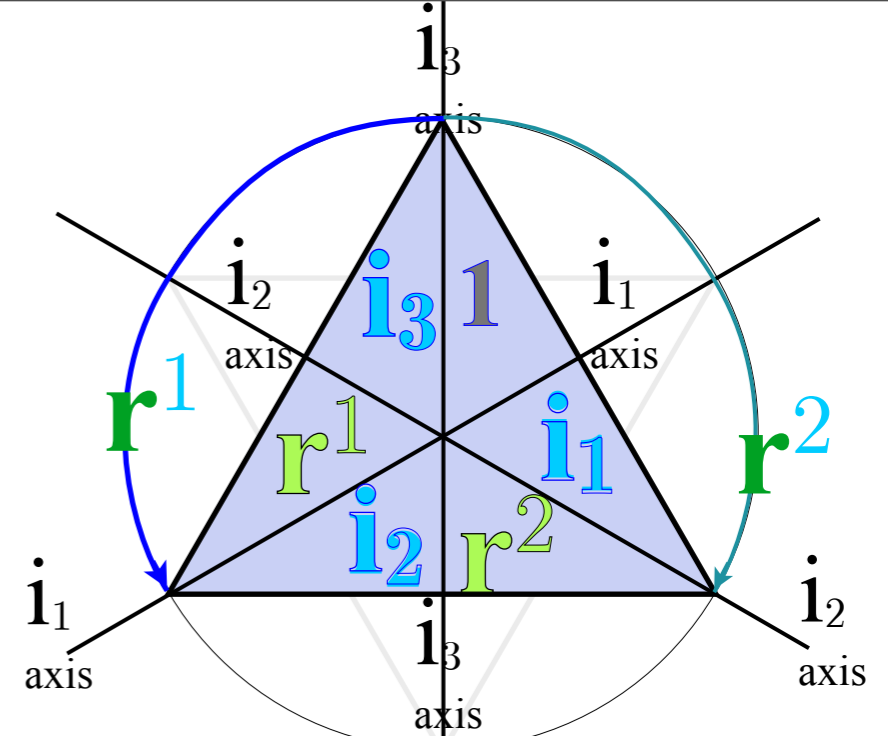
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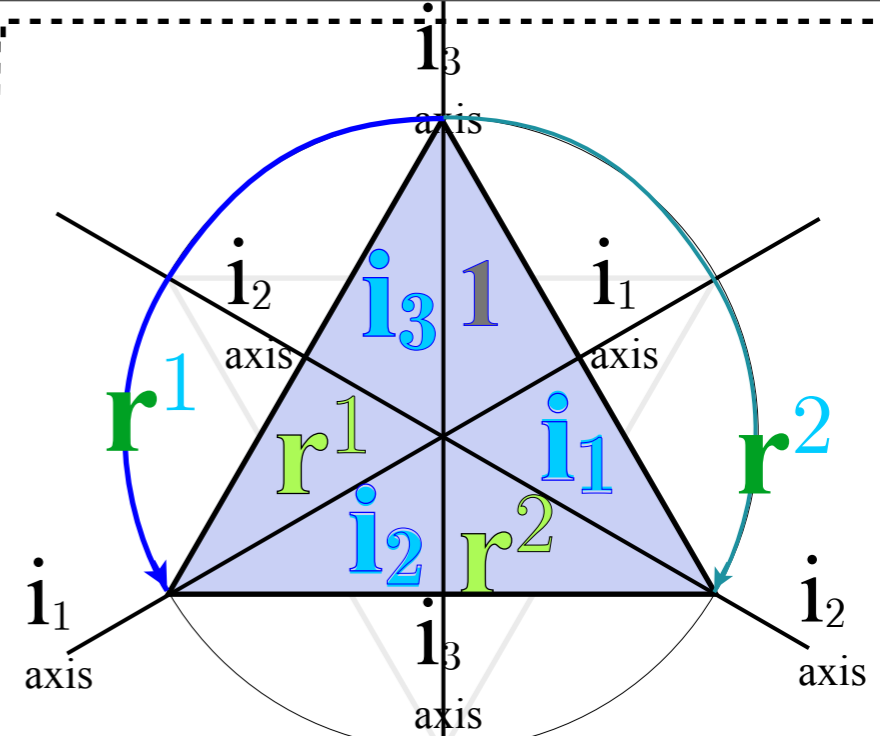
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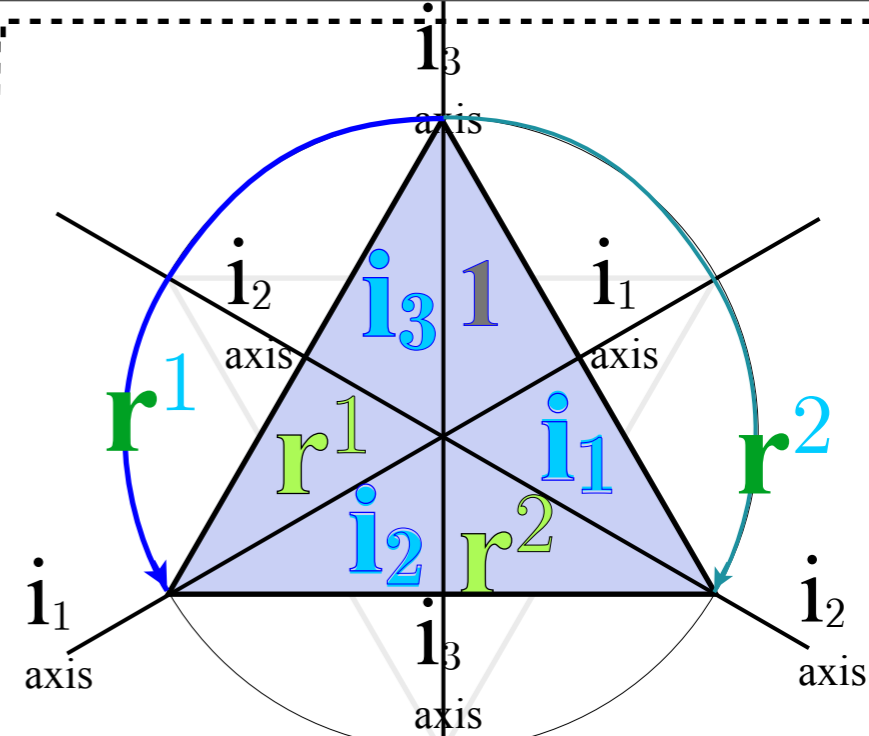
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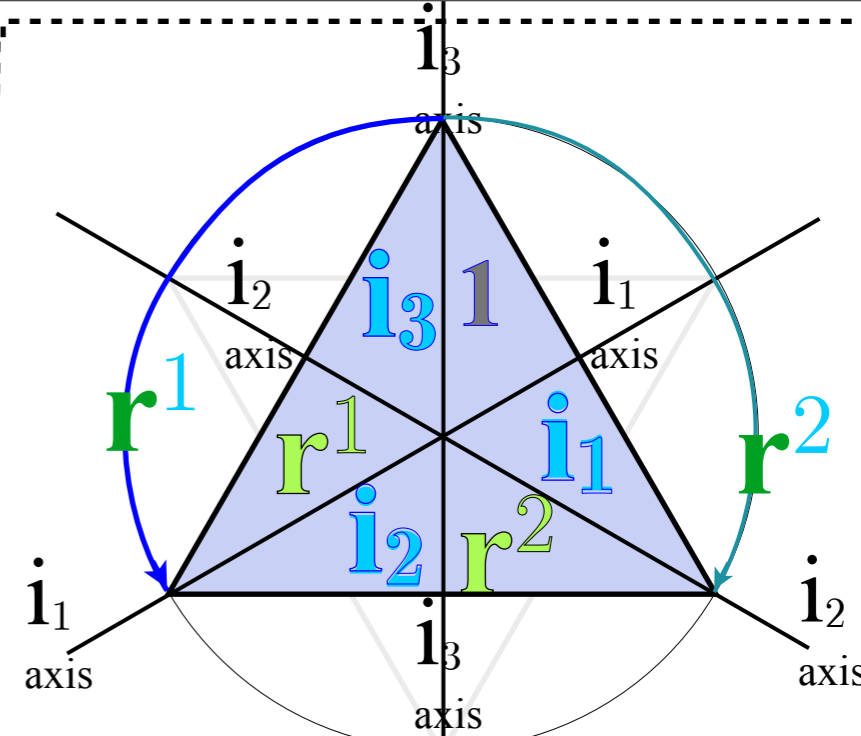
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Solving for (?) -factor: $(?) = \pm \sqrt{3}/6$ Gives all \mathbf{P}^E and D^E to \pm

$$(?)^2 \cdot 4 = \frac{1}{3} = \frac{1}{3} D_{0_2 0_2}^{E*}(1) \quad \pm \mathbf{P}_{0_2 1_2}^E = \frac{1}{3} \left(\frac{\sqrt{3}}{2} \mathbf{r} - \frac{\sqrt{3}}{2} \mathbf{r}^2 - \frac{\sqrt{3}}{2} \mathbf{i}_1 + \frac{\sqrt{3}}{2} \mathbf{i}_2 \right)$$

$$\pm D_{0_2 1_2}^{E*}(r) = \frac{\sqrt{3}}{2}, \text{ etc.}$$

$\pm \mathbf{P}_{0_2 1_2}^E = \frac{1}{3} \left(\frac{\sqrt{3}}{2} \mathbf{r} - \frac{\sqrt{3}}{2} \mathbf{r}^2 - \frac{\sqrt{3}}{2} \mathbf{i}_1 + \frac{\sqrt{3}}{2} \mathbf{i}_2 \right)$ Now, to set \pm signs of off-diagonal components...

$\pm D_{0_2 1_2}^{E*}(r) = \frac{\sqrt{3}}{2}, etc.$

Irreducible nilpotent projectors $\mathbf{P}^\mu_{m,n}$

Review of $D_3 \supset C_2 \sim C_{3v} \supset C_v$

$D_3 : \chi_k^\alpha$	χ_1^α	χ_r^α	χ_i^α
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Given: $\mathbf{P}^E = \frac{1}{3}(2\mathbf{c}_1 - \mathbf{c}_r + 0)$
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$$\mathbf{P}_{0_2 0_2}^E = \mathbf{P}^E \mathbf{p}_{0_2} = \frac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2) \frac{1}{2}(\mathbf{1} + \mathbf{i}_3) = \frac{1}{6}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 - \mathbf{i}_2 + 2\mathbf{i}_3)$$

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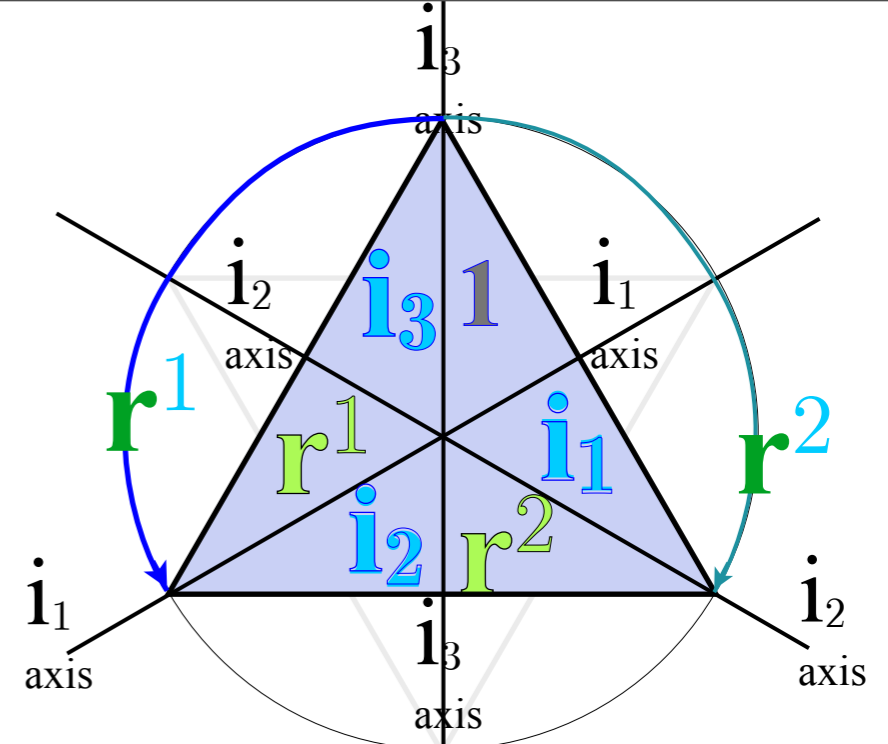
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Make group space vectors:

$$|\mathbf{P}_{0_2 0_2}^E\rangle = \frac{1}{2\sqrt{3}}(2|\mathbf{1}\rangle - |\mathbf{r}\rangle - |\mathbf{r}^2\rangle - |\mathbf{i}_1\rangle - |\mathbf{i}_2\rangle + 2|\mathbf{i}_3\rangle)$$

$$|\mathbf{P}_{1_2 0_2}^E\rangle = \frac{1}{2}(0|\mathbf{1}\rangle + |\mathbf{r}\rangle - |\mathbf{r}^2\rangle - |\mathbf{i}_1\rangle + |\mathbf{i}_2\rangle + 0|\mathbf{i}_3\rangle)$$



$$\begin{pmatrix} & \mathbf{r} & +\mathbf{r}\mathbf{i}_3 \\ \mathbf{1} & \mathbf{r} & +\mathbf{r}\mathbf{i}_3 \\ -\mathbf{i}_3 & -\mathbf{i}_3\mathbf{r} & -\mathbf{i}_3\mathbf{r}\mathbf{i}_3 \end{pmatrix} = \frac{1}{4} \mathbf{P}^E \begin{pmatrix} & \mathbf{r} & +\mathbf{r}\mathbf{i}_3 \\ \mathbf{1} & \mathbf{r} & +\mathbf{i}_2 \\ -\mathbf{i}_3 & -\mathbf{i}_1 & -\mathbf{r}^2 \end{pmatrix}$$

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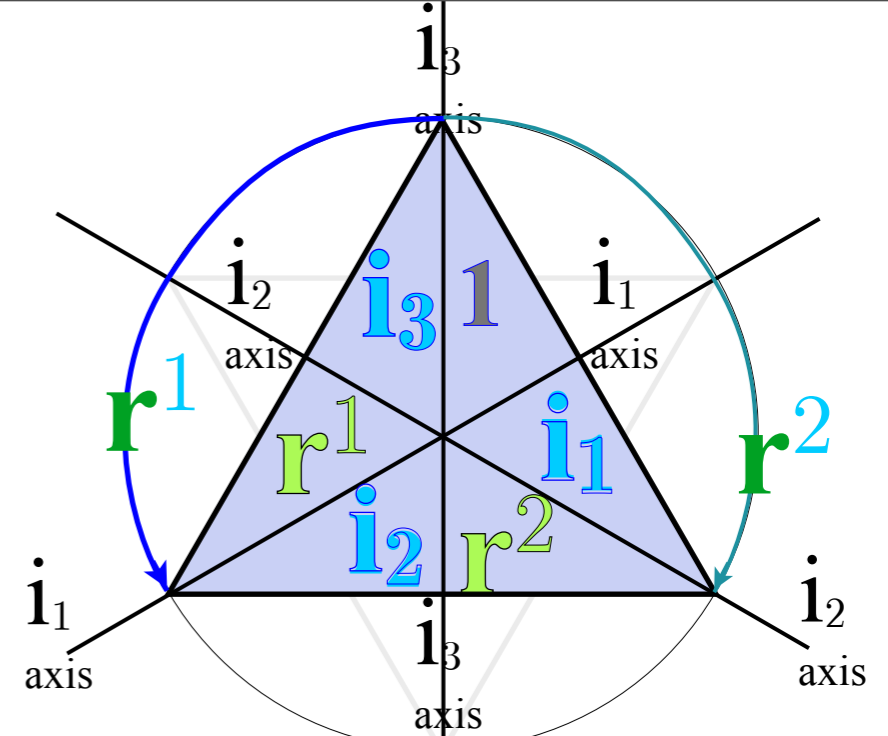
$$|\mathbf{P}_{0_2 0_2}^E\rangle = \frac{1}{2\sqrt{3}}(2|\mathbf{1}\rangle - |\mathbf{r}\rangle - |\mathbf{r}^2\rangle - |\mathbf{i}_1\rangle - |\mathbf{i}_2\rangle + 2|\mathbf{i}_3\rangle)$$

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$$\mathbf{r}|\mathbf{P}_{0_2 0_2}^E\rangle = \frac{1}{2\sqrt{3}}(2|\mathbf{r}\rangle - |\mathbf{r}^2\rangle - |\mathbf{1}\rangle - |\mathbf{i}_3\rangle - |\mathbf{i}_1\rangle + 2|\mathbf{i}_2\rangle)$$

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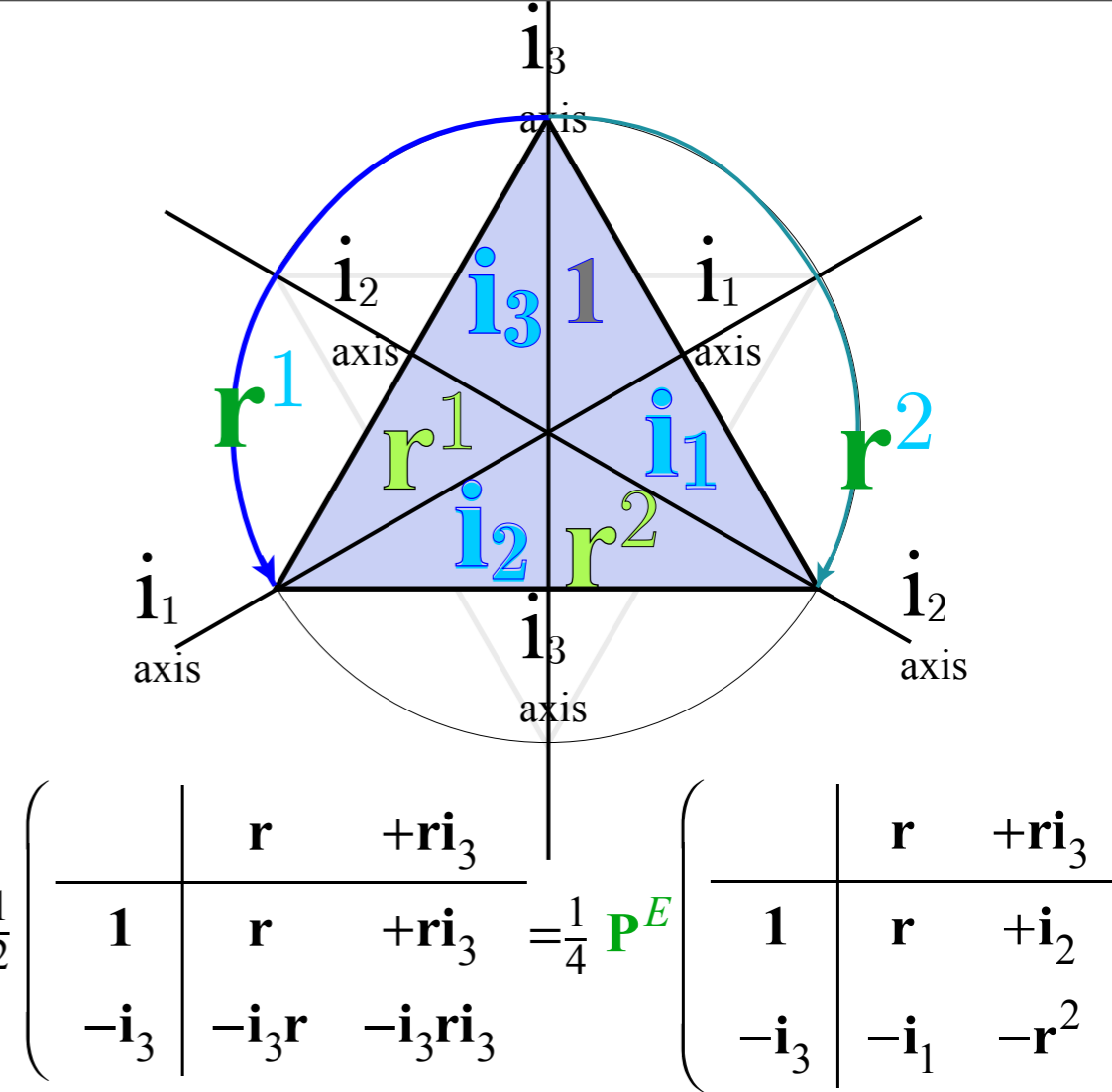
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$$\mathbf{r}|\mathbf{P}_{1_2 0_2}^E\rangle = \frac{1}{2}(-|\mathbf{1}\rangle + 0|\mathbf{r}\rangle + |\mathbf{r}^2\rangle + |\mathbf{i}_1\rangle + 0|\mathbf{i}_3\rangle - |\mathbf{i}_3\rangle)$$

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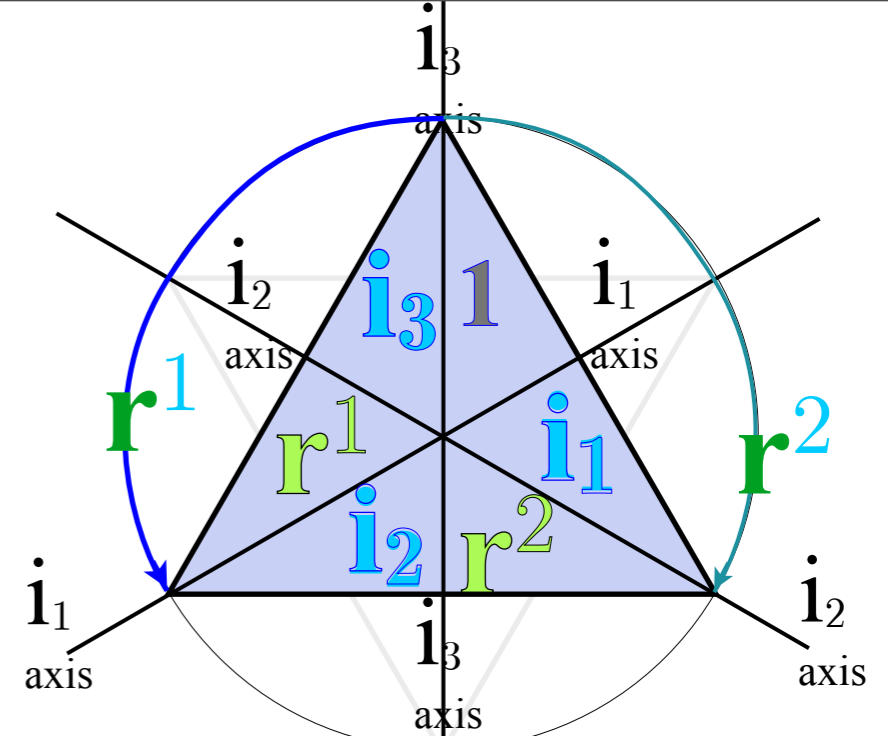
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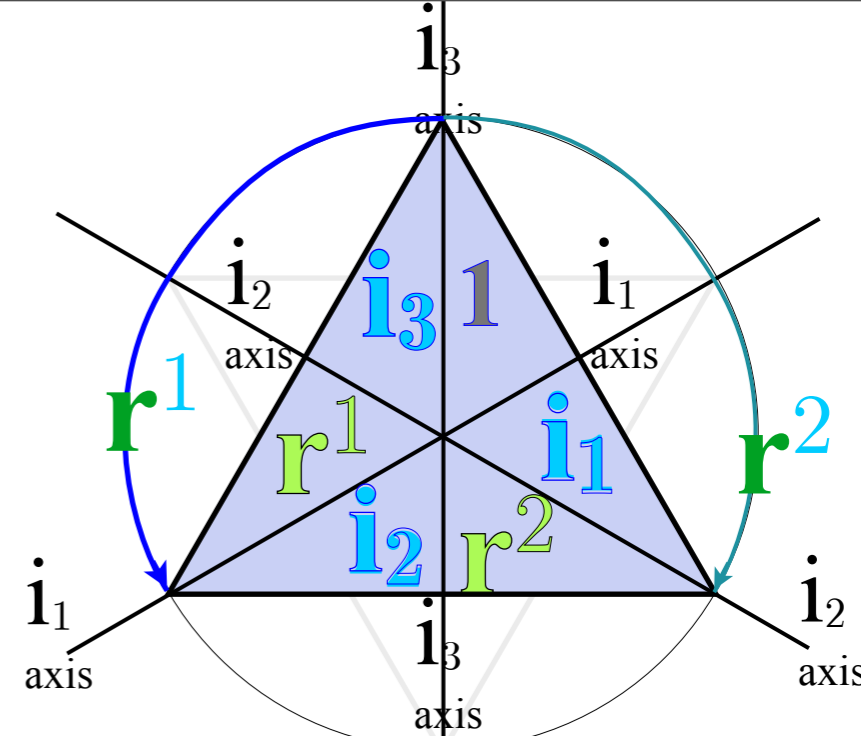
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The $D_{01} \pm$ sign was $(-)$.



$$\begin{pmatrix} & \mathbf{r} & +\mathbf{r}\mathbf{i}_3 \\ \mathbf{1} & \mathbf{r} & +\mathbf{r}\mathbf{i}_3 \\ -\mathbf{i}_3 & -\mathbf{i}_3\mathbf{r} & -\mathbf{i}_3\mathbf{r}\mathbf{i}_3 \end{pmatrix} = \frac{1}{4} \mathbf{P}^E \begin{pmatrix} & \mathbf{r} & +\mathbf{r}\mathbf{i}_3 \\ \mathbf{1} & \mathbf{r} & +\mathbf{i}_2 \\ -\mathbf{i}_3 & -\mathbf{i}_1 & -\mathbf{r}^2 \end{pmatrix}$$

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Review Coset factored splitting of $O \supset D_4 \supset C_4$ projectors and levels

Irreducible idempotent projectors $\mathbf{P}^\mu_{m,m}$ of $O \supset C_4 \sim T_d \supset C_{4i}$

Calculating \mathbf{P}^E_{0404} \mathbf{P}^E_{2424} $\mathbf{P}^{T_1}_{0404}$ $\mathbf{P}^{T_1}_{1414}$ $\mathbf{P}^{T_2}_{2424}$

Factoring out $O \supset C_4$ subgroup cosets:

Factoring \mathbf{P}^E_{0404} \mathbf{P}^E_{2424} $\mathbf{P}^{T_1}_{0404}$ $\mathbf{P}^{T_1}_{1414}$ $\mathbf{P}^{T_2}_{2424}$

Irreducible nilpotent projectors $\mathbf{P}^\mu_{m,n}$

Fundamental $\mathbf{P}^\mu_{m,n}$ definitions:

Review of $D_3 \supset C_2 \sim C_{3v} \supset C_v$

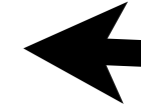
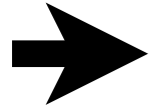
Calculating and Factoring $\mathbf{P}^{T_1}_{1404}$

Structure and applications of various subgroup chain ireps

$O_h \supset D_{4h} \supset C_{4v}$

$O_h \supset D_{3h} \supset C_{3v}$

$O_h \supset C_{2v}$



Coset-factored T_1 -sum:

$$\mathbf{P}_{1_4 1_4}^{T_1} = \frac{1}{8}[(1) \cdot \mathbf{1} \mathbf{p}_{1_4} + (0) \cdot \rho_x \mathbf{p}_{1_4} + (+\frac{i}{2}) \cdot \mathbf{r}_1 \mathbf{p}_{1_4} + (+\frac{i}{2}) \cdot \mathbf{r}_2 \mathbf{p}_{1_4} + (-\frac{i}{2}) \cdot \tilde{\mathbf{r}}_1 \mathbf{p}_{1_4} + (-\frac{i}{2}) \cdot \tilde{\mathbf{r}}_2 \mathbf{p}_{1_4}]$$

$$\mathbf{P}_{3_4 3_4}^{T_1} = \frac{1}{8}[(1) \cdot \mathbf{1} \mathbf{p}_{3_4} + (0) \cdot \rho_x \mathbf{p}_{3_4} + (-\frac{i}{2}) \cdot \mathbf{r}_1 \mathbf{p}_{3_4} + (-\frac{i}{2}) \cdot \mathbf{r}_2 \mathbf{p}_{3_4} + (+\frac{i}{2}) \cdot \tilde{\mathbf{r}}_1 \mathbf{p}_{3_4} + (+\frac{i}{2}) \cdot \tilde{\mathbf{r}}_2 \mathbf{p}_{3_4}]$$

$$\mathbf{P}_{0_4 0_4}^{T_1} = \frac{1}{8}[(1) \cdot \mathbf{1} \mathbf{p}_{0_4} + (-1) \cdot \rho_x \mathbf{p}_{0_4} + (0) \cdot \mathbf{r}_1 \mathbf{p}_{0_4} + (0) \cdot \mathbf{r}_2 \mathbf{p}_{0_4} + (0) \cdot \tilde{\mathbf{r}}_1 \mathbf{p}_{0_4} + (0) \cdot \tilde{\mathbf{r}}_2 \mathbf{p}_{0_4}]$$

Calculating: $\mathbf{P}_{1_4 1_4}^{T_1} \mathbf{r}_1 \mathbf{P}_{0_4 0_4}^{T_1} = D_{1_4 0_4}^{T_1} (\mathbf{r}_1) \mathbf{P}_{1_4 0_4}^{T_1} = \mathbf{P}_{1_4}^{T_1} \mathbf{p}_{1_4} \mathbf{r}_1 \mathbf{p}_{0_4}$

Coset-factored T_1 -sum:

$$\mathbf{P}^{T_1}_{1_4 1_4} = \frac{1}{8}[(1) \cdot \mathbf{1p}_{1_4} + (0) \cdot \rho_x \mathbf{p}_{1_4} + (+\frac{i}{2}) \cdot \mathbf{r}_1 \mathbf{p}_{1_4} + (+\frac{i}{2}) \cdot \mathbf{r}_2 \mathbf{p}_{1_4} + (-\frac{i}{2}) \cdot \tilde{\mathbf{r}}_1 \mathbf{p}_{1_4} + (-\frac{i}{2}) \cdot \tilde{\mathbf{r}}_2 \mathbf{p}_{1_4}]$$

$$\mathbf{P}^{T_1}_{3_4 3_4} = \frac{1}{8}[(1) \cdot \mathbf{1p}_{3_4} + (0) \cdot \rho_x \mathbf{p}_{3_4} + (-\frac{i}{2}) \cdot \mathbf{r}_1 \mathbf{p}_{3_4} + (-\frac{i}{2}) \cdot \mathbf{r}_2 \mathbf{p}_{3_4} + (+\frac{i}{2}) \cdot \tilde{\mathbf{r}}_1 \mathbf{p}_{3_4} + (+\frac{i}{2}) \cdot \tilde{\mathbf{r}}_2 \mathbf{p}_{3_4}]$$

$$\mathbf{P}^{T_1}_{0_4 0_4} = \frac{1}{8}[(1) \cdot \mathbf{1p}_{0_4} + (-1) \cdot \rho_x \mathbf{p}_{0_4} + (0) \cdot \mathbf{r}_1 \mathbf{p}_{0_4} + (0) \cdot \mathbf{r}_2 \mathbf{p}_{0_4} + (0) \cdot \tilde{\mathbf{r}}_1 \mathbf{p}_{0_4} + (0) \cdot \tilde{\mathbf{r}}_2 \mathbf{p}_{0_4}]$$

Calculating: $\mathbf{P}^{T_1}_{1_4 1_4} \mathbf{r}_1 \mathbf{P}^{T_1}_{0_4 0_4} = D^{T_1}_{1_4 0_4} (\mathbf{r}_1) \mathbf{P}^{T_1}_{1_4 0_4} = \mathbf{P}^{T_1} \mathbf{p}_{1_4} \mathbf{r}_1 \mathbf{p}_{0_4}$

Then find nilpotent proportional to: $\mathbf{p}_{1_4} \mathbf{r}_1 \mathbf{p}_{0_4}$

Coset-factored T_1 -sum:

$$\begin{aligned} \mathbf{P}_{1_4 1_4}^{T_1} &= \frac{1}{8}[(1) \cdot \mathbf{1} \mathbf{p}_{1_4} + (0) \cdot \rho_x \mathbf{p}_{1_4} + (+\frac{i}{2}) \cdot \mathbf{r}_1 \mathbf{p}_{1_4} + (+\frac{i}{2}) \cdot \mathbf{r}_2 \mathbf{p}_{1_4} + (-\frac{i}{2}) \cdot \tilde{\mathbf{r}}_1 \mathbf{p}_{1_4} + (-\frac{i}{2}) \cdot \tilde{\mathbf{r}}_2 \mathbf{p}_{1_4}] \\ \mathbf{P}_{3_4 3_4}^{T_1} &= \frac{1}{8}[(1) \cdot \mathbf{1} \mathbf{p}_{3_4} + (0) \cdot \rho_x \mathbf{p}_{3_4} + (-\frac{i}{2}) \cdot \mathbf{r}_1 \mathbf{p}_{3_4} + (-\frac{i}{2}) \cdot \mathbf{r}_2 \mathbf{p}_{3_4} + (+\frac{i}{2}) \cdot \tilde{\mathbf{r}}_1 \mathbf{p}_{3_4} + (+\frac{i}{2}) \cdot \tilde{\mathbf{r}}_2 \mathbf{p}_{3_4}] \\ \mathbf{P}_{0_4 0_4}^{T_1} &= \frac{1}{8}[(1) \cdot \mathbf{1} \mathbf{p}_{0_4} + (-1) \cdot \rho_x \mathbf{p}_{0_4} + (0) \cdot \mathbf{r}_1 \mathbf{p}_{0_4} + (0) \cdot \mathbf{r}_2 \mathbf{p}_{0_4} + (0) \cdot \tilde{\mathbf{r}}_1 \mathbf{p}_{0_4} + (0) \cdot \tilde{\mathbf{r}}_2 \mathbf{p}_{0_4}] \end{aligned}$$

Calculating: $\mathbf{P}_{1_4 1_4}^{T_1} \mathbf{r}_1 \mathbf{P}_{0_4 0_4}^{T_1} = D_{1_4 0_4}^{T_1} (\mathbf{r}_1) \mathbf{P}_{1_4 0_4}^{T_1} = \mathbf{P}_{1_4}^{T_1} \mathbf{p}_{1_4} \mathbf{r}_1 \mathbf{p}_{0_4}$

Then find nilpotent proportional to: $\mathbf{p}_{1_4} \mathbf{r}_1 \mathbf{p}_{0_4} =$

	\mathbf{r}_1	\mathbf{r}_4	\mathbf{i}_1	\mathbf{R}_y
$\mathbf{1}$	\mathbf{r}_1	\mathbf{r}_4	\mathbf{i}_1	\mathbf{R}_y
$-\rho_z$	$-\mathbf{r}_3$	$-\mathbf{r}_2$	$-\tilde{\mathbf{R}}_y$	$-\mathbf{i}_2$
$+i\mathbf{R}_z$	$+i\mathbf{i}_6$	$+i\tilde{\mathbf{R}}_x$	$+i\tilde{\mathbf{r}}_1$	$+i\tilde{\mathbf{r}}_3$
$-i\tilde{\mathbf{R}}_z$	$-i\mathbf{R}_x$	$-i\mathbf{i}_5$	$-i\tilde{\mathbf{r}}_4$	$-i\tilde{\mathbf{r}}_2$

Coset-factored T_1 -sum:

$$\begin{aligned} \mathbf{P}_{1_4 1_4}^{T_1} &= \frac{1}{8}[(1) \cdot \mathbf{1} \mathbf{p}_{1_4} + (0) \cdot \rho_x \mathbf{p}_{1_4} + (+\frac{i}{2}) \cdot \mathbf{r}_1 \mathbf{p}_{1_4} + (+\frac{i}{2}) \cdot \mathbf{r}_2 \mathbf{p}_{1_4} + (-\frac{i}{2}) \cdot \tilde{\mathbf{r}}_1 \mathbf{p}_{1_4} + (-\frac{i}{2}) \cdot \tilde{\mathbf{r}}_2 \mathbf{p}_{1_4}] \\ \mathbf{P}_{3_4 3_4}^{T_1} &= \frac{1}{8}[(1) \cdot \mathbf{1} \mathbf{p}_{3_4} + (0) \cdot \rho_x \mathbf{p}_{3_4} + (-\frac{i}{2}) \cdot \mathbf{r}_1 \mathbf{p}_{3_4} + (-\frac{i}{2}) \cdot \mathbf{r}_2 \mathbf{p}_{3_4} + (+\frac{i}{2}) \cdot \tilde{\mathbf{r}}_1 \mathbf{p}_{3_4} + (+\frac{i}{2}) \cdot \tilde{\mathbf{r}}_2 \mathbf{p}_{3_4}] \\ \mathbf{P}_{0_4 0_4}^{T_1} &= \frac{1}{8}[(1) \cdot \mathbf{1} \mathbf{p}_{0_4} + (-1) \cdot \rho_x \mathbf{p}_{0_4} + (0) \cdot \mathbf{r}_1 \mathbf{p}_{0_4} + (0) \cdot \mathbf{r}_2 \mathbf{p}_{0_4} + (0) \cdot \tilde{\mathbf{r}}_1 \mathbf{p}_{0_4} + (0) \cdot \tilde{\mathbf{r}}_2 \mathbf{p}_{0_4}] \end{aligned}$$

Calculating: $\mathbf{P}_{1_4 1_4}^{T_1} \mathbf{r}_1 \mathbf{P}_{0_4 0_4}^{T_1} = D_{1_4 0_4}^{T_1} (\mathbf{r}_1) \mathbf{P}_{1_4 0_4}^{T_1} = \mathbf{P}_{1_4}^{T_1} \mathbf{p}_{1_4} \mathbf{r}_1 \mathbf{p}_{0_4}$

Then find nilpotent proportional to: $\mathbf{p}_{1_4} \mathbf{r}_1 \mathbf{p}_{0_4} =$

	\mathbf{r}_1	\mathbf{r}_4	\mathbf{i}_1	\mathbf{R}_y
$\mathbf{1}$	\mathbf{r}_1	\mathbf{r}_4	\mathbf{i}_1	\mathbf{R}_y
$-\rho_z$	$-\mathbf{r}_3$	$-\mathbf{r}_2$	$-\tilde{\mathbf{R}}_y$	$-\mathbf{i}_2$
$+i\mathbf{R}_z$	$+i\mathbf{i}_6$	$+i\tilde{\mathbf{R}}_x$	$+i\tilde{\mathbf{r}}_1$	$+i\tilde{\mathbf{r}}_3$
$-i\tilde{\mathbf{R}}_z$	$-i\mathbf{R}_x$	$-i\mathbf{i}_5$	$-i\tilde{\mathbf{r}}_4$	$-i\tilde{\mathbf{r}}_2$

Coset-factored T_1 -sum:

$$\begin{aligned} \mathbf{P}_{1_4 1_4}^{T_1} &= \frac{1}{8}[(1) \cdot \mathbf{1} \mathbf{p}_{1_4} + (0) \cdot \rho_x \mathbf{p}_{1_4} + (+\frac{i}{2}) \cdot \mathbf{r}_1 \mathbf{p}_{1_4} + (+\frac{i}{2}) \cdot \mathbf{r}_2 \mathbf{p}_{1_4} + (-\frac{i}{2}) \cdot \tilde{\mathbf{r}}_1 \mathbf{p}_{1_4} + (-\frac{i}{2}) \cdot \tilde{\mathbf{r}}_2 \mathbf{p}_{1_4}] \\ \mathbf{P}_{3_4 3_4}^{T_1} &= \frac{1}{8}[(1) \cdot \mathbf{1} \mathbf{p}_{3_4} + (0) \cdot \rho_x \mathbf{p}_{3_4} + (-\frac{i}{2}) \cdot \mathbf{r}_1 \mathbf{p}_{3_4} + (-\frac{i}{2}) \cdot \mathbf{r}_2 \mathbf{p}_{3_4} + (+\frac{i}{2}) \cdot \tilde{\mathbf{r}}_1 \mathbf{p}_{3_4} + (+\frac{i}{2}) \cdot \tilde{\mathbf{r}}_2 \mathbf{p}_{3_4}] \\ \mathbf{P}_{0_4 0_4}^{T_1} &= \frac{1}{8}[(1) \cdot \mathbf{1} \mathbf{p}_{0_4} + (-1) \cdot \rho_x \mathbf{p}_{0_4} + (0) \cdot \mathbf{r}_1 \mathbf{p}_{0_4} + (0) \cdot \mathbf{r}_2 \mathbf{p}_{0_4} + (0) \cdot \tilde{\mathbf{r}}_1 \mathbf{p}_{0_4} + (0) \cdot \tilde{\mathbf{r}}_2 \mathbf{p}_{0_4}] \end{aligned}$$

Calculating: $\mathbf{P}_{1_4 1_4}^{T_1} \mathbf{r}_1 \mathbf{P}_{0_4 0_4}^{T_1} = D_{1_4 0_4}^{T_1} (\mathbf{r}_1) \mathbf{P}_{1_4 0_4}^{T_1} = \mathbf{P}_{1_4}^{T_1} \mathbf{p}_{1_4} \mathbf{r}_1 \mathbf{p}_{0_4}$

	\mathbf{r}_1	\mathbf{r}_4	\mathbf{i}_1	\mathbf{R}_y
$\mathbf{1}$	\mathbf{r}_1	\mathbf{r}_4	\mathbf{i}_1	\mathbf{R}_y
$-\rho_z$	$-\mathbf{r}_3$	$-\mathbf{r}_2$	$-\tilde{\mathbf{R}}_y$	$-\mathbf{i}_2$
$+i\mathbf{R}_z$	$+i\mathbf{i}_6$	$+i\tilde{\mathbf{R}}_x$	$+i\tilde{\mathbf{r}}_1$	$+i\tilde{\mathbf{r}}_3$
$-i\tilde{\mathbf{R}}_z$	$-i\mathbf{R}_x$	$-i\mathbf{i}_5$	$-i\tilde{\mathbf{r}}_4$	$-i\tilde{\mathbf{r}}_2$

$$\begin{aligned} &= (\mathbf{r}_1 + \mathbf{r}_4 + \mathbf{i}_1 + \mathbf{R}_y) - (\mathbf{r}_2 + \mathbf{r}_3 + \mathbf{i}_2 + \tilde{\mathbf{R}}_y) + i(\tilde{\mathbf{r}}_1 + \tilde{\mathbf{r}}_3 + \tilde{\mathbf{R}}_x + \mathbf{i}_6) - i(\tilde{\mathbf{r}}_2 + \tilde{\mathbf{r}}_4 + \mathbf{R}_x + \mathbf{i}_5) \\ &= \mathbf{r}_1 \mathbf{p}_{0_4} - \mathbf{r}_2 \mathbf{p}_{0_4} + i\tilde{\mathbf{r}}_1 \mathbf{p}_{0_4} - i\tilde{\mathbf{r}}_2 \mathbf{p}_{0_4} \end{aligned}$$

Coset-factored T_1 -sum:

$$\begin{aligned} \mathbf{P}_{1_4 1_4}^{T_1} &= \frac{1}{8}[(1) \cdot \mathbf{1p}_{1_4} + (0) \cdot \rho_x \mathbf{p}_{1_4} + (+\frac{i}{2}) \cdot \mathbf{r}_1 \mathbf{p}_{1_4} + (+\frac{i}{2}) \cdot \mathbf{r}_2 \mathbf{p}_{1_4} + (-\frac{i}{2}) \cdot \tilde{\mathbf{r}}_1 \mathbf{p}_{1_4} + (-\frac{i}{2}) \cdot \tilde{\mathbf{r}}_2 \mathbf{p}_{1_4}] \\ \mathbf{P}_{3_4 3_4}^{T_1} &= \frac{1}{8}[(1) \cdot \mathbf{1p}_{3_4} + (0) \cdot \rho_x \mathbf{p}_{3_4} + (-\frac{i}{2}) \cdot \mathbf{r}_1 \mathbf{p}_{3_4} + (-\frac{i}{2}) \cdot \mathbf{r}_2 \mathbf{p}_{3_4} + (+\frac{i}{2}) \cdot \tilde{\mathbf{r}}_1 \mathbf{p}_{3_4} + (+\frac{i}{2}) \cdot \tilde{\mathbf{r}}_2 \mathbf{p}_{3_4}] \\ \mathbf{P}_{0_4 0_4}^{T_1} &= \frac{1}{8}[(1) \cdot \mathbf{1p}_{0_4} + (-1) \cdot \rho_x \mathbf{p}_{0_4} + (0) \cdot \mathbf{r}_1 \mathbf{p}_{0_4} + (0) \cdot \mathbf{r}_2 \mathbf{p}_{0_4} + (0) \cdot \tilde{\mathbf{r}}_1 \mathbf{p}_{0_4} + (0) \cdot \tilde{\mathbf{r}}_2 \mathbf{p}_{0_4}] \end{aligned}$$

Calculating: $\mathbf{P}_{1_4 1_4}^{T_1} \mathbf{r}_1 \mathbf{P}_{0_4 0_4}^{T_1} = D_{1_4 0_4}^{T_1} (\mathbf{r}_1) \mathbf{P}_{1_4 0_4}^{T_1} = \mathbf{P}_{1_4}^{T_1} \mathbf{p}_{1_4} \mathbf{r}_1 \mathbf{p}_{0_4}$

	\mathbf{r}_1	\mathbf{r}_4	\mathbf{i}_1	\mathbf{R}_y
$\mathbf{1}$	\mathbf{r}_1	\mathbf{r}_4	\mathbf{i}_1	\mathbf{R}_y
$-\rho_z$	$-\mathbf{r}_3$	$-\mathbf{r}_2$	$-\tilde{\mathbf{R}}_y$	$-\mathbf{i}_2$
$+i\mathbf{R}_z$	$+i\mathbf{i}_6$	$+i\tilde{\mathbf{R}}_x$	$+i\tilde{\mathbf{r}}_1$	$+i\tilde{\mathbf{r}}_3$
$-i\tilde{\mathbf{R}}_z$	$-i\mathbf{R}_x$	$-i\mathbf{i}_5$	$-i\tilde{\mathbf{r}}_4$	$-i\tilde{\mathbf{r}}_2$

Then find nilpotent proportional to: $\mathbf{p}_{1_4} \mathbf{r}_1 \mathbf{p}_{0_4} =$

$$\begin{aligned} &= (\mathbf{r}_1 + \mathbf{r}_4 + \mathbf{i}_1 + \mathbf{R}_y) - (\mathbf{r}_2 + \mathbf{r}_3 + \mathbf{i}_2 + \tilde{\mathbf{R}}_y) + i(\tilde{\mathbf{r}}_1 + \tilde{\mathbf{r}}_3 + \tilde{\mathbf{R}}_x + \mathbf{i}_6) - i(\tilde{\mathbf{r}}_2 + \tilde{\mathbf{r}}_4 + \mathbf{R}_x + \mathbf{i}_5) \\ &= \mathbf{r}_1 \mathbf{p}_{0_4} - \mathbf{r}_2 \mathbf{p}_{0_4} + i\tilde{\mathbf{r}}_1 \mathbf{p}_{0_4} - i\tilde{\mathbf{r}}_2 \mathbf{p}_{0_4} \end{aligned}$$

Result is nicely factored:

$$\mathbf{P}_{1_4 0_4}^{T_1} = \mathbf{P}_{1_4}^{T_1} \mathbf{p}_{1_4} \mathbf{r}_1 \mathbf{p}_{0_4} \sim (?) \cdot (\mathbf{r}_1 \mathbf{p}_{0_4} - \mathbf{r}_2 \mathbf{p}_{0_4} + i\tilde{\mathbf{r}}_1 \mathbf{p}_{0_4} - i\tilde{\mathbf{r}}_2 \mathbf{p}_{0_4})$$

Coset-factored T_1 -sum:

$$\begin{aligned} \mathbf{P}_{1_4 1_4}^{T_1} &= \frac{1}{8}[(1) \cdot \mathbf{1p}_{1_4} + (0) \cdot \rho_x \mathbf{p}_{1_4} + (+\frac{i}{2}) \cdot \mathbf{r}_1 \mathbf{p}_{1_4} + (+\frac{i}{2}) \cdot \mathbf{r}_2 \mathbf{p}_{1_4} + (-\frac{i}{2}) \cdot \tilde{\mathbf{r}}_1 \mathbf{p}_{1_4} + (-\frac{i}{2}) \cdot \tilde{\mathbf{r}}_2 \mathbf{p}_{1_4}] \\ \mathbf{P}_{3_4 3_4}^{T_1} &= \frac{1}{8}[(1) \cdot \mathbf{1p}_{3_4} + (0) \cdot \rho_x \mathbf{p}_{3_4} + (-\frac{i}{2}) \cdot \mathbf{r}_1 \mathbf{p}_{3_4} + (-\frac{i}{2}) \cdot \mathbf{r}_2 \mathbf{p}_{3_4} + (+\frac{i}{2}) \cdot \tilde{\mathbf{r}}_1 \mathbf{p}_{3_4} + (+\frac{i}{2}) \cdot \tilde{\mathbf{r}}_2 \mathbf{p}_{3_4}] \\ \mathbf{P}_{0_4 0_4}^{T_1} &= \frac{1}{8}[(1) \cdot \mathbf{1p}_{0_4} + (-1) \cdot \rho_x \mathbf{p}_{0_4} + (0) \cdot \mathbf{r}_1 \mathbf{p}_{0_4} + (0) \cdot \mathbf{r}_2 \mathbf{p}_{0_4} + (0) \cdot \tilde{\mathbf{r}}_1 \mathbf{p}_{0_4} + (0) \cdot \tilde{\mathbf{r}}_2 \mathbf{p}_{0_4}] \end{aligned}$$

Calculating: $\mathbf{P}_{1_4 1_4}^{T_1} \mathbf{r}_1 \mathbf{P}_{3_4 3_4}^{T_1} = D_{1_4 3_4}^{T_1} (\mathbf{r}_1) \mathbf{P}_{1_4 3_4}^{T_1} = \mathbf{P}^{T_1} \mathbf{p}_{1_4} \mathbf{r}_1 \mathbf{p}_{3_4}$

	\mathbf{r}_1	$-\mathbf{r}_4$	$-i\mathbf{i}_1$	$+i\mathbf{R}_y$
$\mathbf{1}$	\mathbf{r}_1	$-\mathbf{r}_4$	$-i\mathbf{i}_1$	$+i\mathbf{R}_y$
$-\rho_z$	$-\mathbf{r}_3$	$+\mathbf{r}_2$	$+i\tilde{\mathbf{R}}_y$	$-i\mathbf{i}_2$
$+i\mathbf{R}_z$	$+i\mathbf{i}_6$	$-i\tilde{\mathbf{R}}_x$	$+\tilde{\mathbf{r}}_1$	$-\tilde{\mathbf{r}}_3$
$-i\tilde{\mathbf{R}}_z$	$-i\mathbf{R}_x$	$+i\mathbf{i}_5$	$-\tilde{\mathbf{r}}_4$	$+\tilde{\mathbf{r}}_2$

$= (\mathbf{r}_1 - \mathbf{r}_4 - i\mathbf{i}_1 + i\mathbf{R}_y) + (\mathbf{r}_2 - \mathbf{r}_3 - i\mathbf{i}_2 + i\tilde{\mathbf{R}}_y) + (\tilde{\mathbf{r}}_1 - \tilde{\mathbf{r}}_3 - i\tilde{\mathbf{R}}_x + i\mathbf{i}_6) + (\tilde{\mathbf{r}}_2 - \tilde{\mathbf{r}}_4 - i\mathbf{R}_x + i\mathbf{i}_5)$
 $= \mathbf{r}_1 \mathbf{p}_{3_4} + \mathbf{r}_2 \mathbf{p}_{3_4} + \tilde{\mathbf{r}}_1 \mathbf{p}_{3_4} + \tilde{\mathbf{r}}_2 \mathbf{p}_{3_4}$

Result is nicely factored:

$$\mathbf{P}_{1_4 3_4}^{T_1} = \mathbf{P}^{T_1} \mathbf{p}_{1_4} \mathbf{r}_1 \mathbf{p}_{3_4} \sim (?) \cdot (\mathbf{r}_1 \mathbf{p}_{3_4} + \mathbf{r}_2 \mathbf{p}_{3_4} + \tilde{\mathbf{r}}_1 \mathbf{p}_{3_4} + \tilde{\mathbf{r}}_2 \mathbf{p}_{3_4})$$

Review Coset factored splitting of $O \supset D_4 \supset C_4$ projectors and levels

Irreducible idempotent projectors $P^{\mu}_{m,m}$ of $O \supset C_4 \sim T_d \supset C_{4i}$

Calculating $P^{E_{0404}}$ $P^{E_{2424}}$ $P^{T_1_{0404}}$ $P^{T_1_{1414}}$ $P^{T_2_{2424}}$

Factoring out $O \supset C_4$ subgroup cosets:

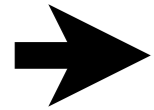
Factoring $P^{E_{0404}}$ $P^{E_{2424}}$ $P^{T_1_{0404}}$ $P^{T_1_{1414}}$ $P^{T_2_{2424}}$

Irreducible nilpotent projectors $P^{\mu}_{m,n}$

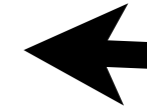
Fundamental $P^{\mu}_{m,n}$ definitions:

Review of $D_3 \supset C_2 \sim C_{3v} \supset C_v$

Calculating and Factoring $P^{T_1_{1404}}$



Structure and applications of various subgroup chain ireps



$O_h \supset D_{4h} \supset C_{4v}$

$O_h \supset D_{3h} \supset C_{3v}$

$O_h \supset C_{2v}$

Ireps for $O \supset D_4 \supset C_4$ subgroup chain

(a) Vector T_1 Representation

$\mathcal{D}^{T_1}(1) =$ $\begin{pmatrix} 1 & & \\ & 1 & \\ & & 1 \end{pmatrix}$	$R_1^2 =$ $\begin{pmatrix} & -1 & \\ -1 & & \\ & & -1 \end{pmatrix}$	$r_1 =$ $\begin{pmatrix} -i & i & -1 \\ 2 & 2 & \sqrt{2} \end{pmatrix}$	$r_2 =$ $\begin{pmatrix} -i & i & 1 \\ 2 & 2 & \sqrt{2} \end{pmatrix}$	$r_1^2 =$ $\begin{pmatrix} i & i & i \\ 2 & 2 & \sqrt{2} \end{pmatrix}$	$r_2^2 =$ $\begin{pmatrix} i & i & -i \\ 2 & 2 & \sqrt{2} \end{pmatrix}$	T₁ Vector x, y, z
$\mathcal{D}^{T_1}(R_3^2) =$ $\begin{pmatrix} -1 & & \\ & -1 & \\ & & 1 \end{pmatrix}$	$R_2^2 =$ $\begin{pmatrix} & 1 & \\ 1 & & \\ & & -1 \end{pmatrix}$	$r_4 =$ $\begin{pmatrix} i & -i & -1 \\ 2 & 2 & \sqrt{2} \end{pmatrix}$	$r_3 =$ $\begin{pmatrix} i & -i & 1 \\ 2 & 2 & \sqrt{2} \end{pmatrix}$	$r_3^2 =$ $\begin{pmatrix} -i & -i & i \\ 2 & 2 & \sqrt{2} \end{pmatrix}$	$r_4^2 =$ $\begin{pmatrix} -i & -i & -i \\ 2 & 2 & \sqrt{2} \end{pmatrix}$	
$\mathcal{D}^{T_1}(R_3) =$ $\begin{pmatrix} -i & & \\ & i & \\ & & 1 \end{pmatrix}$	$i_4 =$ $\begin{pmatrix} & -i & \\ i & & \\ & & -1 \end{pmatrix}$	$i_1 =$ $\begin{pmatrix} -1 & -1 & -1 \\ 2 & 2 & \sqrt{2} \end{pmatrix}$	$i_2 =$ $\begin{pmatrix} -1 & -1 & 1 \\ 2 & 2 & \sqrt{2} \end{pmatrix}$	$R_1^3 =$ $\begin{pmatrix} 1 & -1 & i \\ 2 & 2 & \sqrt{2} \end{pmatrix}$	$R_1 =$ $\begin{pmatrix} 1 & -1 & -i \\ 2 & 2 & \sqrt{2} \end{pmatrix}$	
$\mathcal{D}^{T_1}(R_3^3) =$ $\begin{pmatrix} i & & \\ & -i & \\ & & 1 \end{pmatrix}$	$i_3 =$ $\begin{pmatrix} & i & \\ -i & & \\ & & -1 \end{pmatrix}$	$R_2 =$ $\begin{pmatrix} 1 & 1 & -1 \\ 2 & 2 & \sqrt{2} \end{pmatrix}$	$R_2^3 =$ $\begin{pmatrix} 1 & 1 & 1 \\ 2 & 2 & \sqrt{2} \end{pmatrix}$	$i_6 =$ $\begin{pmatrix} -1 & 1 & i \\ 2 & 2 & \sqrt{2} \end{pmatrix}$	$i_5 =$ $\begin{pmatrix} -1 & 1 & -i \\ 2 & 2 & \sqrt{2} \end{pmatrix}$	basis $O: \begin{pmatrix} T_1 \\ D_4: E \\ C_4: 1_4 \end{pmatrix} \left \begin{pmatrix} T_1 \\ E \\ 3_4 \end{pmatrix} \right \begin{pmatrix} T_1 \\ A_2 \\ 0_4 \end{pmatrix} \right\rangle$

(b) Tensor T_2 Representation

$\mathcal{D}^{T_2}(1) =$ $\begin{pmatrix} 1 & & \\ & 1 & \\ & & 1 \end{pmatrix}$	$R_1^2 =$ $\begin{pmatrix} & -1 & \\ -1 & & \\ & & -1 \end{pmatrix}$	$r_1 =$ $\begin{pmatrix} i & -i & -1 \\ 2 & 2 & \sqrt{2} \end{pmatrix}$	$r_2 =$ $\begin{pmatrix} i & -i & 1 \\ 2 & 2 & \sqrt{2} \end{pmatrix}$	$r_1^2 =$ $\begin{pmatrix} -i & -i & -i \\ 2 & 2 & \sqrt{2} \end{pmatrix}$	$r_2^2 =$ $\begin{pmatrix} -i & -i & i \\ 2 & 2 & \sqrt{2} \end{pmatrix}$	T₂ Tensor yz, xz, xy
$\mathcal{D}^{T_2}(R_3^2) =$ $\begin{pmatrix} -1 & & \\ & -1 & \\ & & 1 \end{pmatrix}$	$R_2^2 =$ $\begin{pmatrix} & 1 & \\ 1 & & \\ & & -1 \end{pmatrix}$	$r_4 =$ $\begin{pmatrix} -i & i & -1 \\ 2 & 2 & \sqrt{2} \end{pmatrix}$	$r_3 =$ $\begin{pmatrix} -i & i & 1 \\ 2 & 2 & \sqrt{2} \end{pmatrix}$	$r_3^2 =$ $\begin{pmatrix} i & i & -i \\ 2 & 2 & \sqrt{2} \end{pmatrix}$	$r_4^2 =$ $\begin{pmatrix} i & i & i \\ 2 & 2 & \sqrt{2} \end{pmatrix}$	
$\mathcal{D}^{T_2}(R_3) =$ $\begin{pmatrix} -i & & \\ & i & \\ & & 1 \end{pmatrix}$	$i_4 =$ $\begin{pmatrix} & -i & \\ i & & \\ & & -1 \end{pmatrix}$	$i_1 =$ $\begin{pmatrix} 1 & 1 & 1 \\ 2 & 2 & \sqrt{2} \end{pmatrix}$	$i_2 =$ $\begin{pmatrix} 1 & 1 & -1 \\ 2 & 2 & \sqrt{2} \end{pmatrix}$	$R_1^3 =$ $\begin{pmatrix} -1 & 1 & i \\ 2 & 2 & \sqrt{2} \end{pmatrix}$	$R_1 =$ $\begin{pmatrix} -1 & 1 & -i \\ 2 & 2 & \sqrt{2} \end{pmatrix}$	
$\mathcal{D}^{T_2}(R_3^3) =$ $\begin{pmatrix} i & & \\ & -i & \\ & & 1 \end{pmatrix}$	$i_3 =$ $\begin{pmatrix} & i & \\ -i & & \\ & & -1 \end{pmatrix}$	$R_2 =$ $\begin{pmatrix} -1 & -1 & 1 \\ 2 & 2 & \sqrt{2} \end{pmatrix}$	$R_2^3 =$ $\begin{pmatrix} -1 & -1 & -1 \\ 2 & 2 & \sqrt{2} \end{pmatrix}$	$i_6 =$ $\begin{pmatrix} 1 & -1 & i \\ 2 & 2 & \sqrt{2} \end{pmatrix}$	$i_5 =$ $\begin{pmatrix} 1 & -1 & -i \\ 2 & 2 & \sqrt{2} \end{pmatrix}$	basis $O: \begin{pmatrix} T_2 \\ D_4: E \\ C_4: 1_4 \end{pmatrix} \left \begin{pmatrix} T_2 \\ E \\ 3_4 \end{pmatrix} \right \begin{pmatrix} T_2 \\ B_2 \\ 2_4 \end{pmatrix} \right\rangle$

$1 = [1][2][3][4]$	$R_1^2 = [13][24]$	$r_1 = [132]$	$r_2 = [124]$	$r_1^2 = [123]$	$r_2^2 = [142]$
$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ +\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ +\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & +\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & +\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$
$R_3^2 = [12][34]$	$R_2^2 = [14][23]$	$r_4 = [234]$	$r_3 = [124]$	$r_3^2 = [134]$	$r_4^2 = [243]$
$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ +\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ +\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & +\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & +\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$
$R_3 = [1423]$	$i_4 = [12]$	$i_1 = [14]$	$i_2 = [23]$	$R_1^3 = [1432]$	$R_1 = [1234]$
$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & +\frac{\sqrt{3}}{2} \\ +\frac{\sqrt{3}}{2} & +\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & +\frac{\sqrt{3}}{2} \\ +\frac{\sqrt{3}}{2} & +\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & +\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & +\frac{1}{2} \end{pmatrix}$
$R_3^3 = [1324]$	$i_3 = [34]$	$R_2 = [1243]$	$R_2^3 = [1342]$	$i_6 = [24]$	$i_5 = [13]$
$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & +\frac{\sqrt{3}}{2} \\ +\frac{\sqrt{3}}{2} & +\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & +\frac{\sqrt{3}}{2} \\ +\frac{\sqrt{3}}{2} & +\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & +\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & +\frac{1}{2} \end{pmatrix}$

E
Tensor
 $x^2 + y^2 - 2z^2$
 $(x^2 - y^2)\sqrt{3}$

basis: $O: \begin{pmatrix} E \\ D_4: A_1 \\ C_4: 0_4 \end{pmatrix} \left| \begin{pmatrix} E \\ B_1 \\ 2_4 \end{pmatrix} \right\rangle$

$O: \chi_g^\mu$	$g=1$	r_{1-4} \tilde{r}_{1-4}	ρ_{xyz} \tilde{R}_{xyz}	R_{xyz} \tilde{R}_{xyz}	i_{1-6}
$\mu=A_1$	1	1	1	1	1
A_2	1	1	1	-1	-1
E	2	-1	2	0	0
T_1	3	0	-1	1	-1
T_2	3	0	-1	-1	1

Ireps for $O \supset D_3 \supset C_2$ subgroup chain

$$\mathcal{D}^{T_1(1)} = \quad i_4 = [12]$$

$$C_2 \quad \begin{vmatrix} 1 & & \\ & 1 & \\ & & -1 \end{vmatrix}$$

$$r_1 = [132] \quad i_5 = [13]$$

$$\begin{vmatrix} -1 & -\sqrt{3} & \\ 2 & 2 & \\ \sqrt{3} & -1 & \\ & & 1 \end{vmatrix} \quad \begin{vmatrix} -1 & -\sqrt{3} & \\ 2 & 2 & \\ -\sqrt{3} & 1 & \\ & & -1 \end{vmatrix}$$

$$r_1^2 = [123] \quad i_2 = [23]$$

$$\begin{vmatrix} -1 & \sqrt{3} & \\ 2 & 2 & \\ -\sqrt{3} & -1 & \\ & & 1 \end{vmatrix} \quad \begin{vmatrix} -1 & \sqrt{3} & \\ 2 & 2 & \\ \sqrt{3} & 1 & \\ & & -1 \end{vmatrix}$$

$$R_1^2 = [13][24] \quad R_3 = [1423]$$

$$\begin{vmatrix} & \sqrt{3} & \sqrt{6} \\ & 3 & 3 \\ \sqrt{3} & -2 & \sqrt{2} \\ 3 & 3 & 3 \\ \sqrt{6} & \sqrt{2} & -1 \\ 3 & 3 & 3 \end{vmatrix} \quad \begin{vmatrix} & -\sqrt{3} & -\sqrt{6} \\ & 3 & 3 \\ \sqrt{3} & 2 & -\sqrt{2} \\ 3 & 3 & 3 \\ \sqrt{6} & -\sqrt{2} & 1 \\ 3 & 3 & 3 \end{vmatrix}$$

$$r_4 = [234] \quad i_6 = [24]$$

$$\begin{vmatrix} 1 & -\sqrt{3} & \sqrt{6} \\ 2 & 6 & 3 \\ -\sqrt{3} & -1 & \sqrt{2} \\ 2 & 6 & 3 \\ & -\sqrt{8} & -1 \\ 3 & 3 & 3 \end{vmatrix} \quad \begin{vmatrix} -1 & \sqrt{3} & -\sqrt{6} \\ 2 & 6 & 3 \\ \sqrt{3} & -5 & -\sqrt{2} \\ 6 & 6 & 3 \\ -\sqrt{6} & -\sqrt{2} & 1 \\ 3 & 3 & 3 \end{vmatrix}$$

$$r_2^2 = [142] \quad R_2^3 = [1342]$$

$$\begin{vmatrix} -1 & -\sqrt{3} & \sqrt{6} \\ 2 & 6 & 3 \\ \sqrt{3} & 5 & \sqrt{2} \\ 6 & 6 & 3 \\ -\sqrt{6} & \sqrt{2} & -1 \\ 3 & 3 & 3 \end{vmatrix} \quad \begin{vmatrix} 1 & \sqrt{3} & -\sqrt{6} \\ 2 & 6 & 3 \\ -\sqrt{3} & 1 & -\sqrt{2} \\ 2 & 6 & 3 \\ & \sqrt{8} & 1 \\ 3 & 3 & 3 \end{vmatrix}$$

$$R_2^2 = [14][23] \quad R_3^3 = [1324]$$

$$\begin{vmatrix} & -\sqrt{3} & -\sqrt{6} \\ & 3 & 3 \\ -\sqrt{3} & -2 & \sqrt{2} \\ 3 & 3 & 3 \\ -\sqrt{6} & \sqrt{2} & -1 \\ 3 & 3 & 3 \end{vmatrix} \quad \begin{vmatrix} & \sqrt{3} & \sqrt{6} \\ & 3 & 3 \\ -\sqrt{3} & 2 & -\sqrt{2} \\ 3 & 3 & 3 \\ -\sqrt{6} & -\sqrt{2} & 1 \\ 3 & 3 & 3 \end{vmatrix}$$

$$r_2 = [124] \quad R_1 = [1234]$$

$$\begin{vmatrix} -1 & \sqrt{3} & -\sqrt{6} \\ 2 & 6 & 3 \\ -\sqrt{3} & 5 & \sqrt{2} \\ 6 & 6 & 3 \\ \sqrt{6} & \sqrt{2} & -1 \\ 3 & 3 & 3 \end{vmatrix} \quad \begin{vmatrix} 1 & -\sqrt{3} & \sqrt{6} \\ 2 & 6 & 3 \\ \sqrt{3} & 1 & -\sqrt{2} \\ 2 & 6 & 3 \\ & \sqrt{8} & 1 \\ 3 & 3 & 3 \end{vmatrix}$$

$$r_3^2 = [134] \quad i_1 = [14]$$

$$\begin{vmatrix} 1 & \sqrt{3} & -\sqrt{6} \\ 2 & 6 & 3 \\ \sqrt{3} & -1 & \sqrt{2} \\ 2 & 6 & 3 \\ & -\sqrt{8} & -1 \\ 3 & 3 & 3 \end{vmatrix} \quad \begin{vmatrix} -1 & -\sqrt{3} & \sqrt{6} \\ 2 & 6 & 3 \\ -\sqrt{3} & -5 & -\sqrt{2} \\ 6 & 6 & 3 \\ \sqrt{6} & -\sqrt{2} & 1 \\ 3 & 3 & 3 \end{vmatrix}$$

$$R_2^3 = [12][34] \quad i_3 = [34]$$

$$\begin{vmatrix} -1 & & \\ & 1 & -\sqrt{8} \\ & 3 & 3 \\ & -\sqrt{8} & -1 \\ & 3 & 3 \end{vmatrix} \quad \begin{vmatrix} -1 & & \\ & -1 & \sqrt{8} \\ & 3 & 3 \\ & \sqrt{8} & 1 \\ & 3 & 3 \end{vmatrix}$$

$$r_3 = [143] \quad R_1^3 = [1432]$$

$$\begin{vmatrix} 1 & \sqrt{3} & \\ 2 & 6 & \\ \sqrt{3} & -1 & -\sqrt{8} \\ 6 & 6 & 3 \\ -\sqrt{6} & \sqrt{2} & -1 \\ 3 & 3 & 3 \end{vmatrix} \quad \begin{vmatrix} 1 & \sqrt{3} & \\ 2 & 6 & \\ -\sqrt{3} & 1 & \sqrt{8} \\ 6 & 6 & 3 \\ \sqrt{6} & -\sqrt{2} & 1 \\ 3 & 3 & 3 \end{vmatrix}$$

$$r_4^2 = [243] \quad R_2 = [1243]$$

$$\begin{vmatrix} 1 & -\sqrt{3} & \\ 2 & 6 & \\ -\sqrt{3} & -1 & -\sqrt{8} \\ 6 & 6 & 3 \\ \sqrt{6} & \sqrt{2} & -1 \\ 3 & 3 & 3 \end{vmatrix} \quad \begin{vmatrix} 1 & -\sqrt{3} & \\ 2 & 6 & \\ \sqrt{3} & 1 & \sqrt{8} \\ 6 & 6 & 3 \\ -\sqrt{6} & -\sqrt{2} & 1 \\ 3 & 3 & 3 \end{vmatrix}$$

T₁ Vector
u, v, w

$$\text{basis: } \begin{matrix} O \\ D_3 \\ C_2 \end{matrix} \left| \begin{matrix} T_1 \\ E \\ O_2 \end{matrix} \right\rangle \left| \begin{matrix} T_1 \\ E \\ I_2 \end{matrix} \right\rangle \left| \begin{matrix} T_1 \\ A_2 \\ I_2 \end{matrix} \right\rangle$$

$$\mathcal{D}^{T_2(1)} = \quad i_4 = [12]$$

$$\begin{vmatrix} 1 & & \\ & 1 & \\ & & -1 \end{vmatrix}$$

$$r_1 = [132] \quad i_5 = [13]$$

$$\begin{vmatrix} 1 & & \\ & -1 & -\sqrt{3} \\ & 2 & 2 \\ \sqrt{3} & -1 & \\ & & 1 \end{vmatrix} \quad \begin{vmatrix} 1 & & \\ & -1 & -\sqrt{3} \\ & 2 & 2 \\ -\sqrt{3} & 1 & \\ & & 1 \end{vmatrix}$$

$$r_1^2 = [123] \quad i_2 = [23]$$

$$\begin{vmatrix} 1 & & \\ & -1 & \sqrt{3} \\ & 2 & 2 \\ -\sqrt{3} & -1 & \\ & & 1 \end{vmatrix} \quad \begin{vmatrix} 1 & & \\ & -1 & \sqrt{3} \\ & 2 & 2 \\ \sqrt{3} & 1 & \\ & & 1 \end{vmatrix}$$

$$R_2^2 = [14][23] \quad R_3^3 = [1324]$$

$$\begin{vmatrix} -1 & -\sqrt{2} & -\sqrt{6} \\ 3 & 3 & 3 \\ -\sqrt{2} & -2 & \sqrt{3} \\ 3 & 3 & 3 \\ -\sqrt{6} & \sqrt{3} & \\ 3 & 3 & 3 \end{vmatrix} \quad \begin{vmatrix} -1 & -\sqrt{2} & \sqrt{6} \\ 3 & 3 & 3 \\ -\sqrt{2} & -2 & \sqrt{3} \\ 3 & 3 & 3 \\ -\sqrt{6} & \sqrt{3} & \\ 3 & 3 & 3 \end{vmatrix}$$

$$r_2 = [124] \quad R_1 = [1234]$$

$$\begin{vmatrix} -1 & -\sqrt{2} & \sqrt{6} \\ 3 & 3 & 3 \\ -\sqrt{2} & 5 & \sqrt{3} \\ 6 & 6 & 6 \\ -\sqrt{6} & -\sqrt{3} & -1 \\ 3 & 6 & 2 \end{vmatrix} \quad \begin{vmatrix} -1 & \sqrt{8} & \\ 3 & 3 & \\ -\sqrt{2} & -1 & \sqrt{3} \\ 3 & 6 & 2 \\ -\sqrt{6} & -\sqrt{3} & -1 \\ 3 & 6 & 2 \end{vmatrix}$$

$$r_3^2 = [134] \quad i_1 = [14]$$

$$\begin{vmatrix} -1 & \sqrt{8} & \\ 3 & 3 & \\ -\sqrt{2} & -1 & -\sqrt{3} \\ 3 & 6 & 2 \\ -\sqrt{6} & -\sqrt{3} & 1 \\ 3 & 6 & 2 \end{vmatrix} \quad \begin{vmatrix} -1 & -\sqrt{2} & -\sqrt{6} \\ 3 & 3 & 3 \\ -\sqrt{2} & 5 & -\sqrt{3} \\ 3 & 6 & 6 \\ -\sqrt{6} & -\sqrt{3} & 1 \\ 3 & 6 & 2 \end{vmatrix}$$

T₂ Tensor
vw, uw, uv

$$\text{basis: } \begin{matrix} O \\ D_3 \\ C_2 \end{matrix} \left| \begin{matrix} T_2 \\ B_2 \\ O_2 \end{matrix} \right\rangle \left| \begin{matrix} T_2 \\ E \\ O_2 \end{matrix} \right\rangle \left| \begin{matrix} T_2 \\ E \\ I_2 \end{matrix} \right\rangle$$

$$\mathcal{D}^{E(1)} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad C_2 \quad \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad i_4 = [12]$$

$$r_1 = [132] \quad i_5 = [13] \\ \begin{pmatrix} -1 & -\sqrt{3} \\ 2 & 2 \end{pmatrix} \quad \begin{pmatrix} -1 & -\sqrt{3} \\ 2 & 2 \end{pmatrix}$$

$$r_1^2 = [123] \quad i_2 = [23] \\ \begin{pmatrix} -1 & \sqrt{3} \\ 2 & 2 \end{pmatrix} \quad \begin{pmatrix} -1 & \sqrt{3} \\ 2 & 2 \end{pmatrix}$$

$$R_2^2 = [14][23] \quad R_3^3 = [1324] \\ \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$r_2 = [124] \quad R_1 = [1234] \\ \begin{pmatrix} -1 & -\sqrt{3} \\ 2 & 2 \end{pmatrix} \quad \begin{pmatrix} -1 & -\sqrt{3} \\ 2 & 2 \end{pmatrix}$$

$$r_3^2 = [134] \quad i_1 = [14] \\ \begin{pmatrix} -1 & \sqrt{3} \\ 2 & 2 \end{pmatrix} \quad \begin{pmatrix} -1 & \sqrt{3} \\ 2 & 2 \end{pmatrix}$$

$$R_1^2 = [13][24] \quad R_3 = [1423] \\ \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$r_4 = [234] \quad i_6 = [24] \\ \begin{pmatrix} -1 & -\sqrt{3} \\ 2 & 2 \end{pmatrix} \quad \begin{pmatrix} -1 & -\sqrt{3} \\ 2 & 2 \end{pmatrix}$$

$$r_2^2 = [142] \quad R_2^3 = [1342] \\ \begin{pmatrix} -1 & \sqrt{3} \\ 2 & 2 \end{pmatrix} \quad \begin{pmatrix} -1 & \sqrt{3} \\ 2 & 2 \end{pmatrix}$$

$$R_3^2 = [12][34] \quad i_3 = [34] \\ \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

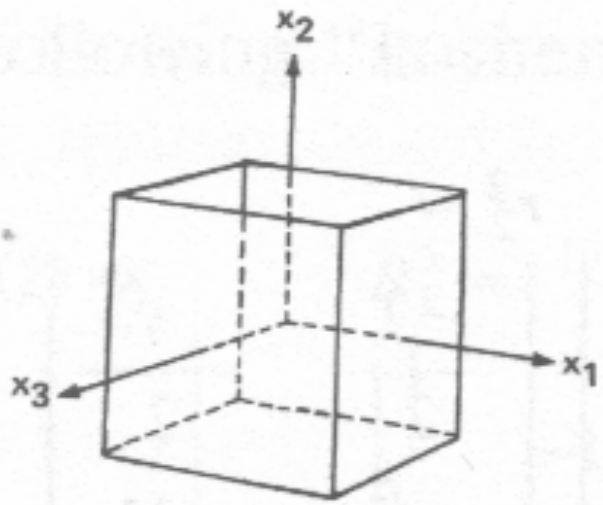
$$r_3 = [143] \quad R_1^3 = [1432] \\ \begin{pmatrix} -1 & -\sqrt{3} \\ 2 & 2 \end{pmatrix} \quad \begin{pmatrix} -1 & -\sqrt{3} \\ 2 & 2 \end{pmatrix}$$

$$r_4^2 = [243] \quad R_2 = [1243] \\ \begin{pmatrix} -1 & \sqrt{3} \\ 2 & 2 \end{pmatrix} \quad \begin{pmatrix} -1 & \sqrt{3} \\ 2 & 2 \end{pmatrix}$$

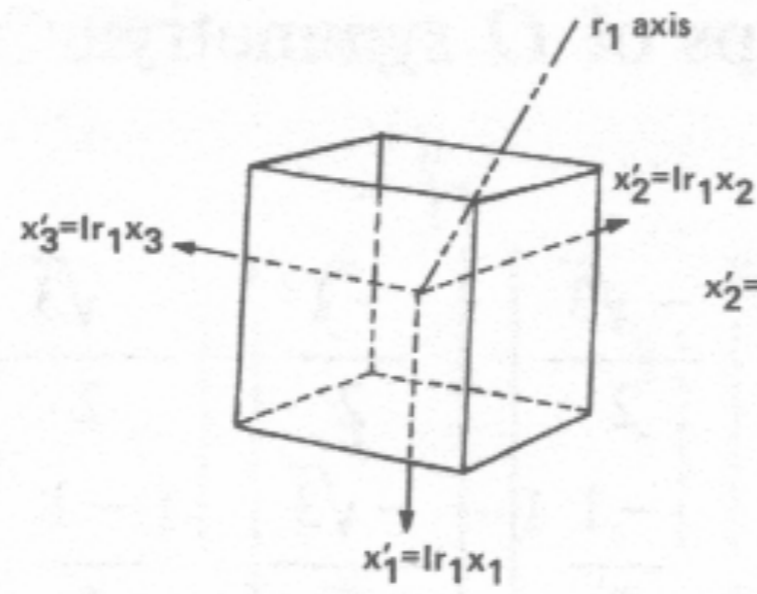
E *Tensor*
 $u^2 + v^2 - 2w^2$
 $(u^2 - v^2)\sqrt{3}$

basis: $O \left| \begin{matrix} E \\ E \\ 0_2 \end{matrix} \right\rangle \left| \begin{matrix} E \\ E \\ 1_2 \end{matrix} \right\rangle$

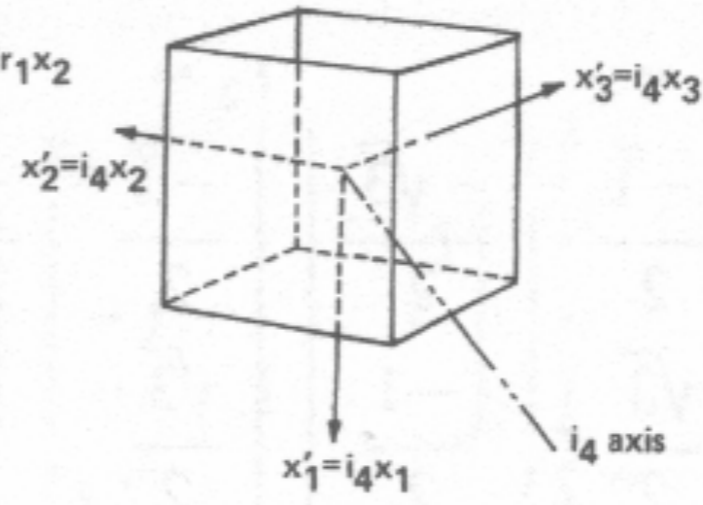
O: χ_g^μ	$g=1$	r_{1-4} \tilde{r}_{1-4}	ρ_{xyz}	R_{xyz} \tilde{R}_{xyz}	i_{1-6}
$\mu=A_1$	1	1	1	1	1
A_2	1	1	1	-1	-1
E	2	-1	2	0	0
T_1	3	0	-1	1	-1
T_2	3	0	-1	-1	1



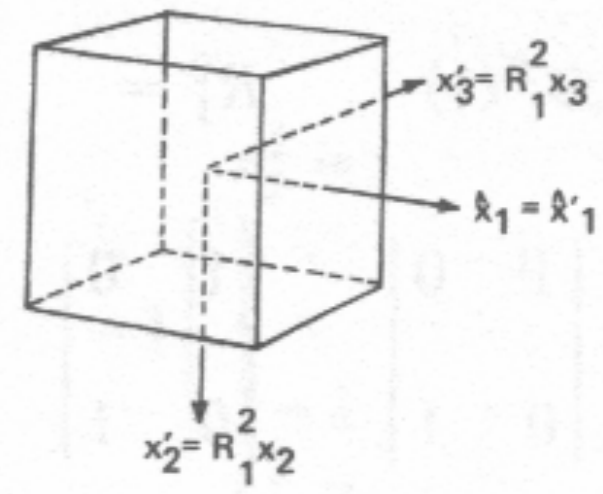
TETRAGONAL BASES



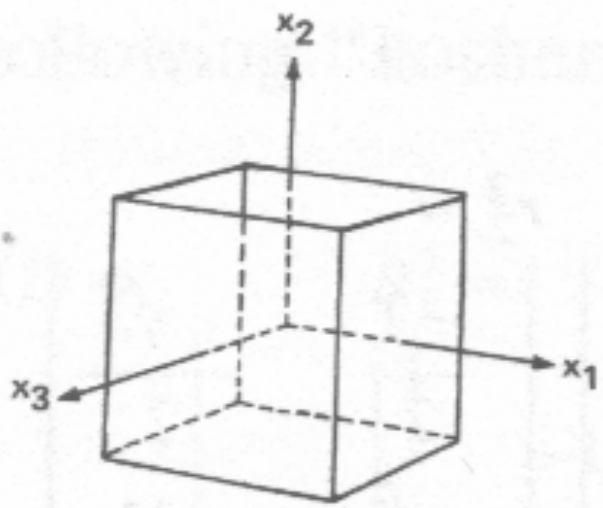
$$D^{T1u(lr_1)} = \begin{pmatrix} 0 & 0 & -1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix}$$



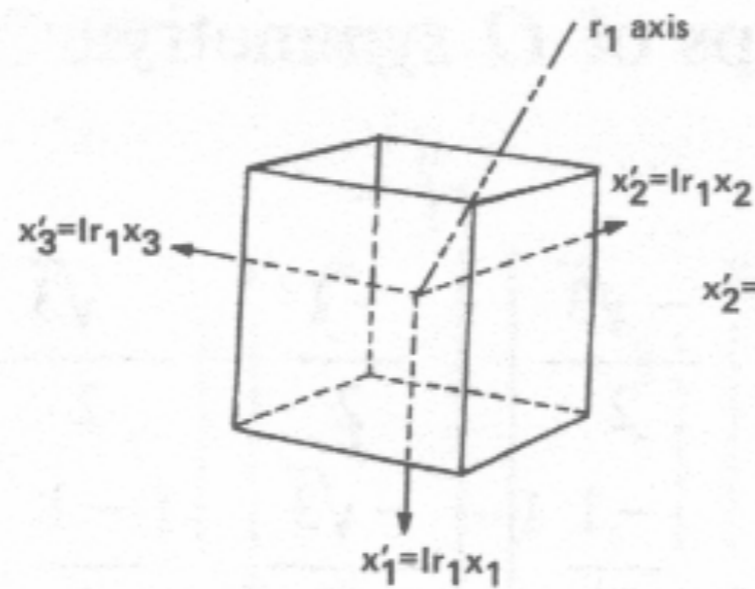
$$D^{T1u(i_4)} = \begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$



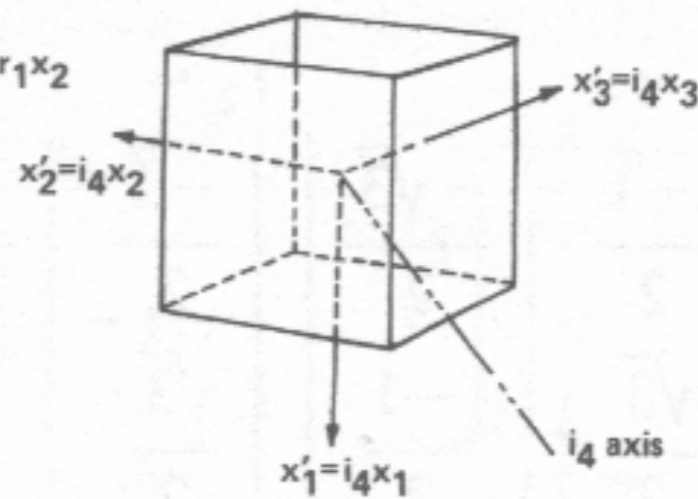
$$D^{T1u(R_1^2)} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$



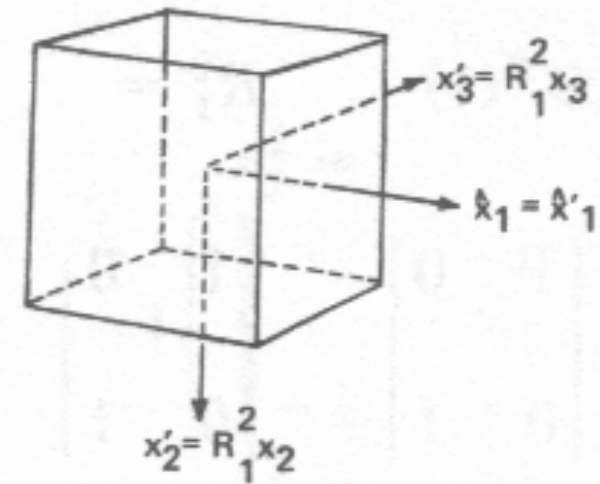
TETRAGONAL BASES



$$D^{T1u(lr_1)} = \begin{pmatrix} 0 & 0 & -1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix}$$



$$D^{T1u(i_4)} = \begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$



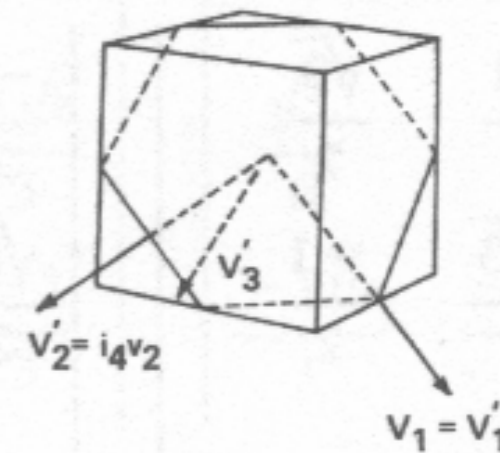
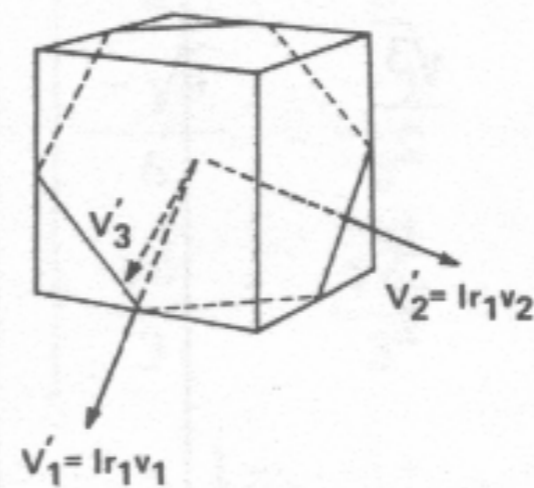
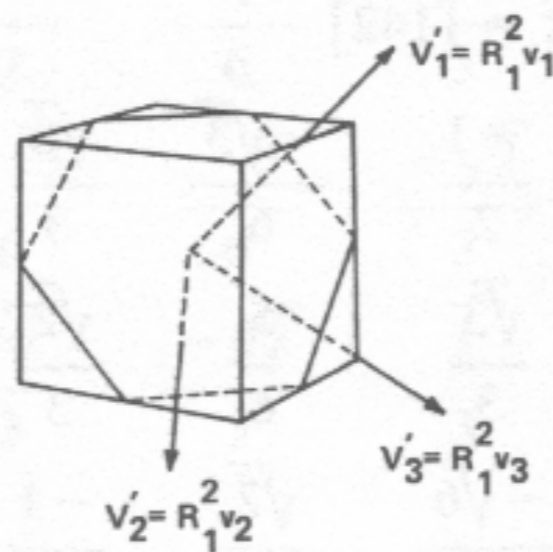
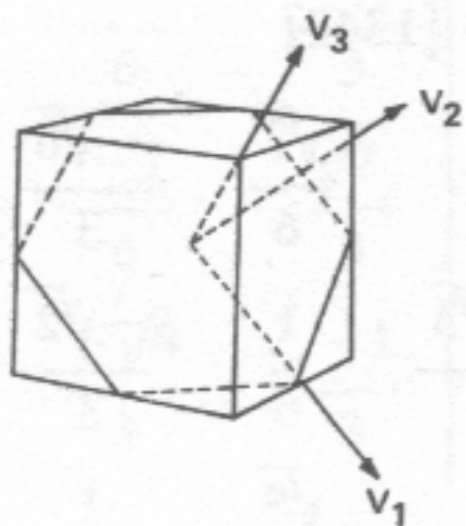
$$D^{T1u(R_1^2)} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

TRIGONAL BASES

$$D^{T1u(R_1^2)} = \begin{pmatrix} 0 & \sqrt{3}/3 & \sqrt{6}/3 \\ \sqrt{3}/3 & -2/3 & \sqrt{2}/3 \\ \sqrt{6}/3 & \sqrt{2}/3 & -1/3 \end{pmatrix}$$

$$D^{T1u(lr_1)} = \begin{pmatrix} 1/2 & \sqrt{3}/2 & 0 \\ -\sqrt{3}/2 & 1/2 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

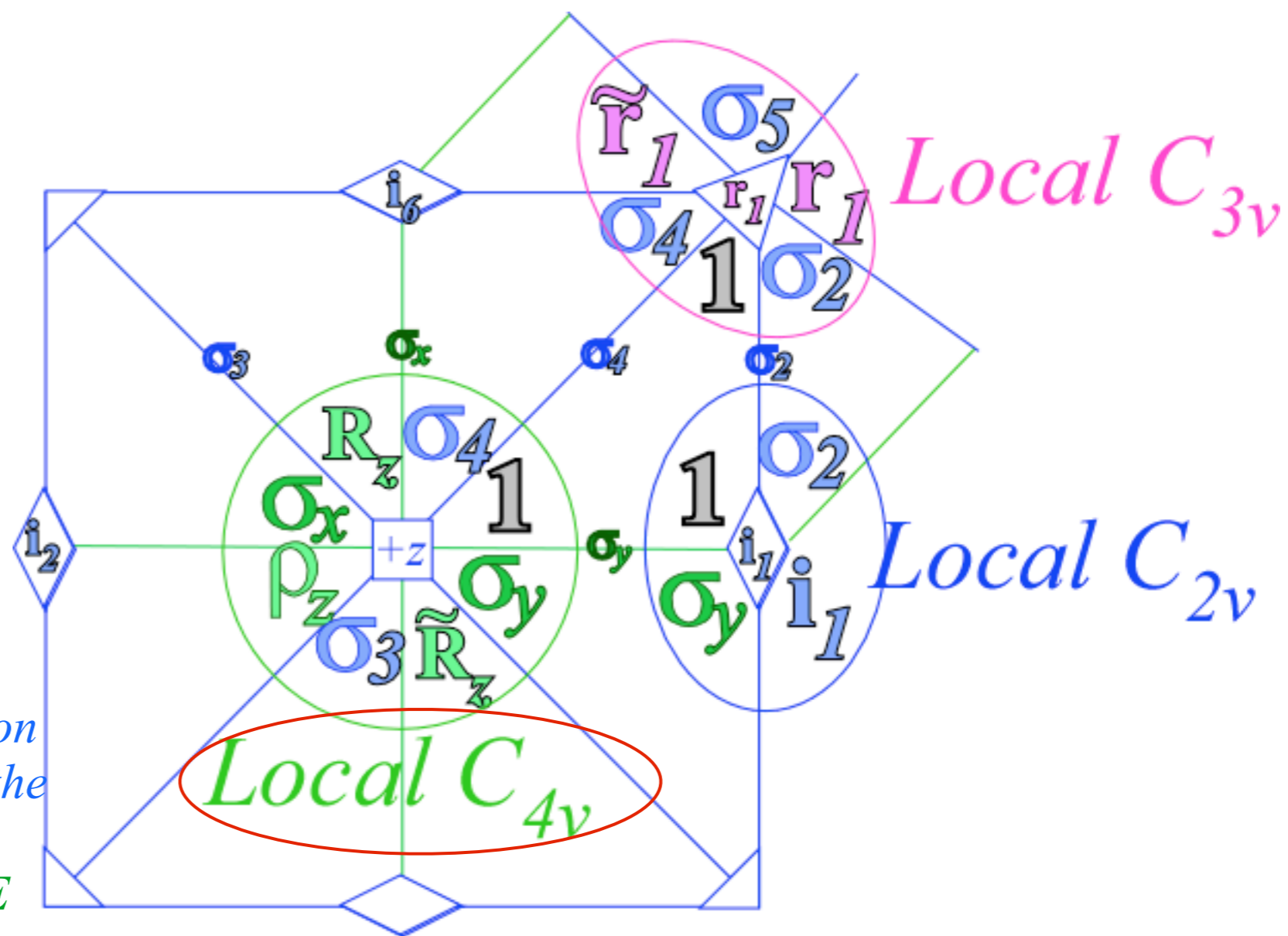
$$D^{T1u(i_4)} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$



$O \supset C_4$	0_4	1_4	2_4	3_4
$A_1 \downarrow C_4$	1	.	.	.
$A_2 \downarrow C_4$.	.	1	.
$E \downarrow C_4$	1	.	1	.
$T_1 \downarrow C_4$	1	1	.	1
$T_2 \downarrow C_4$.	1	1	1

$O_h \supset C_{4v}$	A'	B'	A''	B''	E
$A_{1g} \downarrow C_{4v}$	1
$A_{2g} \downarrow C_{4v}$.	1	.	.	.
$E_g \downarrow C_{4v}$	1	1	.	.	.
$T_{1g} \downarrow C_{4v}$.	.	1	.	1
$T_{2g} \downarrow C_{4v}$.	.	.	1	1
$A_{1u} \downarrow C_{4v}$.	.	1	.	.
$A_{2u} \downarrow C_{4v}$.	.	.	1	.
$E_u \downarrow C_{4v}$.	.	1	1	.
$T_{1u} \downarrow C_{4v}$	1	.	.	.	1
$T_{2u} \downarrow C_{4v}$.	1	.	.	1

$O_h \supset C_{4v}$
 correlation
 predicts the
 parity of
 the $A_1 T_1 E$
 cluster is not
 uniformly
 even (g) or
 odd (u):
 $A_{1g} T_{1u} E_g$



$0_4 \uparrow 0$ cluster

Symmetry parity

$A_{1g} T_{1u} E_g$

$$\begin{pmatrix} \langle 1 | \mathbf{H} | 1 \rangle & \langle 1 | \mathbf{H} | 2 \rangle & \cdots & \langle 1 | \mathbf{H} | 6 \rangle \\ \langle 2 | \mathbf{H} | 1 \rangle & \langle 2 | \mathbf{H} | 2 \rangle & \cdots & \langle 2 | \mathbf{H} | 6 \rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle 6 | \mathbf{H} | 1 \rangle & \langle 6 | \mathbf{H} | 2 \rangle & \cdots & \langle 6 | \mathbf{H} | 6 \rangle \end{pmatrix} = \begin{pmatrix} H & T & S & S & S & S \\ T & H & S & S & S & S \\ S & S & H & T & S & S \\ S & S & T & H & S & S \\ S & S & S & S & H & T \\ S & S & S & S & T & H \end{pmatrix}$$

$$\begin{aligned} E^{A_1} &= H + T + 4S \\ E^{T_1} &= H - T \\ E^E &= H + T - 2S \end{aligned}$$

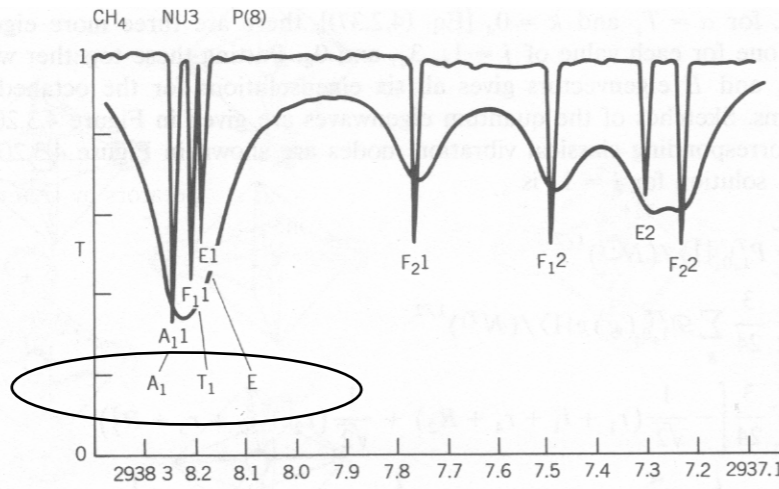
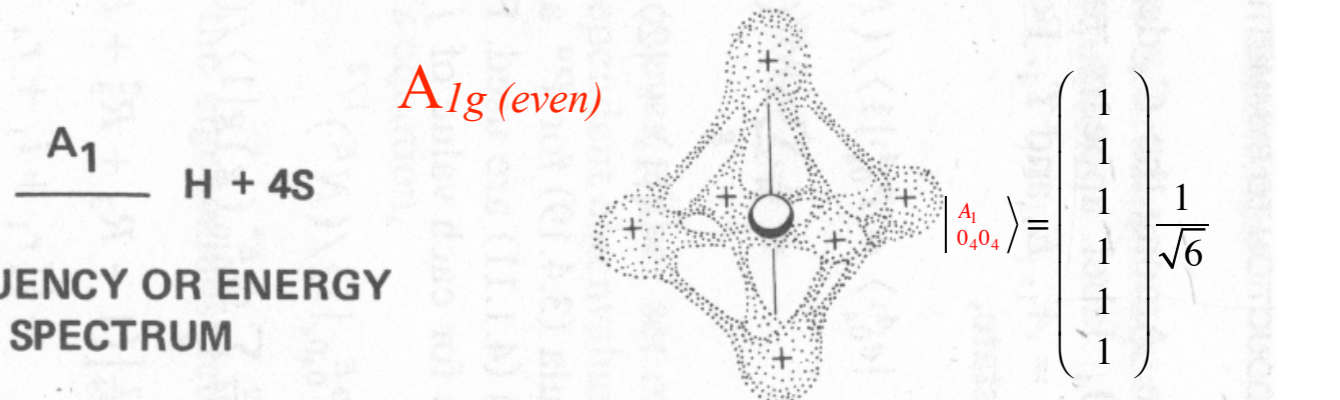
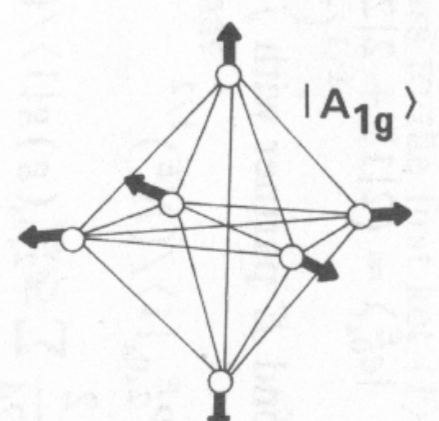
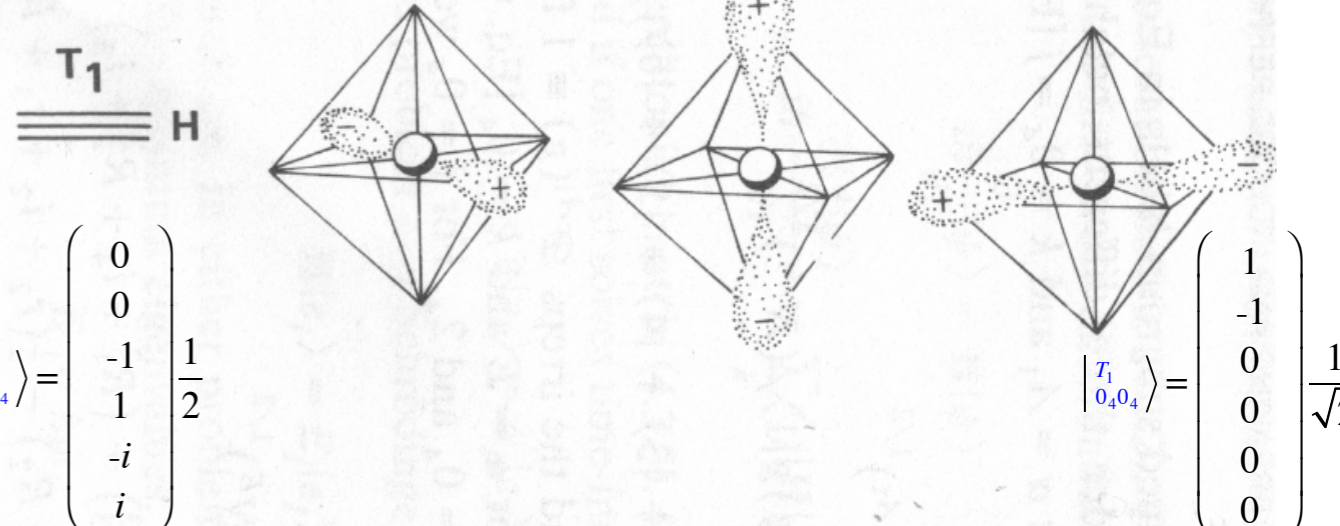
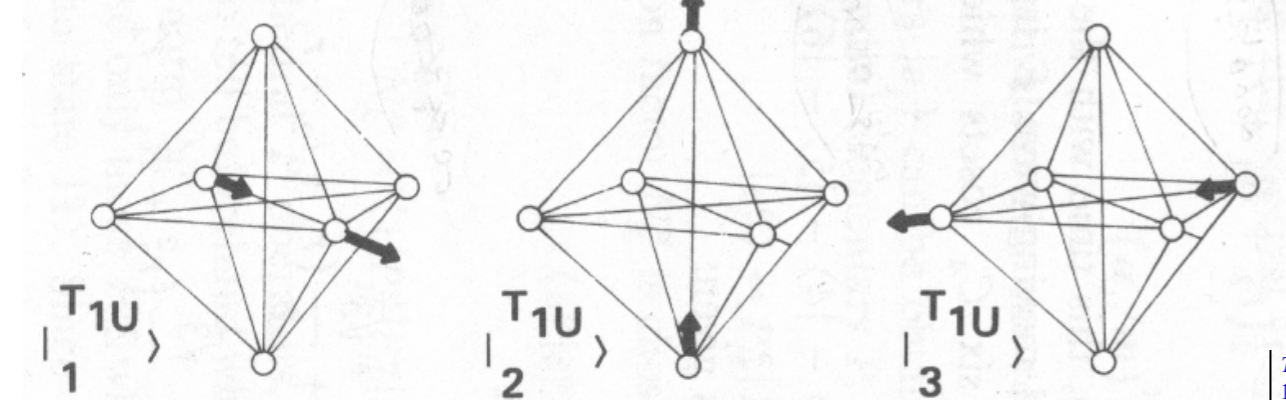
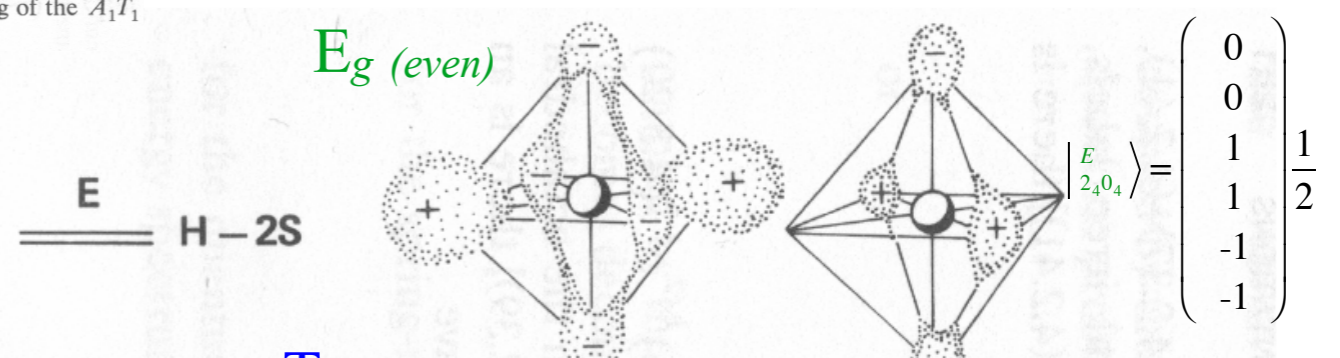
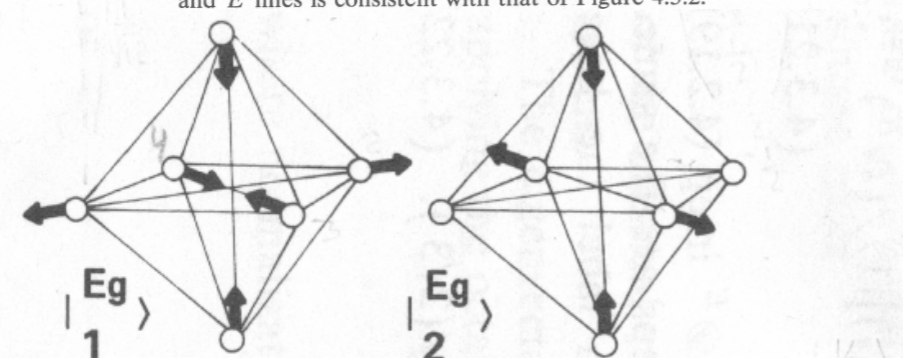


Figure 4.3.3 Evidence of an $(A_1 T_1 E)$ spectral cluster in methane laser spectra. (Courtesy of Dr. Allan Pine, MIT Lincoln Laboratories, from *Journal of Optical Society of America* 66, 97 (1976)). The ordering and approximate spacing of the $A_1 T_1$ and E lines is consistent with that of Figure 4.3.2.

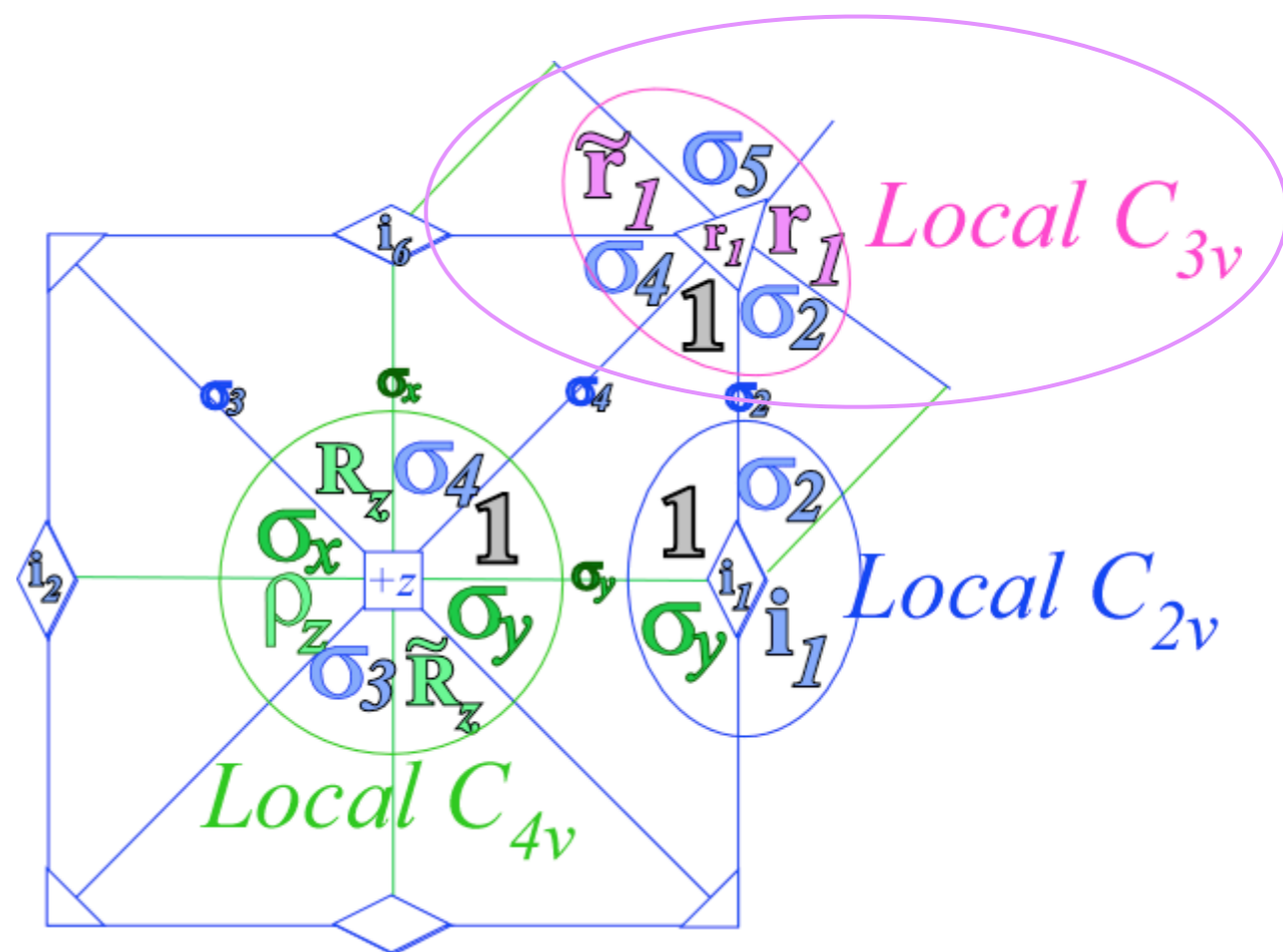
$$|E_{0_4 0_4}\rangle = \frac{1}{2\sqrt{3}} \begin{pmatrix} 2 \\ 2 \\ -1 \\ -1 \\ -1 \\ -1 \end{pmatrix}$$



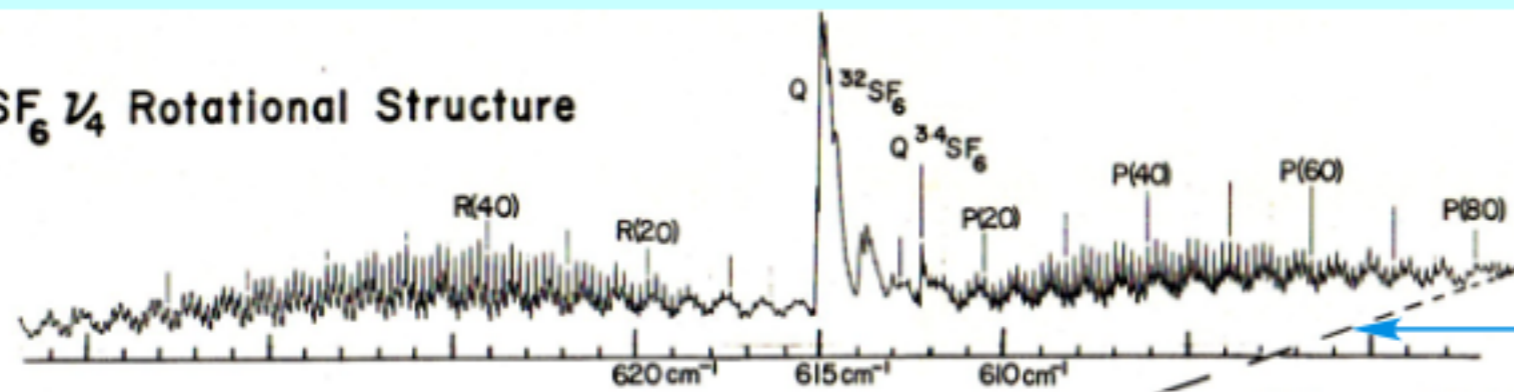
FREQUENCY OR ENERGY SPECTRUM

$O \supset C_3$	0_3	1_3	2_3
$A_1 \downarrow C_3$	1	.	.
$A_2 \downarrow C_3$	1	.	.
$E \downarrow C_3$.	1	1
$T_1 \downarrow C_3$	1	1	1
$T_2 \downarrow C_3$	1	1	1

$O_h \supset C_{3v}$	A'	A''	E
$A_{1g} \downarrow C_{3v}$	1	.	.
$A_{2g} \downarrow C_{3v}$.	1	.
$E_g \downarrow C_{3v}$.	.	1
$T_{1g} \downarrow C_{3v}$.	1	1
$T_{2g} \downarrow C_{3v}$	1	.	1
$A_{1g} \downarrow C_{3v}$.	1	.
$A_{2u} \downarrow C_{3v}$	1	.	.
$E_u \downarrow C_{3v}$.	.	1
$T_{1u} \downarrow C_{3v}$	1	.	1
$T_{2u} \downarrow C_{3v}$.	1	1



(a) SF₆ ν₄ Rotational Structure



FT IR and Laser Diode Spectra
K.C. Kim, W.B. Person, D. Seitz, and B.J. Krohn
J. Mol. Spectrosc. 76, 322 (1979).

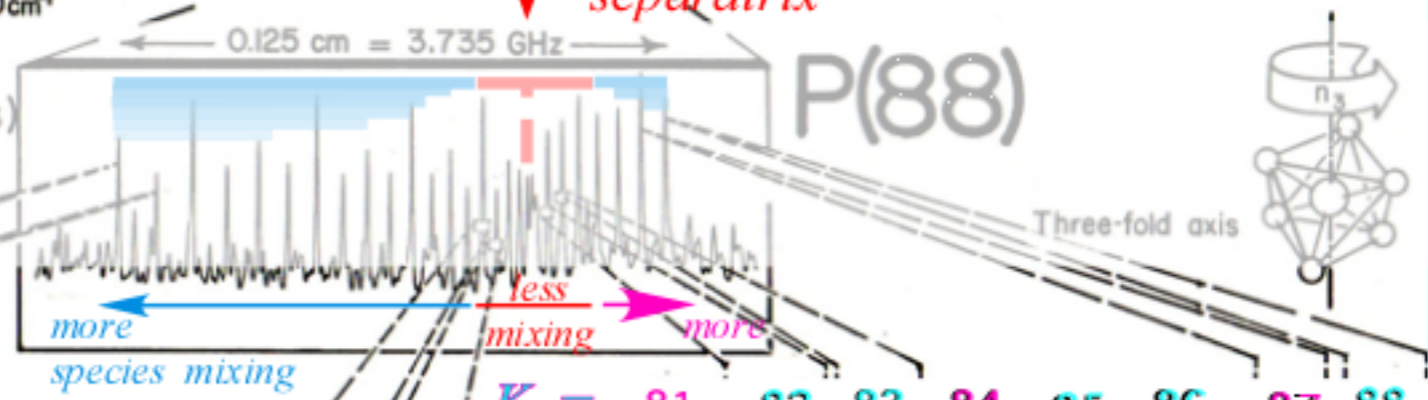
Primary AET species mixing increases with distance from "separatrix"

(b) P(88) Fine Structure (Rotational anisotropy effects)

SF₆ ν₃ P(88) ~ 16m

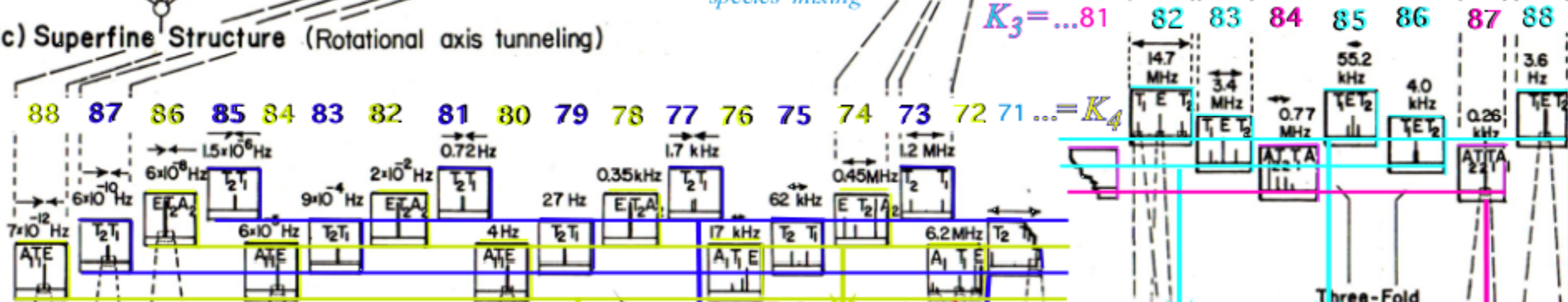


Four fold axis



Three-fold axis

(c) Superfine Structure (Rotational axis tunneling)



Observed repeating sequence(s) .. A₁ T₁ E T₂ T₁ E T₂ A₂ T₂ T₁ A₁ T₁ E T₂ T₁ E T₂ A₂ T₂ T₁ A₁ ..

O=C₄ (0)₄ (1)₄ (2)₄ (3)₄ = (-1)₄

A ₁	1	•	•	•
A ₂	•	•	1	•
E	1	•	1	•
T ₁	1	1	•	1
T ₂	•	1	1	1

O=C₃ (0)₃ (1)₃ (2)₃ = (-1)₃

A ₁	1	•	•
A ₂	1	•	•
E	•	1	1
T ₁	1	1	1
T ₂	1	1	1

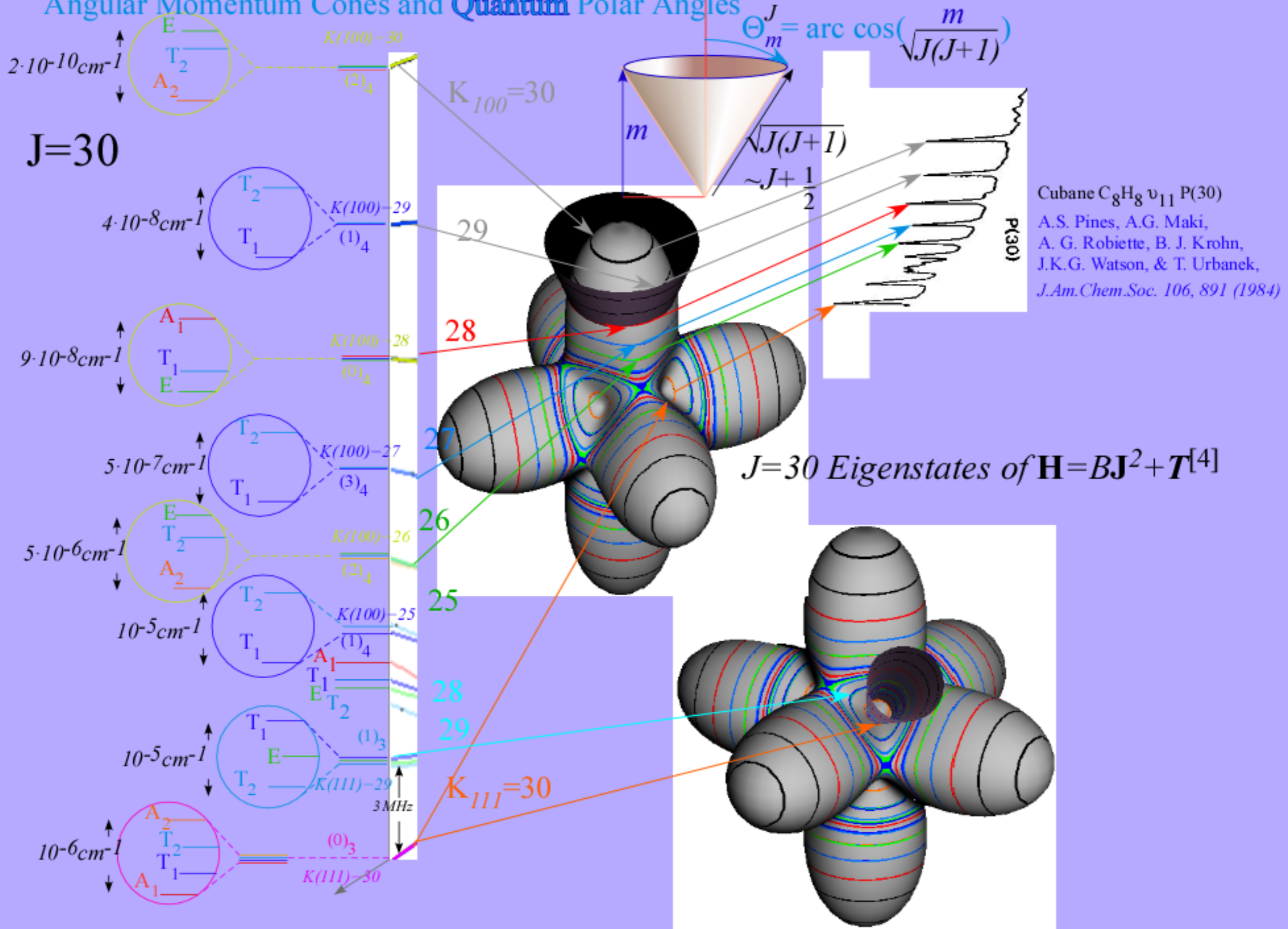
Local correlations explain clustering...
... but what about spacing and ordering?...

...and physical consequences?

major mixing lowest two LUSTERS

(e) Superfine Structure on rotational frame correlation

Angular Momentum Cones and Quantum Polar Angles



$O \supset C_4$	0_4	1_4	2_4	3_4
$A_1 \downarrow C_4$	1	·	·	·
$A_2 \downarrow C_4$	·	·	1	·
$E \downarrow C_4$	1	·	1	·
$T_1 \downarrow C_4$	1	1	·	1
$T_2 \downarrow C_4$	·	1	1	1

$O \supset C_3$	0_3	1_3	2_3
$A_1 \downarrow C_3$	1	·	·
$A_2 \downarrow C_3$	1	·	·
$E \downarrow C_3$	·	1	1
$T_1 \downarrow C_3$	1	1	1
$T_2 \downarrow C_3$	1	1	1

$O \supset C_2(i_1)$	0_2	1_2
$A_1 \downarrow C_2$	1	·
$A_2 \downarrow C_2$	·	1
$E \downarrow C_2$	1	1
$T_1 \downarrow C_2$	1	2
$T_2 \downarrow C_2$	2	1

$O \supset C_2(\rho_z)$	0_2	1_2
$A_1 \downarrow C_2$	1	·
$A_2 \downarrow C_2$	1	·
$E \downarrow C_2$	2	·
$T_1 \downarrow C_2$	1	2
$T_2 \downarrow C_2$	1	2

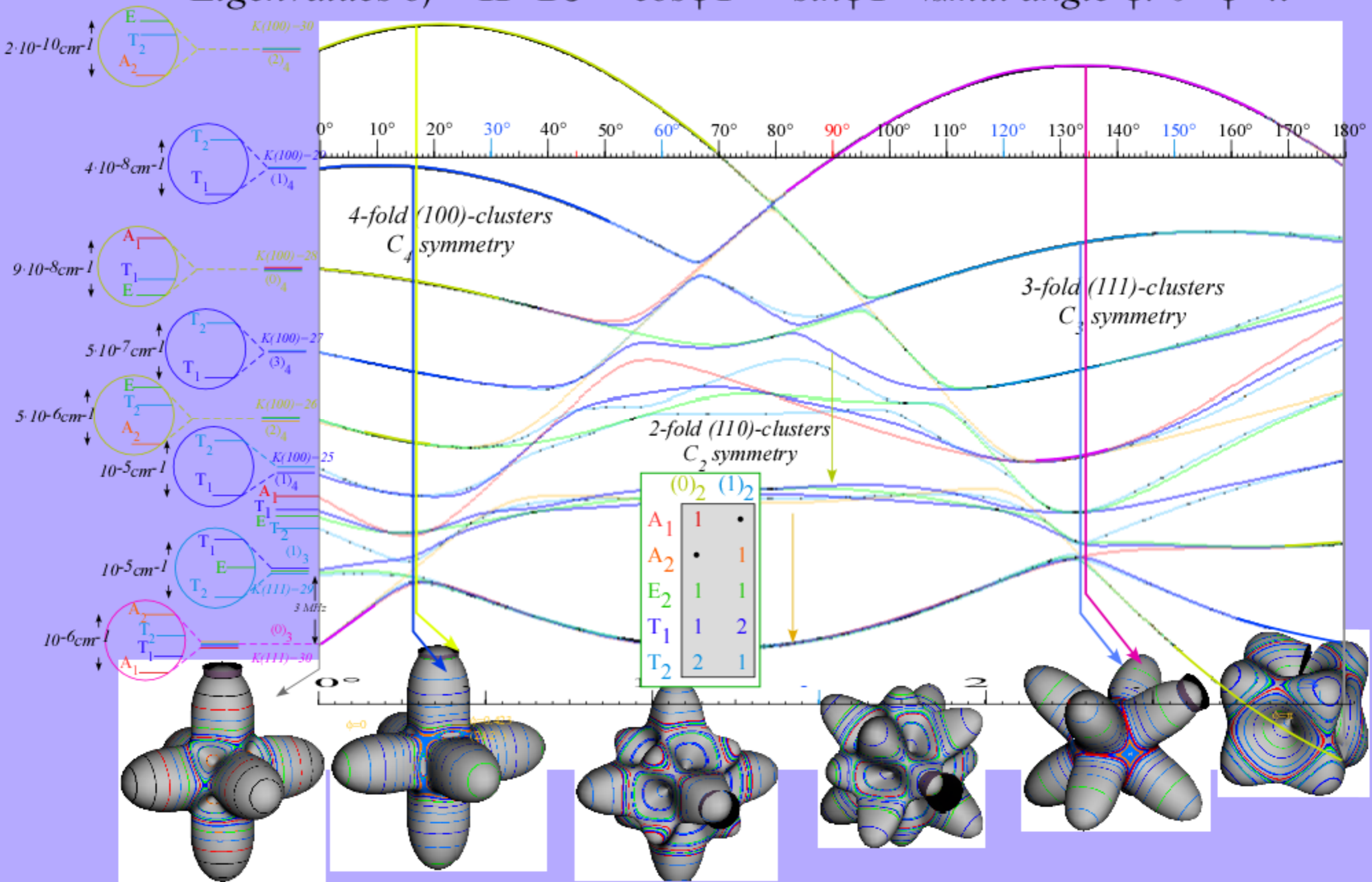
$O_h \supset C_{4v}$	A'	B'	A''	B''	E
$A_{1g} \downarrow C_{4v}$	1	·	·	·	·
$A_{2g} \downarrow C_{4v}$	·	1	·	·	·
$E_g \downarrow C_{4v}$	1	1	·	·	·
$T_{1g} \downarrow C_{4v}$	·	·	1	·	1
$T_{2g} \downarrow C_{4v}$	·	·	·	1	1
$A_{1u} \downarrow C_{4v}$	·	·	1	·	·
$A_{2u} \downarrow C_{4v}$	·	·	·	1	·
$E_u \downarrow C_{4v}$	·	·	1	1	·
$T_{1u} \downarrow C_{4v}$	1	·	·	·	1
$T_{2u} \downarrow C_{4v}$	·	1	·	·	1

$O_h \supset C_{3v}$	A'	A''	E
$A_{1g} \downarrow C_{3v}$	1	·	·
$A_{2g} \downarrow C_{3v}$	·	1	·
$E_g \downarrow C_{3v}$	·	·	1
$T_{1g} \downarrow C_{3v}$	·	1	1
$T_{2g} \downarrow C_{3v}$	1	·	1
$A_{1u} \downarrow C_{3v}$	·	1	·
$A_{2u} \downarrow C_{3v}$	1	·	·
$E_u \downarrow C_{3v}$	·	·	1
$T_{1u} \downarrow C_{3v}$	1	·	1
$T_{2u} \downarrow C_{3v}$	·	1	1

$O_h \supset C_{2v}^i$	A'	B'	A''	B''
$A_{1g} \downarrow C_{2v}^i$	1	·	·	·
$A_{2g} \downarrow C_{2v}^i$	·	1	·	·
$E_g \downarrow C_{2v}^i$	1	1	·	·
$T_{1g} \downarrow C_{2v}^i$	·	1	1	1
$T_{2g} \downarrow C_{2v}^i$	1	·	1	1
$A_{1u} \downarrow C_{2v}^i$	·	·	1	·
$A_{2u} \downarrow C_{2v}^i$	·	·	·	1
$E_u \downarrow C_{2v}^i$	·	·	1	1
$T_{1u} \downarrow C_{2v}^i$	1	1	·	1
$T_{2u} \downarrow C_{2v}^i$	1	1	1	·

$O_h \supset C_{2v}^z$	A'	B'	A''	B''
$A_{1g} \downarrow C_{2v}^z$	1	·	·	·
$A_{2g} \downarrow C_{2v}^z$	1	·	·	·
$E_g \downarrow C_{2v}^z$	2	·	·	·
$T_{1g} \downarrow C_{2v}^z$	·	1	1	1
$T_{2g} \downarrow C_{2v}^z$	·	1	1	1
$A_{1u} \downarrow C_{2v}^z$	·	·	1	·
$A_{2u} \downarrow C_{2v}^z$	·	·	1	·
$E_u \downarrow C_{2v}^z$	·	·	2	·
$T_{1u} \downarrow C_{2v}^z$	1	1	·	1
$T_{2u} \downarrow C_{2v}^z$	1	1	·	1

Eigenvalues of $\mathbf{H} = B\mathbf{J}^2 + \cos\phi\mathbf{T}^{[4]} + \sin\phi\mathbf{T}^{[6]}$ vs. mix angle $\phi: 0 < \phi < \pi$



	$(0)_2$	$(1)_2$
A_1	1	•
A_2	•	1
E_2	1	1
T_1	1	2
T_2	2	1

Ireps for $O \supset D_4 \supset C_4$ subgroup chain

T₁

Vector
x,y,z

T₂

Tensor
yz,xz,xy

E

Tensor
 $x^2+y^2-2z^2$
 $(x^2-y^2)\sqrt{3}$

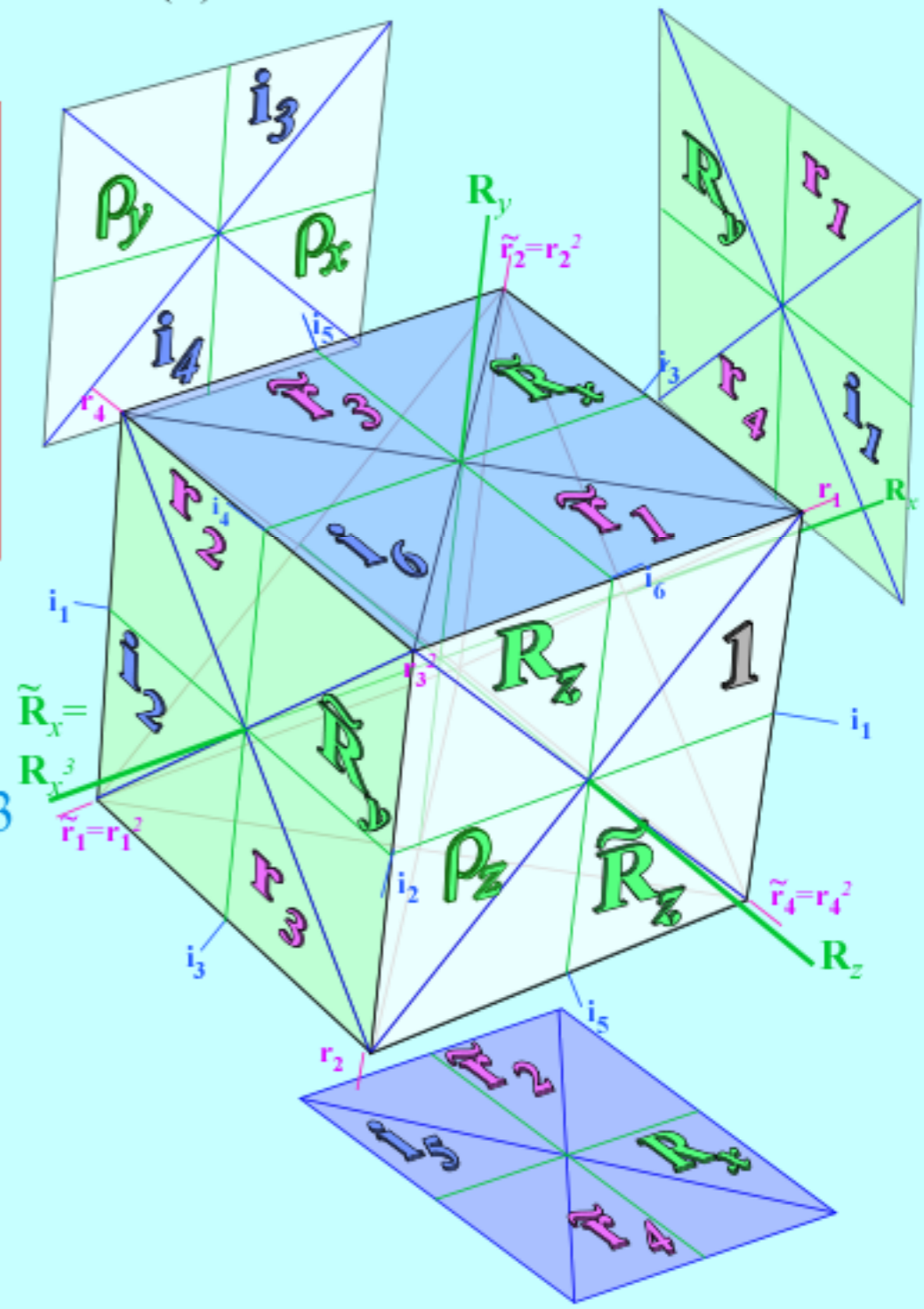
$$\begin{aligned} \ell^{A_1} &= 1 \\ \ell^{A_2} &= 1 \\ \ell^E &= 2 \\ \ell^{T_1} &= 3 \\ \ell^{T_2} &= 3 \end{aligned}$$

Example: $G=O$ Centrum: $\kappa(O) = \sum_{(\alpha)} (\ell^\alpha)^0 = 1^0 + 1^0 + 2^0 + 3^0 + 3^0 = 5$
 Cubic-Octahedral Group O

Rank: $\rho(O) = \sum_{(\alpha)} (\ell^\alpha)^1 = 1^1 + 1^1 + 2^1 + 3^1 + 3^1 = 10$

Order: $o(O) = \sum_{(\alpha)} (\ell^\alpha)^2 = 1^2 + 1^2 + 2^2 + 3^2 + 3^2 = 24$

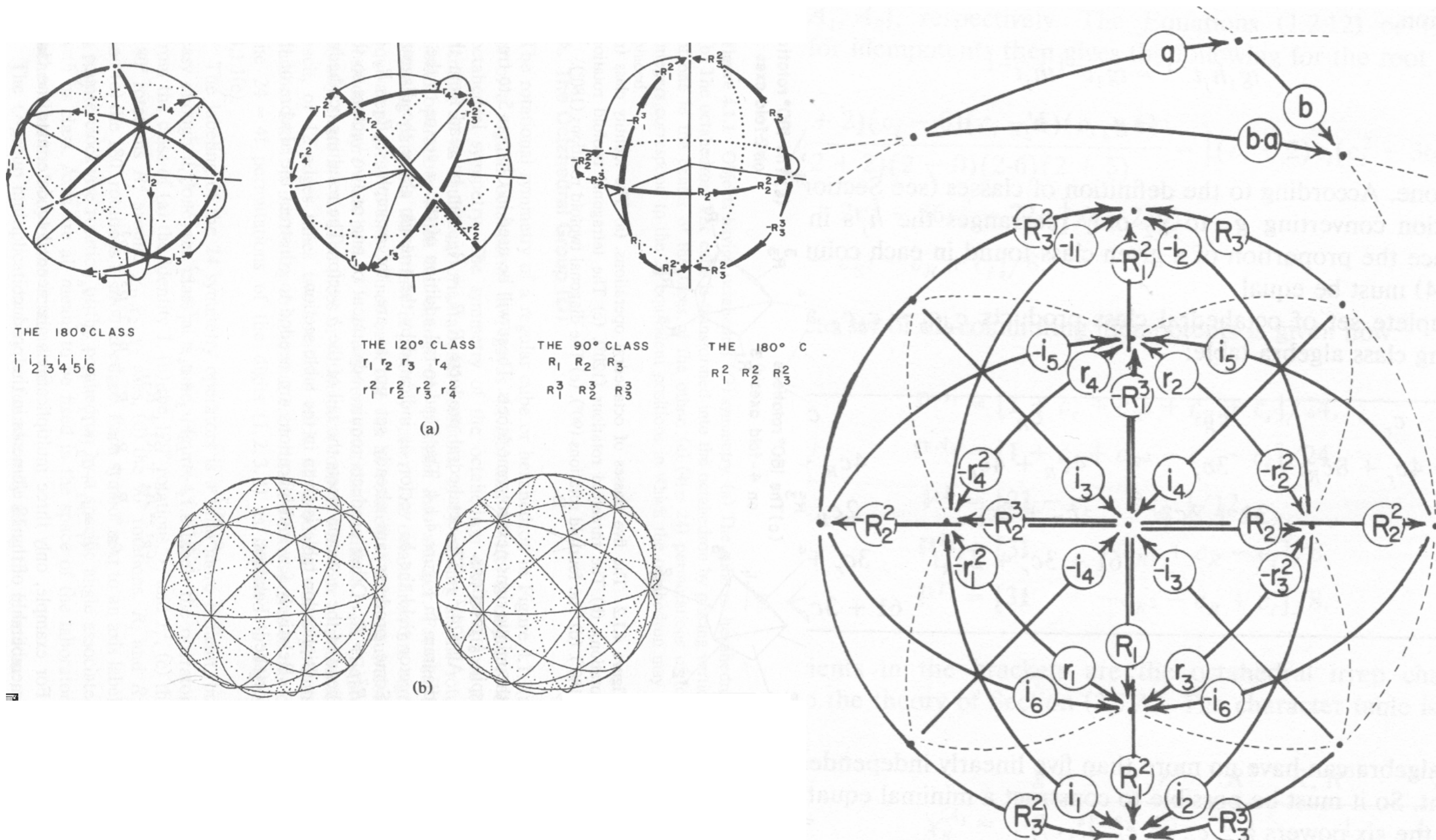
O group	$g = 1$	r_{1-4}	ρ_{xyz}	R_{xyz}	i_{1-6}
$\chi_{\kappa_g}^\alpha$		\tilde{r}_{1-4}		\tilde{R}_{xyz}	
$\alpha = A_1$ <i>s-orbital r^2</i>	1	1	1	1	1
A_2 <i>d-orbitals</i>	1	1	1	-1	-1
E $\{x^2+y^2-2z^2, x^2-y^2\}$	2	-1	2	0	0
T_1 $\{x, y, z\}$ <i>p-orbitals</i>	3	0	-1	1	-1
T_2 $\{xz, yz, xy\}$ <i>d-orbitals</i>	3	0	-1	-1	1



$O \supset C_4$ $(0)_4 (1)_4 (2)_4 (3)_4 = (-1)_4$ $O \supset C_3$ $(0)_3 (1)_3 (2)_3 = (-1)_3$

A_1	1	•	•	•
A_2	•	•	1	•
E	1	•	1	•
T_1	1	1	•	1
T_2	•	1	1	1

A_1	1	•	•
A_2	1	•	•
E	•	1	1
T_1	1	1	1
T_2	1	1	1



Octahedral $O \supset D_4 \supset C_4$ subgroup correlations

$O \downarrow D_4$ subduction

D_4 : $1, \rho_{z180^\circ}, R_{z\pm 90^\circ}, \rho_{z180^\circ}, i_{3,4}$

$\chi_g^\mu(O)$	$g=1$	$r_{1..4}$	180° ρ_{xyz}	90° R_{xyz}	180° $i_{1..6}$
A_1	1	1	1	1	1
A_2	1	1	1	-1	-1
E	2	-1	2	0	0
T_1	3	0	-1	1	-1
T_2	3	0	-1	-1	1

$A_1(O) \downarrow D_4 = 1, 1, 1, 1, 1$
 $A_2(O) \downarrow D_4 = 1, 1, -1, 1, -1$
 $E(O) \downarrow D_4 = 2, 2, 0, 2, 0$
 $T_1(O) \downarrow D_4 = 3, -1, 1, -1, -1$
 $T_2(O) \downarrow D_4 = 3, -1, -1, -1, 1$

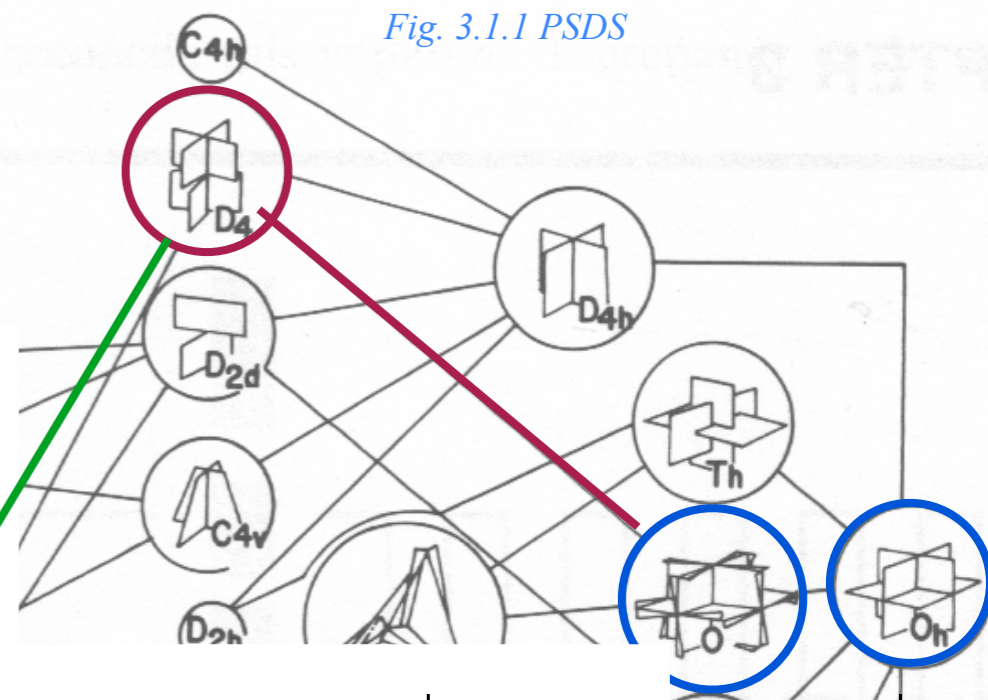


Fig. 3.1.1 PSDS

$\chi_g^\mu(D_4)$	$g=1$	ρ_{z180°	$R_{z\pm 90^\circ}$	$\rho_{x,y180^\circ}$	$i_{3,4}$
A_1	1	1	1	1	1
B_1	1	1	-1	1	-1
A_2	1	1	1	-1	-1
B_2	1	1	-1	-1	1
E	2	-2	0	0	0

$D_4 \downarrow C_4$ subduction

$1, R_{z+90^\circ}, \rho_{z180^\circ}, R_{z-90^\circ}$

$A_1(D_4) \downarrow C_4 = 1, 1, 1, 1 = (0)_4$
 $B_1(D_4) \downarrow C_4 = 1, -1, 1, -1 = (2)_4$
 $A_2(D_4) \downarrow C_4 = 1, 1, 1, 1 = (0)_4$
 $B_2(D_4) \downarrow C_4 = 1, -1, 1, -1 = (2)_4$
 $E(D_4) \downarrow C_4 = 2, 0, -2, 0 = (1)_4 \oplus (3)_4$

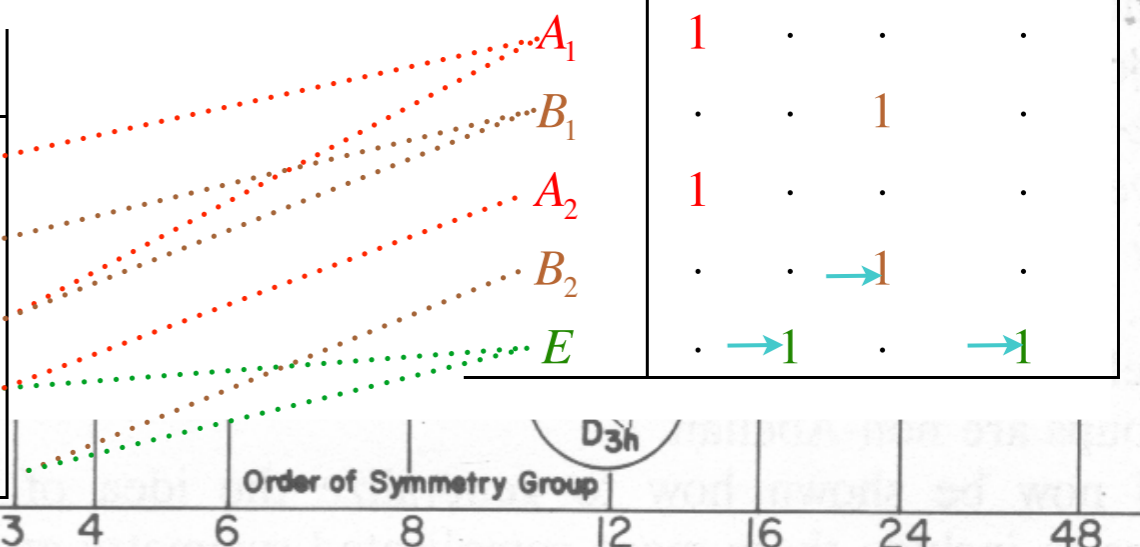
$O \downarrow D_4$	A_1	B_1	A_2	B_2	E
A_1	1
A_2	.	1	.	.	.
E	1	1	.	.	.
T_1	.	.	1	.	1
T_2	.	.	.	1	1

$\chi_g^\mu(C_4)$	$g=1$	R_{z+90°	R_{z+180°	R_{z-90°
$(0)_4$	1	1	1	1
$(1)_4$	1	i	-1	$-i$
$(2)_4$	1	-1	1	-1
$(3)_4$	1	$-i$	-1	i

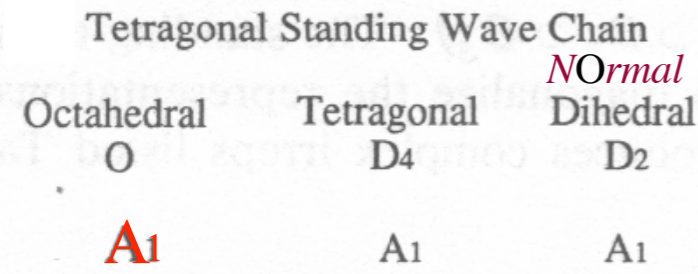
$O \downarrow C_4$ subduction

$O \downarrow C_4$	0_4	1_4	2_4	$3_4 = \bar{1}_4$
A_1	1	.	.	.
A_2	.	.	1	.
E	1	.	1	.
T_1	1	1	.	1
T_2	.	$\rightarrow 1$	$\rightarrow 1$	$\rightarrow 1$

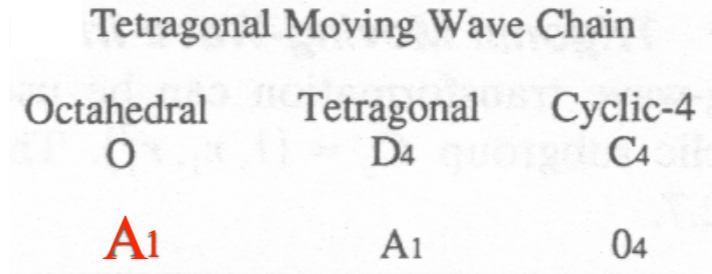
$D_4 \downarrow C_4$	0_4	1_4	2_4	$3_4 = \bar{1}_4$
A_1	1	.	.	.
B_1	.	.	1	.
A_2	1	.	.	.
B_2	.	.	$\rightarrow 1$.
E	.	$\rightarrow 1$.	$\rightarrow 1$



$O_h \supset O \supset D_4 \supset C_4$ subgroup splitting



D_4	1	ρ_z	R_z	$\rho_{x,y}$	$i_{3,4}$
A1	1	1	1	1	1
B1	1	1	-1	1	-1
A2	1	1	1	-1	-1
B2	1	1	-1	-1	1
E	2	-2	0	0	0

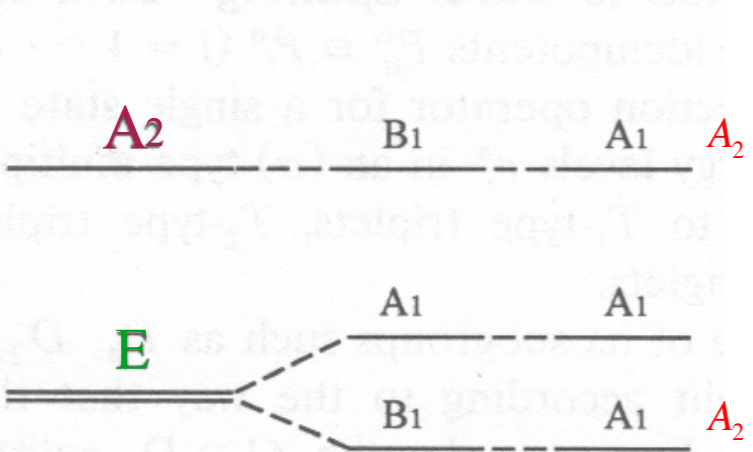


$D_2^{Nm} \{1, R_z^2, R_x^2, R_y^2\}$

$D_2^{Un} \{1, R_z^2, i_3, i_4\}$

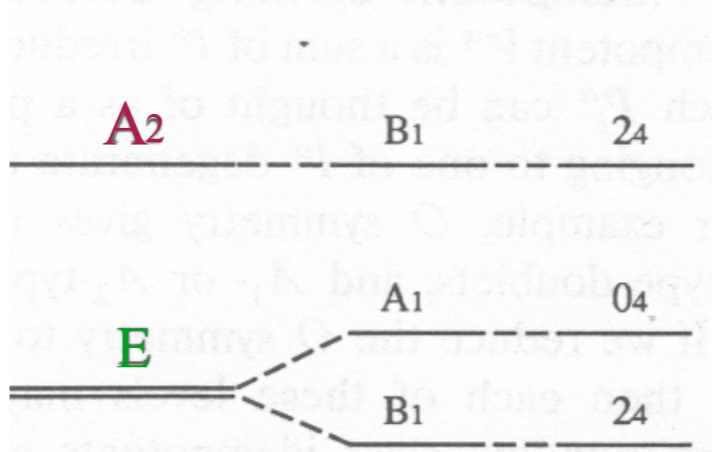
A1	1	1	1	1
B1	1	-1	1	-1
A2	1	1	-1	-1
B2	1	-1	-1	1

$-1_4 =$



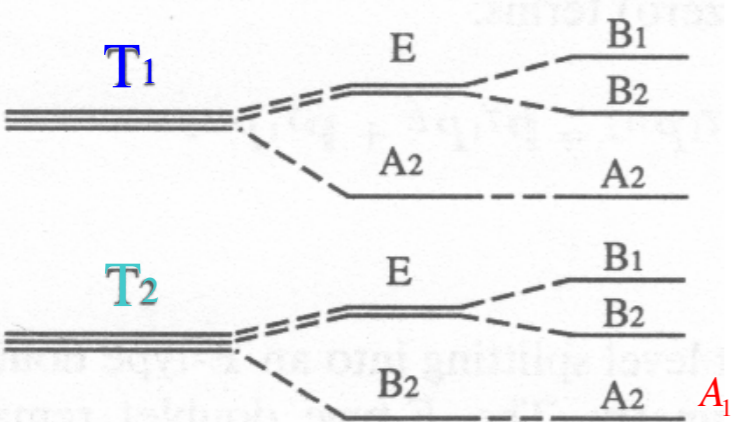
$NORmal D_2 = \{1, R_3^2, R_1^2, R_2^2\}$

$D_4 \downarrow D_2$	A1	B1	A2	B2
A1	1	.	.	.
B1	1	.	.	.
A2	.	.	1	.
B2	.	.	1	.
E	.	1	.	1



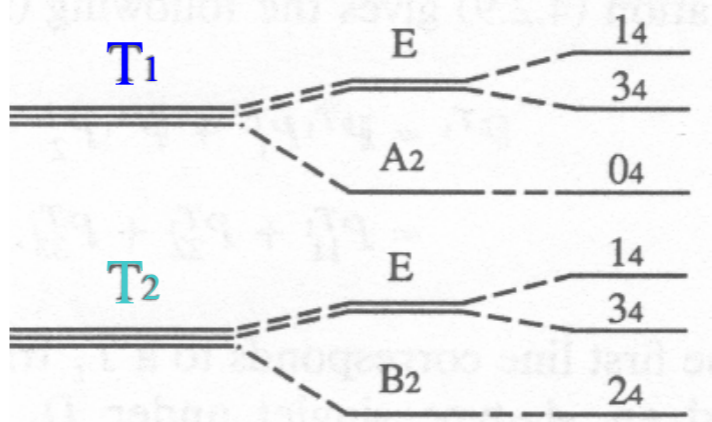
$D_4 \downarrow C_4$

	04	14	24	34
A1	1	.	.	.
B1	.	.	1	.
A2	1	.	.	.
B2	.	.	1	.
E	.	1	.	1



$UnORmal D_2 = \{1, R_3^2, i_3, i_4\}$

$D_4 \downarrow D_2$	A1	B1	A2	B2
A1	1	.	.	.
B1	.	.	1	.
A2	.	.	1	.
B2	1	.	.	.
E	.	1	.	1



$r, \tilde{r}_i \quad \rho_{xyz} \quad R, \tilde{R}_{xyz}$

O	1	r	R^2	R^3	i_k
A1	1	1	1	1	1
A2	1	1	1	-1	-1
E	2	-1	2	0	0
T1	3	0	-1	1	-1
T2	3	0	-1	-1	1

$-1_4 =$

$NORmal D_2 = \{1, R_3^2, R_1^2, R_2^2\}$ $UnORmal D_2 = \{1, R_3^2, i_3, i_4\}$

$O \downarrow D_2$	A1	B1	A2	B2
A1	1	.	.	.
A2	1	.	.	.
E	2	.	.	.
T1	.	1	1	1
T2	.	1	1	1

$O \downarrow D_2$	A1	B1	A2	B2
A1	1	.	.	.
A2	.	.	1	.
E	1	.	1	.
T1	.	1	1	1
T2	1	1	.	1

$O \downarrow D_4$	A1	B1	A2	B2	E
A1	1
A2	.	1	.	.	.
E	1	1	.	.	.
T1	.	.	1	.	1
T2	.	.	.	1	1

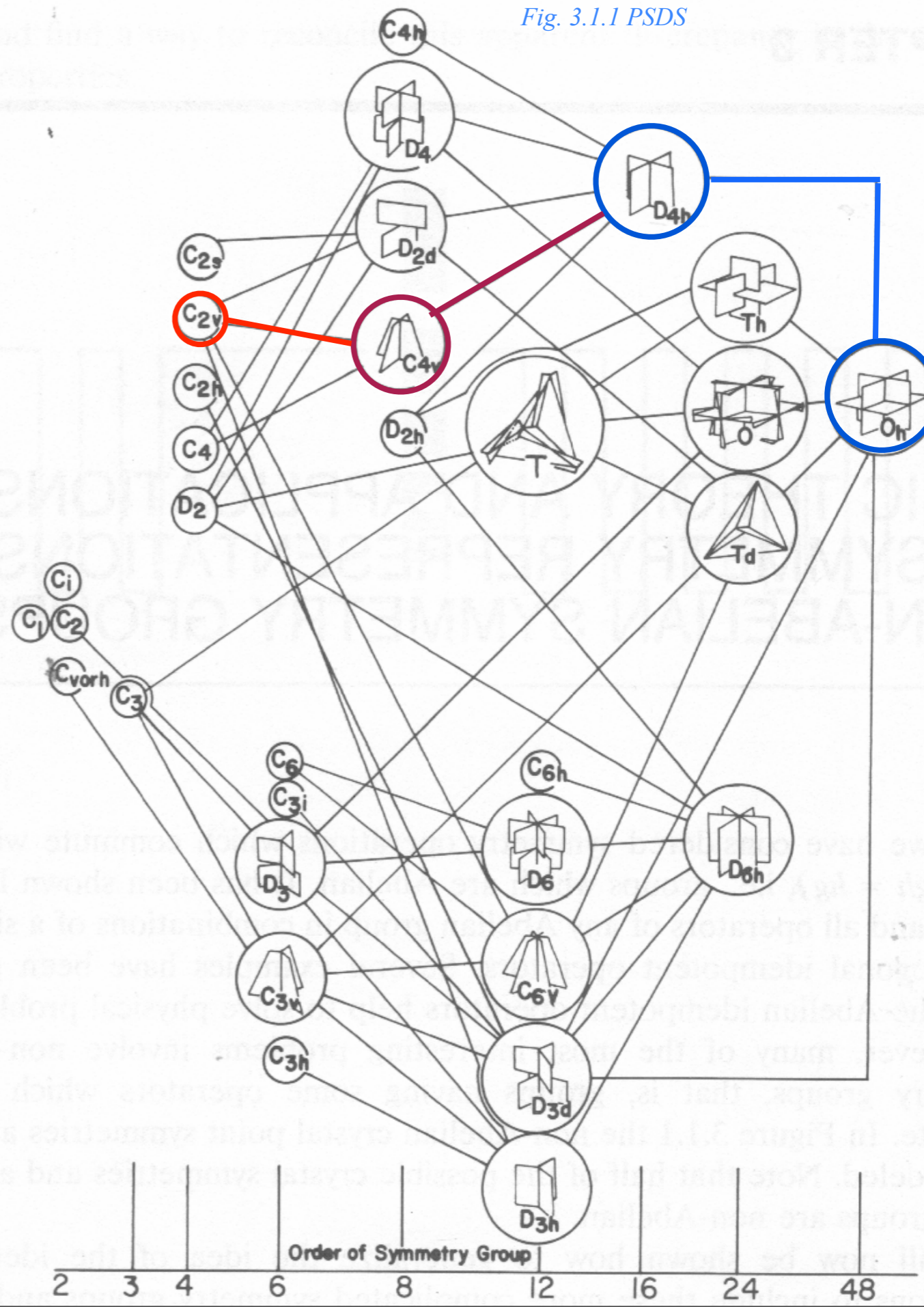
$O \downarrow C_4$	04	14	24	34
A1	1	.	.	.
A2	.	.	1	.
E	1	.	1	.
T1	1	1	.	1
T2	.	1	1	1

$O_h \supset O \supset D_4 \supset C_{4v} \supset C_{2v}$ subgroup splitting

$\downarrow C_{4v}$	A'	B'	A''	B''	E
$\mathcal{D}^{A_{1g}}$	1
$\mathcal{D}^{A_{2g}}$.	1	.	.	.
\mathcal{D}^{E_g}	1	1	.	.	.
$\mathcal{D}^{T_{1g}}$.	.	1	.	1
$\mathcal{D}^{T_{2g}}$.	.	.	1	1
$\mathcal{D}^{A_{1u}}$.	.	1	.	.
$\mathcal{D}^{A_{2u}}$.	.	.	1	.
\mathcal{D}^{E_u}	.	.	1	1	.
$\mathcal{D}^{T_{1u}}$	1	.	.	.	1
$\mathcal{D}^{T_{2u}}$.	1	.	.	1

$\downarrow C_{2v}$	A'	B'	A''	B''
$\mathcal{D}^{A_{1g}}$	1	.	.	.
$\mathcal{D}^{A_{2g}}$.	1	.	.
\mathcal{D}^{E_g}	1	1	.	.
$\mathcal{D}^{T_{1g}}$.	1	1	1
$\mathcal{D}^{T_{2g}}$	1	.	1	1
$\mathcal{D}^{A_{1u}}$.	.	1	.
$\mathcal{D}^{A_{2u}}$.	.	.	1
\mathcal{D}^{E_u}	.	.	1	1
$\mathcal{D}^{T_{1u}}$	1	1	.	1
$\mathcal{D}^{T_{2u}}$	1	1	1	.

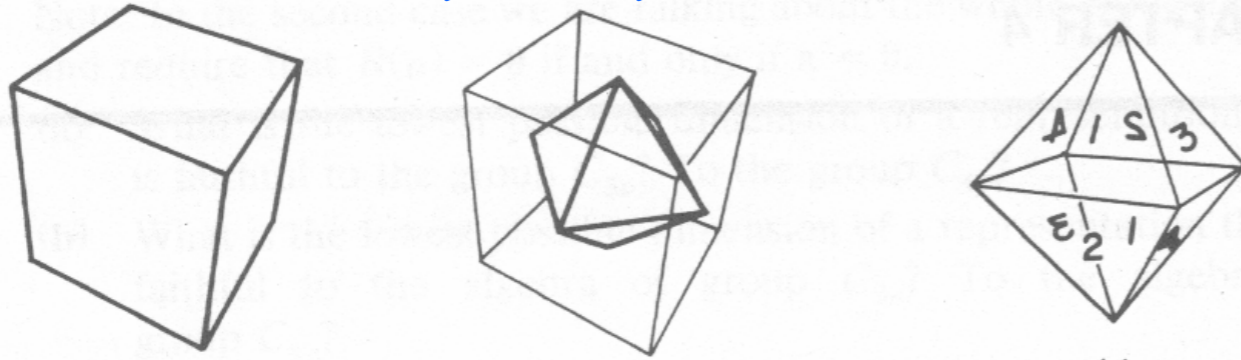
Fig. 3.1.1 PSDS



Introduction to octahedral/ tetrahedral symmetry $O_h \supset O \sim T_d \supset T$

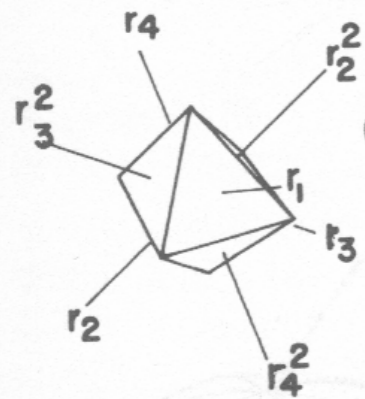
Octahedral-cubic O symmetry

Order $^{\circ}O = 6 \text{ hexahedron squares} \cdot 4 \text{ pts} = 24$
 $= 8 \text{ octahedron triangles} \cdot 3 \text{ pts} = 24$
 $= 12 \text{ lines} \cdot 2 \text{ pts} = 24 \text{ positions}$

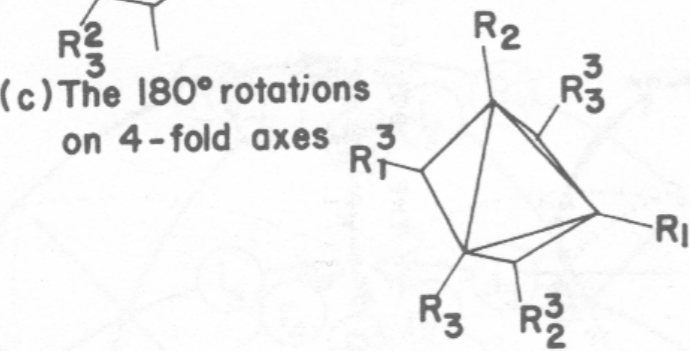


(a) The identity I

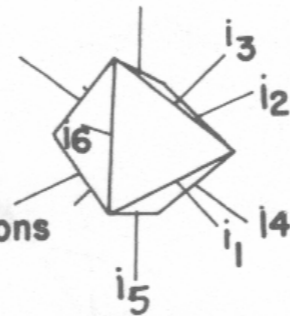
(b) The 120° rotations



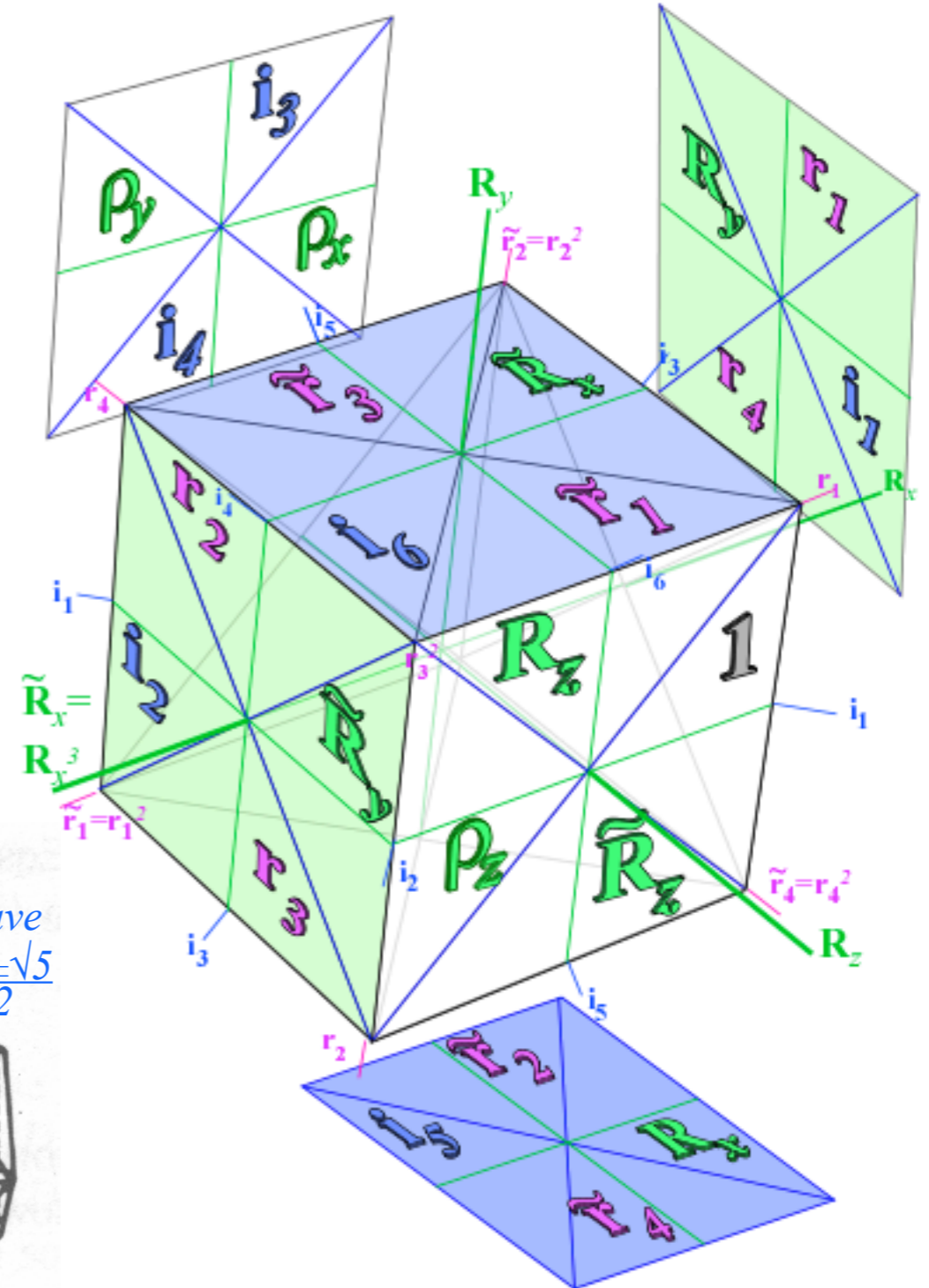
(c) The 180° rotations on 4-fold axes



(d) The 90° rotations



(e) The 180° rotations on 2-fold axes

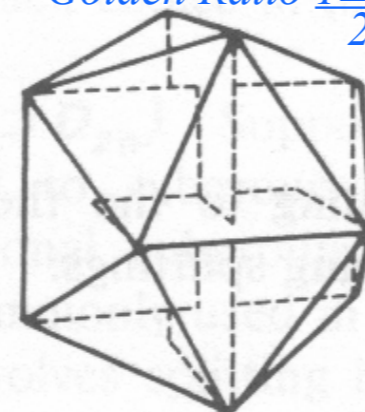
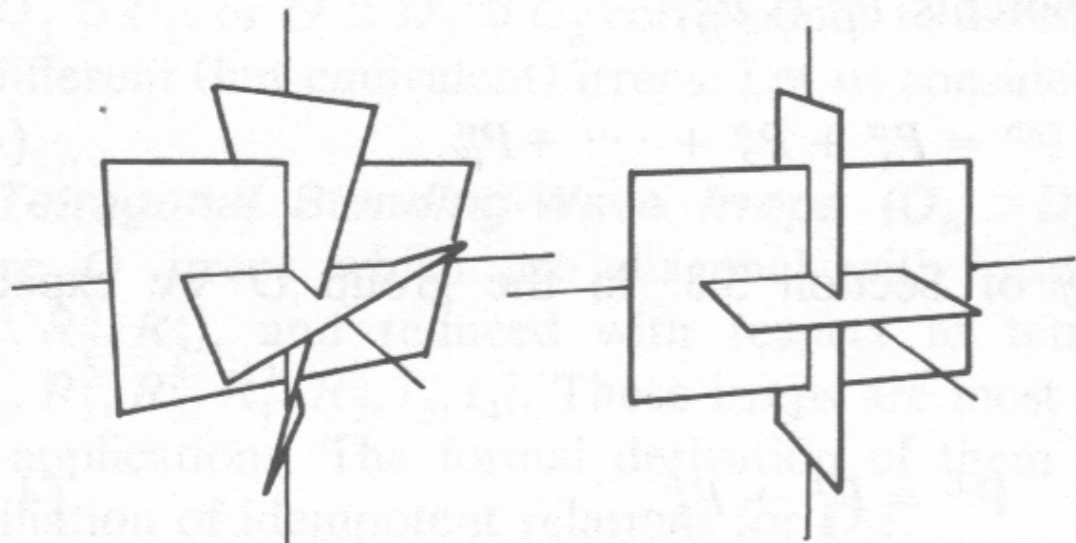


T symmetry

T_h symmetry

I_h symmetry

(If rectangles have Golden Ratio $\frac{1 \pm \sqrt{5}}{2}$)



Introduction to octahedral tetrahedral symmetry $O_h \supset O \sim T_d \supset T$

Octahedral groups $O_h \supset O \sim T_d$ and $O_h \supset T_h \supset T$

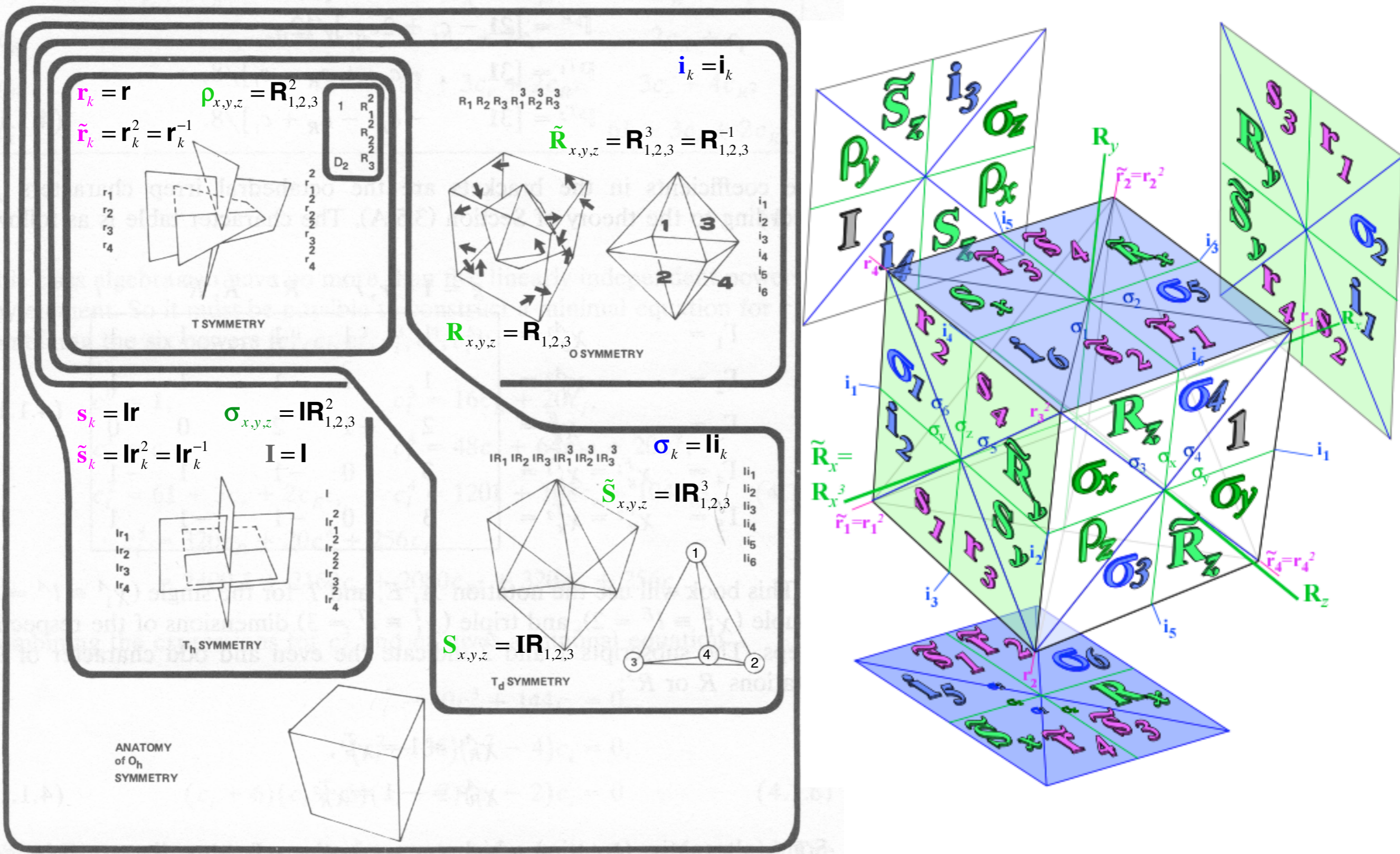
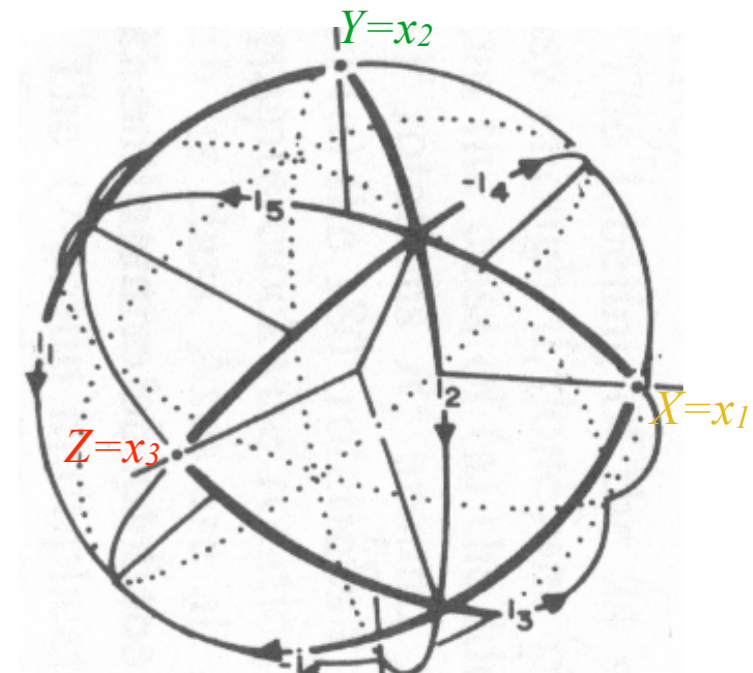
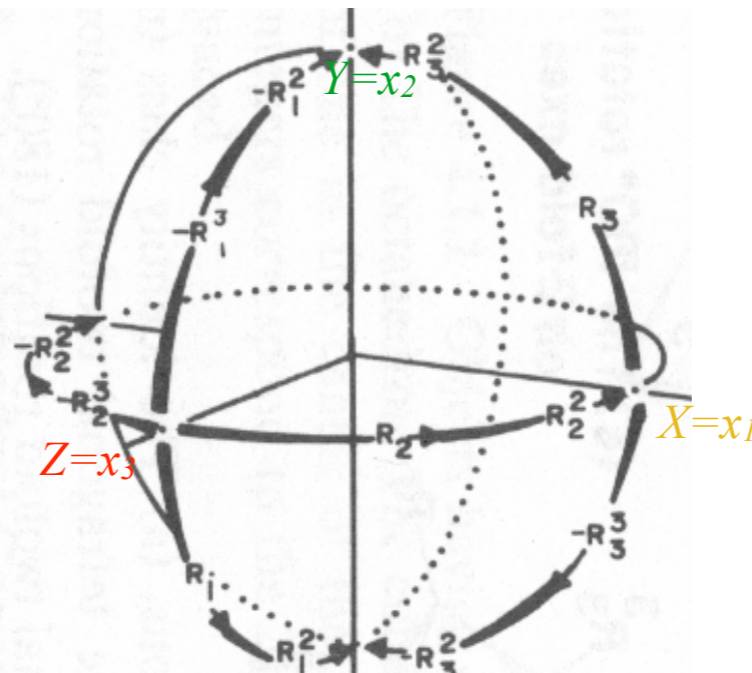
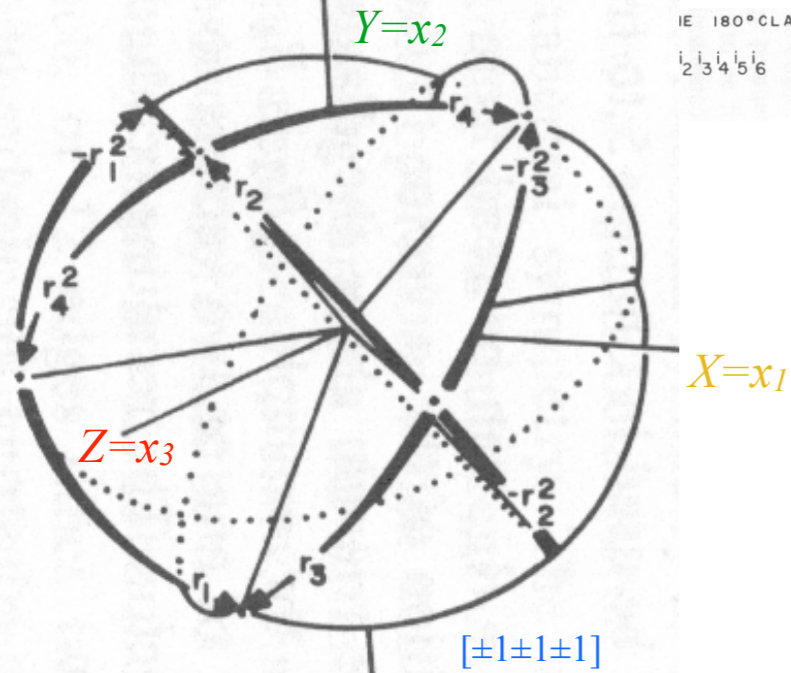


Figure 4.1.5 The full octahedral group (O_h) and four non-Abelian subgroups T , T_h , T_d , and O . The Abelian D_2 subgroup of T is indicated also.

Fig. 4.1.5 from *Principles of Symmetry, Dynamics and Spectroscopy*



$\underbrace{[111][\bar{1}\bar{1}\bar{1}][1\bar{1}\bar{1}][\bar{1}11]}_{+120^\circ}$
 $\underbrace{[\bar{1}\bar{1}\bar{1}][11\bar{1}][\bar{1}11][1\bar{1}\bar{1}]}_{-120^\circ}$
 $\underbrace{[100][010][001]}_{\pm 180^\circ XYZ}$
 $\underbrace{[100][010][001]}_{+90^\circ XYZ}$
 $\underbrace{[\bar{1}00][0\bar{1}0][00\bar{1}]}_{-90^\circ XYZ}$
 $\underbrace{[101][10\bar{1}][110][\bar{1}\bar{1}0][01\bar{1}][011]}_{\pm 180^\circ i_k}$

1	r_1	r_2	r_3	r_4	r_1^2	r_2^2	r_3^2	r_4^2	R_1^2	R_2^2	R_3^2	R_1	R_2	R_3	R_1^3	R_2^3	R_3^3	i_1	i_2	i_3	i_4	i_5	i_6
r_1	r_1^2	$-r_4^2$	$-r_2^2$	$-r_3^2$	-1	$-R_2^2$	$-R_3^2$	$-R_1^2$	$-r_2$	$-r_3$	$-r_4$	i_3	i_6	i_1	$-R_3$	$-R_1$	$-R_2$	R_1^3	i_5	R_2^3	i_2	$-i_4$	R_3^3
r_2	$-r_3^2$	r_2^2	$-r_4^2$	$-r_1^2$	R_2^2	-1	R_1^2	$-R_3^2$	r_1	r_4	$-r_3$	R_3	$-R_1^3$	i_2	i_3	$-i_5$	R_2^3	i_6	$-R_1$	R_2	$-i_1$	R_3^3	i_4
r_3	$-r_4^2$	$-r_1^2$	r_3^2	$-r_2^2$	R_3^2	$-R_1^2$	-1	R_2^2	$-r_4$	r_1	r_2	$-i_4$	R_1	$-R_2^3$	R_3^3	i_6	i_2	i_5	$-R_1^3$	i_1	R_2	$-i_3$	R_3
r_4	$-r_2^2$	$-r_3^2$	$-r_1^2$	r_4^2	R_1^2	R_3^2	$-R_2^2$	-1	r_3	$-r_2$	r_1	$-R_3^3$	$-i_5$	R_2	$-i_4$	R_1^3	i_1	R_1	i_6	$-i_2$	R_2^3	R_3	i_3
r_1^2	-1	R_1^2	R_2^2	R_3^2	$-r_1$	r_3	r_4	r_2	r_4^2	r_2^2	r_3^2	R_2^3	R_3^3	R_1^3	$-i_1$	$-i_3$	$-i_6$	$-R_3$	$-i_4$	$-R_1$	i_5	$-i_2$	$-R_2$
r_2^2	$-R_1^2$	-1	R_3^2	$-R_2^2$	r_4	$-r_2$	r_1	r_3	$-r_3^2$	$-r_1^2$	r_4^2	i_2	$-i_3$	$-R_1$	R_2	$-R_3^3$	$-i_5$	i_4	$-R_3$	$-R_1^3$	$-i_6$	R_2^3	$-i_1$
r_3^2	$-R_2^2$	$-R_3^2$	-1	R_1^2	r_2	r_4	$-r_3$	r_1	r_2^2	$-r_4^2$	$-r_1^2$	$-R_2$	$-i_4$	$-i_6$	i_2	R_3	$-R_1^3$	$-i_3$	$-R_3^3$	i_5	R_1	$-i_1$	$-R_2^3$
r_4^2	$-R_3^2$	R_2^2	$-R_1^2$	-1	r_3	r_1	r_2	$-r_4$	$-r_1^2$	r_3^2	$-r_2^2$	$-i_1$	$-R_3$	$-i_5$	$-R_2^3$	$-i_4$	R_1	$-R_3^3$	i_3	$-i_6$	R_1^3	R_2	$-i_2$
R_1^2	$-r_4$	r_3	$-r_2$	r_1	r_2^2	$-r_1^2$	r_4^2	$-r_3^2$	-1	R_3^2	$-R_2^2$	R_1^3	i_1	$-i_4$	$-R_1$	i_2	$-i_3$	$-R_2$	$-R_2^3$	R_3^3	R_3	$-i_6$	i_5
R_2^2	$-r_2$	r_1	r_4	$-r_3$	r_3^2	$-r_4^2$	$-r_1^2$	r_2^2	$-R_3^2$	-1	R_1^2	$-i_5$	R_2^3	i_3	$-i_6$	$-R_2$	$-i_4$	$-i_2$	i_1	$-R_3$	R_3^3	R_1	R_1^3
R_3^2	$-r_3$	$-r_4$	r_1	r_2	r_4^2	r_3^2	$-r_2^2$	$-r_1^2$	R_2^2	$-R_1^2$	-1	i_6	i_2	R_3^3	$-i_5$	$-i_1$	$-R_3$	R_2^3	$-R_2$	i_4	$-i_3$	R_1^3	$-R_1$
R_1	i_1	$-R_2^3$	$-i_2$	R_2	R_3^3	$-i_3$	$-R_3$	i_4	R_1^3	i_6	i_5	R_1^2	r_1	$-r_4^2$	-1	$-r_3$	r_2^2	$-r_4$	r_2	r_1^2	$-r_3^2$	$-R_2^2$	R_3^2
R_2	i_3	R_3	$-R_3^3$	i_4	R_1^3	i_5	$-i_6$	$-R_1$	$-i_2$	R_2^3	i_1	$-r_2^2$	R_2^2	r_1	r_3^2	-1	$-r_4$	R_1^2	R_3^3	$-r_2$	$-r_3$	$-r_4^2$	r_1^2
R_3	i_6	i_5	R_1	$-R_1^3$	R_2^3	$-R_2$	$-i_2$	$-i_1$	i_3	i_4	R_3^3	r_1	$-r_3^2$	R_3^2	$-r_2$	r_4^2	-1	r_1^2	r_2^2	R_2^2	$-R_1^2$	$-r_4$	$-r_3$
R_1^3	$-R_2$	$-i_2$	R_2^3	i_1	$-i_3$	$-R_3^3$	i_4	R_3	$-R_1$	i_5	$-i_6$	-1	$-r_4$	r_3^2	$-R_1^2$	r_2	$-r_1^2$	$-r_1$	r_3	r_2^2	$-r_4^2$	$-R_2^3$	$-R_2^2$
R_2^3	$-R_3$	i_3	i_4	R_3^3	$-i_6$	R_1	$-R_1^3$	i_5	$-i_1$	$-R_2$	$-i_2$	r_4^2	-1	$-r_2$	$-r_1^2$	$-R_2^2$	r_3	$-R_3^2$	R_1^2	$-r_1$	$-r_4$	$-r_2^2$	r_3^2
R_3^3	$-R_1$	R_1^3	i_6	i_5	$-i_1$	$-i_2$	R_2	$-R_2^3$	i_4	$-i_3$	$-R_3$	$-r_3$	r_2^2	-1	r_4	$-r_1^2$	$-R_3^2$	r_4^2	r_3^2	$-R_1^2$	$-R_2^2$	$-r_2$	$-r_1$
i_1	R_3^3	$-i_4$	i_3	R_3	$-R_1$	$-i_6$	$-i_5$	$-R_1^3$	R_2^3	i_2	$-R_2$	r_1^2	R_3^2	$-r_4$	r_4^2	$-R_1^2$	$-r_1$	-1	$-R_2^2$	$-r_3$	r_2	r_3^2	r_2^2
i_2	i_4	R_3^3	R_3	$-i_3$	$-i_5$	R_1^3	R_1	$-i_6$	R_2	$-i_1$	R_2^2	$-r_3^2$	$-R_1^2$	$-r_3$	$-r_2^2$	$-R_3^2$	$-r_2$	R_2^2	-1	r_4	$-r_1$	r_1^2	r_4^2
i_3	R_1^3	R_1	$-i_5$	i_6	$-R_2$	$-R_2^3$	$-i_1$	i_2	$-R_3$	R_3^3	$-i_4$	$-r_2$	r_1^2	R_1^2	$-r_1$	r_2^2	$-R_2^2$	r_3^2	$-r_4^2$	-1	R_3^2	r_3	$-r_4$
i_4	$-i_5$	i_6	$-R_1^3$	$-R_1$	$-i_2$	i_1	$-R_2^2$	$-R_2$	$-R_3^3$	$-R_3$	i_3	r_4	r_4^2	R_2^2	r_3	r_3^2	R_1^2	$-r_2^2$	r_1^2	$-R_3^3$	-1	r_1	$-r_2$
i_5	i_2	$-R_2$	i_1	$-R_2^3$	i_4	$-R_3$	i_3	$-R_3^3$	i_6	$-R_1^3$	$-R_1$	R_3^2	r_2	r_2^2	R_2^2	r_4	r_4^2	$-r_3$	$-r_1$	$-r_3^2$	$-r_1^2$	-1	$-R_1^2$
i_6	R_2^3	i_1	R_2	i_2	$-R_3$	$-i_4$	$-R_3^3$	$-i_3$	$-i_5$	$-R_1$	R_1^3	R_2^2	$-r_3$	r_1^2	$-R_3^2$	$-r_1$	r_3^2	$-r_2$	$-r_4$	r_4^2	r_2^2	R_1^2	-1

Octahedral O and spin-OCU(2) rotation product Table F.2.1 from Principles of Symmetry, Dynamics and Spectroscopy