Group Theory in Quantum Mechanics

Lecture 21 (4.09.15)

Octahedral $O_h \supset$subgroup tunneling parameter modeling

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

Review Calculating idempotent projectors $\mathbf{P}^{\mu}_{m,m}$ of $O \supset C_4$ $\mathbf{P}^{E}_{0_4 0_4}$ $\mathbf{P}^{E}_{2_4 2_4}$ $\mathbf{P}^{T_1}_{0_4 0_4}$ $\mathbf{P}^{T_1}_{1_4 1_4}$ $\mathbf{P}^{T_2}_{2_4 2_4}$

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

Review Broken-class-ordered splitting of $O \supset D_4 \supset C_4$ projectors and levels

Subgroup-defined tunneling parameter modeling

Comparing two diagonal $O \supset C_4$ parameter sets to SF_6 spectra

Comparing two diagonal $O \supset C_3$ parameter sets to SF_6 spectra

Why $O \supset C_2$ parameter sets require off-diagonal nilpotent $\mathbf{P}^{\mu}_{m,n}$ $(m \neq n)$

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

Using fundamental $\mathbf{g} \rightleftarrows \mathbf{P}^{\mu}_{m,n}$ relations: (from Lecture 16)

(a) $\mathbf{P}^{\mu}_{m,m}\mathbf{g}\mathbf{P}^{\mu}_{n,n} = D^{\mu}_{m,n}(\mathbf{g})\mathbf{P}^{\mu}_{m,n}$ (b) $\mathbf{g} = \Sigma_{\mu}\Sigma_{m,n} D^{\mu}_{m,n}(\mathbf{g})\mathbf{P}^{\mu}_{m,n}$ (c) $\mathbf{P}^{\mu}_{n,n} = (\ell^{\mu}/{}^{\circ}G)\Sigma_{\mathbf{g}} D^{\mu *}_{m,n}(\mathbf{g})\mathbf{g}$

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

Calculating and Factoring $\mathbf{P}^{T_1}_{1_4 0_4}$ and $\mathbf{P}^{T_1}_{1_4 3_4}$

Structure and applications of various subgroup chain irreducible representations

$O_h \supset D_{4h} \supset C_{4v}$, $O_h \supset D_{3h} \supset C_{3v}$, $O_h \supset C_{2v}$

Comparing $O_h \supset D_{4h} \supset D_{2h}$ and $O_h \supset D_{3d} \supset C_2$ representations (T_1 vector-type)

Examples of off-diagonal tunneling coefficients $D^{E}_{0_4 2_4}$

Comparing Local C_4, C_3, and C_2 symmetric spectra

When Local C_2 symmetry dominates

Comparing off-diagonal $O \supset C_2$ parameter sets to CH_4 models with "cluster-crossings"

Review Calculating idempotent projectors $\mathbf{P}^{\mu}_{m,m}$ *of* $O\supset C_4$ $\mathbf{P}^{E}_{0_4 0_4}$ $\mathbf{P}^{E}_{2_4 2_4}$ $\mathbf{P}^{T_1}_{0_4 0_4}$ $\mathbf{P}^{T_1}_{1_4 1_4}$ $\mathbf{P}^{T_2}_{2_4 2_4}$

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

Review Broken-class-ordered splitting of $O\supset D_4\supset C_4$ *projectors and levels*

Subgroup-defined tunneling parameter modeling

Comparing two diagonal $O\supset C_4$ *parameter sets to* SF_6 *spectra*

Comparing two diagonal $O\supset C_3$ *parameter sets to* SF_6 *spectra*

Why $O\supset C_2$ *parameter sets require off-diagonal nilpotent* $\mathbf{P}^{\mu}_{m,n}$ $(m\neq n)$

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

Using fundamental $\mathbf{g}\rightleftarrows\mathbf{P}^{\mu}_{m,n}$ *relations: (from Lecture 16)*

(a) $\mathbf{P}^{\mu}_{m,m}\,\mathbf{g}\mathbf{P}^{\mu}_{n,n}=D^{\mu}_{m,n}(\mathbf{g})\mathbf{P}^{\mu}_{m,n}$ (b) $\mathbf{g}=\Sigma_{\mu}\Sigma_{m,n}D^{\mu}_{m,n}(\mathbf{g})\mathbf{P}^{\mu}_{m,n}$ (c) $\mathbf{P}^{\mu}_{n,n}=(\ell^{\mu}/{}^{\circ}G)\Sigma_{\mathbf{g}}D^{\mu *}_{m,n}(\mathbf{g})\mathbf{g}$

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

Calculating and Factoring $\mathbf{P}^{T_1}_{1_4 0_4}$ *and* $\mathbf{P}^{T_1}_{1_4 3_4}$

Structure and applications of various subgroup chain irreducible representations

$O_h\supset D_{4h}\supset C_{4v}$, $O_h\supset D_{3h}\supset C_{3v}$, $O_h\supset C_{2v}$

Comparing $O_h\supset D_{4h}\supset D_{2h}$ *and* $O_h\supset D_{3d}\supset C_2$ *representations* (T_1 *vector-type*)

Examples of off-diagonal tunneling coefficients $D^{E}_{0_4 2_4}$

Comparing Local C_4, C_3, *and* C_2 *symmetric spectra*

Comparing off-diagonal $O\supset C_2$ *parameter sets to* CH_4 *models with "cluster-crossings"*

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

$O\supset C_4$	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 characters

$O:\chi^{\mu}_{\mathbf{g}}$	$\mathbf{g}=\mathbf{1}$	$\mathbf{r}^{p}_{1-4}$	ρ_{xyz}	$\mathbf{R}^{p}_{xyz}$	$\mathbf{i}_{1-6}$
$\mu=A_1$	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

$$d^{m_4}_{R^p}=e^{\frac{2\pi i\, m_4\cdot p}{4}}$$

C_4 characters

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

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

$$=\sum_{g}^{\circ O}\frac{\ell^{E}}{\circ O}(\chi^{E}_{g})\cdot\mathbf{g}\cdot(\mathbf{p}_{0_4})=\sum_{g}^{\circ O}\frac{2}{96}(\chi^{E}_{g})\cdot\mathbf{g}\cdot(1\cdot\mathbf{1}+1\cdot\rho_z+1\cdot\mathbf{R}_z+1\cdot\tilde{\mathbf{R}}_z)$$

$$\mathbf{1}C_4=\mathbf{1}\{\mathbf{1},\rho_z,\mathbf{R}_z,\tilde{\mathbf{R}}_z\}\quad \rho_x C_4=\{\rho_x,\rho_y,\mathbf{i}_4,\mathbf{i}_3\}\quad \mathbf{r}_1C_4=\{\mathbf{r}_1,\mathbf{r}_4,\mathbf{i}_1,\mathbf{R}_y\}\quad \mathbf{r}_2C_4=\{\mathbf{r}_2,\mathbf{r}_3,\mathbf{i}_2,\tilde{\mathbf{R}}_y\}\quad \tilde{\mathbf{r}}_1C_4=\{\tilde{\mathbf{r}}_1,\tilde{\mathbf{r}}_3,\tilde{\mathbf{R}}_x,\mathbf{i}_6\}\quad \tilde{\mathbf{r}}_2C_4=\{\tilde{\mathbf{r}}_2,\tilde{\mathbf{r}}_4,\mathbf{R}_x,\mathbf{i}_5\}$$

$$=\tfrac{1}{48}\chi^{E}_{\mathbf{1}}(1,d^{0_4}_{\rho_z},d^{0_4}_{R_z},d^{0_4}_{\tilde{R}_z})+\tfrac{1}{48}\chi^{E}_{\rho_x}(1,d^{0_4}_{\rho_z},d^{0_4}_{R_z},d^{0_4}_{\tilde{R}_z})+\tfrac{1}{48}\chi^{E}_{\mathbf{r}_1}(1,d^{0_4}_{\rho_z},d^{0_4}_{R_z},d^{0_4}_{\tilde{R}_z})+\tfrac{1}{48}\chi^{E}_{\mathbf{r}_2}(1,d^{0_4}_{\rho_z},d^{0_4}_{R_z},d^{0_4}_{\tilde{R}_z})+\tfrac{1}{48}\chi^{E}_{\tilde{\mathbf{r}}_1}(1,d^{0_4}_{\rho_z},d^{0_4}_{R_z},d^{0_4}_{\tilde{R}_z})+\tfrac{1}{48}\chi^{E}_{\tilde{\mathbf{r}}_2}(1,d^{0_4}_{\rho_z},d^{0_4}_{R_z},d^{0_4}_{\tilde{R}_z})$$

$$+\tfrac{1}{48}\chi^{E}_{\rho_z}(d^{0_4}_{\rho_z},1,d^{0_4}_{\tilde{R}_z},d^{0_4}_{R_z})+\tfrac{1}{48}\chi^{E}_{\rho_y}(d^{0_4}_{\rho_z},1,d^{0_4}_{\tilde{R}_z},d^{0_4}_{R_z})+\tfrac{1}{48}\chi^{E}_{\mathbf{r}_4}(d^{0_4}_{\rho_z},1,d^{0_4}_{\tilde{R}_z},d^{0_4}_{R_z})+\tfrac{1}{48}\chi^{E}_{\mathbf{r}_3}(d^{0_4}_{\rho_z},1,d^{0_4}_{\tilde{R}_z},d^{0_4}_{R_z})+\tfrac{1}{48}\chi^{E}_{\tilde{\mathbf{r}}_3}(d^{0_4}_{\rho_z},1,d^{0_4}_{\tilde{R}_z},d^{0_4}_{R_z})+\tfrac{1}{48}\chi^{E}_{\tilde{\mathbf{r}}_4}(d^{0_4}_{\rho_z},1,d^{0_4}_{\tilde{R}_z},d^{0_4}_{R_z})$$

$$+\tfrac{1}{48}\chi^{E}_{\mathbf{R}_z}(d^{0_4}_{\tilde{R}_z},d^{0_4}_{R_z},1,d^{0_4}_{\rho_z})+\tfrac{1}{48}\chi^{E}_{\mathbf{i}_4}(d^{0_4}_{\tilde{R}_z},d^{0_4}_{R_z},1,d^{0_4}_{\rho_z})+\tfrac{1}{48}\chi^{E}_{\mathbf{i}_1}(d^{0_4}_{\tilde{R}_z},d^{0_4}_{R_z},1,d^{0_4}_{\rho_z})+\tfrac{1}{48}\chi^{E}_{\mathbf{i}_2}(d^{0_4}_{\tilde{R}_z},d^{0_4}_{R_z},1,d^{0_4}_{\rho_z})+\tfrac{1}{48}\chi^{E}_{\tilde{\mathbf{R}}_x}(d^{0_4}_{\tilde{R}_z},d^{0_4}_{R_z},1,d^{0_4}_{\rho_z})+\tfrac{1}{48}\chi^{E}_{\mathbf{R}_x}(d^{0_4}_{\tilde{R}_z},d^{0_4}_{R_z},1,d^{0_4}_{\rho_z})$$

$$+\tfrac{1}{48}\chi^{E}_{\tilde{\mathbf{R}}_z}(d^{0_4}_{R_z},d^{0_4}_{\tilde{R}_z},d^{0_4}_{\rho_z},1)+\tfrac{1}{48}\chi^{E}_{\mathbf{i}_3}(d^{0_4}_{R_z},d^{0_4}_{\tilde{R}_z},d^{0_4}_{\rho_z},1)+\tfrac{1}{48}\chi^{E}_{\mathbf{R}_y}(d^{0_4}_{R_z},d^{0_4}_{\tilde{R}_z},d^{0_4}_{\rho_z},1)+\tfrac{1}{48}\chi^{E}_{\tilde{\mathbf{R}}_y}(d^{0_4}_{R_z},d^{0_4}_{\tilde{R}_z},d^{0_4}_{\rho_z},1)+\tfrac{1}{48}\chi^{E}_{\mathbf{i}_6}(d^{0_4}_{R_z},d^{0_4}_{\tilde{R}_z},d^{0_4}_{\rho_z},1)+\tfrac{1}{48}\chi^{E}_{\mathbf{i}_5}(d^{0_4}_{R_z},d^{0_4}_{\tilde{R}_z},d^{0_4}_{\rho_z},1)$$

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

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

$$+\tfrac{1}{48}(0)(+1,+1,1,+1)+\tfrac{1}{48}(0)(+1,+1,1,+1)+\tfrac{1}{48}(0)(+1,+1,1,+1)+\tfrac{1}{48}(0)(+1,+1,1,+1)+\tfrac{1}{48}(0)(+1,+1,1,+1)+\tfrac{1}{48}(0)(+1,+1,1,+1)$$

$$+\tfrac{1}{48}(0)(+1,+1,+1,1)+\tfrac{1}{48}(0)(+1,+1,+1,1)+\tfrac{1}{48}(0)(+1,+1,+1,1)+\tfrac{1}{48}(0)(+1,+1,+1,1)+\tfrac{1}{48}(0)(+1,+1,+1,1)+\tfrac{1}{48}(0)(+1,+1,+1,1)$$

4, 4, 4, 4,   4, 4, 4, 4,   -2,-2,-2,-2,   -2,-2,-2,-2,   -2,-2,-2,-2,   -2,-2,-2,-2,

$$\mathbf{P}^{E}_{0_4 0_4}=\tfrac{1}{12}(1\mathbf{1}+1\rho_z+1\mathbf{R}_z+1\tilde{\mathbf{R}}_z+1\rho_x+1\rho_y+1\mathbf{i}_4+1\mathbf{i}_3\ -\tfrac{1}{2}\mathbf{r}_1-\tfrac{1}{2}\mathbf{r}_4-\tfrac{1}{2}\mathbf{i}_1-\tfrac{1}{2}\mathbf{R}_y\ -\tfrac{1}{2}\mathbf{r}_2-\tfrac{1}{2}\mathbf{r}_3-\tfrac{1}{2}\mathbf{i}_2-\tfrac{1}{2}\tilde{\mathbf{R}}_y\ -\tfrac{1}{2}\tilde{\mathbf{r}}_1-\tfrac{1}{2}\tilde{\mathbf{r}}_3-\tfrac{1}{2}\tilde{\mathbf{R}}_x-\tfrac{1}{2}\mathbf{i}_6\ -\tfrac{1}{2}\tilde{\mathbf{r}}_2-\tfrac{1}{2}\tilde{\mathbf{r}}_4-\tfrac{1}{2}\mathbf{R}_x-\tfrac{1}{2}\mathbf{i}_5)$$

Coset-factored sum:

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

Broken-class-ordered sum:

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

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 characters

$O:\chi^{\mu}_{\mathbf{g}}$	$\mathbf{g}$=1	$\mathbf{r}^p_{1-4}$	ρ_{xyz}	$\mathbf{R}^p_{xyz}$	$\mathbf{i}_{1-6}$
$\mu=A_1$	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

$$d^{m_4}_{R^p}=e^{\frac{2\pi i m_4\cdot p}{4}}$$

C_4 characters

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

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

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

$$\mathbf{1}C_4=\mathbf{1}\{\mathbf{1},\rho_z,\mathbf{R}_z,\tilde{\mathbf{R}}_z\}\quad \rho_x C_4=\{\rho_x,\rho_y,\mathbf{i}_4,\mathbf{i}_3\}\quad \mathbf{r}_1C_4=\{\mathbf{r}_1,\mathbf{r}_4,\mathbf{i}_1,\mathbf{R}_y\}\quad \mathbf{r}_2C_4=\{\mathbf{r}_2,\mathbf{r}_3,\mathbf{i}_2,\tilde{\mathbf{R}}_y\}\quad \tilde{\mathbf{r}}_1C_4=\{\tilde{\mathbf{r}}_1,\tilde{\mathbf{r}}_3,\tilde{\mathbf{R}}_x,\mathbf{i}_6\}\quad \tilde{\mathbf{r}}_2C_4=\{\tilde{\mathbf{r}}_2,\tilde{\mathbf{r}}_4,\mathbf{R}_x,\mathbf{i}_5\}$$

$$=\tfrac{1}{32}\chi^{T_1}_{\mathbf{1}}(1,d^{0_4}_{\rho_z},d^{0_4}_{R_z},d^{0_4}_{\tilde{R}_z})+\tfrac{1}{32}\chi^{T_1}_{\rho_x}(1,d^{0_4}_{\rho_z},d^{0_4}_{R_z},d^{0_4}_{\tilde{R}_z})+\tfrac{1}{32}\chi^{T_1}_{\mathbf{r}_1}(1,d^{0_4}_{\rho_z},d^{0_4}_{R_z},d^{0_4}_{\tilde{R}_z})+\tfrac{1}{32}\chi^{T_1}_{\mathbf{r}_2}(1,d^{0_4}_{\rho_z},d^{0_4}_{R_z},d^{0_4}_{\tilde{R}_z})+\tfrac{1}{32}\chi^{T_1}_{\tilde{\mathbf{r}}_1}(1,d^{0_4}_{\rho_z},d^{0_4}_{R_z},d^{0_4}_{\tilde{R}_z})+\tfrac{1}{32}\chi^{T_1}_{\tilde{\mathbf{r}}_2}(1,d^{0_4}_{\rho_z},d^{0_4}_{R_z},d^{0_4}_{\tilde{R}_z})$$

$$+\tfrac{1}{32}\chi^{T_1}_{\rho_z}(d^{0_4}_{\rho_z},1,d^{0_4}_{\tilde{R}_z},d^{0_4}_{R_z})+\tfrac{1}{32}\chi^{T_1}_{\rho_y}(d^{0_4}_{\rho_z},1,d^{0_4}_{\tilde{R}_z},d^{0_4}_{R_z})+\tfrac{1}{32}\chi^{T_1}_{\mathbf{r}_4}(d^{0_4}_{\rho_z},1,d^{0_4}_{\tilde{R}_z},d^{0_4}_{R_z})+\tfrac{1}{32}\chi^{T_1}_{\mathbf{r}_3}(d^{0_4}_{\rho_z},1,d^{0_4}_{\tilde{R}_z},d^{0_4}_{R_z})+\tfrac{1}{32}\chi^{T_1}_{\tilde{\mathbf{r}}_3}(d^{0_4}_{\rho_z},1,d^{0_4}_{\tilde{R}_z},d^{0_4}_{R_z})+\tfrac{1}{32}\chi^{T_1}_{\tilde{\mathbf{r}}_4}(d^{0_4}_{\rho_z},1,d^{0_4}_{\tilde{R}_z},d^{0_4}_{R_z})$$

$$+\tfrac{1}{32}\chi^{T_1}_{\mathbf{R}_z}(d^{0_4}_{\tilde{R}_z},d^{0_4}_{R_z},1,d^{0_4}_{\rho_z})+\tfrac{1}{32}\chi^{T_1}_{\mathbf{i}_4}(d^{0_4}_{\tilde{R}_z},d^{0_4}_{R_z},1,d^{0_4}_{\rho_z})+\tfrac{1}{32}\chi^{T_1}_{\mathbf{i}_1}(d^{0_4}_{\tilde{R}_z},d^{0_4}_{R_z},1,d^{0_4}_{\rho_z})+\tfrac{1}{32}\chi^{T_1}_{\mathbf{i}_2}(d^{0_4}_{\tilde{R}_z},d^{0_4}_{R_z},1,d^{0_4}_{\rho_z})+\tfrac{1}{32}\chi^{T_1}_{\tilde{\mathbf{R}}_x}(d^{0_4}_{\tilde{R}_z},d^{0_4}_{R_z},1,d^{0_4}_{\rho_z})+\tfrac{1}{32}\chi^{T_1}_{\mathbf{R}_x}(d^{0_4}_{\tilde{R}_z},d^{0_4}_{R_z},1,d^{0_4}_{\rho_z})$$

$$+\tfrac{1}{32}\chi^{T_1}_{\tilde{\mathbf{R}}_z}(d^{0_4}_{R_z},d^{0_4}_{\tilde{R}_z},d^{0_4}_{\rho_z},1)+\tfrac{1}{32}\chi^{T_1}_{\mathbf{i}_3}(d^{0_4}_{R_z},d^{0_4}_{\tilde{R}_z},d^{0_4}_{\rho_z},1)+\tfrac{1}{32}\chi^{T_1}_{\mathbf{R}_y}(d^{0_4}_{R_z},d^{0_4}_{\tilde{R}_z},d^{0_4}_{\rho_z},1)+\tfrac{1}{32}\chi^{T_1}_{\tilde{\mathbf{R}}_y}(d^{0_4}_{R_z},d^{0_4}_{\tilde{R}_z},d^{0_4}_{\rho_z},1)+\tfrac{1}{32}\chi^{T_1}_{\mathbf{i}_6}(d^{0_4}_{R_z},d^{0_4}_{\tilde{R}_z},d^{0_4}_{\rho_z},1)+\tfrac{1}{32}\chi^{T_1}_{\mathbf{i}_5}(d^{0_4}_{R_z},d^{0_4}_{\tilde{R}_z},d^{0_4}_{\rho_z},1)$$

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

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

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

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

4, 4, 0, 0,   -4, -4, -4, -4,   0, 0, 0, 0,   0, 0, 0, 0,   0, 0, 0, 0,   0, 0, 0, 0,

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

Coset-factored sum:

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

Broken-class-ordered sum:

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

Calculating $\mathbf{P}^{T_1}{}_{1_4 1_4}$

$O\supset C_4$	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 characters

$O:\chi^{\mu}_{\mathbf{g}}$	$\mathbf{g}$=1	$\mathbf{r}^p_{1-4}$	ρ_{xyz}	$\mathbf{R}^p_{xyz}$	$\mathbf{i}_{1-6}$
$\mu=A_1$	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

$$d^{m_4}_{R^p}=e^{\frac{2\pi i m_4\cdot p}{4}}$$

C_4 characters

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

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

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

$$\mathbf{1}C_4=\mathbf{1}\{\mathbf{1},\rho_z,\mathbf{R}_z,\tilde{\mathbf{R}}_z\}\quad \rho_xC_4=\{\rho_x,\rho_y,\mathbf{i}_4,\mathbf{i}_3\}\quad \mathbf{r}_1C_4=\{\mathbf{r}_1,\mathbf{r}_4,\mathbf{i}_1,\mathbf{R}_y\}\quad \mathbf{r}_2C_4=\{\mathbf{r}_2,\mathbf{r}_3,\mathbf{i}_2,\tilde{\mathbf{R}}_y\}\quad \tilde{\mathbf{r}}_1C_4=\{\tilde{\mathbf{r}}_1,\tilde{\mathbf{r}}_3,\tilde{\mathbf{R}}_x,\mathbf{i}_6\}\quad \tilde{\mathbf{r}}_2C_4=\{\tilde{\mathbf{r}}_2,\tilde{\mathbf{r}}_4,\mathbf{R}_x,\mathbf{i}_5\}$$

$$=\tfrac{1}{32}\chi^{T_1}_{\mathbf{1}}(1,d^{1_4}_{\rho_z},d^{1_4}_{R_z},d^{1_4}_{\tilde{R}_z})+\tfrac{1}{32}\chi^{T_1}_{\rho_x}(1,d^{1_4}_{\rho_z},d^{1_4}_{R_z},d^{1_4}_{\tilde{R}_z})+\tfrac{1}{32}\chi^{T_1}_{\mathbf{r}_1}(1,d^{1_4}_{\rho_z},d^{1_4}_{R_z},d^{1_4}_{\tilde{R}_z})+\tfrac{1}{32}\chi^{T_1}_{\mathbf{r}_2}(1,d^{1_4}_{\rho_z},d^{1_4}_{R_z},d^{1_4}_{\tilde{R}_z})+\tfrac{1}{32}\chi^{T_1}_{\tilde{\mathbf{r}}_1}(1,d^{1_4}_{\rho_z},d^{1_4}_{R_z},d^{1_4}_{\tilde{R}_z})+\tfrac{1}{32}\chi^{T_1}_{\tilde{\mathbf{r}}_2}(1,d^{1_4}_{\rho_z},d^{1_4}_{R_z},d^{1_4}_{\tilde{R}_z})$$

$$+\tfrac{1}{32}\chi^{T_1}_{\rho_z}(d^{1_4}_{\rho_z},1,d^{1_4}_{\tilde{R}_z},d^{1_4}_{R_z})+\tfrac{1}{32}\chi^{T_1}_{\rho_y}(d^{1_4}_{\rho_z},1,d^{1_4}_{\tilde{R}_z},d^{1_4}_{R_z})+\tfrac{1}{32}\chi^{T_1}_{\mathbf{r}_4}(d^{1_4}_{\rho_z},1,d^{1_4}_{\tilde{R}_z},d^{1_4}_{R_z})+\tfrac{1}{32}\chi^{T_1}_{\mathbf{r}_3}(d^{1_4}_{\rho_z},1,d^{1_4}_{\tilde{R}_z},d^{1_4}_{R_z})+\tfrac{1}{32}\chi^{T_1}_{\tilde{\mathbf{r}}_3}(d^{1_4}_{\rho_z},1,d^{1_4}_{\tilde{R}_z},d^{1_4}_{R_z})+\tfrac{1}{32}\chi^{T_1}_{\tilde{\mathbf{r}}_4}(d^{1_4}_{\rho_z},1,d^{1_4}_{\tilde{R}_z},d^{1_4}_{R_z})$$

$$+\tfrac{1}{32}\chi^{T_1}_{\mathbf{R}_z}(d^{1_4}_{\tilde{R}_z},d^{1_4}_{R_z},1,d^{1_4}_{\rho_z})+\tfrac{1}{32}\chi^{T_1}_{\mathbf{i}_4}(d^{1_4}_{\tilde{R}_z},d^{1_4}_{R_z},1,d^{1_4}_{\rho_z})+\tfrac{1}{32}\chi^{T_1}_{\mathbf{i}_1}(d^{1_4}_{\tilde{R}_z},d^{1_4}_{R_z},1,d^{1_4}_{\rho_z})+\tfrac{1}{32}\chi^{T_1}_{\mathbf{i}_2}(d^{1_4}_{\tilde{R}_z},d^{1_4}_{R_z},1,d^{1_4}_{\rho_z})+\tfrac{1}{32}\chi^{T_1}_{\tilde{\mathbf{R}}_x}(d^{1_4}_{\tilde{R}_z},d^{1_4}_{R_z},1,d^{1_4}_{\rho_z})+\tfrac{1}{32}\chi^{T_1}_{\mathbf{R}_x}(d^{1_4}_{\tilde{R}_z},d^{1_4}_{R_z},1,d^{1_4}_{\rho_z})$$

$$+\tfrac{1}{32}\chi^{T_1}_{\tilde{\mathbf{R}}_z}(d^{1_4}_{R_z},d^{1_4}_{\tilde{R}_z},d^{1_4}_{\rho_z},1)+\tfrac{1}{32}\chi^{T_1}_{\mathbf{i}_3}(d^{1_4}_{R_z},d^{1_4}_{\tilde{R}_z},d^{1_4}_{\rho_z},1)+\tfrac{1}{32}\chi^{T_1}_{\mathbf{R}_y}(d^{1_4}_{R_z},d^{1_4}_{\tilde{R}_z},d^{1_4}_{\rho_z},1)+\tfrac{1}{32}\chi^{T_1}_{\tilde{\mathbf{R}}_y}(d^{1_4}_{R_z},d^{1_4}_{\tilde{R}_z},d^{1_4}_{\rho_z},1)+\tfrac{1}{32}\chi^{T_1}_{\mathbf{i}_6}(d^{1_4}_{R_z},d^{1_4}_{\tilde{R}_z},d^{1_4}_{\rho_z},1)+\tfrac{1}{32}\chi^{T_1}_{\mathbf{i}_5}(d^{1_4}_{R_z},d^{1_4}_{\tilde{R}_z},d^{1_4}_{\rho_z},1)$$

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

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

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

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

+4,-4, 4i,-4i, 0, 0, 0, 0, +2i, -2i,-2, +2, +2i, -2i,-2, +2, -2i,+2i,+2, -2 -2i,+2i,+2, -2.

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

Coset-factored sum:

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

Broken-class-ordered sum:

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

Review Calculating idempotent projectors $\mathbf{P}^{\mu}_{m,m}$ *of* $O\supset C_4$ $\mathbf{P}^{E}_{0_4 0_4}$ $\mathbf{P}^{E}_{2_4 2_4}$ $\mathbf{P}^{T_1}_{0_4 0_4}$ $\mathbf{P}^{T_1}_{1_4 1_4}$ $\mathbf{P}^{T_2}_{2_4 2_4}$

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

Review Broken-class-ordered splitting of $O\supset D_4\supset C_4$ *projectors and levels*

Subgroup-defined tunneling parameter modeling

Comparing two diagonal $O\supset C_4$ *parameter sets to* SF_6 *spectra*

Comparing two diagonal $O\supset C_3$ *parameter sets to* SF_6 *spectra*

Why $O\supset C_2$ *parameter sets require off-diagonal nilpotent* $\mathbf{P}^{\mu}_{m,n}$ $(m\neq n)$

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

Using fundamental $\mathbf{g}\rightleftarrows\mathbf{P}^{\mu}_{m,n}$ *relations: (from Lecture 16)*

(a) $\mathbf{P}^{\mu}_{m,m}\mathbf{g}\mathbf{P}^{\mu}_{n,n}=D^{\mu}_{m,n}(\mathbf{g})\mathbf{P}^{\mu}_{m,n}$ (b) $\mathbf{g}=\Sigma_{\mu}\Sigma_{m,n}D^{\mu}_{m,n}(\mathbf{g})\mathbf{P}^{\mu}_{m,n}$ (c) $\mathbf{P}^{\mu}_{n,n}=(\ell^{\mu}/{}^{\circ}G)\Sigma_{\mathbf{g}}D^{\mu*}_{m,n}(\mathbf{g})\mathbf{g}$

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

Calculating and Factoring $\mathbf{P}^{T_1}_{1_4 0_4}$ *and* $\mathbf{P}^{T_1}_{1_4 3_4}$

Structure and applications of various subgroup chain irreducible representations

$O_h\supset D_{4h}\supset C_{4v}$, $O_h\supset D_{3h}\supset C_{3v}$, $O_h\supset C_{2v}$

Comparing $O_h\supset D_{4h}\supset D_{2h}$ *and* $O_h\supset D_{3d}\supset C_2$ *representations (*T_1 *vector-type)*

Examples of off-diagonal tunneling coefficients $D^{E}_{0_4 2_4}$

Comparing Local C_4, C_3, *and* C_2 *symmetric spectra*

Comparing off-diagonal $O\supset C_2$ *parameter sets to* CH_4 *models with "cluster-crossings"*

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:

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

Coset-factored A_1-sum:

$$\mathbf{P}^{A_1}_{0_40_4}=\tfrac{1}{12}[(1)\cdot\mathbf{1}\mathbf{p}_{0_4}+(1)\cdot\boldsymbol{\rho}_x\mathbf{p}_{0_4}+(1)\cdot\mathbf{r}_1\mathbf{p}_{0_4}+(1)\cdot\mathbf{r}_2\mathbf{p}_{0_4}+(1)\cdot\tilde{\mathbf{r}}_1\mathbf{p}_{0_4}+(1)\cdot\tilde{\mathbf{r}}_2\mathbf{p}_{0_4}]$$

Coset-factored A_2-sum:

$$\mathbf{P}^{A_2}_{2_42_4}=\tfrac{1}{12}[(1)\cdot\mathbf{1}\mathbf{p}_{2_4}+(1)\cdot\boldsymbol{\rho}_x\mathbf{p}_{2_4}+(1)\cdot\mathbf{r}_1\mathbf{p}_{2_4}+(1)\cdot\mathbf{r}_2\mathbf{p}_{2_4}+(1)\cdot\tilde{\mathbf{r}}_1\mathbf{p}_{2_4}+(1)\cdot\tilde{\mathbf{r}}_2\mathbf{p}_{2_4}]$$

Coset-factored E-sum:

$$\mathbf{P}^{E}_{0_40_4}=\tfrac{1}{12}[(1)\cdot\mathbf{1}\mathbf{p}_{0_4}+(1)\cdot\boldsymbol{\rho}_x\mathbf{p}_{0_4}+(-\tfrac{1}{2})\cdot\mathbf{r}_1\mathbf{p}_{0_4}+(-\tfrac{1}{2})\cdot\mathbf{r}_2\mathbf{p}_{0_4}+(-\tfrac{1}{2})\cdot\tilde{\mathbf{r}}_1\mathbf{p}_{0_4}+(-\tfrac{1}{2})\cdot\tilde{\mathbf{r}}_2\mathbf{p}_{0_4}]$$

$$\mathbf{P}^{E}_{2_42_4}=\tfrac{1}{12}[(1)\cdot\mathbf{1}\mathbf{p}_{2_4}+(1)\cdot\boldsymbol{\rho}_x\mathbf{p}_{2_4}+(-\tfrac{1}{2})\cdot\mathbf{r}_1\mathbf{p}_{2_4}+(-\tfrac{1}{2})\cdot\mathbf{r}_2\mathbf{p}_{2_4}+(-\tfrac{1}{2})\cdot\tilde{\mathbf{r}}_1\mathbf{p}_{2_4}+(-\tfrac{1}{2})\cdot\tilde{\mathbf{r}}_2\mathbf{p}_{2_4}]$$

Coset-factored T_1-sum:

$$\mathbf{P}^{T_1}_{1_41_4}=\tfrac{1}{8}[(1)\cdot\mathbf{1}\mathbf{p}_{1_4}+(0)\cdot\boldsymbol{\rho}_x\mathbf{p}_{1_4}+(+\tfrac{i}{2})\cdot\mathbf{r}_1\mathbf{p}_{1_4}+(+\tfrac{i}{2})\cdot\mathbf{r}_2\mathbf{p}_{1_4}+(-\tfrac{i}{2})\cdot\tilde{\mathbf{r}}_1\mathbf{p}_{1_4}+(-\tfrac{i}{2})\cdot\tilde{\mathbf{r}}_2\mathbf{p}_{1_4}]$$

$$\mathbf{P}^{T_1}_{3_43_4}=\tfrac{1}{8}[(1)\cdot\mathbf{1}\mathbf{p}_{3_4}+(0)\cdot\boldsymbol{\rho}_x\mathbf{p}_{3_4}+(-\tfrac{i}{2})\cdot\mathbf{r}_1\mathbf{p}_{3_4}+(-\tfrac{i}{2})\cdot\mathbf{r}_2\mathbf{p}_{3_4}+(+\tfrac{i}{2})\cdot\tilde{\mathbf{r}}_1\mathbf{p}_{3_4}+(+\tfrac{i}{2})\cdot\tilde{\mathbf{r}}_2\mathbf{p}_{3_4}]$$

$$\mathbf{P}^{T_1}_{0_40_4}=\tfrac{1}{8}[(1)\cdot\mathbf{1}\mathbf{p}_{0_4}+(-1)\cdot\boldsymbol{\rho}_x\mathbf{p}_{0_4}+(0)\cdot\mathbf{r}_1\mathbf{p}_{0_4}+(0)\cdot\mathbf{r}_2\mathbf{p}_{0_4}+(0)\cdot\tilde{\mathbf{r}}_1\mathbf{p}_{0_4}+(0)\cdot\tilde{\mathbf{r}}_2\mathbf{p}_{0_4}]$$

Coset-factored T_2-sum:

$$\mathbf{P}^{T_2}_{1_41_4}=\tfrac{1}{8}[(1)\cdot\mathbf{1}\mathbf{p}_{1_4}+(0)\cdot\boldsymbol{\rho}_x\mathbf{p}_{1_4}+(-\tfrac{i}{2})\cdot\mathbf{r}_1\mathbf{p}_{1_4}+(-\tfrac{i}{2})\cdot\mathbf{r}_2\mathbf{p}_{1_4}+(-\tfrac{i}{2})\cdot\tilde{\mathbf{r}}_1\mathbf{p}_{1_4}+(-\tfrac{i}{2})\cdot\tilde{\mathbf{r}}_2\mathbf{p}_{1_4}]$$

$$\mathbf{P}^{T_2}_{3_43_4}=\tfrac{1}{8}[(1)\cdot\mathbf{1}\mathbf{p}_{3_4}+(0)\cdot\boldsymbol{\rho}_x\mathbf{p}_{3_4}+(+\tfrac{i}{2})\cdot\mathbf{r}_1\mathbf{p}_{3_4}+(+\tfrac{i}{2})\cdot\mathbf{r}_2\mathbf{p}_{3_4}+(+\tfrac{i}{2})\cdot\tilde{\mathbf{r}}_1\mathbf{p}_{3_4}+(+\tfrac{i}{2})\cdot\tilde{\mathbf{r}}_2\mathbf{p}_{3_4}]$$

$$\mathbf{P}^{T_2}_{2_42_4}=\tfrac{1}{8}[(1)\cdot\mathbf{1}\mathbf{p}_{2_4}+(1)\cdot\boldsymbol{\rho}_x\mathbf{p}_{2_4}+(0)\cdot\mathbf{r}_1\mathbf{p}_{2_4}+(0)\cdot\mathbf{r}_2\mathbf{p}_{2_4}+(0)\cdot\tilde{\mathbf{r}}_1\mathbf{p}_{2_4}+(0)\cdot\tilde{\mathbf{r}}_2\mathbf{p}_{2_4}]$$

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

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

$C_4:\chi^{\mu}_{\mathbf{g}}$	$\mathbf{g}=\mathbf{1}$	$\mathbf{R}_z$	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	$-i$

Review Calculating idempotent projectors $\mathbf{P}^{\mu}_{m,m}$ *of* $O \supset C_4$ $\mathbf{P}^{E}_{0_4 0_4}$ $\mathbf{P}^{E}_{2_4 2_4}$ $\mathbf{P}^{T_1}_{0_4 0_4}$ $\mathbf{P}^{T_1}_{1_4 1_4}$ $\mathbf{P}^{T_2}_{2_4 2_4}$

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

Review Broken-class-ordered splitting of $O \supset D_4 \supset C_4$ *projectors and levels*

Subgroup-defined tunneling parameter modeling

Comparing two diagonal $O \supset C_4$ *parameter sets to* SF_6 *spectra*

Comparing two diagonal $O \supset C_3$ *parameter sets to* SF_6 *spectra*

Why $O \supset C_2$ *parameter sets require off-diagonal nilpotent* $\mathbf{P}^{\mu}_{m,n}$ $(m \neq n)$

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

Using fundamental $\mathbf{g} \rightleftarrows \mathbf{P}^{\mu}_{m,n}$ *relations: (from Lecture 16)*

(a) $\mathbf{P}^{\mu}_{m,m}\mathbf{g}\mathbf{P}^{\mu}_{n,n} = D^{\mu}_{m,n}(\mathbf{g})\mathbf{P}^{\mu}_{m,n}$ (b) $\mathbf{g} = \Sigma_{\mu}\Sigma_{m,n} D^{\mu}_{m,n}(\mathbf{g})\mathbf{P}^{\mu}_{m,n}$ (c) $\mathbf{P}^{\mu}_{n,n} = (\ell^{\mu}/°G)\Sigma_{\mathbf{g}} D^{\mu *}_{m,n}(\mathbf{g})\mathbf{g}$

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

Calculating and Factoring $\mathbf{P}^{T_1}_{1_4 0_4}$ *and* $\mathbf{P}^{T_1}_{1_4 3_4}$

Structure and applications of various subgroup chain irreducible representations

$O_h \supset D_{4h} \supset C_{4v}$, $O_h \supset D_{3h} \supset C_{3v}$, $O_h \supset C_{2v}$

Comparing $O_h \supset D_{4h} \supset D_{2h}$ *and* $O_h \supset D_{3d} \supset C_2$ *representations* (T_1 *vector-type*)

Examples of off-diagonal tunneling coefficients $D^{E}_{0_4 2_4}$

Comparing Local C_4, C_3, *and* C_2 *symmetric spectra*

Comparing off-diagonal $O \supset C_2$ *parameter sets to* CH_4 *models with "cluster-crossings"*

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:*

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

Broken-class-ordered A_2*-sum:*

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

Broken-class-ordered E*-sum:*

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

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

Broken-class-ordered T_1*-sum:*

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

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

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

Broken-class-ordered T_2*-sum:*

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

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

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

O characters

$O:\chi^{\mu}_{\mathbf{g}}$	$\mathbf{g}$=1	$\mathbf{r}^p_{1-4}$	$\boldsymbol{\rho}_{xyz}$	$\mathbf{R}^p_{xyz}$	$\mathbf{i}_{1-6}$
$\mu=A_1$	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

$$d^{m_4}_{R^p} = e^{\frac{2\pi i m_4 \cdot p}{4}}$$

C_4 characters

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

Review Calculating idempotent projectors $\mathbf{P}^{\mu}_{m,m}$ *of* $O \supset C_4$ $\mathbf{P}^{E}_{0_4 0_4}$ $\mathbf{P}^{E}_{2_4 2_4}$ $\mathbf{P}^{T_1}_{0_4 0_4}$ $\mathbf{P}^{T_1}_{1_4 1_4}$ $\mathbf{P}^{T_2}_{2_4 2_4}$

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

Review Broken-class-ordered splitting of $O \supset D_4 \supset C_4$ *projectors and levels*

Subgroup-defined tunneling parameter modeling

Comparing two diagonal $O \supset C_4$ *parameter sets to* SF_6 *spectra*

Comparing two diagonal $O \supset C_3$ *parameter sets to* SF_6 *spectra*

Why $O \supset C_2$ *parameter sets require off-diagonal nilpotent* $\mathbf{P}^{\mu}_{m,n}$ $(m \neq n)$

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

Using fundamental $\mathbf{g} \rightleftarrows \mathbf{P}^{\mu}_{m,n}$ *relations: (from Lecture 16)*

(a) $\mathbf{P}^{\mu}_{m,m}\mathbf{g}\mathbf{P}^{\mu}_{n,n} = D^{\mu}_{m,n}(\mathbf{g})\mathbf{P}^{\mu}_{m,n}$ (b) $\mathbf{g} = \Sigma_{\mu}\Sigma_{m,n} D^{\mu}_{m,n}(\mathbf{g})\mathbf{P}^{\mu}_{m,n}$ (c) $\mathbf{P}^{\mu}_{n,n} = (\ell^{\mu}/{}^{\circ}G)\Sigma_{\mathbf{g}} D^{\mu *}_{m,n}(\mathbf{g})\mathbf{g}$

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

Calculating and Factoring $\mathbf{P}^{T_1}_{1_4 0_4}$ *and* $\mathbf{P}^{T_1}_{1_4 3_4}$

Structure and applications of various subgroup chain irreducible representations

$O_h \supset D_{4h} \supset C_{4v}$, $O_h \supset D_{3h} \supset C_{3v}$, $O_h \supset C_{2v}$

Comparing $O_h \supset D_{4h} \supset D_{2h}$ *and* $O_h \supset D_{3d} \supset C_2$ *representations* (T_1 *vector-type*)

Examples of off-diagonal tunneling coefficients $D^{E}_{0_4 2_4}$

Comparing Local C_4, C_3, *and* C_2 *symmetric spectra*

Comparing off-diagonal $O \supset C_2$ *parameter sets to* CH_4 *models with "cluster-crossings"*

$O\supset C_4$	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

$$\mathbf{1}\cdot\mathbf{P}^{\alpha}=(\mathbf{p}_{0_4}+\mathbf{p}_{1_4}+\mathbf{p}_{2_4}+\mathbf{p}_{3_4})\cdot\mathbf{P}^{\alpha}$$

$$\mathbf{1}\cdot\mathbf{P}^{A_1}=\mathbf{P}^{A_1}_{0_40_4}+0+0+0$$

$$\mathbf{1}\cdot\mathbf{P}^{A_2}=0+0+\mathbf{P}^{A_2}_{2_42_4}+0$$

$$\mathbf{1}\cdot\mathbf{P}^{E}=\mathbf{P}^{E}_{0_40_4}+0+\mathbf{P}^{E}_{2_42_4}+0$$

$$\mathbf{1}\cdot\mathbf{P}^{T_1}=\mathbf{P}^{T_1}_{0_40_4}+\mathbf{P}^{T_1}_{1_41_4}+0+\mathbf{P}^{T_1}_{3_43_4}$$

$$\mathbf{1}\cdot\mathbf{P}^{T_2}=0+\mathbf{P}^{T_2}_{1_41_4}+\mathbf{P}^{T_2}_{2_42_4}+\mathbf{P}^{T_2}_{3_43_4}$$

where: $\mathbf{p}_{m_4}=\frac{1}{4}\sum_{p=0}^{3}e^{im\cdot p/4}\mathbf{R}_z^p$

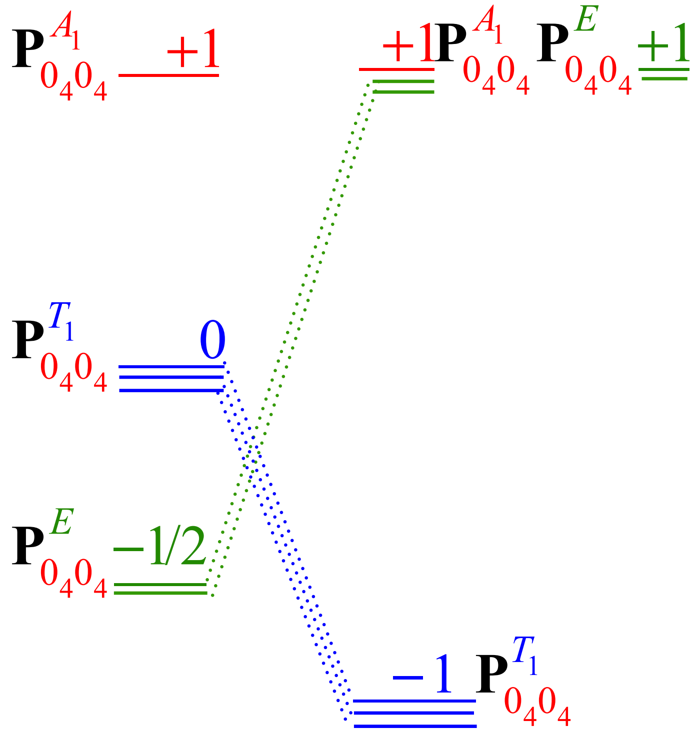
$$\mathbf{p}_{m_4}=\begin{cases}\mathbf{p}_{0_4}=(\mathbf{1}+\mathbf{R}_z+\rho_z+\tilde{\mathbf{R}}_z)/4\\ \mathbf{p}_{1_4}=(\mathbf{1}+i\mathbf{R}_z-\rho_z-i\tilde{\mathbf{R}}_z)/4\\ \mathbf{p}_{2_4}=(\mathbf{1}-\mathbf{R}_z+\rho_z-\tilde{\mathbf{R}}_z)/4\\ \mathbf{p}_{3_4}=(\mathbf{1}-i\mathbf{R}_z-\rho_z+i\tilde{\mathbf{R}}_z)/4\end{cases}$$

Summary of $O\supset C_4$ diagonal (idempotent) projectors $\mathbf{P}^{\mu}_{jj}$

$\mathbf{P}^{(\alpha)}_{n_4n_4}(O\supset C_4)$	$\mathbf{1}$	$r_1r_2\tilde{r}_3\tilde{r}_4$	$\tilde{r}_1\tilde{r}_2r_3r_4$	$\rho_x\rho_y$	ρ_z	$R_x\tilde{R}_xR_y\tilde{R}_y$	R_z	$\tilde{R}_z$	$i_1i_2i_5i_6$	i_3i_4
$24\cdot\mathbf{P}^{A_1}_{0_40_4}$	1	1	1	1	1	1	1	1	+1	+1
$24\cdot\mathbf{P}^{A_2}_{2_42_4}$	1	1	1	1	1	−1	−1	−1	−1	−1
$12\cdot\mathbf{P}^{E}_{0_40_4}$	1	$-\frac{1}{2}$	$-\frac{1}{2}$	1	1	$-\frac{1}{2}$	1	1	$-\frac{1}{2}$	+1
$12\cdot\mathbf{P}^{E}_{2_42_4}$	1	$-\frac{1}{2}$	$-\frac{1}{2}$	1	1	$+\frac{1}{2}$	−1	−1	$+\frac{1}{2}$	−1
$8\cdot\mathbf{P}^{T_1}_{1_41_4}$	1	$-\frac{i}{2}$	$+\frac{i}{2}$	0	−1	$+\frac{1}{2}$	$-i$	$+i$	$-\frac{1}{2}$	0
$8\cdot\mathbf{P}^{T_1}_{3_43_4}$	1	$+\frac{i}{2}$	$-\frac{i}{2}$	0	−1	$+\frac{1}{2}$	$+i$	$-i$	$-\frac{1}{2}$	0
$8\cdot\mathbf{P}^{T_1}_{0_40_4}$	1	0	0	−1	1	0	1	1	0	−1
$8\cdot\mathbf{P}^{T_2}_{1_41_4}$	1	$+\frac{i}{2}$	$-\frac{i}{2}$	0	−1	$-\frac{1}{2}$	$-i$	$+i$	$+\frac{1}{2}$	0
$8\cdot\mathbf{P}^{T_2}_{3_43_4}$	1	$-\frac{i}{2}$	$+\frac{i}{2}$	0	−1	$-\frac{1}{2}$	$+i$	$-i$	$+\frac{1}{2}$	0
$8\cdot\mathbf{P}^{T_2}_{2_42_4}$	1	0	0	−1	1	0	−1	−1	0	1

The $0_4\uparrow$ cluster

i_{16} split *i_{34} split*



5 class sums (Each commutes with all 24 operators in O)

O characters $O:\chi^{\mu}_{\mathbf{g}}$	**g=1**	$\mathbf{r}_{1-4}$ $\tilde{\mathbf{r}}_{1-4}$	$\boldsymbol{\rho}_{xyz}$	$\mathbf{R}_{xyz}$ $\tilde{\mathbf{R}}_{xyz}$	$\mathbf{i}_{1-6}$
$\mu=A_1$	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

5 $\mathbf{P}^{\mu}$ projectors

where: $\mathbf{p}_{m_4}=\frac{1}{4}\sum_{p=0}^{3}e^{im\cdot p/4}\mathbf{R}_z^p$

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

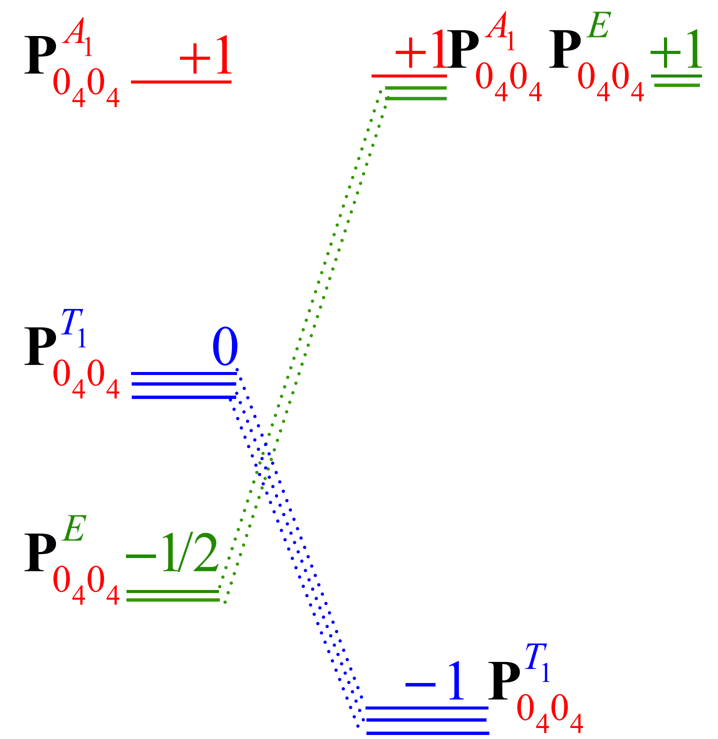
10 split-class sums (Each commutes with all 4 operators in C_4)

$\mathbf{P}^{(\alpha)}_{n_4n_4}(O\supset C_4)$		**1**	2 $r_1r_2\tilde{r}_3\tilde{r}_4$	3 $\tilde{r}_1\tilde{r}_2r_3r_4$	4 $\rho_x\rho_y$	5 ρ_z	6 $R_x\tilde{R}_xR_y\tilde{R}_y$	7 R_z	8 $\tilde{R}_z$	9 $i_1i_2i_5i_6$	10 i_3i_4
$24\cdot\mathbf{P}^{A_1}_{0_40_4}$	1	1	1	1	1	1	1	1	1	+1	(+1)
$24\cdot\mathbf{P}^{A_2}_{2_42_4}$	2	1	1	1	1	1	−1	−1	−1	−1	−1
$12\cdot\mathbf{P}^{E}_{0_40_4}$	3	1	$-\frac{1}{2}$	$-\frac{1}{2}$	1	1	$-\frac{1}{2}$	1	1	$-\frac{1}{2}$	(+1)
$12\cdot\mathbf{P}^{E}_{2_42_4}$	4	1	$-\frac{1}{2}$	$-\frac{1}{2}$	1	1	$+\frac{1}{2}$	−1	−1	$+\frac{1}{2}$	−1
$8\cdot\mathbf{P}^{T_1}_{1_41_4}$	5	1	$-\frac{i}{2}$	$+\frac{i}{2}$	0	−1	$+\frac{1}{2}$	$-i$	$+i$	$-\frac{1}{2}$	0
$8\cdot\mathbf{P}^{T_1}_{3_43_4}$	6	1	$+\frac{i}{2}$	$-\frac{i}{2}$	0	−1	$+\frac{1}{2}$	$+i$	$-i$	$-\frac{1}{2}$	0
$8\cdot\mathbf{P}^{T_1}_{0_40_4}$	7	1	0	0	−1	1	0	1	1	0	(−1)
$8\cdot\mathbf{P}^{T_2}_{1_41_4}$	8	1	$+\frac{i}{2}$	$-\frac{i}{2}$	0	−1	$-\frac{1}{2}$	$-i$	$+i$	$+\frac{1}{2}$	0
$8\cdot\mathbf{P}^{T_2}_{3_43_4}$	9	1	$-\frac{i}{2}$	$+\frac{i}{2}$	0	−1	$-\frac{1}{2}$	$+i$	$-i$	$+\frac{1}{2}$	0
$8\cdot\mathbf{P}^{T_2}_{2_42_4}$	10	1	0	0	−1	1	0	−1	−1	0	1

10 $\mathbf{P}^{\mu}{}_{kk}$ projectors

The 0_4↑cluster

i_{16} split *i_{34} split*



5 class sums (Each commutes with all 24 operators in O)

O characters

5 $\mathbf{P}^\mu$ projectors

$O:\chi^{\mu}_{\mathbf{g}}$	$\mathbf{g}=1$	$\mathbf{r}_{1-4}$, $\tilde{\mathbf{r}}_{1-4}$	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

where: $\mathbf{p}_{m_4}=\frac{1}{4}\sum_{p=0}^{3}e^{im\cdot p/4}\mathbf{R}_z^p$

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

10 split-class sums (Each commutes with all 4 operators in C_4)

10 $\mathbf{P}^{\mu}{}_{kk}$ projectors

$\mathbf{P}^{(\alpha)}_{n_4 n_4}(O\supset C_4)$		1	2: $r_1r_2\tilde{r}_3\tilde{r}_4$	3: $\tilde{r}_1\tilde{r}_2r_3r_4$	4: $\rho_x\rho_y$	5: ρ_z	6: $R_x\tilde{R}_xR_y\tilde{R}_y$	7: R_z	8: $\tilde{R}_z$	9: $i_1i_2i_5i_6$	10: i_3i_4
$24\cdot\mathbf{P}^{A_1}_{0_4 0_4}$	1	1	1	1	1	1	1	1	1	+1	+1
(sum)		1	1		1		1			1	
$24\cdot\mathbf{P}^{A_2}_{2_4 2_4}$	2	1	1	1	1	1	-1	-1	-1	-1	-1
(sum)		1	1		1		1			1	
$12\cdot\mathbf{P}^{E}_{0_4 0_4}$	3	1	$-\frac{1}{2}$	$-\frac{1}{2}$	1	1	$-\frac{1}{2}$	1	1	$-\frac{1}{2}$	+1
$12\cdot\mathbf{P}^{E}_{2_4 2_4}$	4	1	$-\frac{1}{2}$	$-\frac{1}{2}$	1	1	$+\frac{1}{2}$	-1	-1	$+\frac{1}{2}$	-1
(sum)		2	-1		2		0			0	
$8\cdot\mathbf{P}^{T_1}_{1_4 1_4}$	5	1	$-\frac{i}{2}$	$+\frac{i}{2}$	0	-1	$+\frac{1}{2}$	$-i$	$+i$	$-\frac{1}{2}$	0
$8\cdot\mathbf{P}^{T_1}_{3_4 3_4}$	6	1	$+\frac{i}{2}$	$-\frac{i}{2}$	0	-1	$+\frac{1}{2}$	$+i$	$-i$	$-\frac{1}{2}$	0
$8\cdot\mathbf{P}^{T_1}_{0_4 0_4}$	7	1	0	0	-1	1	0	1	1	0	-1
(sum)		3	0		-1		1			-1	
$8\cdot\mathbf{P}^{T_2}_{1_4 1_4}$	8	1	$+\frac{i}{2}$	$-\frac{i}{2}$	0	-1	$-\frac{1}{2}$	$-i$	$+i$	$+\frac{1}{2}$	0
$8\cdot\mathbf{P}^{T_2}_{3_4 3_4}$	9	1	$-\frac{i}{2}$	$+\frac{i}{2}$	0	-1	$-\frac{1}{2}$	$+i$	$-i$	$+\frac{1}{2}$	0
$8\cdot\mathbf{P}^{T_2}_{2_4 2_4}$	10	1	0	0	-1	1	0	-1	-1	0	1
(sum)		3	0		-1		-1			1	

Adding rows of eigenvalue table collapses it back to O-characters

Review Calculating idempotent projectors $\mathbf{P}^{\mu}_{m,m}$ *of* $O\supset C_4$ $\mathbf{P}^{E}_{0_4 0_4}$ $\mathbf{P}^{E}_{2_4 2_4}$ $\mathbf{P}^{T_1}_{0_4 0_4}$ $\mathbf{P}^{T_1}_{1_4 1_4}$ $\mathbf{P}^{T_2}_{2_4 2_4}$

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

Review Broken-class-ordered splitting of $O\supset D_4\supset C_4$ *projectors and levels*

Subgroup-defined tunneling parameter modeling

- *Comparing two diagonal* $O\supset C_4$ *parameter sets to* SF_6 *spectra*
- *Comparing two diagonal* $O\supset C_3$ *parameter sets to* SF_6 *spectra*
- *Why* $O\supset C_2$ *parameter sets require off-diagonal nilpotent* $\mathbf{P}^{\mu}_{m,n}$ $(m\neq n)$

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

Using fundamental $\mathbf{g}\rightleftarrows\mathbf{P}^{\mu}_{m,n}$ *relations: (from Lecture 16)*

(a) $\mathbf{P}^{\mu}_{m,m}\mathbf{g}\mathbf{P}^{\mu}_{n,n}=D^{\mu}_{m,n}(\mathbf{g})\mathbf{P}^{\mu}_{m,n}$ (b) $\mathbf{g}=\Sigma_{\mu}\Sigma_{m,n}D^{\mu}_{m,n}(\mathbf{g})\mathbf{P}^{\mu}_{m,n}$ (c) $\mathbf{P}^{\mu}_{n,n}=(\ell^{\mu}/{}^{\circ}G)\Sigma_{\mathbf{g}}D^{\mu *}_{m,n}(\mathbf{g})\mathbf{g}$

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

Calculating and Factoring $\mathbf{P}^{T_1}_{1_4 0_4}$ *and* $\mathbf{P}^{T_1}_{1_4 3_4}$

Structure and applications of various subgroup chain irreducible representations

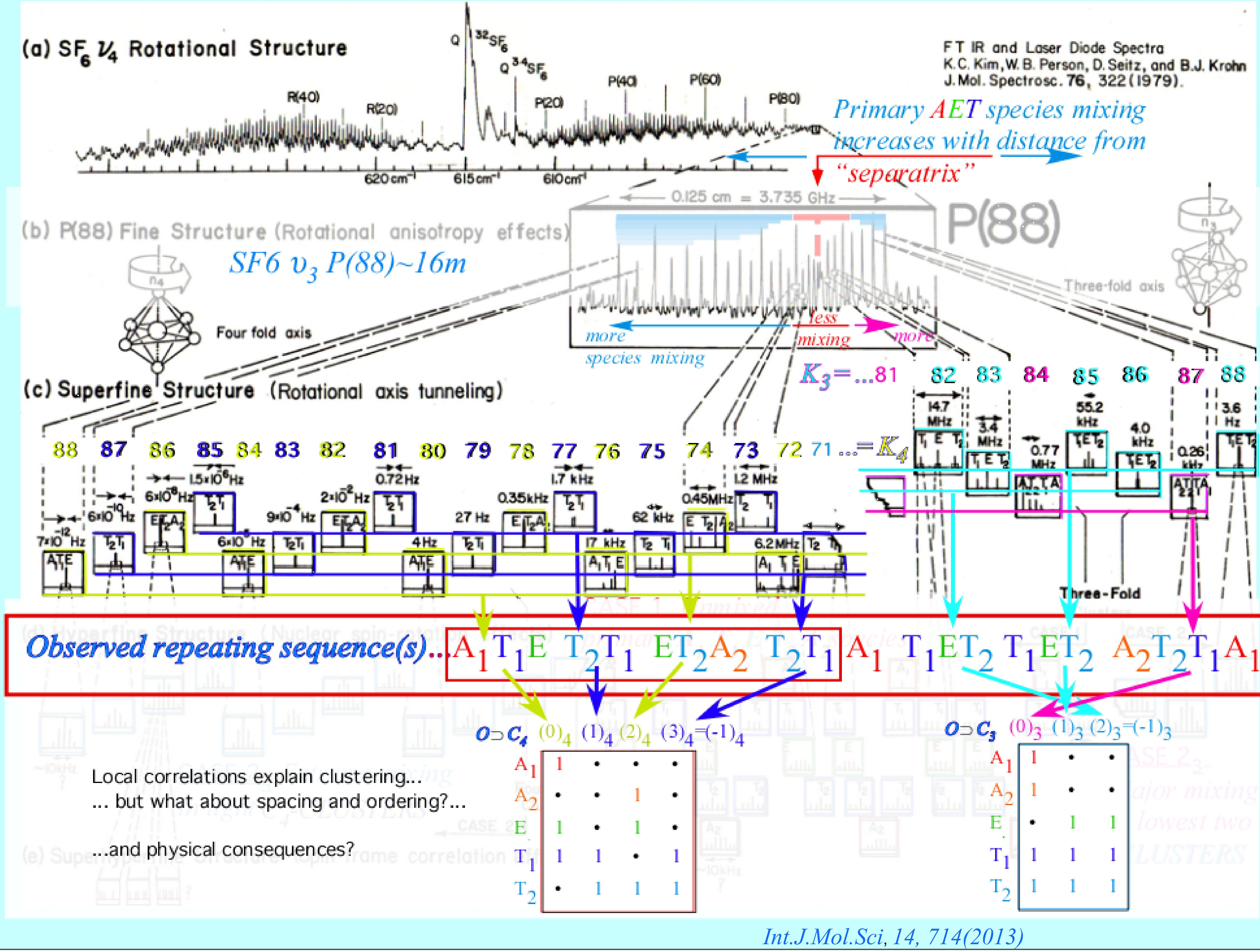
$O_h\supset D_{4h}\supset C_{4v}$, $O_h\supset D_{3h}\supset C_{3v}$, $O_h\supset C_{2v}$

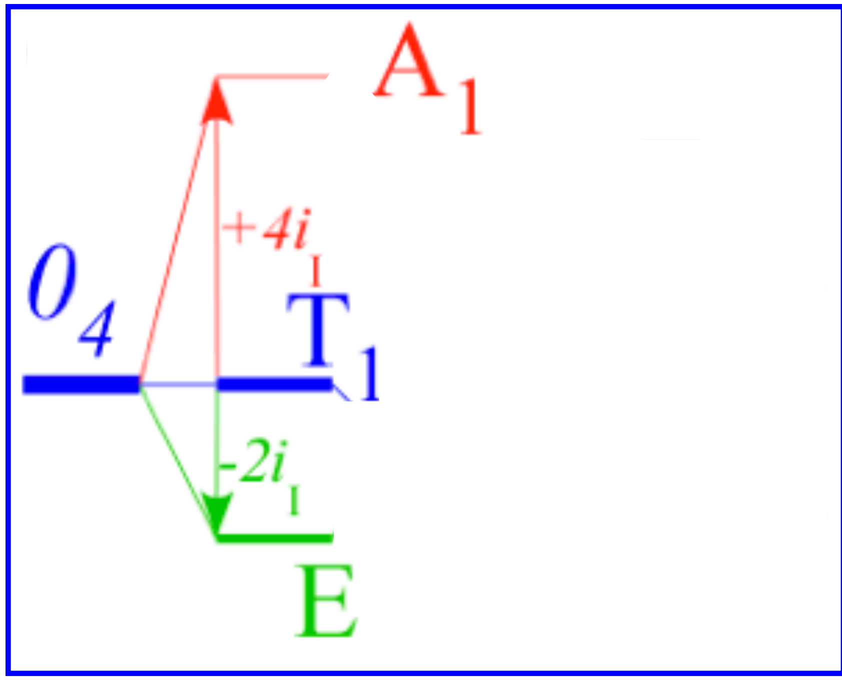
Comparing $O_h\supset D_{4h}\supset D_{2h}$ *and* $O_h\supset D_{3d}\supset C_2$ *representations* (T_1 *vector-type)*

Examples of off-diagonal tunneling coefficients $D^{E}_{0_4 2_4}$

Comparing Local C_4, C_3, *and* C_2 *symmetric spectra*

Comparing off-diagonal $O\supset C_2$ *parameter sets to* CH_4 *models with "cluster-crossings"*


(a) SF6 ν4 Rotational Structure
F T IR and Laser Diode Spectra
K.C. Kim, W.B. Person, D. Seitz, and B.J. Krohn
J. Mol. Spectrosc. 76, 322 (1979).
Q 32SF6
Q 34SF6
R(40) R(20) P(20) P(40) P(60) P(80)
620cm-1 615cm-1 610cm-1
Primary AET species mixing increases with distance from "separatrix"
0.125 cm = 3.735 GHz
P(88)
(b) P(88) Fine Structure (Rotational anisotropy effects)
SF6 υ3 P(88)~16m
Four fold axis
Three-fold axis
more species mixing
less mixing
more
K3=...81 82 83 84 85 86 87 88
(c) Superfine Structure (Rotational axis tunneling)
88 87 86 85 84 83 82 81 80 79 78 77 76 75 74 73 72 71 ...=K4
Three-Fold
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
O⊃C3 (0)3 (1)3 (2)3=(-1)3
Local correlations explain clustering...
... but what about spacing and ordering?...
...and physical consequences?
Int.J.Mol.Sci, 14, 714(2013)



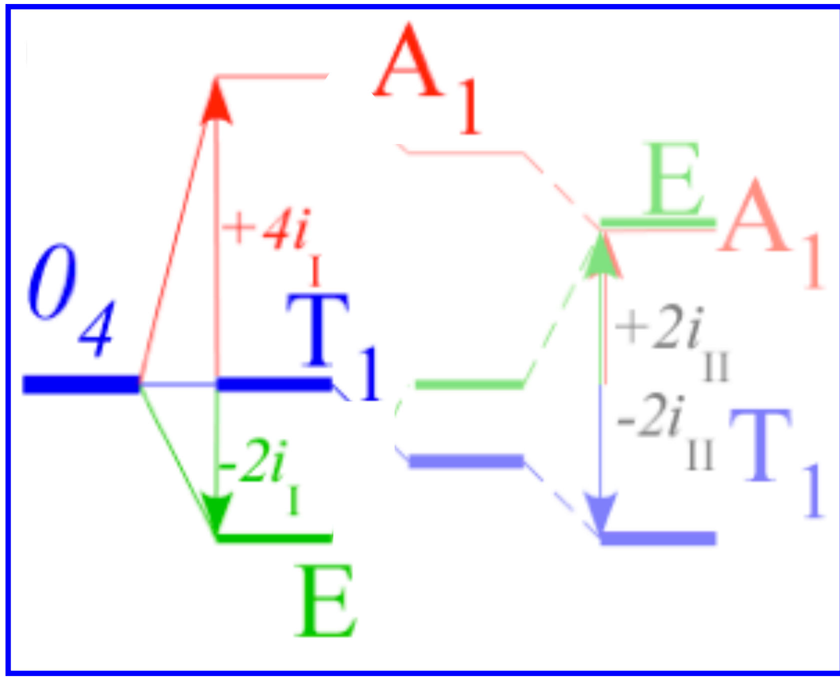
1_4 2_4 3_4

C_4 Subgroup-defined tunneling parameter modeling

Table 11. Splittings of $O \supset C_4$ given sub-class structure.

$O \supset C_4$	$0°$	$r_n 120°$	$\rho_n 180°$	$R_n 90°$	$i_n 180°$
0_4	$\cdot$	$r_{\rm I} = {\rm Re}\, r_{1234}$ $m_{\rm I} = {\rm Im}\, r_{1234}$	$\cdot$	$R_z = {\rm Re} R_z$ $I_z = {\rm Im} R_z$	$i_{\rm I} = i_{1256}$ $i_{\rm II} = i_{34}$
$\varepsilon^{A_1}_{0_4} =$	g_0	$+8r_{\rm I}$	$+2\rho_{xy} + \rho_z$	$+4R_{xy} + 2R_z$	$+4i_{\rm I} + 2i_{\rm II}$
$\varepsilon^{T_1}_{0_4}$	g_0	0	$-2\rho_{xy} + \rho_z$	$+2R_z$	$-2i_{\rm II}$
$\varepsilon^{E}_{0_4}$	g_0	$-2r_{\rm I}$	$+2\rho_{xy} + \rho_z$	$-2R_{xy} - R_z$	$-2i_{\rm I} + 2i_{\rm II}$
1_4	$\cdot$	$\cdot$	$\cdot$	$\cdot$	$\cdot$
$\varepsilon^{T_2}_{1_4}$	g_0	$+2m_{\rm I}$	$-\rho_z$	$-R_{xy} - 2I_z$	$+2i_{\rm I}$
$\varepsilon^{T_1}_{1_4}$	g_0	$-2m_{\rm I}$	$-\rho_z$	$+R_{xy} - 2I_z$	$-2i_{\rm I}$
2_4	$\cdot$	$\cdot$	$\cdot$	$\cdot$	$\cdot$
$\varepsilon^{E}_{2_4}$	g_0	$-2r_{\rm I}$	$+2\rho_{xy} + \rho_z$	$+2R_{xy} - R_z$	$+2i_{\rm I} - 2i_{\rm II}$
$\varepsilon^{T_2}_{2_4}$	g_0	0	$-2\rho_{xy} + \rho_z$	$-2R_z$	$+2i_{\rm II}$
$\varepsilon^{A_2}_{2_4}$	g_0	$+8r_{\rm I}$	$+2\rho_{xy} + \rho_z$	$-4R_{xy} - 2R_z$	$-4i_{\rm I} - 2i_{\rm II}$
3_4	$\cdot$	$\cdot$	$\cdot$	$\cdot$	$\cdot$
$\varepsilon^{T_2}_{3_4}$	g_0	$-2m_{\rm I}$	$-\rho_z$	$-R_{xy} + 2I_z$	$+2i_{\rm I}$
$\varepsilon^{T_1}_{3_4}$	g_0	$+2m_{\rm I}$	$-\rho_z$	$+R_{xy} + 2I_z$	$-2i_{\rm I}$

Int.J.Mol.Sci, 14, 714(2013)



1_4

2_4

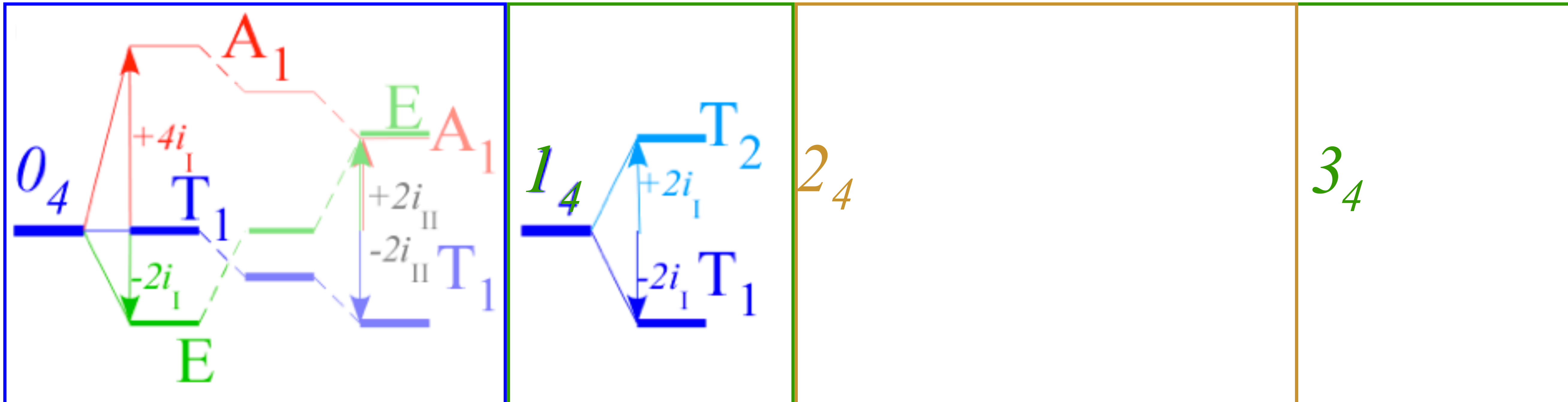
3_4

C_4 Subgroup-defined tunneling parameter modeling

Table 11. Splittings of $O \supset C_4$ given sub-class structure.

$O \supset C_4$	$0°$	$r_n 120°$	$\rho_n 180°$	$R_n 90°$	$i_n 180°$
0_4	$\cdot$	$r_{\rm I} = {\rm Re}\, r_{1234}$ $m_{\rm I} = {\rm Im}\, r_{1234}$	$\cdot$	$R_z = {\rm Re} R_z$ $I_z = {\rm Im} R_z$	$i_{\rm I} = i_{1256}$ $i_{\rm II} = i_{34}$
$\varepsilon_{0_4}^{A_1} =$	g_0	$+8r_{\rm I}$	$+2\rho_{xy} + \rho_z$	$+4R_{xy} + 2R_z$	$+4i_{\rm I} + 2i_{\rm II}$
$\varepsilon_{0_4}^{T_1}$	g_0	0	$-2\rho_{xy} + \rho_z$	$+2R_z$	$-2i_{\rm II}$
$\varepsilon_{0_4}^{E}$	g_0	$-2r_{\rm I}$	$+2\rho_{xy} + \rho_z$	$-2R_{xy} - R_z$	$-2i_{\rm I} + 2i_{\rm II}$
1_4	$\cdot$	$\cdot$	$\cdot$	$\cdot$	$\cdot$
$\varepsilon_{1_4}^{T_2}$	g_0	$+2m_{\rm I}$	$-\rho_z$	$-R_{xy} - 2I_z$	$+2i_{\rm I}$
$\varepsilon_{1_4}^{T_1}$	g_0	$-2m_{\rm I}$	$-\rho_z$	$+R_{xy} - 2I_z$	$-2i_{\rm I}$
2_4	$\cdot$	$\cdot$	$\cdot$	$\cdot$	$\cdot$
$\varepsilon_{2_4}^{E}$	g_0	$-2r_{\rm I}$	$+2\rho_{xy} + \rho_z$	$+2R_{xy} - R_z$	$+2i_{\rm I} - 2i_{\rm II}$
$\varepsilon_{2_4}^{T_2}$	g_0	0	$-2\rho_{xy} + \rho_z$	$-2R_z$	$+2i_{\rm II}$
$\varepsilon_{2_4}^{A_2}$	g_0	$+8r_{\rm I}$	$+2\rho_{xy} + \rho_z$	$-4R_{xy} - 2R_z$	$-4i_{\rm I} - 2i_{\rm II}$
3_4	$\cdot$	$\cdot$	$\cdot$	$\cdot$	$\cdot$
$\varepsilon_{3_4}^{T_2}$	g_0	$-2m_{\rm I}$	$-\rho_z$	$-R_{xy} + 2I_z$	$+2i_{\rm I}$
$\varepsilon_{3_4}^{T_1}$	g_0	$+2m_{\rm I}$	$-\rho_z$	$+R_{xy} + 2I_z$	$-2i_{\rm I}$

Int.J.Mol.Sci, 14, 714(2013)

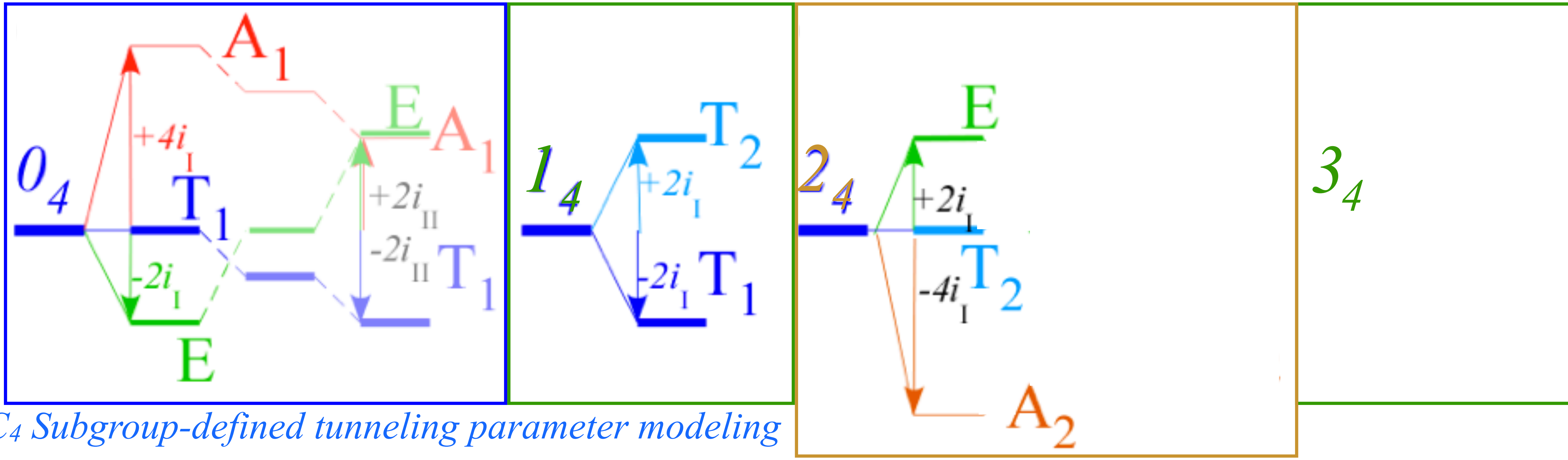


C_4 Subgroup-defined tunneling parameter modeling

Table 11. Splittings of $O \supset C_4$ given sub-class structure.

$O \supset C_4$	$0°$	$r_n 120°$	$\rho_n 180°$	$R_n 90°$	$i_n 180°$
0_4	.	$r_{\rm I} = {\rm Re}\, r_{1234}$ $m_{\rm I} = {\rm Im}\, r_{1234}$	.	$R_z = {\rm Re} R_z$ $I_z = {\rm Im} R_z$	$i_{\rm I} = i_{1256}$ $i_{\rm II} = i_{34}$
$\varepsilon_{0_4}^{A_1} =$	g_0	$+8r_{\rm I}$	$+2\rho_{xy} + \rho_z$	$+4R_{xy} + 2R_z$	$+4i_{\rm I} + 2i_{\rm II}$
$\varepsilon_{0_4}^{T_1}$	g_0	0	$-2\rho_{xy} + \rho_z$	$+2R_z$	$-2i_{\rm II}$
$\varepsilon_{0_4}^{E}$	g_0	$-2r_{\rm I}$	$+2\rho_{xy} + \rho_z$	$-2R_{xy} - R_z$	$-2i_{\rm I} + 2i_{\rm II}$
1_4	.	.	.	.	.
$\varepsilon_{1_4}^{T_2}$	g_0	$+2m_{\rm I}$	$-\rho_z$	$-R_{xy} - 2I_z$	$+2i_{\rm I}$
$\varepsilon_{1_4}^{T_1}$	g_0	$-2m_{\rm I}$	$-\rho_z$	$+R_{xy} - 2I_z$	$-2i_{\rm I}$
2_4	.	.	.	.	.
$\varepsilon_{2_4}^{E}$	g_0	$-2r_{\rm I}$	$+2\rho_{xy} + \rho_z$	$+2R_{xy} - R_z$	$+2i_{\rm I} - 2i_{\rm II}$
$\varepsilon_{2_4}^{T_2}$	g_0	0	$-2\rho_{xy} + \rho_z$	$-2R_z$	$+2i_{\rm II}$
$\varepsilon_{2_4}^{A_2}$	g_0	$+8r_{\rm I}$	$+2\rho_{xy} + \rho_z$	$-4R_{xy} - 2R_z$	$-4i_{\rm I} - 2i_{\rm II}$
3_4	.	.	.	.	.
$\varepsilon_{3_4}^{T_2}$	g_0	$-2m_{\rm I}$	$-\rho_z$	$-R_{xy} + 2I_z$	$+2i_{\rm I}$
$\varepsilon_{3_4}^{T_1}$	g_0	$+2m_{\rm I}$	$-\rho_z$	$+R_{xy} + 2I_z$	$-2i_{\rm I}$

Int.J.Mol.Sci, 14, 714(2013)

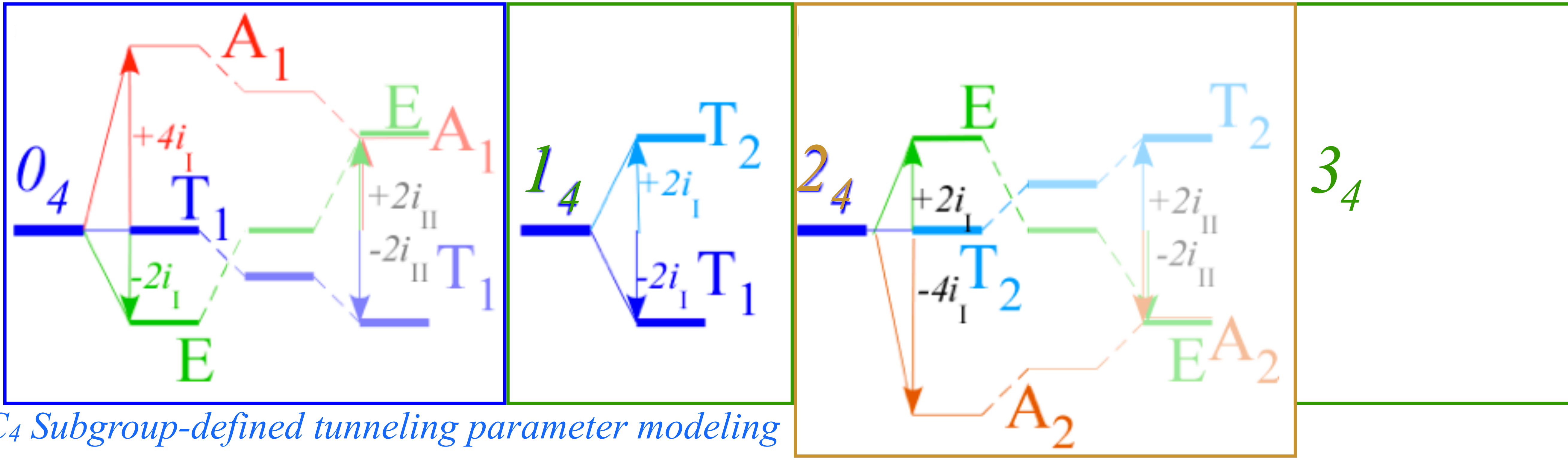


C_4 Subgroup-defined tunneling parameter modeling

Table 11. Splittings of $O \supset C_4$ given sub-class structure.

$O \supset C_4$	$0°$	$r_n 120°$	$\rho_n 180°$	$R_n 90°$	$i_n 180°$
0_4	.	$r_{\text{I}} = \text{Re}\, r_{1234}$ $m_{\text{I}} = \text{Im}\, r_{1234}$	.	$R_z = \text{Re}R_z$ $I_z = \text{Im}R_z$	$i_{\text{I}} = i_{1256}$ $i_{\text{II}} = i_{34}$
$\varepsilon_{0_4}^{A_1} =$	g_0	$+8r_{\text{I}}$	$+2\rho_{xy} + \rho_z$	$+4R_{xy} + 2R_z$	$+4i_{\text{I}} + 2i_{\text{II}}$
$\varepsilon_{0_4}^{T_1}$	g_0	0	$-2\rho_{xy} + \rho_z$	$+2R_z$	$-2i_{\text{II}}$
$\varepsilon_{0_4}^{E}$	g_0	$-2r_{\text{I}}$	$+2\rho_{xy} + \rho_z$	$-2R_{xy} - R_z$	$-2i_{\text{I}} + 2i_{\text{II}}$
1_4	.	.	.	.	.
$\varepsilon_{1_4}^{T_2}$	g_0	$+2m_{\text{I}}$	$-\rho_z$	$-R_{xy} - 2I_z$	$+2i_{\text{I}}$
$\varepsilon_{1_4}^{T_1}$	g_0	$-2m_{\text{I}}$	$-\rho_z$	$+R_{xy} - 2I_z$	$-2i_{\text{I}}$
2_4	.	.	.	.	.
$\varepsilon_{2_4}^{E}$	g_0	$-2r_{\text{I}}$	$+2\rho_{xy} + \rho_z$	$+2R_{xy} - R_z$	$+2i_{\text{I}} - 2i_{\text{II}}$
$\varepsilon_{2_4}^{T_2}$	g_0	0	$-2\rho_{xy} + \rho_z$	$-2R_z$	$+2i_{\text{II}}$
$\varepsilon_{2_4}^{A_2}$	g_0	$+8r_{\text{I}}$	$+2\rho_{xy} + \rho_z$	$-4R_{xy} - 2R_z$	$-4i_{\text{I}} - 2i_{\text{II}}$
3_4	.	.	.	.	.
$\varepsilon_{3_4}^{T_2}$	g_0	$-2m_{\text{I}}$	$-\rho_z$	$-R_{xy} + 2I_z$	$+2i_{\text{I}}$
$\varepsilon_{3_4}^{T_1}$	g_0	$+2m_{\text{I}}$	$-\rho_z$	$+R_{xy} + 2I_z$	$-2i_{\text{I}}$

Int.J.Mol.Sci, 14, 714(2013)

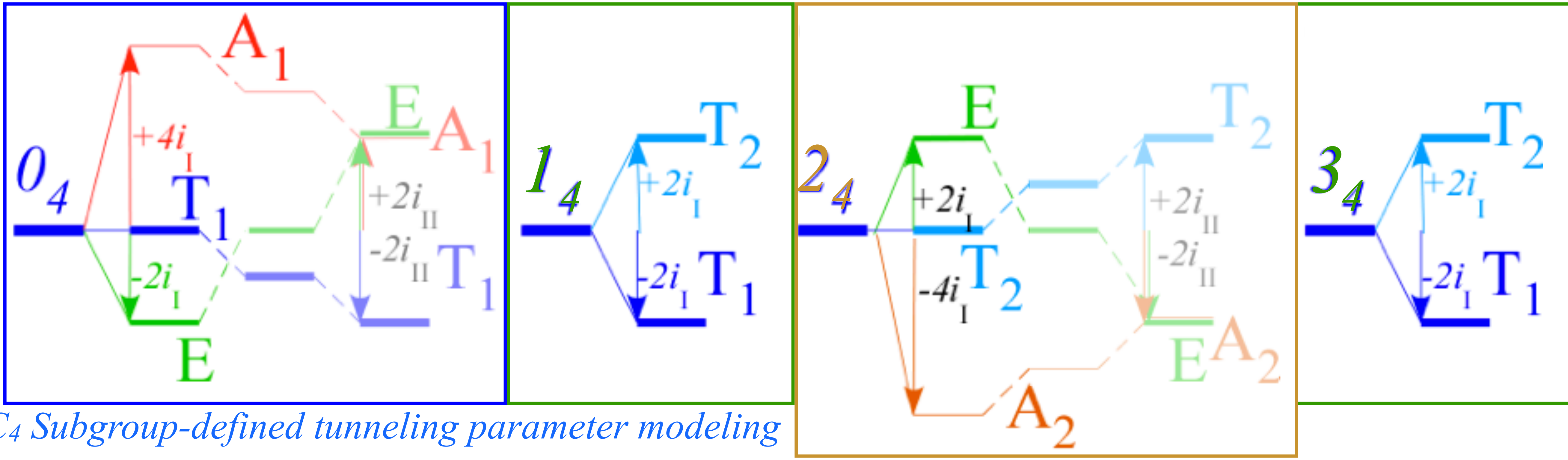


C_4 Subgroup-defined tunneling parameter modeling

Table 11. Splittings of $O \supset C_4$ given sub-class structure.

$O \supset C_4$	$0°$	$r_n 120°$	$\rho_n 180°$	$R_n 90°$	$i_n 180°$
0_4	.	$r_I = \text{Re}\, r_{1234}$ $m_I = \text{Im}\, r_{1234}$	.	$R_z = \text{Re}R_z$ $I_z = \text{Im}R_z$	$i_I = i_{1256}$ $i_{II} = i_{34}$
$\varepsilon_{0_4}^{A_1} =$	g_0	$+8r_I$	$+2\rho_{xy} + \rho_z$	$+4R_{xy} + 2R_z$	$+4i_I + 2i_{II}$
$\varepsilon_{0_4}^{T_1}$	g_0	0	$-2\rho_{xy} + \rho_z$	$+2R_z$	$-2i_{II}$
$\varepsilon_{0_4}^{E}$	g_0	$-2r_I$	$+2\rho_{xy} + \rho_z$	$-2R_{xy} - R_z$	$-2i_I + 2i_{II}$
1_4	.	.	.	.	.
$\varepsilon_{1_4}^{T_2}$	g_0	$+2m_I$	$-\rho_z$	$-R_{xy} - 2I_z$	$+2i_I$
$\varepsilon_{1_4}^{T_1}$	g_0	$-2m_I$	$-\rho_z$	$+R_{xy} - 2I_z$	$-2i_I$
2_4	.	.	.	.	.
$\varepsilon_{2_4}^{E}$	g_0	$-2r_I$	$+2\rho_{xy} + \rho_z$	$+2R_{xy} - R_z$	$+2i_I - 2i_{II}$
$\varepsilon_{2_4}^{T_2}$	g_0	0	$-2\rho_{xy} + \rho_z$	$-2R_z$	$+2i_{II}$
$\varepsilon_{2_4}^{A_2}$	g_0	$+8r_I$	$+2\rho_{xy} + \rho_z$	$-4R_{xy} - 2R_z$	$-4i_I - 2i_{II}$
3_4	.	.	.	.	.
$\varepsilon_{3_4}^{T_2}$	g_0	$-2m_I$	$-\rho_z$	$-R_{xy} + 2I_z$	$+2i_I$
$\varepsilon_{3_4}^{T_1}$	g_0	$+2m_I$	$-\rho_z$	$+R_{xy} + 2I_z$	$-2i_I$

Int.J.Mol.Sci, 14, 714(2013)



C_4 Subgroup-defined tunneling parameter modeling

Table 11. Splittings of $O \supset C_4$ given sub-class structure.

$O \supset C_4$	$0°$	$r_n 120°$	$\rho_n 180°$	$R_n 90°$	$i_n 180°$
0_4	$\cdot$	$r_I = \mathrm{Re}\, r_{1234}$ $m_I = \mathrm{Im}\, r_{1234}$	$\cdot$	$R_z = \mathrm{Re} R_z$ $I_z = \mathrm{Im} R_z$	$i_I = i_{1256}$ $i_{II} = i_{34}$
$\varepsilon_{0_4}^{A_1} =$	g_0	$+8r_I$	$+2\rho_{xy} + \rho_z$	$+4R_{xy} + 2R_z$	$+4i_I + 2i_{II}$
$\varepsilon_{0_4}^{T_1}$	g_0	0	$-2\rho_{xy} + \rho_z$	$+2R_z$	$-2i_{II}$
$\varepsilon_{0_4}^{E}$	g_0	$-2r_I$	$+2\rho_{xy} + \rho_z$	$-2R_{xy} - R_z$	$-2i_I + 2i_{II}$
1_4	$\cdot$	$\cdot$	$\cdot$	$\cdot$	$\cdot$
$\varepsilon_{1_4}^{T_2}$	g_0	$+2m_I$	$-\rho_z$	$-R_{xy} - 2I_z$	$+2i_I$
$\varepsilon_{1_4}^{T_1}$	g_0	$-2m_I$	$-\rho_z$	$+R_{xy} - 2I_z$	$-2i_I$
2_4	$\cdot$	$\cdot$	$\cdot$	$\cdot$	$\cdot$
$\varepsilon_{2_4}^{E}$	g_0	$-2r_I$	$+2\rho_{xy} + \rho_z$	$+2R_{xy} - R_z$	$+2i_I - 2i_{II}$
$\varepsilon_{2_4}^{T_2}$	g_0	0	$-2\rho_{xy} + \rho_z$	$-2R_z$	$+2i_{II}$
$\varepsilon_{2_4}^{A_2}$	g_0	$+8r_I$	$+2\rho_{xy} + \rho_z$	$-4R_{xy} - 2R_z$	$-4i_I - 2i_{II}$
3_4	$\cdot$	$\cdot$	$\cdot$	$\cdot$	$\cdot$
$\varepsilon_{3_4}^{T_2}$	g_0	$-2m_I$	$-\rho_z$	$-R_{xy} + 2I_z$	$+2i_I$
$\varepsilon_{3_4}^{T_1}$	g_0	$+2m_I$	$-\rho_z$	$+R_{xy} + 2I_z$	$-2i_I$

Int.J.Mol.Sci, 14, 714(2013)

Review Calculating idempotent projectors $\mathbf{P}^{\mu}_{m,m}$ *of* $O \supset C_4$ $\mathbf{P}^{E}_{0_4 0_4}$ $\mathbf{P}^{E}_{2_4 2_4}$ $\mathbf{P}^{T_1}_{0_4 0_4}$ $\mathbf{P}^{T_1}_{1_4 1_4}$ $\mathbf{P}^{T_2}_{2_4 2_4}$

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

Review Broken-class-ordered splitting of $O \supset D_4 \supset C_4$ *projectors and levels*

Subgroup-defined tunneling parameter modeling

Comparing two diagonal $O \supset C_4$ *parameter sets to* SF_6 *spectra*

Comparing two diagonal $O \supset C_3$ *parameter sets to* SF_6 *spectra*

Why $O \supset C_2$ *parameter sets require off-diagonal nilpotent* $\mathbf{P}^{\mu}_{m,n}$ $(m \neq n)$

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

Using fundamental $\mathbf{g} \rightleftarrows \mathbf{P}^{\mu}_{m,n}$ *relations: (from Lecture 16)*

(a) $\mathbf{P}^{\mu}_{m,m}\mathbf{g}\mathbf{P}^{\mu}_{n,n} = D^{\mu}_{m,n}(\mathbf{g})\mathbf{P}^{\mu}_{m,n}$ (b) $\mathbf{g} = \Sigma_{\mu}\Sigma_{m,n} D^{\mu}_{m,n}(\mathbf{g})\mathbf{P}^{\mu}_{m,n}$ (c) $\mathbf{P}^{\mu}_{n,n} = (\ell^{\mu}/°G)\Sigma_{\mathbf{g}} D^{\mu *}_{m,n}(\mathbf{g})\mathbf{g}$

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

Calculating and Factoring $\mathbf{P}^{T_1}_{1_4 0_4}$ *and* $\mathbf{P}^{T_1}_{1_4 3_4}$

Structure and applications of various subgroup chain irreducible representations

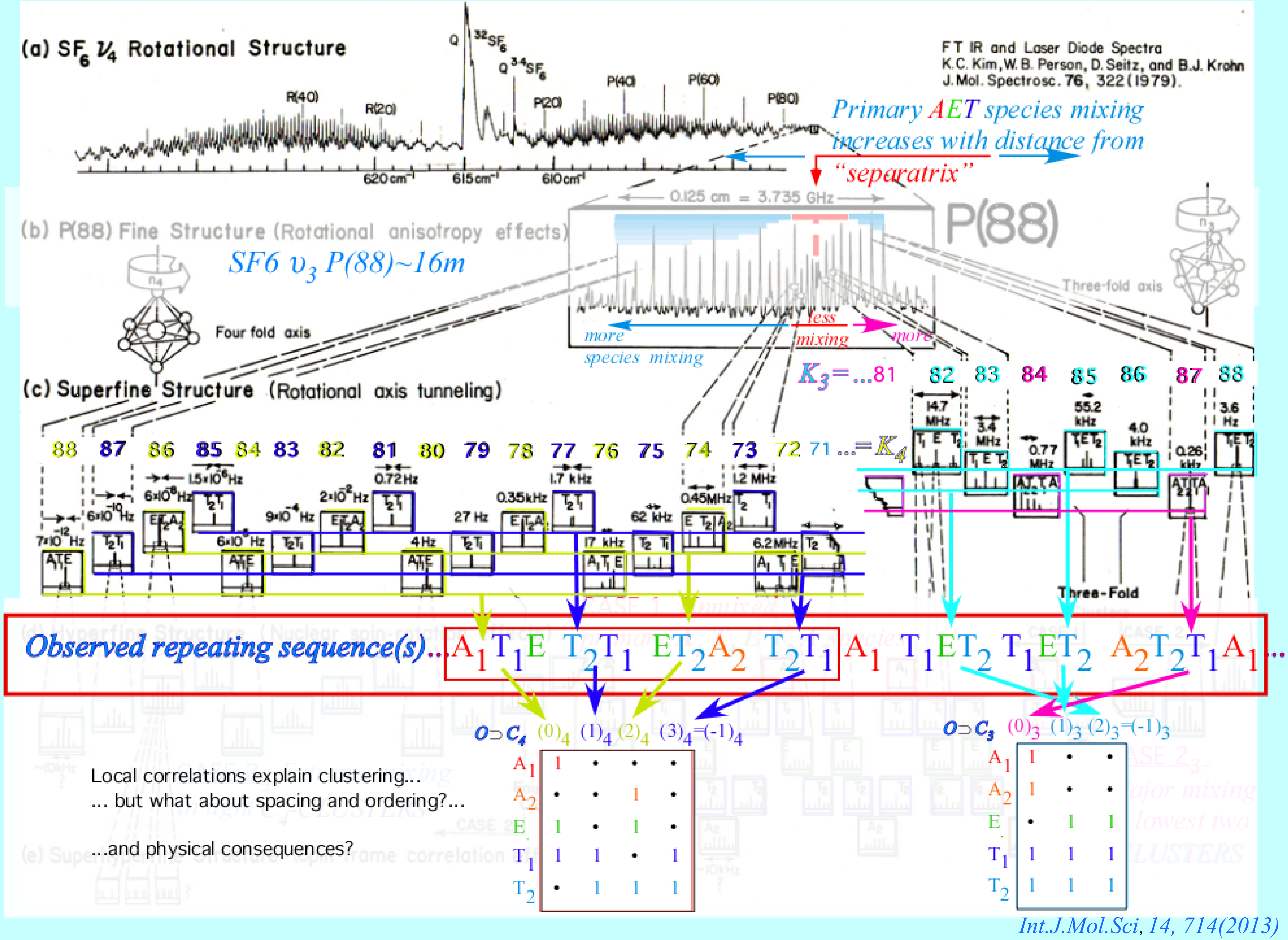
$O_h \supset D_{4h} \supset C_{4v}$, $O_h \supset D_{3h} \supset C_{3v}$, $O_h \supset C_{2v}$

Comparing $O_h \supset D_{4h} \supset D_{2h}$ *and* $O_h \supset D_{3d} \supset C_2$ *representations (*T_1 *vector-type)*

Examples of off-diagonal tunneling coefficients $D^{E}_{0_4 2_4}$

Comparing Local C_4, C_3, *and* C_2 *symmetric spectra*

Comparing off-diagonal $O \supset C_2$ *parameter sets to* CH_4 *models with "cluster-crossings"*



(a) SF6 ν4 Rotational Structure
F T IR and Laser Diode Spectra
K.C. Kim, W.B. Person, D. Seitz, and B.J. Krohn
J. Mol. Spectrosc. 76, 322 (1979).
Q 32SF6
Q 34SF6
R(40)
R(20)
P(20)
P(40)
P(60)
P(80)
620 cm-1
615 cm-1
610 cm-1
Primary AET species mixing
increases with distance from
"separatrix"
0.125 cm = 3.735 GHz
P(88)
(b) P(88) Fine Structure (Rotational anisotropy effects)
SF6 υ3 P(88)~16m
Four fold axis
Three-fold axis
more
species mixing
less
mixing
more
K3=...81 82 83 84 85 86 87 88
(c) Superfine Structure (Rotational axis tunneling)
88 87 86 85 84 83 82 81 80 79 78 77 76 75 74 73 72 71 ...=K4
Three-Fold
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
O⊃C3 (0)3 (1)3 (2)3=(-1)3
Local correlations explain clustering...
... but what about spacing and ordering?...
...and physical consequences?
Int.J.Mol.Sci, 14, 714(2013)

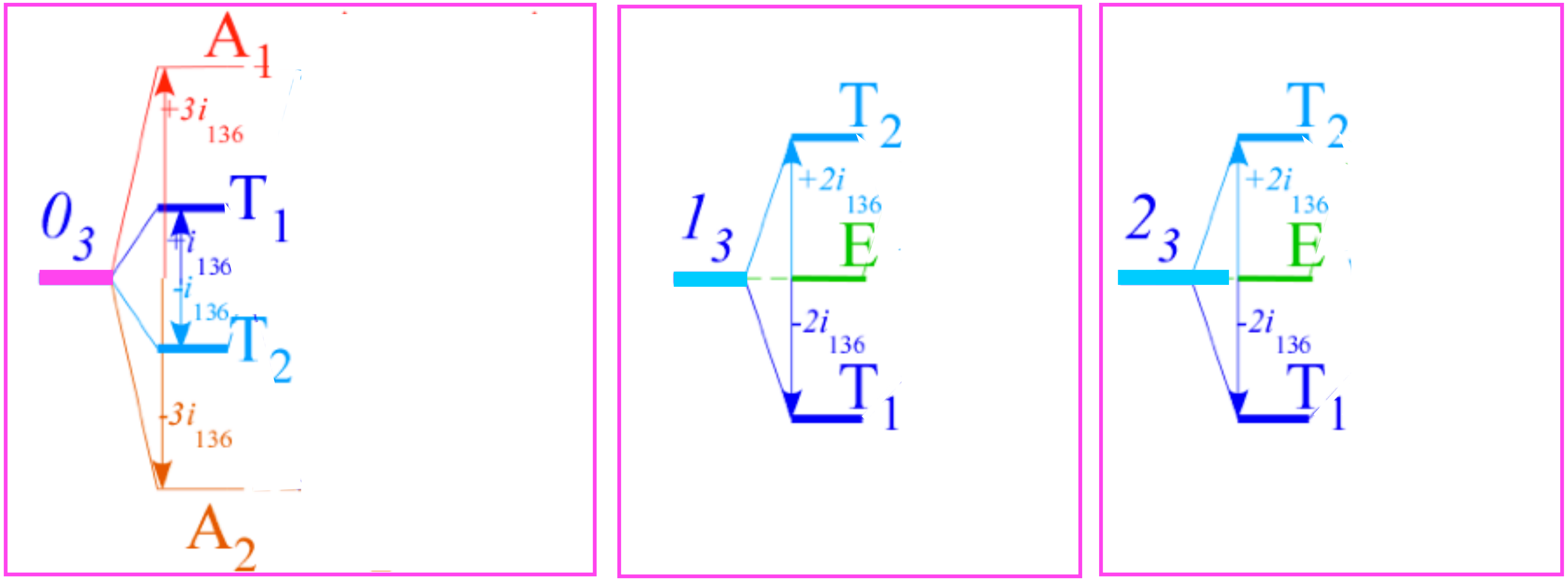


Table 12. Splittings of $O \supset C_3$ given sub-class structure.

C_3 *Subgroup-defined tunneling parameter modeling*

$O \supset C_3$	$0°$	$r_n 120°$	$\rho_n 180°$	$R_n 90°$	$i_n 180°$
0_3	$\cdot$	$r_{\mathrm{I}} = Re(r_1)$ $i_{\mathrm{I}} = Im(r_1)$ $r_{\mathrm{II}} = Re(r_{234})$ $i_{\mathrm{I}} = Im(r_{234})$	$\rho = \rho_{xyz}$	$R_n = Re(R_{xyz})$ $I_n = Im(R_{xyz})$	$i_{\mathrm{I}} = i_{136}$ $i_{\mathrm{II}} = i_{245}$
$\varepsilon_{0_3}^{A_1}$	g_0	$2r_{\mathrm{I}} + 6r_{\mathrm{II}}$	3ρ	$6R_n$	$3i_{\mathrm{I}} + 3i_{\mathrm{I}}$
$\varepsilon_{0_3}^{A_2}$	g_0	$2r_{\mathrm{I}} + 6r_{\mathrm{II}}$	3ρ	$-6R_n$	$-3i_{\mathrm{I}} - 3i_{\mathrm{II}}$
$\varepsilon_{0_3}^{T_1}$	g_0	$2r_{\mathrm{I}} - 2r_{\mathrm{II}}$	$-\rho$	$2R_n$	$i_{\mathrm{I}} - 3i_{\mathrm{II}}$
$\varepsilon_{0_3}^{T_2}$	g_0	$2r_{\mathrm{I}} - 2r_{\mathrm{II}}$	$-\rho$	$-2R_n$	$-i_{\mathrm{I}} + 3i_{\mathrm{II}}$
1_3					
$\varepsilon_{1_3}^{E}$	g_0	$-r_{\mathrm{I}} + \sqrt{3}i_{\mathrm{I}} - 3r_{\mathrm{II}} + 3\sqrt{3}i_{\mathrm{II}}$	3ρ	0	0
$\varepsilon_{1_3}^{T_1}$	g_0	$-r_{\mathrm{I}} + \sqrt{3}i_{\mathrm{I}} + r_{\mathrm{II}} - \sqrt{3}i_{\mathrm{II}}$	$-\rho$	$2R_n + 2\sqrt{3}I_n$	$-2i_{\mathrm{I}}$
$\varepsilon_{1_3}^{T_2}$	g_0	$-r_{\mathrm{I}} + \sqrt{3}i_{\mathrm{I}} + r_{\mathrm{II}} - \sqrt{3}i_{\mathrm{II}}$	$-\rho$	$-2R_n - 2\sqrt{3}I_n$	$2i_{\mathrm{I}}$
2_3					
$\varepsilon_{2_3}^{E}$	g_0	$-r_{\mathrm{I}} - \sqrt{3}i_{\mathrm{I}} - 3r_{\mathrm{II}} - 3\sqrt{3}i_{\mathrm{II}}$	3ρ	0	0
$\varepsilon_{2_3}^{T_1}$	g_0	$-r_{\mathrm{I}} - \sqrt{3}i_{\mathrm{I}} + r_{\mathrm{II}} + \sqrt{3}i_{\mathrm{II}}$	$-\rho$	$2R_n - 2\sqrt{3}I_n$	$-2i_{\mathrm{I}}$
$\varepsilon_{2_3}^{T_2}$	g_0	$-r_{\mathrm{I}} - \sqrt{3}i_{\mathrm{I}} + r_{\mathrm{II}} + \sqrt{3}i_{\mathrm{II}})$	$-\rho$	$-2R_n + 2\sqrt{3}I_n$	$2i_{\mathrm{I}}$

Int.J.Mol.Sci, 14, 714(2013)

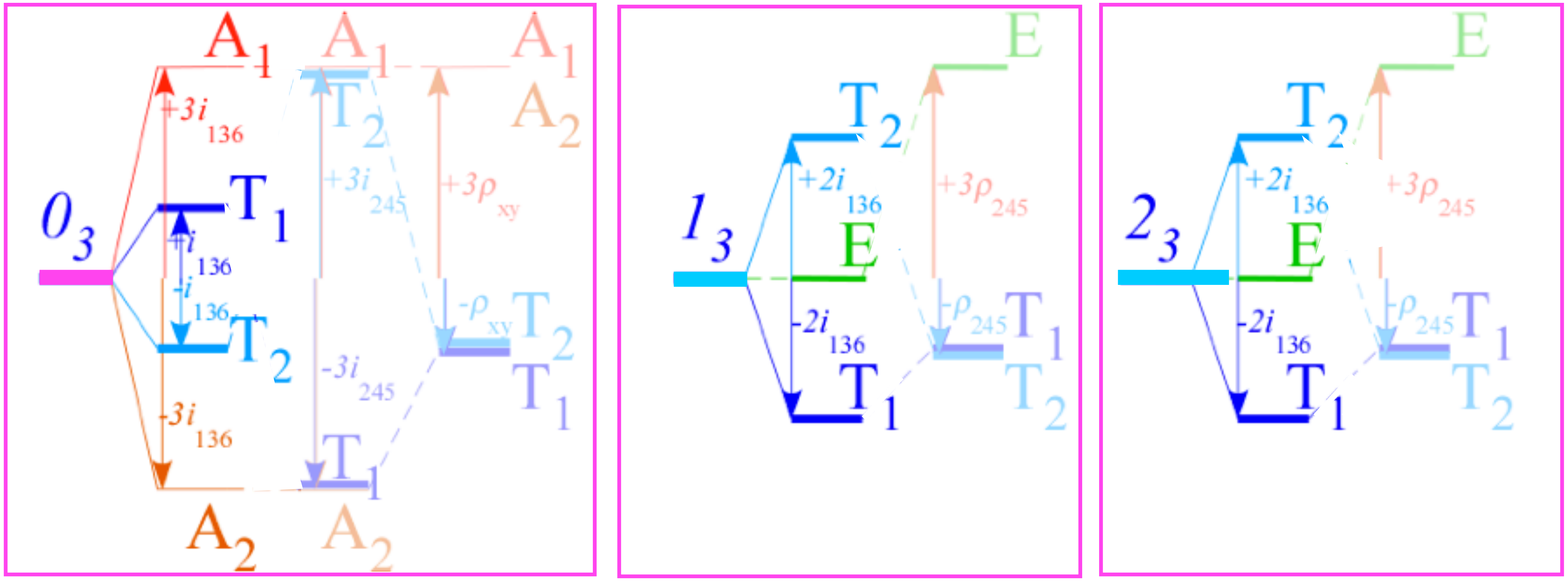


Table 12. Splittings of $O \supset C_3$ given sub-class structure.

C_3 *Subgroup-defined tunneling parameter modeling*

$O \supset C_3$	$0°$	$r_n 120°$	$\rho_n 180°$	$R_n 90°$	$i_n 180°$
0_3	$\cdot$	$r_I = Re(r_1)$ $i_I = Im(r_1)$ $r_{II} = Re(r_{234})$ $i_I = Im(r_{234})$	$\rho = \rho_{xyz}$	$R_n = Re(R_{xyz})$ $I_n = Im(R_{xyz})$	$i_I = i_{136}$ $i_{II} = i_{245}$
$\varepsilon_{0_3}^{A_1}$	g_0	$2r_I + 6r_{II}$	3ρ	$6R_n$	$3i_I + 3i_I$
$\varepsilon_{0_3}^{A_2}$	g_0	$2r_I + 6r_{II}$	3ρ	$-6R_n$	$-3i_I - 3i_{II}$
$\varepsilon_{0_3}^{T_1}$	g_0	$2r_I - 2r_{II}$	$-\rho$	$2R_n$	$i_I - 3i_{II}$
$\varepsilon_{0_3}^{T_2}$	g_0	$2r_I - 2r_{II}$	$-\rho$	$-2R_n$	$-i_I + 3i_{II}$
1_3					
$\varepsilon_{1_3}^{E}$	g_0	$-r_I + \sqrt{3}i_I - 3r_{II} + 3\sqrt{3}i_{II}$	3ρ	0	0
$\varepsilon_{1_3}^{T_1}$	g_0	$-r_I + \sqrt{3}i_I + r_{II} - \sqrt{3}i_{II}$	$-\rho$	$2R_n + 2\sqrt{3}I_n$	$-2i_I$
$\varepsilon_{1_3}^{T_2}$	g_0	$-r_I + \sqrt{3}i_I + r_{II} - \sqrt{3}i_{II}$	$-\rho$	$-2R_n - 2\sqrt{3}I_n$	$2i_I$
2_3					
$\varepsilon_{2_3}^{E}$	g_0	$-r_I - \sqrt{3}i_I - 3r_{II} - 3\sqrt{3}i_{II}$	3ρ	0	0
$\varepsilon_{2_3}^{T_1}$	g_0	$-r_I - \sqrt{3}i_I + r_{II} + \sqrt{3}i_{II}$	$-\rho$	$2R_n - 2\sqrt{3}I_n$	$-2i_I$
$\varepsilon_{2_3}^{T_2}$	g_0	$-r_I - \sqrt{3}i_I + r_{II} + \sqrt{3}i_{II})$	$-\rho$	$-2R_n + 2\sqrt{3}I_n$	$2i_I$

Int.J.Mol.Sci, 14, 714(2013)

Review Calculating idempotent projectors $\mathbf{P}^{\mu}_{m,m}$ *of* $O\supset C_4$ $\mathbf{P}^{E}_{0_4 0_4}$ $\mathbf{P}^{E}_{2_4 2_4}$ $\mathbf{P}^{T_1}_{0_4 0_4}$ $\mathbf{P}^{T_1}_{1_4 1_4}$ $\mathbf{P}^{T_2}_{2_4 2_4}$

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

Review Broken-class-ordered splitting of $O\supset D_4\supset C_4$ *projectors and levels*

Subgroup-defined tunneling parameter modeling

Comparing two diagonal $O\supset C_4$ *parameter sets to* SF_6 *spectra*

Comparing two diagonal $O\supset C_3$ *parameter sets to* SF_6 *spectra*

Why $O\supset C_2$ *parameter sets require off-diagonal nilpotent* $\mathbf{P}^{\mu}_{m,n}$ $(m\neq n)$

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

Using fundamental $\mathbf{g}\rightleftarrows\mathbf{P}^{\mu}_{m,n}$ *relations: (from Lecture 16)*

(a) $\mathbf{P}^{\mu}_{m,m}\mathbf{g}\mathbf{P}^{\mu}_{n,n}=D^{\mu}_{m,n}(\mathbf{g})\mathbf{P}^{\mu}_{m,n}$ (b) $\mathbf{g}=\Sigma_{\mu}\Sigma_{m,n}D^{\mu}_{m,n}(\mathbf{g})\mathbf{P}^{\mu}_{m,n}$ (c) $\mathbf{P}^{\mu}_{n,n}=(\ell^{\mu}/°G)\Sigma_{\mathbf{g}}D^{\mu*}_{m,n}(\mathbf{g})\mathbf{g}$

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

Calculating and Factoring $\mathbf{P}^{T_1}_{1_4 0_4}$ *and* $\mathbf{P}^{T_1}_{1_4 3_4}$

Structure and applications of various subgroup chain irreducible representations

$O_h\supset D_{4h}\supset C_{4v}$, $O_h\supset D_{3h}\supset C_{3v}$, $O_h\supset C_{2v}$

Comparing $O_h\supset D_{4h}\supset D_{2h}$ *and* $O_h\supset D_{3d}\supset C_2$ *representations (*T_1 *vector-type)*

Examples of off-diagonal tunneling coefficients $D^{E}_{0_4 2_4}$

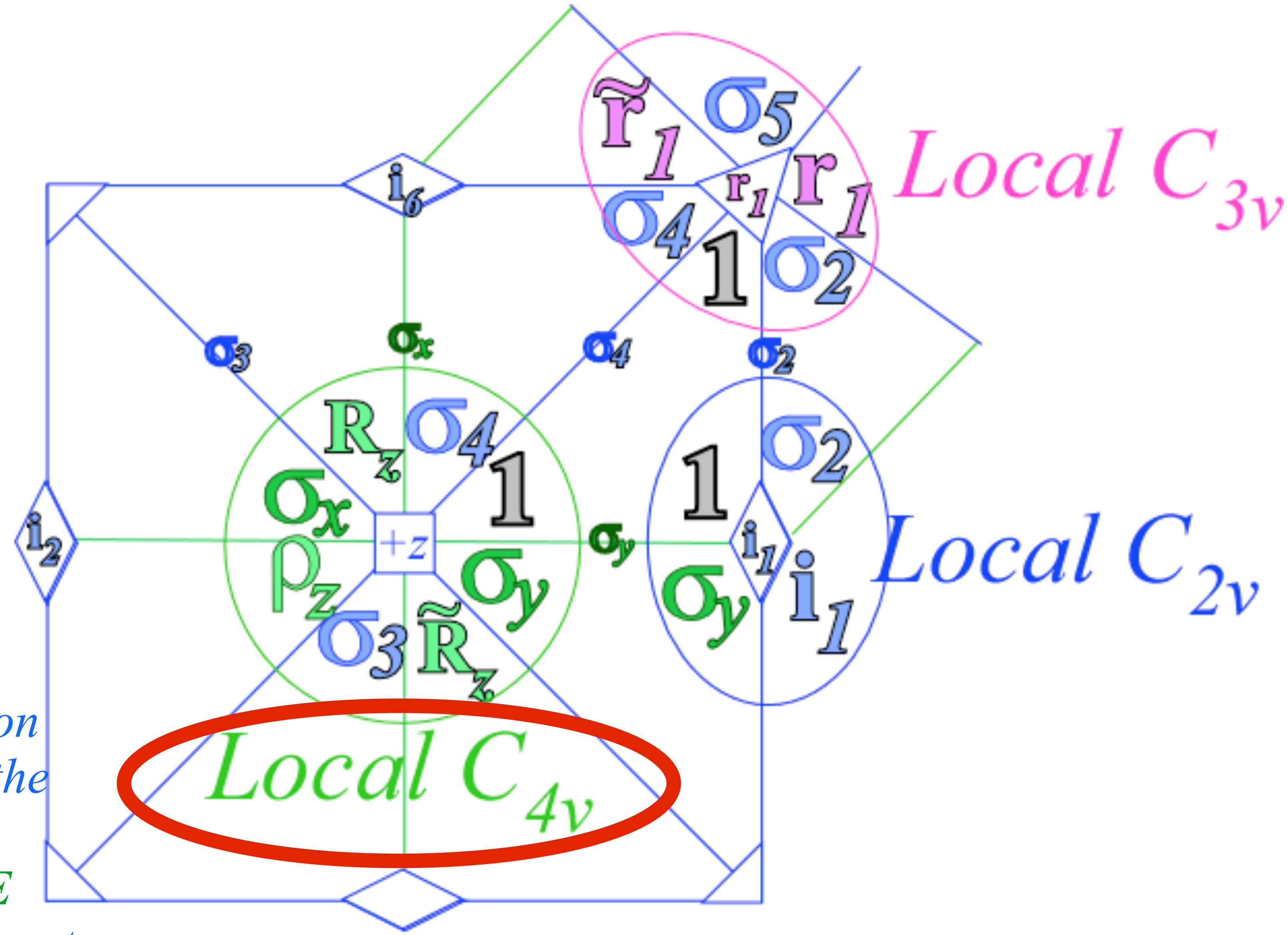
Comparing Local C_4, C_3, *and* C_2 *symmetric spectra*

Comparing off-diagonal $O\supset C_2$ *parameter sets to* CH_4 *models with "cluster-crossings"*

$O \supset C_4$	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
$A_{1g} \downarrow C_{4v}$	·	·	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

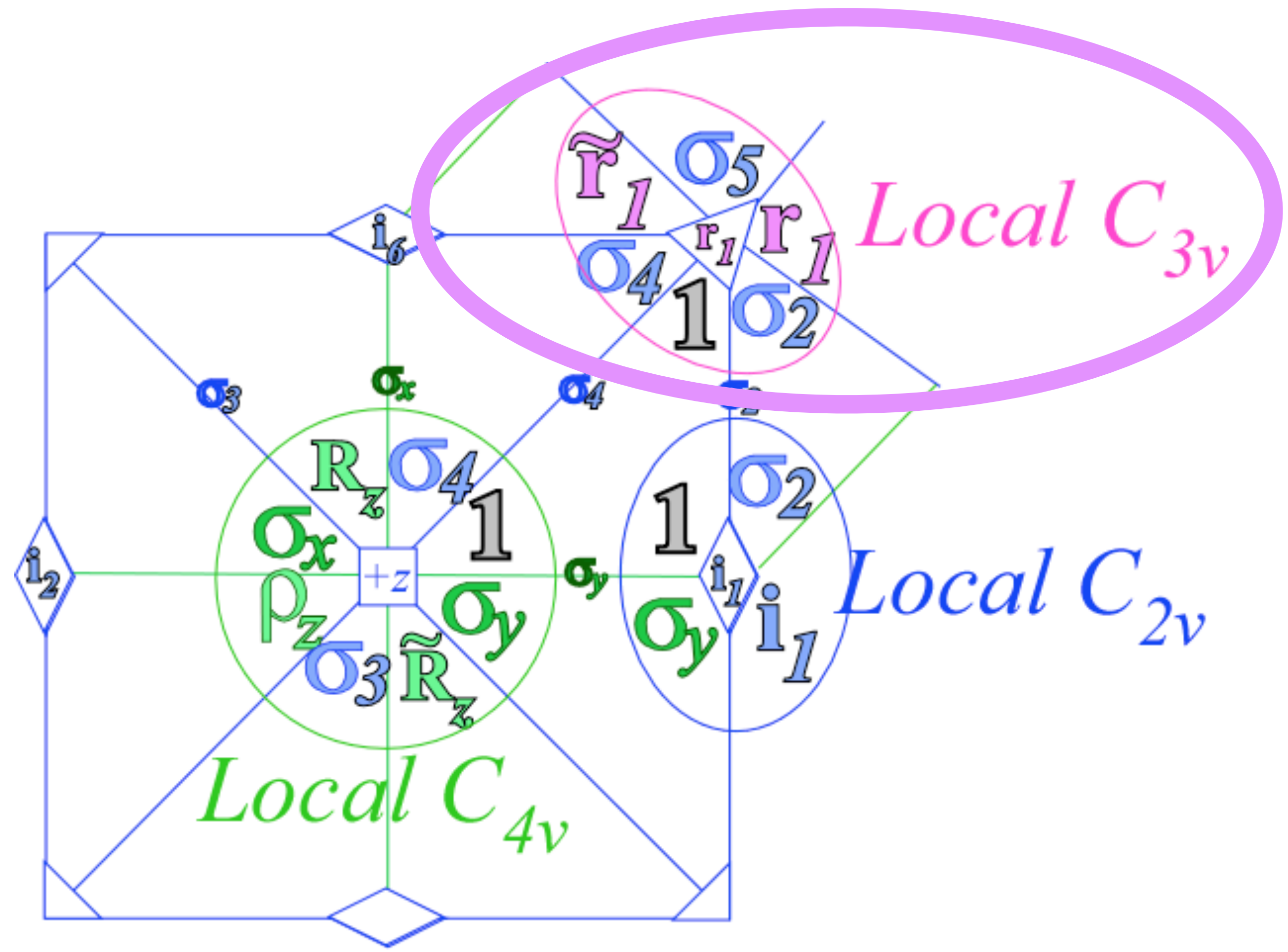
$O_h \supset C_{4v}$ correlation predicts the parity of the A_1T_1E cluster is not uniformly even (g) or odd (u): $A_{1g}T_{1u}E_g$



Int.J.Mol.Sci, 14, 714(2013)

$O \supset C_3$	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



Int.J.Mol.Sci, 14, 714(2013)

Why O⊃C₂ parameter sets require off-diagonal nilpotent $\mathbf{P}^{\mu}_{m,n}$ (m≠n)

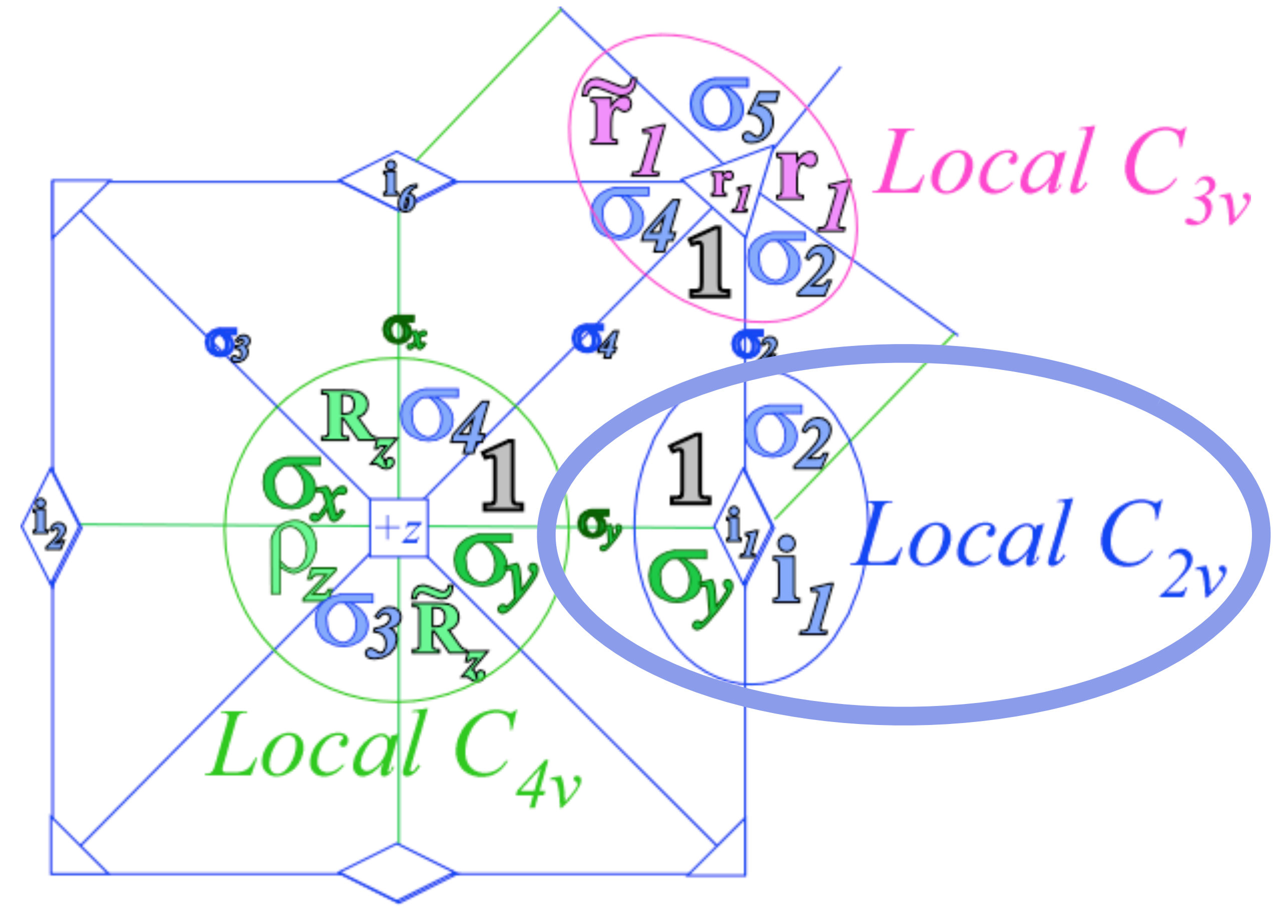
$O\supset C_2(\mathbf{i}_1)$	0_2	1_2
$A_1\downarrow C_2$	1	·
$A_2\downarrow C_2$	·	1
$E\downarrow C_2$	1	1
$T_1\downarrow C_2$	1	2
$T_2\downarrow C_2$	2	1

$O\supset C_2(\rho_z)$	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

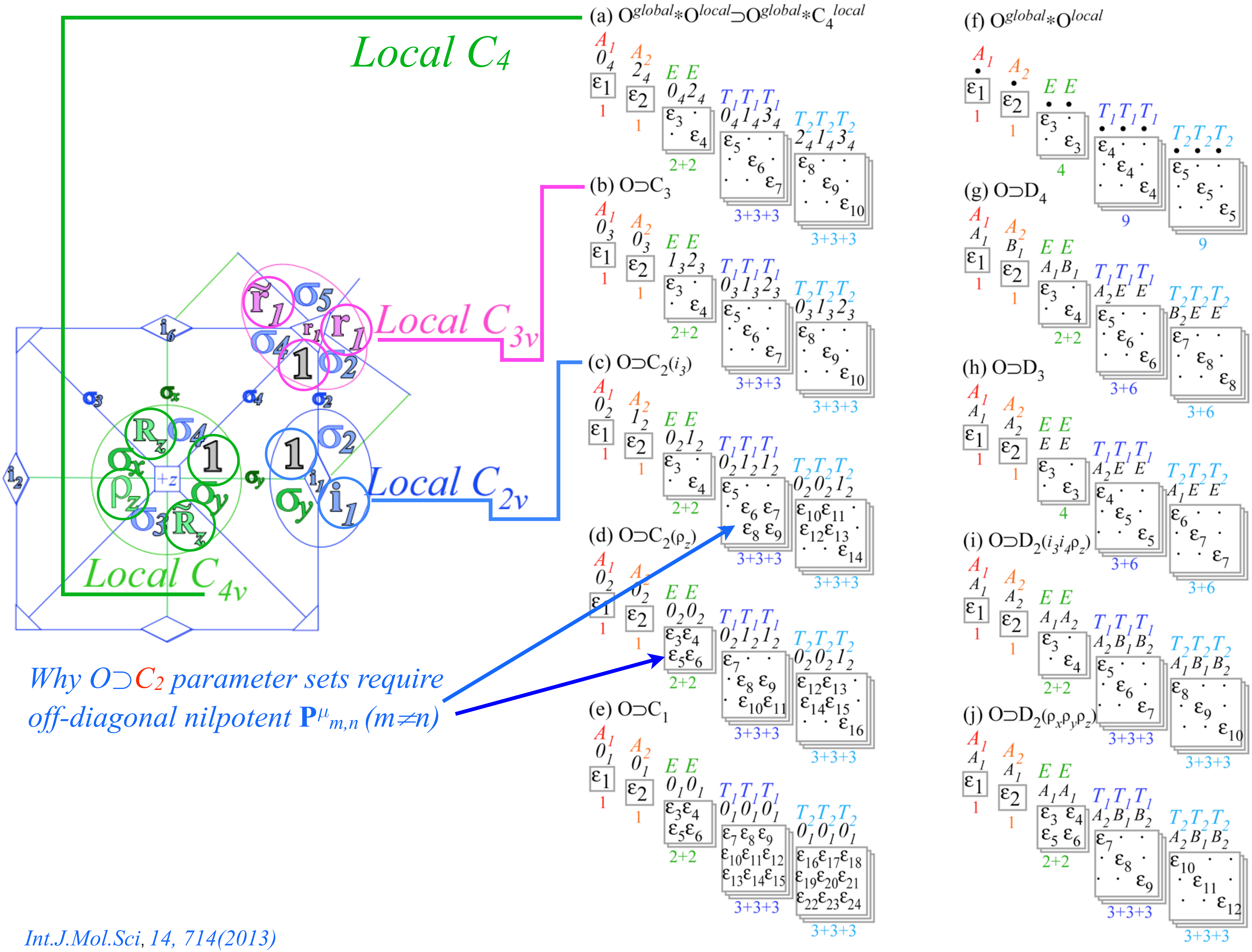
$O_h\supset C^i_{2v}$	A'	B'	A''	B''
$A_{1g}\downarrow C^i_{2v}$	1	·	·	·
$A_{2g}\downarrow C^i_{2v}$	·	1	·	·
$E_g\downarrow C^i_{2v}$	1	1	·	·
$T_{1g}\downarrow C^i_{2v}$	·	1	1	1
$T_{2g}\downarrow C^i_{2v}$	1	·	1	1
$A_{1g}\downarrow C^i_{2v}$	·	·	1	·
$A_{2u}\downarrow C^i_{2v}$	·	·	·	1
$E_u\downarrow C^i_{2v}$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

,

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



Int.J.Mol.Sci, 14, 714(2013)



Int.J.Mol.Sci, *14, 714(2013)*

Review Calculating idempotent projectors $\mathbf{P}^{\mu}{}_{m,m}$ *of* $O\supset C_4$ $\mathbf{P}^{E}{}_{0_4 0_4}$ $\mathbf{P}^{E}{}_{2_4 2_4}$ $\mathbf{P}^{T_1}{}_{0_4 0_4}$ $\mathbf{P}^{T_1}{}_{1_4 1_4}$ $\mathbf{P}^{T_2}{}_{2_4 2_4}$

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

Review Broken-class-ordered splitting of $O\supset D_4\supset C_4$ *projectors and levels*

Subgroup-defined tunneling parameter modeling

- *Comparing two diagonal* $O\supset C_4$ *parameter sets to* SF_6 *spectra*
- *Comparing two diagonal* $O\supset C_3$ *parameter sets to* SF_6 *spectra*
- *Why* $O\supset C_2$ *parameter sets require off-diagonal nilpotent* $\mathbf{P}^{\mu}{}_{m,n}$ $(m\neq n)$

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

- *Using fundamental* $\mathbf{g}\rightleftarrows\mathbf{P}^{\mu}{}_{m,n}$ *relations: (from Lecture 16)*
  - (a) $\mathbf{P}^{\mu}{}_{m,m}\,\mathbf{g}\mathbf{P}^{\mu}{}_{n,n}=D^{\mu}{}_{m,n}(\mathbf{g})\mathbf{P}^{\mu}{}_{m,n}$ (b) $\mathbf{g}=\Sigma_{\mu}\Sigma_{m,n}D^{\mu}{}_{m,n}(\mathbf{g})\mathbf{P}^{\mu}{}_{m,n}$ (c) $\mathbf{P}^{\mu}{}_{n,n}=(\ell^{\mu}/{}^{\circ}G)\Sigma_{\mathbf{g}}D^{\mu*}{}_{m,n}(\mathbf{g})\mathbf{g}$
- *Review of* $D_3\supset C_2\sim C_{3v}\supset C_v$
- *Calculating and Factoring* $\mathbf{P}^{T_1}{}_{1_4 0_4}$ *and* $\mathbf{P}^{T_1}{}_{1_4 3_4}$

Structure and applications of various subgroup chain irreducible representations

- $O_h\supset D_{4h}\supset C_{4v}$, $O_h\supset D_{3h}\supset C_{3v}$, $O_h\supset C_{2v}$
- *Comparing* $O_h\supset D_{4h}\supset D_{2h}$ *and* $O_h\supset D_{3d}\supset C_2$ *representations (*T_1 *vector-type)*
  - *Examples of off-diagonal tunneling coefficients* $D^{E}{}_{0_4 2_4}$
- *Comparing Local* C_4, C_3, *and* C_2 *symmetric spectra*
- *Comparing off-diagonal* $O\supset C_2$ *parameter sets to* CH_4 *models with "cluster-crossings"*

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

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

(from Lecture 16 p.34 and p.50)

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

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

Fundamental $\mathbf{P}^{\mu}{}_{m,n}$ *definitions:* *(from Lecture 6 p.34 and p.50)*

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

Problem: Need to derive *both* $\mathbf{P}^{\mu}{}_{m,n}$ *and* $D^{\mu}{}_{m,n}(\mathrm{g})$ for unequal *(m≠n)* values.

Irreducible nilpotent projectors $\mathbf{P}^{\mu}_{m,n}$ *(m≠n)*

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

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

Problem: Need to derive *both* $\mathbf{P}^{\mu}_{m,n}$ *and* $D^{\mu}_{m,n}$(g) for unequal *(m≠n)* values.

Solution: First use $\mathbf{P}^{\mu}_{m,m}$ in (1) to get something proportional to $\mathbf{P}^{\mu}_{m,n}$

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

Irreducible nilpotent projectors $\mathbf{P}^{\mu}_{m,n}$ *(m≠n)*

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

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

Problem: Need to derive *both* $\mathbf{P}^{\mu}_{m,n}$ *and* $D^{\mu}_{m,n}$(g) for unequal *(m≠n)* values.

Solution: First use $\mathbf{P}^{\mu}_{m,m}$ in (1) to get something proportional to $\mathbf{P}^{\mu}_{m,n}$

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

Then find $D^{\mu}_{m,n}$(g) by operator transformations:

$$\mathbf{g}\mathbf{P}^{\mu}_{mn} = \sum_{k}^{\ell^{\mu}} D^{\mu}_{km}(\mathbf{g})\mathbf{P}^{\mu}_{kn}$$

Irreducible nilpotent projectors $\mathbf{P}^{\mu}_{m,n}$ *(m≠n)*

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

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

Problem: Need to derive *both* $\mathbf{P}^{\mu}_{m,n}$ *and* $D^{\mu}_{m,n}$(g) for unequal *(m≠n)* values.

Solution: First use $\mathbf{P}^{\mu}_{m,m}$ in (1) to get something proportional to $\mathbf{P}^{\mu}_{m,n}$ $\boxed{\mathbf{P}^{\mu}_{mm}\mathbf{g}\mathbf{P}^{\mu}_{nn} = (?)\cdot\mathbf{P}^{\mu}_{mn}}$

Then find $D^{\mu}_{m,n}$(g) by operator transformations: $\mathbf{g}\mathbf{P}^{\mu}_{mn} = \sum_{k}^{\ell^{\mu}} D^{\mu}_{km}(\mathbf{g})\mathbf{P}^{\mu}_{kn}$

or by projector nomalization: $\mathbf{P}^{\mu}_{mn}\mathbf{P}^{\mu\dagger}_{mn} = \mathbf{P}^{\mu}_{mn}\mathbf{P}^{\mu}_{nm} = \mathbf{P}^{\mu}_{mm}$

Irreducible nilpotent projectors $\mathbf{P}^{\mu}_{m,n}$ *(m≠n)*

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

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

Problem: Need to derive *both* $\mathbf{P}^{\mu}_{m,n}$ *and* $D^{\mu}_{m,n}$(g) for unequal *(m≠n)* values.

Solution: First use $\mathbf{P}^{\mu}_{m,m}$ in (1) to get something proportional to $\mathbf{P}^{\mu}_{m,n}$ $\boxed{\mathbf{P}^{\mu}_{mm}\mathbf{g}\mathbf{P}^{\mu}_{nn} = (?)\cdot\mathbf{P}^{\mu}_{mn}}$

Then find $D^{\mu}_{m,n}$(g) by operator transformations: $\mathbf{g}\mathbf{P}^{\mu}_{mn} = \sum_{k}^{\ell^{\mu}} D^{\mu}_{km}(\mathbf{g})\mathbf{P}^{\mu}_{kn}$

or by projector nomalization: $\mathbf{P}^{\mu}_{mn}\mathbf{P}^{\mu\dagger}_{mn} = \mathbf{P}^{\mu}_{mn}\mathbf{P}^{\mu}_{nm} = \mathbf{P}^{\mu}_{mm}$

or by ket-vector transformations: $\mathbf{g}\left|\mathbf{P}^{\mu}_{mn}\right\rangle = \sum_{k}^{\ell^{\mu}} D^{\mu}_{km}(\mathbf{g})\left|\mathbf{P}^{\mu}_{kn}\right\rangle$

Irreducible nilpotent projectors $\mathbf{P}^{\mu}_{m,n}$ *(m≠n)*

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

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

Problem: Need to derive *both* $\mathbf{P}^{\mu}_{m,n}$ *and* $D^{\mu}_{m,n}$(g) for unequal *(m≠n)* values.

Solution: First use $\mathbf{P}^{\mu}_{m,m}$ in (1) to get something proportional to $\mathbf{P}^{\mu}_{m,n}$ $\boxed{\mathbf{P}^{\mu}_{mm}\mathbf{g}\mathbf{P}^{\mu}_{nn} = (?)\cdot\mathbf{P}^{\mu}_{mn}}$

Then find $D^{\mu}_{m,n}$(g) by operator transformations: $\mathbf{g}\mathbf{P}^{\mu}_{mn} = \sum_{k}^{\ell^{\mu}} D^{\mu}_{km}(\mathbf{g})\mathbf{P}^{\mu}_{kn}$

or by projector nomalization: $\mathbf{P}^{\mu}_{mn}\mathbf{P}^{\mu\dagger}_{mn} = \mathbf{P}^{\mu}_{mn}\mathbf{P}^{\mu}_{nm} = \mathbf{P}^{\mu}_{mm}$

or by ket-vector transformations: $\mathbf{g}\left|\mathbf{P}^{\mu}_{mn}\right\rangle = \sum_{k}^{\ell^{\mu}} D^{\mu}_{km}(\mathbf{g})\left|\mathbf{P}^{\mu}_{kn}\right\rangle$

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

Irreducible nilpotent projectors $\mathbf{P}^{\mu}_{m,n}$ *(m≠n)*

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

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

Problem: Need to derive *both* $\mathbf{P}^{\mu}_{m,n}$ *and* $D^{\mu}_{m,n}$(g) for unequal *(m≠n)* values.

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

Solution: First use $\mathbf{P}^{\mu}_{m,m}$ in (1) to get something proportional to $\mathbf{P}^{\mu}_{m,n}$

Then find $D^{\mu}_{m,n}$(g) by operator transformations: $\mathbf{g}\mathbf{P}^{\mu}_{mn} = \sum_{k}^{\ell^{\mu}} D^{\mu}_{km}(\mathbf{g})\mathbf{P}^{\mu}_{kn}$

or by projector nomalization: $\mathbf{P}^{\mu}_{mn}\mathbf{P}^{\mu\dagger}_{mn} = \mathbf{P}^{\mu}_{mn}\mathbf{P}^{\mu}_{nm} = \mathbf{P}^{\mu}_{mm}$

or by ket-vector transformations: $\mathbf{g}\left|\mathbf{P}^{\mu}_{mn}\right\rangle = \sum_{k}^{\ell^{\mu}} D^{\mu}_{km}(\mathbf{g})\left|\mathbf{P}^{\mu}_{kn}\right\rangle$

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

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

Irreducible nilpotent projectors $\mathbf{P}^{\mu}{}_{m,n}$ *(m≠n)*

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

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

Problem: Need to derive *both* $\mathbf{P}^{\mu}{}_{m,n}$ *and* $D^{\mu}{}_{m,n}$(g) for unequal *(m≠n)* values.

Solution: First use $\mathbf{P}^{\mu}{}_{m,m}$ in (1) to get something proportional to $\mathbf{P}^{\mu}{}_{m,n}$ $\mathbf{P}^{\mu}_{mm}\mathbf{g}\mathbf{P}^{\mu}_{nn} = (?)\cdot\mathbf{P}^{\mu}_{mn}$

Then find $D^{\mu}{}_{m,n}$(g) by operator transformations: $\mathbf{g}\mathbf{P}^{\mu}_{mn} = \sum_{k}^{\ell^{\mu}} D^{\mu}_{km}(\mathbf{g})\mathbf{P}^{\mu}_{kn}$

or by projector nomalization: $\mathbf{P}^{\mu}_{mn}\mathbf{P}^{\mu\dagger}_{mn} = \mathbf{P}^{\mu}_{mn}\mathbf{P}^{\mu}_{nm} = \mathbf{P}^{\mu}_{mm}$

or by ket-vector transformations: $\mathbf{g}\left|\mathbf{P}^{\mu}_{mn}\right\rangle = \sum_{k}^{\ell^{\mu}} D^{\mu}_{km}(\mathbf{g})\left|\mathbf{P}^{\mu}_{kn}\right\rangle$

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

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

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

Review Calculating idempotent projectors $\mathbf{P}^{\mu}_{m,m}$ *of* $O\supset C_4$ $\mathbf{P}^{E}_{0_4 0_4}$ $\mathbf{P}^{E}_{2_4 2_4}$ $\mathbf{P}^{T_1}_{0_4 0_4}$ $\mathbf{P}^{T_1}_{1_4 1_4}$ $\mathbf{P}^{T_2}_{2_4 2_4}$

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

Review Broken-class-ordered splitting of $O\supset D_4\supset C_4$ *projectors and levels*

Subgroup-defined tunneling parameter modeling

Comparing two diagonal $O\supset C_4$ *parameter sets to* SF_6 *spectra*

Comparing two diagonal $O\supset C_3$ *parameter sets to* SF_6 *spectra*

Why $O\supset C_2$ *parameter sets require off-diagonal nilpotent* $\mathbf{P}^{\mu}_{m,n}$ $(m\neq n)$

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

Using fundamental $\mathbf{g}\rightleftarrows\mathbf{P}^{\mu}_{m,n}$ *relations: (from Lecture 16)*

(a) $\mathbf{P}^{\mu}_{m,m}\,\mathbf{g}\mathbf{P}^{\mu}_{n,n}=D^{\mu}_{m,n}(\mathbf{g})\mathbf{P}^{\mu}_{m,n}$ (b) $\mathbf{g}=\Sigma_{\mu}\Sigma_{m,n}D^{\mu}_{m,n}(\mathbf{g})\mathbf{P}^{\mu}_{m,n}$ (c) $\mathbf{P}^{\mu}_{n,n}=(\ell^{\mu}/{}^{\circ}G)\Sigma_{\mathbf{g}}D^{\mu *}_{m,n}(\mathbf{g})\mathbf{g}$

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

Calculating and Factoring $\mathbf{P}^{T_1}_{1_4 0_4}$ *and* $\mathbf{P}^{T_1}_{1_4 3_4}$

Structure and applications of various subgroup chain irreducible representations

$O_h\supset D_{4h}\supset C_{4v}$, $O_h\supset D_{3h}\supset C_{3v}$, $O_h\supset C_{2v}$

Comparing $O_h\supset D_{4h}\supset D_{2h}$ *and* $O_h\supset D_{3d}\supset C_2$ *representations (*T_1 *vector-type)*

Examples of off-diagonal tunneling coefficients $D^{E}_{0_4 2_4}$

Comparing Local C_4, C_3, *and* C_2 *symmetric spectra*

Comparing off-diagonal $O\supset C_2$ *parameter sets to* CH_4 *models with "cluster-crossings"*

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

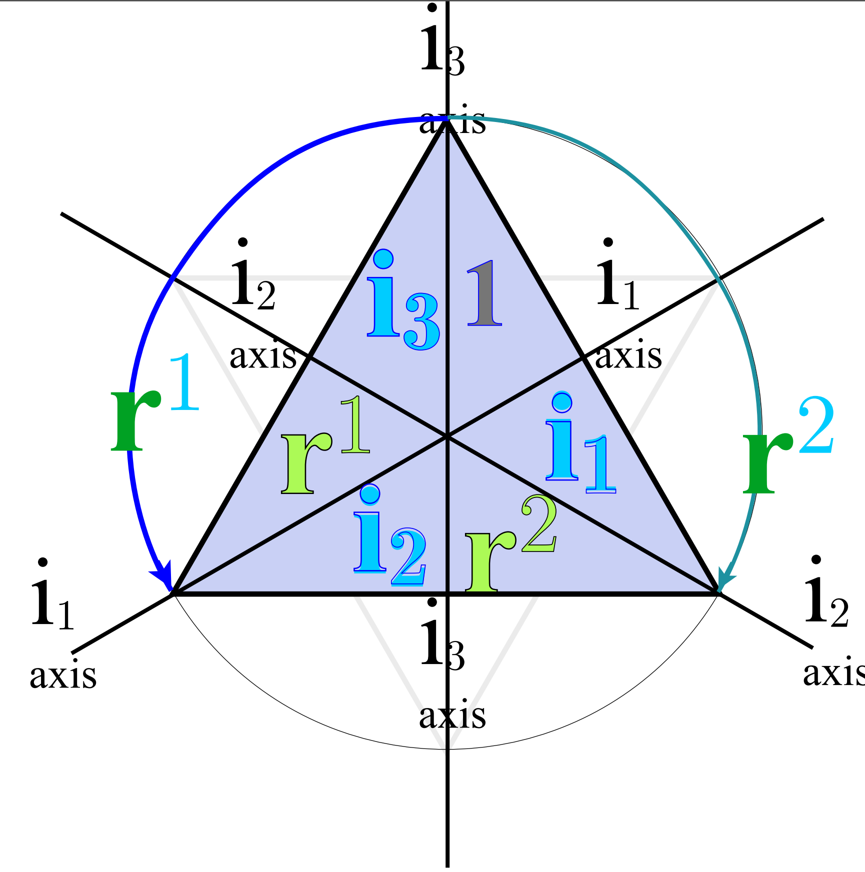
Review of $D_3 \supset C_2 \sim C_{3v} \supset C_v$

$$\mathbf{P}^{\mu}_{mn} = \frac{\ell^{\mu}}{°G} \sum_{\mathbf{g}}^{°G} D^{\mu *}_{mn}(\mathbf{g})\mathbf{g}$$

$D_3 : \chi^{\alpha}_k$	χ^{α}_1	χ^{α}_r	χ^{α}_i
$\alpha = A_1$	1	1	1
$\alpha = A_2$	1	1	-1
$\alpha = E$	2	-1	0

Given: $\mathbf{P}^{E} = \frac{1}{3}(2\mathbf{c}_1 - \mathbf{c}_r + 0)$

$= \frac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)$



First do $C_2 = \{\mathbf{1}, \mathbf{i}_3\}$ splitting:

$$\mathbf{P}^{E}_{0_2 0_2} = \mathbf{P}^{E}\mathbf{p}_{0_2} = \tfrac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)\tfrac{1}{2}(\mathbf{1} + \mathbf{i}_3) = \tfrac{1}{6}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 - \mathbf{i}_2 + 2\mathbf{i}_3)$$

$$\mathbf{P}^{E}_{1_2 1_2} = \mathbf{P}^{E}\mathbf{p}_{1_2} = \tfrac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)\tfrac{1}{2}(\mathbf{1} - \mathbf{i}_3) = \tfrac{1}{6}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 + \mathbf{i}_1 + \mathbf{i}_2 - 2\mathbf{i}_3)$$

Then find nilpotent proportional to: $\mathbf{P}^{E}_{1_2 0_2} = \mathbf{P}^{E}\mathbf{p}_{1_2}\mathbf{r}\mathbf{p}_{0_2}$

Irreducible nilpotent projectors $\mathbf{P}^{\mu}_{m,n}$ *(m≠n)*

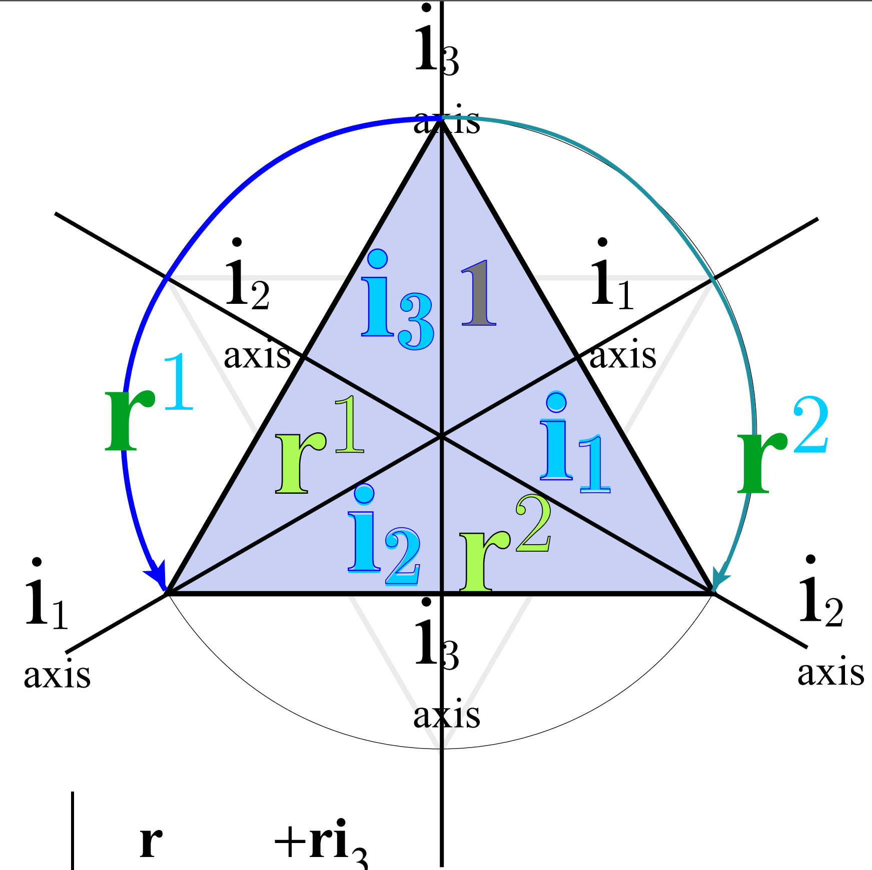
Review of $D_3 \supset C_2 \sim C_{3v} \supset C_v$

$$\mathbf{P}^{\mu}_{mn} = \frac{\ell^{\mu}}{°G} \sum_{\mathbf{g}}^{°G} D^{\mu *}_{mn}(\mathbf{g})\mathbf{g}$$

$D_3 : \chi^{\alpha}_{k}$	χ^{α}_{1}	χ^{α}_{r}	χ^{α}_{i}
$\alpha = A_1$	1	1	1
$\alpha = A_2$	1	1	−1
$\alpha = E$	2	−1	0

Given: $\mathbf{P}^{E} = \frac{1}{3}(2\mathbf{c}_1 - \mathbf{c}_r + 0)$

$= \frac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)$



First do $C_2 = \{\mathbf{1}, \mathbf{i}_3\}$ splitting:

$$\mathbf{P}^{E}_{0_2 0_2} = \mathbf{P}^{E}\mathbf{p}_{0_2} = \tfrac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)\tfrac{1}{2}(\mathbf{1} + \mathbf{i}_3) = \tfrac{1}{6}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 - \mathbf{i}_2 + 2\mathbf{i}_3)$$

$$\mathbf{P}^{E}_{1_2 1_2} = \mathbf{P}^{E}\mathbf{p}_{1_2} = \tfrac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)\tfrac{1}{2}(\mathbf{1} - \mathbf{i}_3) = \tfrac{1}{6}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 + \mathbf{i}_1 + \mathbf{i}_2 - 2\mathbf{i}_3)$$

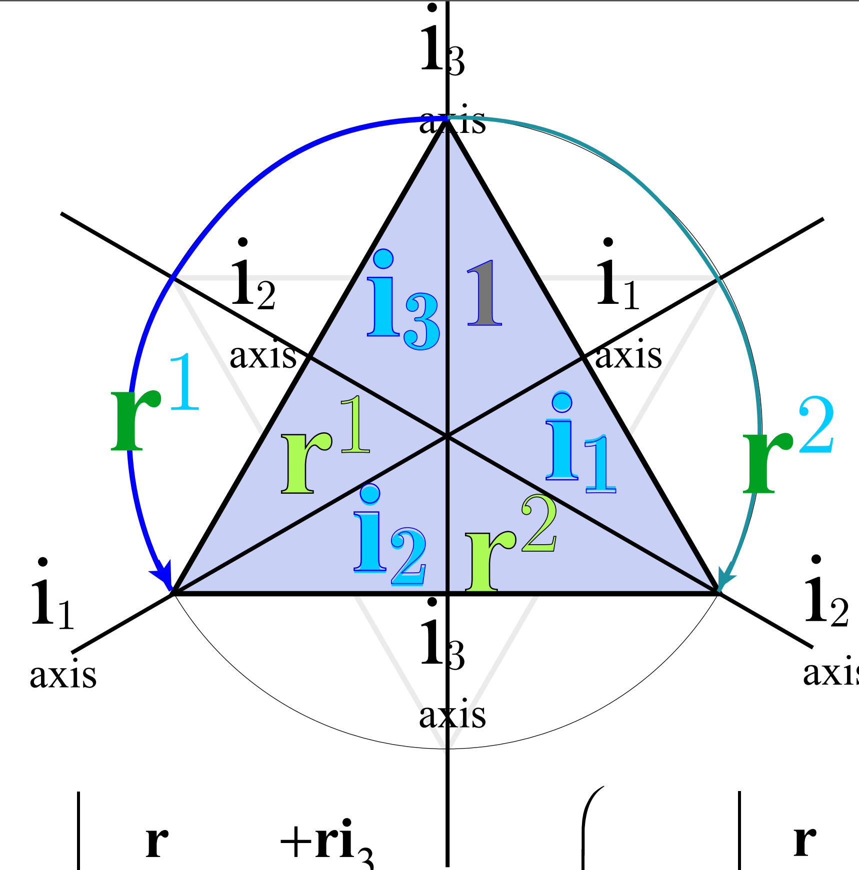
Then find nilpotent proportional to: $\mathbf{P}^{E}_{1_2 0_2} = \mathbf{P}^{E}\mathbf{p}_{1_2}\mathbf{r}\mathbf{p}_{0_2} = \mathbf{P}^{E}\,\frac{1}{2}\cdot\frac{1}{2}\Big($

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

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

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

$$\mathbf{P}^{\mu}_{mn} = \frac{\ell^{\mu}}{{}^{\circ}G} \sum_{\mathbf{g}}^{{}^{\circ}G} D^{\mu *}_{mn}(\mathbf{g})\mathbf{g}$$



$D_3 : \chi^{\alpha}_{k}$	χ^{α}_{1}	χ^{α}_{r}	χ^{α}_{i}
$\alpha = A_1$	1	1	1
$\alpha = A_2$	1	1	−1
$\alpha = E$	2	−1	0

Given: $\mathbf{P}^{E} = \frac{1}{3}(2\mathbf{c}_1 - \mathbf{c}_r + 0)$

$= \frac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)$

First do $C_2 = \{\mathbf{1}, \mathbf{i}_3\}$ splitting:

$$\mathbf{P}^{E}_{0_2 0_2} = \mathbf{P}^{E}\mathbf{p}_{0_2} = \tfrac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)\tfrac{1}{2}(\mathbf{1} + \mathbf{i}_3) = \tfrac{1}{6}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 - \mathbf{i}_2 + 2\mathbf{i}_3)$$

$$\mathbf{P}^{E}_{1_2 1_2} = \mathbf{P}^{E}\mathbf{p}_{1_2} = \tfrac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)\tfrac{1}{2}(\mathbf{1} - \mathbf{i}_3) = \tfrac{1}{6}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 + \mathbf{i}_1 + \mathbf{i}_2 - 2\mathbf{i}_3)$$

Then find nilpotent proportional to: $\mathbf{P}^{E}_{1_2 0_2} = \mathbf{P}^{E}\mathbf{p}_{1_2}\mathbf{r}\mathbf{p}_{0_2} = \mathbf{P}^{E}\,\frac{1}{2}\cdot\frac{1}{2}\left(\begin{array}{c|cc} & \mathbf{r} & +\mathbf{r}\mathbf{i}_3 \\ \hline \mathbf{1} & \mathbf{r} & +\mathbf{r}\mathbf{i}_3 \\ -\mathbf{i}_3 & -\mathbf{i}_3\mathbf{r} & -\mathbf{i}_3\mathbf{r}\mathbf{i}_3 \end{array}\right) = \frac{1}{4}\mathbf{P}^{E}\left(\begin{array}{c|cc} & \mathbf{r} & +\mathbf{r}\mathbf{i}_3 \\ \hline \mathbf{1} & \mathbf{r} & +\mathbf{i}_2 \\ -\mathbf{i}_3 & -\mathbf{i}_1 & -\mathbf{r}^2 \end{array}\right)$

Irreducible nilpotent projectors $\mathbf{P}^{\mu}{}_{m,n}$ *($m \neq n$)*

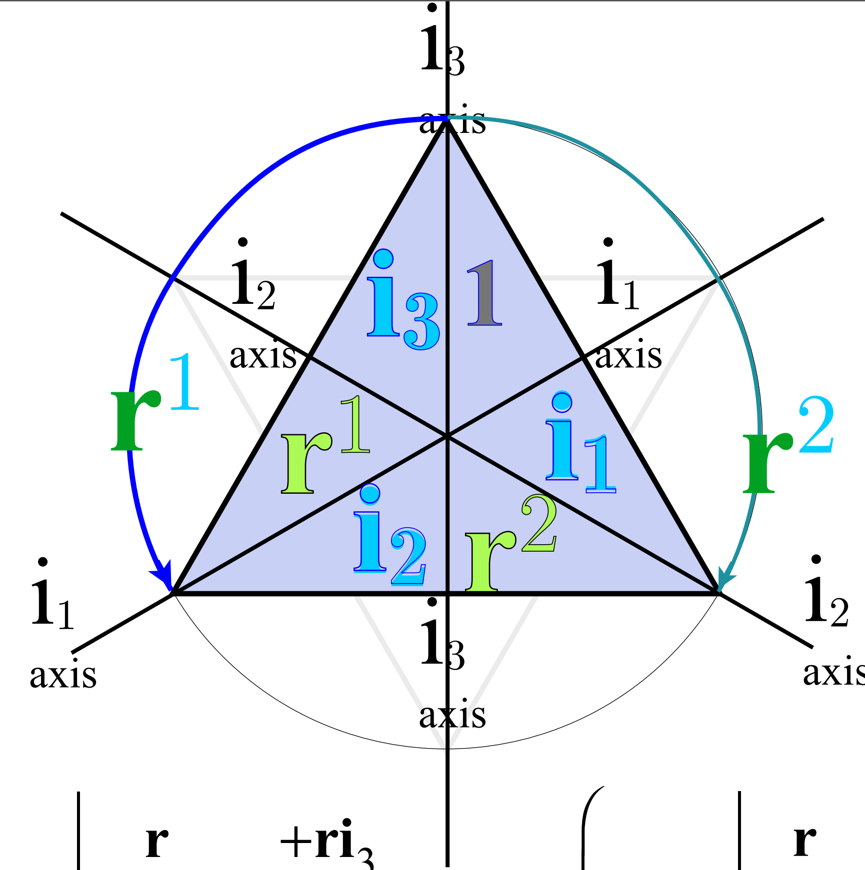
$$\mathbf{P}^{\mu}_{mn} = \frac{\ell^{\mu}}{{}^{\circ}G} \sum_{\mathbf{g}}^{{}^{\circ}G} D^{\mu *}_{mn}(\mathbf{g})\mathbf{g}$$

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

$D_3 : \chi^{\alpha}_{k}$	χ^{α}_{1}	χ^{α}_{r}	χ^{α}_{i}
$\alpha = A_1$	1	1	1
$\alpha = A_2$	1	1	-1
$\alpha = E$	2	-1	0

Given: $\mathbf{P}^{E} = \frac{1}{3}(2\mathbf{c}_1 - \mathbf{c}_r + 0)$

$= \frac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)$



First do $C_2 = \{\mathbf{1}, \mathbf{i}_3\}$ splitting:

$$\mathbf{P}^{E}_{0_2 0_2} = \mathbf{P}^{E}\mathbf{p}_{0_2} = \tfrac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)\tfrac{1}{2}(\mathbf{1} + \mathbf{i}_3) = \tfrac{1}{6}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 - \mathbf{i}_2 + 2\mathbf{i}_3)$$

$$\mathbf{P}^{E}_{1_2 1_2} = \mathbf{P}^{E}\mathbf{p}_{1_2} = \tfrac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)\tfrac{1}{2}(\mathbf{1} - \mathbf{i}_3) = \tfrac{1}{6}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 + \mathbf{i}_1 + \mathbf{i}_2 - 2\mathbf{i}_3)$$

Then find nilpotent proportional to: $\mathbf{P}^{E}_{1_2 0_2} = \mathbf{P}^{E}\mathbf{p}_{1_2}\mathbf{r}\mathbf{p}_{0_2} = \mathbf{P}^{E}\,\frac{1}{2}\cdot\frac{1}{2}$

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

$= \frac{1}{4}\,\mathbf{P}^{E}$

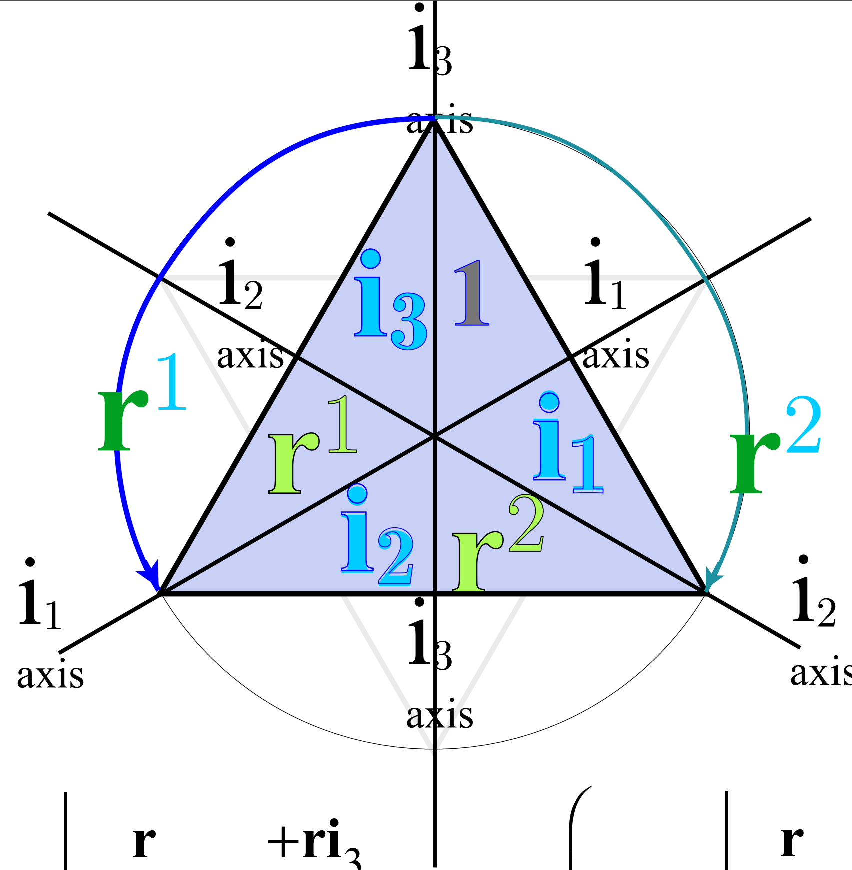
	$\mathbf{r}$	$+\mathbf{r}\mathbf{i}_3$
$\mathbf{1}$	$\mathbf{r}$	$+\mathbf{i}_2$
$-\mathbf{i}_3$	$-\mathbf{i}_1$	$-\mathbf{r}^2$

or: $\mathbf{P}^{E}_{1_2 0_2} = (?) \cdot (\mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 + \mathbf{i}_2)$

Irreducible nilpotent projectors $\mathbf{P}^{\mu}{}_{m,n}$ *($m \neq n$)*

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

$$\mathbf{P}^{\mu}_{mn} = \frac{\ell^{\mu}}{{}^{\circ}G} \sum_{\mathbf{g}}^{{}^{\circ}G} D^{\mu *}_{mn}(\mathbf{g})\mathbf{g}$$



$D_3 : \chi^{\alpha}_{k}$	χ^{α}_{1}	χ^{α}_{r}	χ^{α}_{i}
$\alpha = A_1$	1	1	1
$\alpha = A_2$	1	1	-1
$\alpha = E$	2	-1	0

Given: $\mathbf{P}^{E} = \frac{1}{3}(2\mathbf{c}_1 - \mathbf{c}_r + 0)$

$= \frac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)$

First do $C_2 = \{\mathbf{1}, \mathbf{i}_3\}$ splitting:

$$\mathbf{P}^{E}_{0_2 0_2} = \mathbf{P}^{E}\mathbf{p}_{0_2} = \frac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)\frac{1}{2}(\mathbf{1} + \mathbf{i}_3) = \frac{1}{6}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 - \mathbf{i}_2 + 2\mathbf{i}_3)$$

$$\mathbf{P}^{E}_{1_2 1_2} = \mathbf{P}^{E}\mathbf{p}_{1_2} = \frac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)\frac{1}{2}(\mathbf{1} - \mathbf{i}_3) = \frac{1}{6}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 + \mathbf{i}_1 + \mathbf{i}_2 - 2\mathbf{i}_3)$$

Then find nilpotent proportional to: $\mathbf{P}^{E}_{1_2 0_2} = \mathbf{P}^{E}\mathbf{p}_{1_2}\mathbf{r}\mathbf{p}_{0_2} = \mathbf{P}^{E}\,\frac{1}{2}\cdot\frac{1}{2}$

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

$= \frac{1}{4}\,\mathbf{P}^{E}$

	$\mathbf{r}$	$+\mathbf{r}\mathbf{i}_3$
$\mathbf{1}$	$\mathbf{r}$	$+\mathbf{i}_2$
$-\mathbf{i}_3$	$-\mathbf{i}_1$	$-\mathbf{r}^2$

or: $\mathbf{P}^{E}_{1_2 0_2} = (?)\cdot(\mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 + \mathbf{i}_2)$

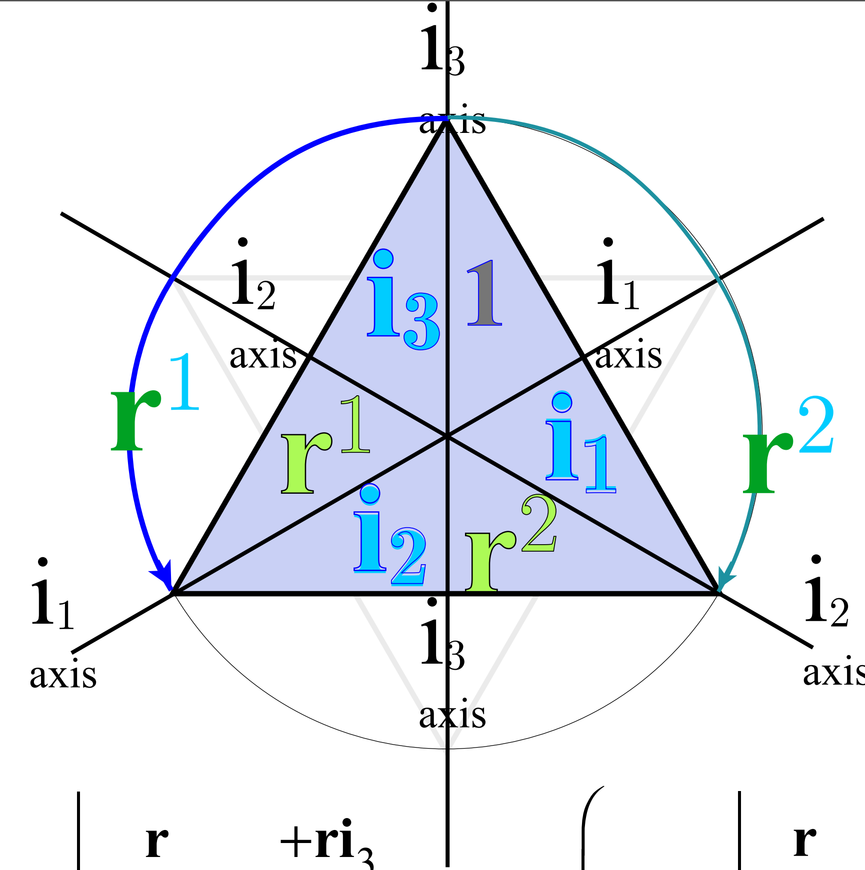
† conjugation: $(\mathbf{r}^{\dagger} = \mathbf{r}^2, \mathbf{r}^{2\dagger} = \mathbf{r}, \mathbf{i}_1^{\dagger} = \mathbf{i}_1, \mathbf{i}_2^{\dagger} = \mathbf{i}_2)$

so: $\mathbf{P}^{E\dagger}_{1_2 0_2} = \mathbf{P}^{E}_{0_2 1_2} = (?)^{*}(\mathbf{r}^2 - \mathbf{r} - \mathbf{i}_1 + \mathbf{i}_2)$

Irreducible nilpotent projectors $\mathbf{P}^{\mu}_{m,n}$ *(m≠n)*

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

$$\mathbf{P}^{\mu}_{mn} = \frac{\ell^{\mu}}{{}^{\circ}G} \sum_{\mathbf{g}}^{{}^{\circ}G} D^{\mu *}_{mn}(\mathbf{g})\mathbf{g}$$



$D_3 : \chi^{\alpha}_k$	χ^{α}_1	χ^{α}_r	χ^{α}_i
$\alpha = A_1$	1	1	1
$\alpha = A_2$	1	1	−1
$\alpha = E$	2	−1	0

Given: $\mathbf{P}^E = \frac{1}{3}(2\mathbf{c}_1 - \mathbf{c}_r + 0)$

$= \frac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)$

First do $C_2 = \{\mathbf{1}, \mathbf{i}_3\}$ splitting:

$$\mathbf{P}^E_{0_2 0_2} = \mathbf{P}^E \mathbf{p}_{0_2} = \tfrac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)\tfrac{1}{2}(\mathbf{1} + \mathbf{i}_3) = \tfrac{1}{6}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 - \mathbf{i}_2 + 2\mathbf{i}_3)$$

$$\mathbf{P}^E_{1_2 1_2} = \mathbf{P}^E \mathbf{p}_{1_2} = \tfrac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)\tfrac{1}{2}(\mathbf{1} - \mathbf{i}_3) = \tfrac{1}{6}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 + \mathbf{i}_1 + \mathbf{i}_2 - 2\mathbf{i}_3)$$

Then find nilpotent proportional to: $\mathbf{P}^E_{1_2 0_2} = \mathbf{P}^E \mathbf{p}_{1_2} \mathbf{r} \mathbf{p}_{0_2} = \mathbf{P}^E \frac{1}{2}\cdot\frac{1}{2}$

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

$= \frac{1}{4}\mathbf{P}^E$

	$\mathbf{r}$	$+\mathbf{r}\mathbf{i}_3$
$\mathbf{1}$	$\mathbf{r}$	$+\mathbf{i}_2$
$-\mathbf{i}_3$	$-\mathbf{i}_1$	$-\mathbf{r}^2$

or: $\mathbf{P}^E_{1_2 0_2} = (?)\cdot(\mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 + \mathbf{i}_2)$

† conjugation: $(\mathbf{r}^{\dagger} = \mathbf{r}^2, \mathbf{r}^{2\dagger} = \mathbf{r}, \mathbf{i}_1^{\dagger} = \mathbf{i}_1, \mathbf{i}_2^{\dagger} = \mathbf{i}_2)$

so: $\mathbf{P}^{E\dagger}_{1_2 0_2} = \mathbf{P}^E_{0_2 1_2} = (?)^*(\mathbf{r}^2 - \mathbf{r} - \mathbf{i}_1 + \mathbf{i}_2)$

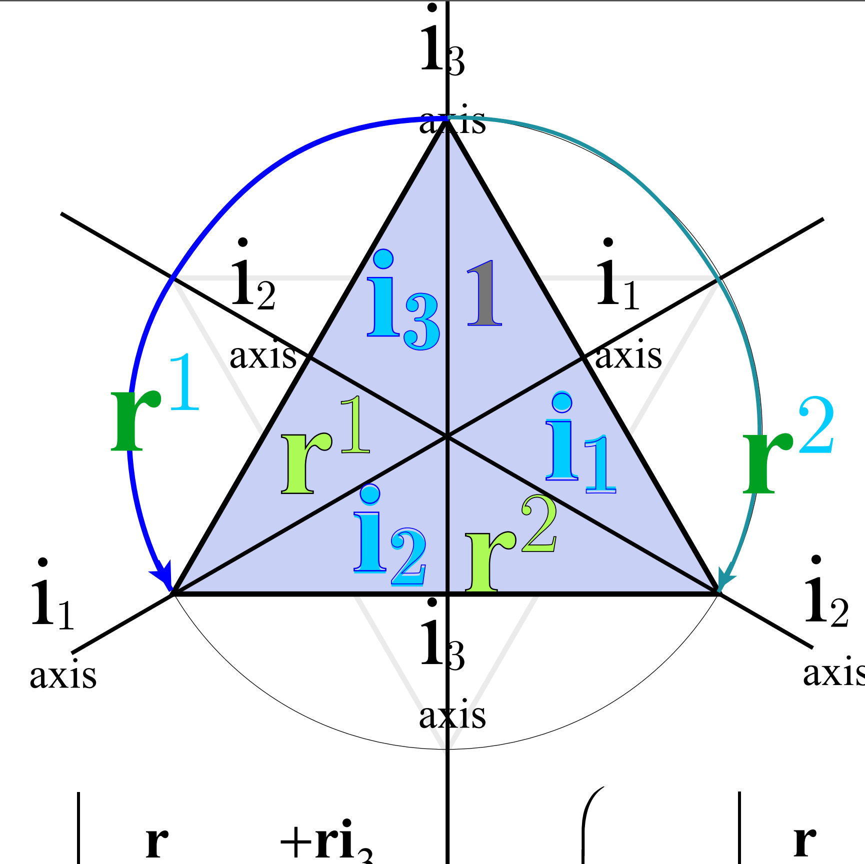
Definition (1): $\mathbf{P}^E_{1_2 1_2}\mathbf{r}\mathbf{P}^E_{0_2 0_2} = D^E_{1_2 0_2}(r)\mathbf{P}^E_{1_2 0_2} = \mathbf{P}^E \mathbf{p}_{1_2}\mathbf{r}\mathbf{p}_{0_2}$

gives equation for (?)-factor: $\mathbf{P}^E_{0_2 1_2} \cdot \mathbf{P}^E_{1_2 0_2} = \mathbf{P}^E_{0_2 0_2} = (?)^2 \cdot (\mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 + \mathbf{i}_2)(\mathbf{r}^2 - \mathbf{r} - \mathbf{i}_1 + \mathbf{i}_2)$

Irreducible nilpotent projectors $\mathbf{P}^{\mu}{}_{m,n}$ *($m \neq n$)*

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

$$\mathbf{P}^{\mu}_{mn} = \frac{\ell^{\mu}}{°G} \sum_{\mathbf{g}}^{°G} D^{\mu *}_{mn}(\mathbf{g})\mathbf{g}$$



$D_3 : \chi^{\alpha}_{k}$	χ^{α}_{1}	χ^{α}_{r}	χ^{α}_{i}
$\alpha = A_1$	1	1	1
$\alpha = A_2$	1	1	−1
$\alpha = E$	2	−1	0

Given: $\mathbf{P}^{E} = \frac{1}{3}(2\mathbf{c}_1 - \mathbf{c}_r + 0)$

$= \frac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)$

First do $C_2 = \{\mathbf{1}, \mathbf{i}_3\}$ splitting:

$$\mathbf{P}^{E}_{0_2 0_2} = \mathbf{P}^{E}\mathbf{p}_{0_2} = \frac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)\frac{1}{2}(\mathbf{1} + \mathbf{i}_3) = \frac{1}{6}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 - \mathbf{i}_2 + 2\mathbf{i}_3)$$

$$\mathbf{P}^{E}_{1_2 1_2} = \mathbf{P}^{E}\mathbf{p}_{1_2} = \frac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)\frac{1}{2}(\mathbf{1} - \mathbf{i}_3) = \frac{1}{6}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 + \mathbf{i}_1 + \mathbf{i}_2 - 2\mathbf{i}_3)$$

Then find nilpotent proportional to: $\mathbf{P}^{E}_{1_2 0_2} = \mathbf{P}^{E}\mathbf{p}_{1_2}\mathbf{r}\mathbf{p}_{0_2} = \mathbf{P}^{E}\,\frac{1}{2}\cdot\frac{1}{2}$

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

$= \frac{1}{4}\,\mathbf{P}^{E}$

	$\mathbf{r}$	$+\mathbf{r}\mathbf{i}_3$
$\mathbf{1}$	$\mathbf{r}$	$+\mathbf{i}_2$
$-\mathbf{i}_3$	$-\mathbf{i}_1$	$-\mathbf{r}^2$

or: $\mathbf{P}^{E}_{1_2 0_2} = (?)\cdot(\mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 + \mathbf{i}_2)$

† conjugation: $(\mathbf{r}^{\dagger} = \mathbf{r}^2, \mathbf{r}^{2\dagger} = \mathbf{r}, \mathbf{i}_1^{\dagger} = \mathbf{i}_1, \mathbf{i}_2^{\dagger} = \mathbf{i}_2)$

so: $\mathbf{P}^{E\dagger}_{1_2 0_2} = \mathbf{P}^{E}_{0_2 1_2} = (?)^{*}(\mathbf{r}^2 - \mathbf{r} - \mathbf{i}_1 + \mathbf{i}_2)$

gives equation for (?)-factor: $\mathbf{P}^{E}_{0_2 1_2}\cdot\mathbf{P}^{E}_{1_2 0_2} = \mathbf{P}^{E}_{0_2 0_2} = (?)^2\cdot(\mathbf{r}^2 - \mathbf{r} - \mathbf{i}_1 + \mathbf{i}_2)(\mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 + \mathbf{i}_2)$

$$= \frac{1}{6}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 - \mathbf{i}_2 + 2\mathbf{i}_3) = (\tfrac{\ell^{E}}{°O} = \tfrac{1}{3})(D^{E*}_{0_2 0_2}(1)\mathbf{1} + D^{E*}_{0_2 0_2}(r)\mathbf{r} + \ldots)$$

Irreducible nilpotent projectors $\mathbf{P}^{\mu}{}_{m,n}$ *(m≠n)*

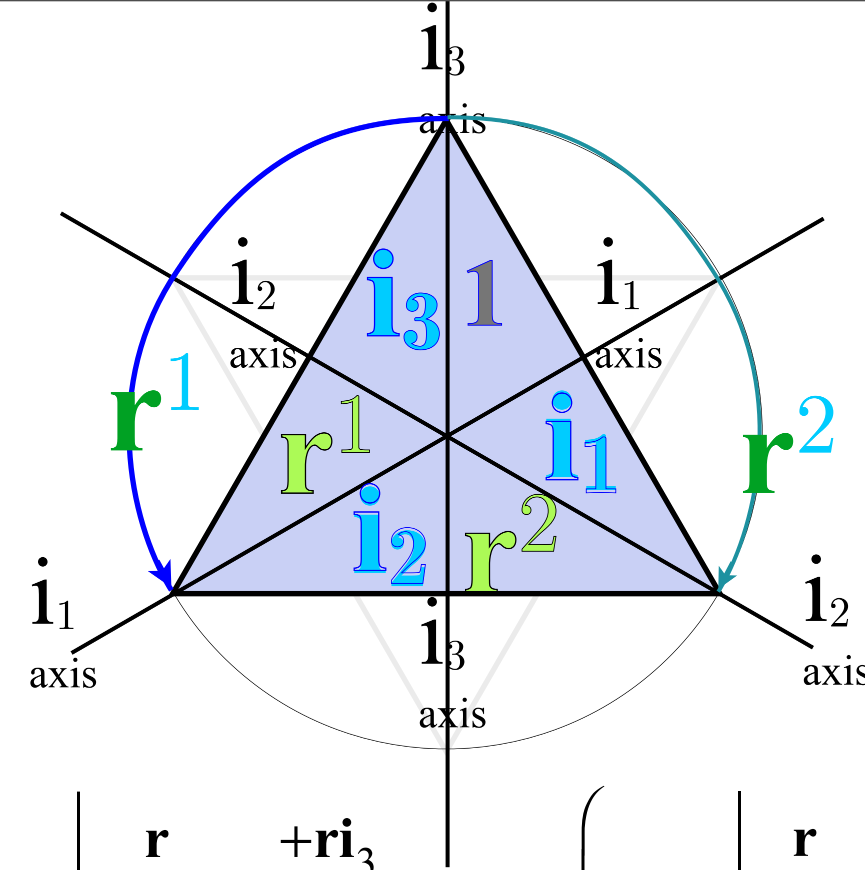
Review of $D_3 \supset C_2 \sim C_{3v} \supset C_v$

$$\mathbf{P}^{\mu}_{mn} = \frac{\ell^{\mu}}{{}^{\circ}G} \sum_{\mathbf{g}}^{{}^{\circ}G} D^{\mu *}_{mn}(\mathbf{g})\mathbf{g}$$

$D_3 : \chi^{\alpha}_{k}$	χ^{α}_{1}	χ^{α}_{r}	χ^{α}_{i}
$\alpha = A_1$	1	1	1
$\alpha = A_2$	1	1	−1
$\alpha = E$	2	−1	0

Given: $\mathbf{P}^{E} = \frac{1}{3}(2\mathbf{c}_1 - \mathbf{c}_r + 0)$

$= \frac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)$



First do $C_2 = \{\mathbf{1},\mathbf{i}_3\}$ splitting:

$$\mathbf{P}^{E}_{0_2 0_2} = \mathbf{P}^{E}\mathbf{p}_{0_2} = \tfrac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)\tfrac{1}{2}(\mathbf{1} + \mathbf{i}_3) = \tfrac{1}{6}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 - \mathbf{i}_2 + 2\mathbf{i}_3)$$

$$\mathbf{P}^{E}_{1_2 1_2} = \mathbf{P}^{E}\mathbf{p}_{1_2} = \tfrac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)\tfrac{1}{2}(\mathbf{1} - \mathbf{i}_3) = \tfrac{1}{6}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 + \mathbf{i}_1 + \mathbf{i}_2 - 2\mathbf{i}_3)$$

Then find nilpotent proportional to: $\mathbf{P}^{E}_{1_2 0_2} = \mathbf{P}^{E}\mathbf{p}_{1_2}\mathbf{r}\mathbf{p}_{0_2} = \mathbf{P}^{E}\,\frac{1}{2}\cdot\frac{1}{2}\left(\begin{array}{c|cc} & \mathbf{r} & +\mathbf{r}\mathbf{i}_3 \\ \hline \mathbf{1} & \mathbf{r} & +\mathbf{r}\mathbf{i}_3 \\ -\mathbf{i}_3 & -\mathbf{i}_3\mathbf{r} & -\mathbf{i}_3\mathbf{r}\mathbf{i}_3 \end{array}\right) = \frac{1}{4}\mathbf{P}^{E}\left(\begin{array}{c|cc} & \mathbf{r} & +\mathbf{r}\mathbf{i}_3 \\ \hline \mathbf{1} & \mathbf{r} & +\mathbf{i}_2 \\ -\mathbf{i}_3 & -\mathbf{i}_1 & -\mathbf{r}^2 \end{array}\right)$

or: $\mathbf{P}^{E}_{1_2 0_2} = (?)\cdot(\mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 + \mathbf{i}_2)$

† conjugation: $(\mathbf{r}^{\dagger} = \mathbf{r}^2, \mathbf{r}^{2\dagger} = \mathbf{r}, \mathbf{i}_1^{\dagger} = \mathbf{i}_1, \mathbf{i}_2^{\dagger} = \mathbf{i}_2)$

so: $\mathbf{P}^{E\dagger}_{1_2 0_2} = \mathbf{P}^{E}_{0_2 1_2} = (?)^{*}(\mathbf{r}^2 - \mathbf{r} - \mathbf{i}_1 + \mathbf{i}_2)$

Note diagonal D^{E}

$D^{E*}_{0_2 0_2}(\mathbf{1}) = 1$

$D^{E*}_{0_2 0_2}(\mathbf{r}) = -\frac{1}{2}$

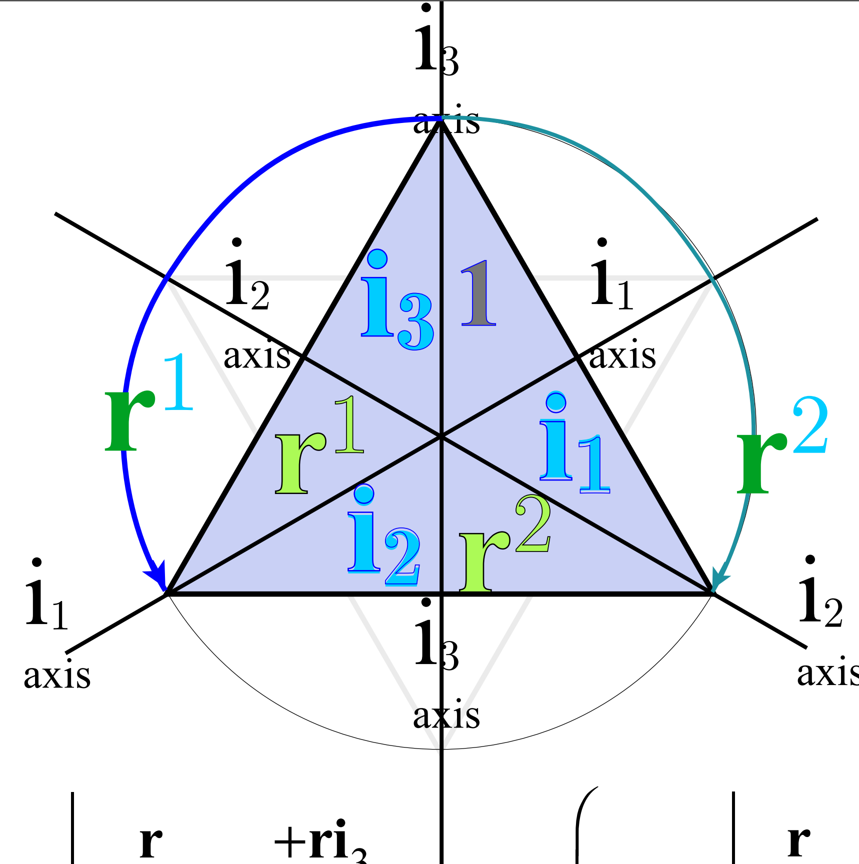
gives equation for (?)-factor: $\mathbf{P}^{E}_{0_2 1_2}\cdot\mathbf{P}^{E}_{1_2 0_2} = \mathbf{P}^{E}_{0_2 0_2} = (?)^2\cdot(\mathbf{r}^2 - \mathbf{r} - \mathbf{i}_1 + \mathbf{i}_2)(\mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 + \mathbf{i}_2)$

$$= \tfrac{1}{6}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 - \mathbf{i}_2 + 2\mathbf{i}_3) = \left(\tfrac{\ell^{E}}{{}^{\circ}O} = \tfrac{1}{3}\right)\left(D^{E*}_{0_2 0_2}(1)\mathbf{1} + D^{E*}_{0_2 0_2}(r)\mathbf{r} + \ldots\right)$$

Irreducible nilpotent projectors $\mathbf{P}^{\mu}_{m,n}$ *(m≠n)*

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

$$\mathbf{P}^{\mu}_{mn} = \frac{\ell^{\mu}}{{}^{\circ}G}\sum_{\mathbf{g}}^{{}^{\circ}G} D^{\mu *}_{mn}(\mathbf{g})\mathbf{g}$$



$D_3 : \chi^{\alpha}_{k}$	χ^{α}_{1}	χ^{α}_{r}	χ^{α}_{i}
$\alpha = A_1$	1	1	1
$\alpha = A_2$	1	1	−1
$\alpha = E$	2	−1	0

Given: $\mathbf{P}^{E} = \frac{1}{3}(2\mathbf{c}_1 - \mathbf{c}_r + 0)$
$= \frac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)$

First do $C_2 = \{\mathbf{1}, \mathbf{i}_3\}$ splitting:

$$\mathbf{P}^{E}_{0_2 0_2} = \mathbf{P}^{E}\mathbf{p}_{0_2} = \tfrac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)\tfrac{1}{2}(\mathbf{1} + \mathbf{i}_3) = \tfrac{1}{6}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 - \mathbf{i}_2 + 2\mathbf{i}_3)$$

$$\mathbf{P}^{E}_{1_2 1_2} = \mathbf{P}^{E}\mathbf{p}_{1_2} = \tfrac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)\tfrac{1}{2}(\mathbf{1} - \mathbf{i}_3) = \tfrac{1}{6}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 + \mathbf{i}_1 + \mathbf{i}_2 - 2\mathbf{i}_3)$$

Then find nilpotent proportional to: $\mathbf{P}^{E}_{1_2 0_2} = \mathbf{P}^{E}\mathbf{p}_{1_2}\mathbf{r}\mathbf{p}_{0_2} = \mathbf{P}^{E}\,\frac{1}{2}\cdot\frac{1}{2}$

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

$= \frac{1}{4}\mathbf{P}^{E}$

	$\mathbf{r}$	$+\mathbf{r}\mathbf{i}_3$
$\mathbf{1}$	$\mathbf{r}$	$+\mathbf{i}_2$
$-\mathbf{i}_3$	$-\mathbf{i}_1$	$-\mathbf{r}^2$

or: $\mathbf{P}^{E}_{1_2 0_2} = (?)\cdot(\mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 + \mathbf{i}_2)$

† conjugation: $(\mathbf{r}^{\dagger} = \mathbf{r}^2, \mathbf{r}^{2\dagger} = \mathbf{r}, \mathbf{i}_1^{\dagger} = \mathbf{i}_1, \mathbf{i}_2^{\dagger} = \mathbf{i}_2)$

so: $\mathbf{P}^{E\dagger}_{1_2 0_2} = \mathbf{P}^{E}_{0_2 1_2} = (?)^{*}(\mathbf{r}^2 - \mathbf{r} - \mathbf{i}_1 + \mathbf{i}_2)$

Note diagonal D^E

$D^{E*}_{0_2 0_2}(\mathbf{1}) = 1$

$D^{E*}_{0_2 0_2}(\mathbf{r}) = -\frac{1}{2}$

gives equation for (?)-factor: $\mathbf{P}^{E}_{0_2 1_2}\cdot\mathbf{P}^{E}_{1_2 0_2} = \mathbf{P}^{E}_{0_2 0_2} = (?)^2\cdot(\mathbf{r}^2 - \mathbf{r} - \mathbf{i}_1 + \mathbf{i}_2)(\mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 + \mathbf{i}_2)$

$$= \tfrac{1}{6}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 - \mathbf{i}_2 + 2\mathbf{i}_3) = (\tfrac{\ell^E}{{}^{\circ}O} = \tfrac{1}{3})(D^{E*}_{0_2 0_2}(1)\mathbf{1} + D^{E*}_{0_2 0_2}(r)\mathbf{r} + \ldots)$$

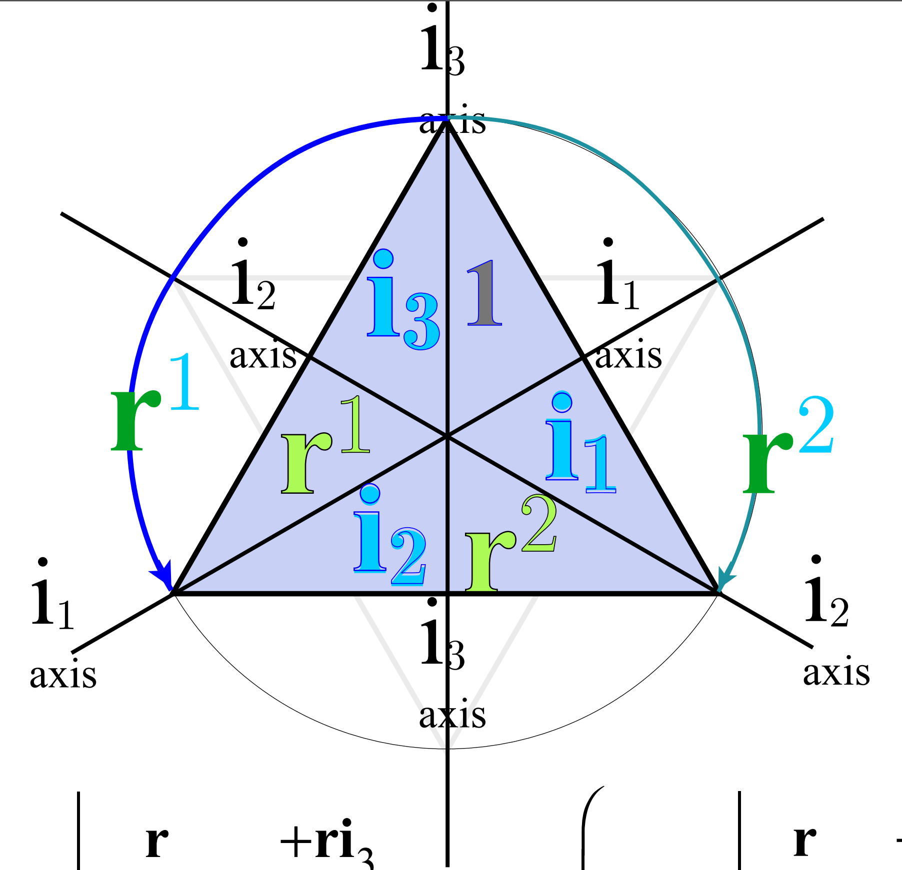
$\mathbf{P}^{E}_{0_2 0_2} = (?)^2 \cdot$

	$+\mathbf{r}$	$-\mathbf{r}^2$	$-\mathbf{i}_1$	$+\mathbf{i}_2$
$+\mathbf{r}^2$	$+\mathbf{1}$	$-\mathbf{r}$	$-\mathbf{i}_2$	$+\mathbf{i}_3$
$-\mathbf{r}$	$-\mathbf{r}^2$	$+\mathbf{1}$	$+\mathbf{i}_3$	$-\mathbf{i}_1$
$-\mathbf{i}_1$	$-\mathbf{i}_2$	$+\mathbf{i}_3$	$+\mathbf{1}$	$-\mathbf{r}$
$+\mathbf{i}_2$	$+\mathbf{i}_3$	$-\mathbf{i}_1$	$-\mathbf{r}^2$	$+\mathbf{1}$

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

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

$$\mathbf{P}^{\mu}_{mn} = \frac{\ell^{\mu}}{{}^{\circ}G}\sum_{\mathbf{g}}^{{}^{\circ}G} D^{\mu *}_{mn}(\mathbf{g})\mathbf{g}$$



$D_3 : \chi^{\alpha}_k$	χ^{α}_1	χ^{α}_r	χ^{α}_i
$\alpha = A_1$	1	1	1
$\alpha = A_2$	1	1	−1
$\alpha = E$	2	−1	0

Given: $\mathbf{P}^E = \frac{1}{3}(2\mathbf{c}_1 - \mathbf{c}_r + 0)$

$= \frac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)$

First do $C_2 = \{\mathbf{1}, \mathbf{i}_3\}$ splitting:

$$\mathbf{P}^E_{0_2 0_2} = \mathbf{P}^E \mathbf{p}_{0_2} = \tfrac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)\tfrac{1}{2}(\mathbf{1} + \mathbf{i}_3) = \tfrac{1}{6}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 - \mathbf{i}_2 + 2\mathbf{i}_3)$$

$$\mathbf{P}^E_{1_2 1_2} = \mathbf{P}^E \mathbf{p}_{1_2} = \tfrac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)\tfrac{1}{2}(\mathbf{1} - \mathbf{i}_3) = \tfrac{1}{6}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 + \mathbf{i}_1 + \mathbf{i}_2 - 2\mathbf{i}_3)$$

Then find nilpotent proportional to: $\mathbf{P}^E_{1_2 0_2} = \mathbf{P}^E \mathbf{p}_{1_2} \mathbf{r} \mathbf{p}_{0_2} = \mathbf{P}^E \frac{1}{2}\cdot\frac{1}{2}$

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

$= \frac{1}{4}\mathbf{P}^E$

	$\mathbf{r}$	$+\mathbf{r}\mathbf{i}_3$
$\mathbf{1}$	$\mathbf{r}$	$+\mathbf{i}_2$
$-\mathbf{i}_3$	$-\mathbf{i}_1$	$-\mathbf{r}^2$

or: $\mathbf{P}^E_{1_2 0_2} = (?)\cdot(\mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 + \mathbf{i}_2)$

† conjugation: $(\mathbf{r}^{\dagger} = \mathbf{r}^2, \mathbf{r}^{2\dagger} = \mathbf{r}, \mathbf{i}_1^{\dagger} = \mathbf{i}_1, \mathbf{i}_2^{\dagger} = \mathbf{i}_2)$

so: $\mathbf{P}^{E\dagger}_{1_2 0_2} = \mathbf{P}^E_{0_2 1_2} = (?)^*(\mathbf{r}^2 - \mathbf{r} - \mathbf{i}_1 + \mathbf{i}_2)$

gives equation for (?)-factor: $\mathbf{P}^E_{0_2 1_2}\cdot\mathbf{P}^E_{1_2 0_2} = \mathbf{P}^E_{0_2 0_2} = (?)^2\cdot(\mathbf{r}^2 - \mathbf{r} - \mathbf{i}_1 + \mathbf{i}_2)(\mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 + \mathbf{i}_2)$

Note diagonal D^E

$D^{E*}_{0_2 0_2}(\mathbf{1}) = 1$

$D^{E*}_{0_2 0_2}(\mathbf{r}) = -\frac{1}{2}$

$$= \tfrac{1}{6}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 - \mathbf{i}_2 + 2\mathbf{i}_3) = \left(\tfrac{\ell^E}{{}^{\circ}O} = \tfrac{1}{3}\right)(D^{E*}_{0_2 0_2}(1)\mathbf{1} + D^{E*}_{0_2 0_2}(r)\mathbf{r} + \ldots)$$

$\mathbf{P}^E_{0_2 0_2} = (?)^2 \cdot$

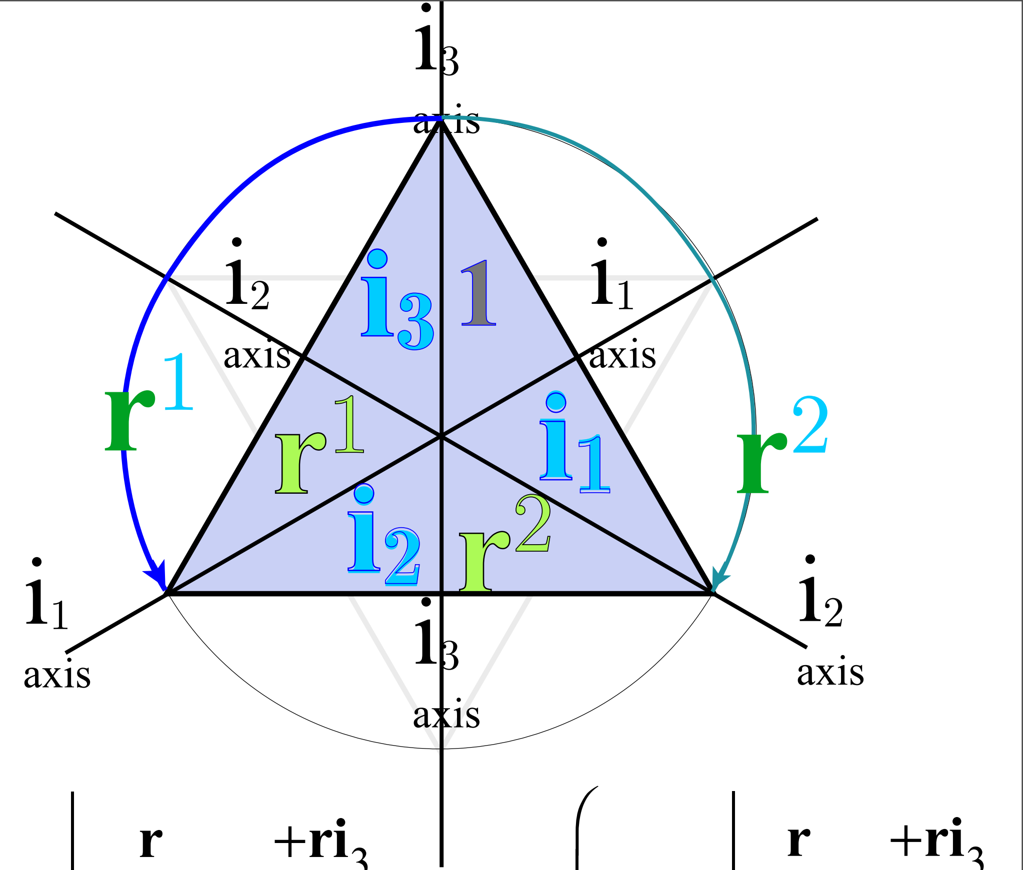
	$+\mathbf{r}$	$-\mathbf{r}^2$	$-\mathbf{i}_1$	$+\mathbf{i}_2$
$+\mathbf{r}^2$	$+\mathbf{1}$	$-\mathbf{r}$	$-\mathbf{i}_2$	$+\mathbf{i}_3$
$-\mathbf{r}$	$-\mathbf{r}^2$	$+\mathbf{1}$	$+\mathbf{i}_3$	$-\mathbf{i}_1$
$-\mathbf{i}_1$	$-\mathbf{i}_2$	$+\mathbf{i}_3$	$+\mathbf{1}$	$-\mathbf{r}$
$+\mathbf{i}_2$	$+\mathbf{i}_3$	$-\mathbf{i}_1$	$-\mathbf{r}^2$	$+\mathbf{1}$

$= (?)^2\cdot(+4\mathbf{1} - 2\mathbf{r} - 2\mathbf{r}^2 - 2\mathbf{i}_1 - 2\mathbf{i}_2 + 4\mathbf{i}_3)$

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

$$\mathbf{P}^{\mu}_{mn} = \frac{\ell^{\mu}}{{}^{\circ}G}\sum_{\mathbf{g}}^{{}^{\circ}G} D^{\mu *}_{mn}(\mathbf{g})\mathbf{g}$$

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



$D_3 : \chi^{\alpha}_k$	χ^{α}_1	χ^{α}_r	χ^{α}_i
$\alpha = A_1$	1	1	1
$\alpha = A_2$	1	1	−1
$\alpha = E$	2	−1	0

Given: $\mathbf{P}^E = \frac{1}{3}(2\mathbf{c}_1 - \mathbf{c}_r + 0)$

$= \frac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)$

First do $C_2 = \{\mathbf{1},\mathbf{i}_3\}$ splitting:

$$\mathbf{P}^E_{0_2 0_2} = \mathbf{P}^E\mathbf{p}_{0_2} = \tfrac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)\tfrac{1}{2}(\mathbf{1} + \mathbf{i}_3) = \tfrac{1}{6}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 - \mathbf{i}_2 + 2\mathbf{i}_3)$$

$$\mathbf{P}^E_{1_2 1_2} = \mathbf{P}^E\mathbf{p}_{1_2} = \tfrac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)\tfrac{1}{2}(\mathbf{1} - \mathbf{i}_3) = \tfrac{1}{6}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 + \mathbf{i}_1 + \mathbf{i}_2 - 2\mathbf{i}_3)$$

Then find nilpotent proportional to: $\mathbf{P}^E_{1_2 0_2} = \mathbf{P}^E\mathbf{p}_{1_2}\mathbf{r}\mathbf{p}_{0_2} = \mathbf{P}^E \frac{1}{2}\cdot\frac{1}{2}$

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

$= \frac{1}{4}\mathbf{P}^E$

	$\mathbf{r}$	$+\mathbf{r}\mathbf{i}_3$
$\mathbf{1}$	$\mathbf{r}$	$+\mathbf{i}_2$
$-\mathbf{i}_3$	$-\mathbf{i}_1$	$-\mathbf{r}^2$

or: $\mathbf{P}^E_{1_2 0_2} = (?)\cdot(\mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 + \mathbf{i}_2)$

† conjugation: $(\mathbf{r}^{\dagger} = \mathbf{r}^2, \mathbf{r}^{2\dagger} = \mathbf{r}, \mathbf{i}_1^{\dagger} = \mathbf{i}_1, \mathbf{i}_2^{\dagger} = \mathbf{i}_2)$

so: $\mathbf{P}^{E\dagger}_{1_2 0_2} = \mathbf{P}^E_{0_2 1_2} = (?)^*(\mathbf{r}^2 - \mathbf{r} - \mathbf{i}_1 + \mathbf{i}_2)$

Note diagonal D^E

$D^{E*}_{0_2 0_2}(\mathbf{1}) = 1$

$D^{E*}_{0_2 0_2}(\mathbf{r}) = -\frac{1}{2}$

gives equation for (?)-factor: $\mathbf{P}^E_{0_2 1_2}\cdot\mathbf{P}^E_{1_2 0_2} = \mathbf{P}^E_{0_2 0_2} = (?)^2\cdot(\mathbf{r}^2 - \mathbf{r} - \mathbf{i}_1 + \mathbf{i}_2)(\mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 + \mathbf{i}_2)$

$= \frac{1}{6}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 - \mathbf{i}_2 + 2\mathbf{i}_3) = (\frac{\ell^E}{{}^{\circ}G} = \frac{1}{3})(D^{E*}_{0_2 0_2}(1)\mathbf{1} + D^{E*}_{0_2 0_2}(r)\mathbf{r} + \ldots)$

$(?)^2 \cdot 4 = \frac{1}{3}$

$\mathbf{P}^E_{0_2 0_2} = (?)^2 \cdot$

	$+\mathbf{r}$	$-\mathbf{r}^2$	$-\mathbf{i}_1$	$+\mathbf{i}_2$
$+\mathbf{r}^2$	$+\mathbf{1}$	$-\mathbf{r}$	$-\mathbf{i}_2$	$+\mathbf{i}_3$
$-\mathbf{r}$	$-\mathbf{r}^2$	$+\mathbf{1}$	$+\mathbf{i}_3$	$-\mathbf{i}_1$
$-\mathbf{i}_1$	$-\mathbf{i}_2$	$+\mathbf{i}_3$	$+\mathbf{1}$	$-\mathbf{r}$
$+\mathbf{i}_2$	$+\mathbf{i}_3$	$-\mathbf{i}_1$	$-\mathbf{r}^2$	$+\mathbf{1}$

$= (?)^2\cdot(+4\mathbf{1} - 2\mathbf{r} - 2\mathbf{r}^2 - 2\mathbf{i}_1 - 2\mathbf{i}_2 + 4\mathbf{i}_3)$

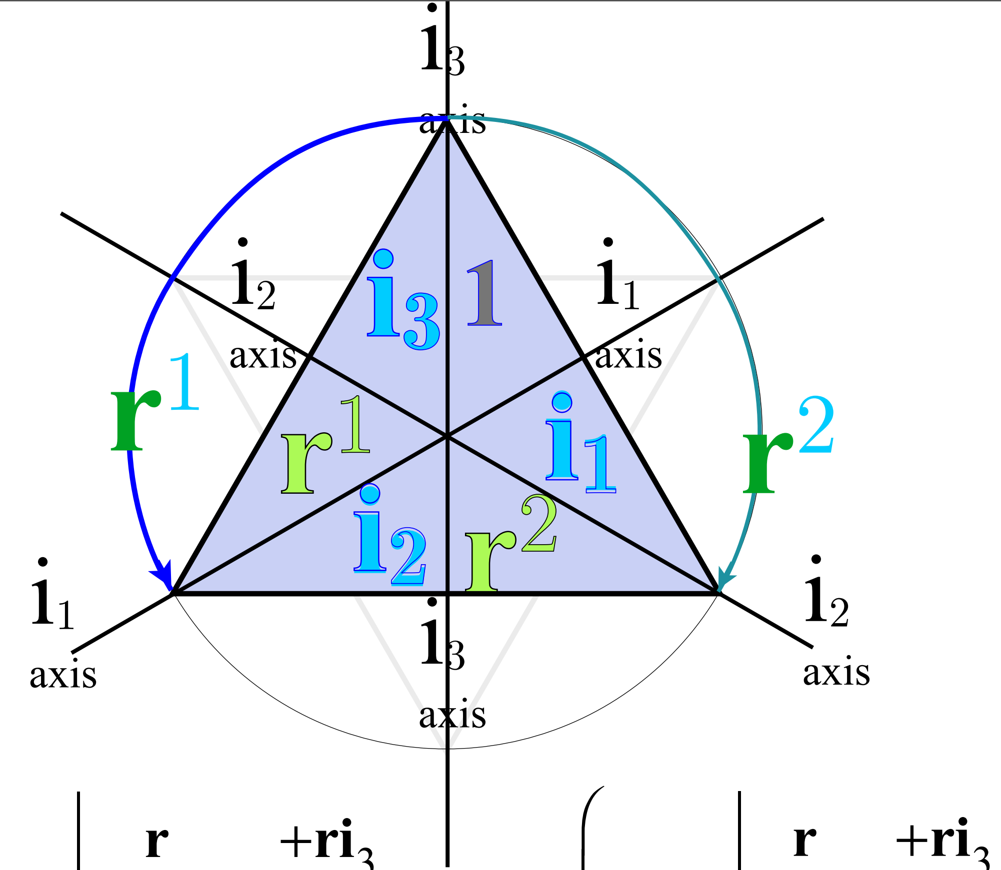
Irreducible nilpotent projectors $\mathbf{P}^{\mu}_{m,n}$ *(m≠n)*

$$\mathbf{P}^{\mu}_{mn} = \frac{\ell^{\mu}}{{}^{\circ}G}\sum_{\mathbf{g}}^{{}^{\circ}G} D^{\mu *}_{mn}(\mathbf{g})\mathbf{g}$$

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

$D_3 : \chi^{\alpha}_{k}$	χ^{α}_{1}	χ^{α}_{r}	χ^{α}_{i}
$\alpha = A_1$	1	1	1
$\alpha = A_2$	1	1	−1
$\alpha = E$	2	−1	0

Given: $\mathbf{P}^{E} = \frac{1}{3}(2\mathbf{c}_1 - \mathbf{c}_r + 0)$
$= \frac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)$



First do $C_2 = \{\mathbf{1}, \mathbf{i}_3\}$ splitting:

$$\mathbf{P}^{E}_{0_2 0_2} = \mathbf{P}^{E}\mathbf{p}_{0_2} = \tfrac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)\tfrac{1}{2}(\mathbf{1} + \mathbf{i}_3) = \tfrac{1}{6}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 - \mathbf{i}_2 + 2\mathbf{i}_3)$$

$$\mathbf{P}^{E}_{1_2 1_2} = \mathbf{P}^{E}\mathbf{p}_{1_2} = \tfrac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)\tfrac{1}{2}(\mathbf{1} - \mathbf{i}_3) = \tfrac{1}{6}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 + \mathbf{i}_1 + \mathbf{i}_2 - 2\mathbf{i}_3)$$

Then find nilpotent proportional to: $\mathbf{P}^{E}_{1_2 0_2} = \mathbf{P}^{E}\mathbf{p}_{1_2}\mathbf{r}\mathbf{p}_{0_2} = \mathbf{P}^{E}\,\frac{1}{2}\cdot\frac{1}{2}$

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

$= \frac{1}{4}\mathbf{P}^{E}$

	$\mathbf{r}$	$+\mathbf{r}\mathbf{i}_3$
$\mathbf{1}$	$\mathbf{r}$	$+\mathbf{i}_2$
$-\mathbf{i}_3$	$-\mathbf{i}_1$	$-\mathbf{r}^2$

or: $\mathbf{P}^{E}_{1_2 0_2} = (?)\cdot(\mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 + \mathbf{i}_2)$

† conjugation: $(\mathbf{r}^{\dagger} = \mathbf{r}^2, \mathbf{r}^{2\dagger} = \mathbf{r}, \mathbf{i}_1^{\dagger} = \mathbf{i}_1, \mathbf{i}_2^{\dagger} = \mathbf{i}_2)$

so: $\mathbf{P}^{E\dagger}_{1_2 0_2} = \mathbf{P}^{E}_{0_2 1_2} = (?)^{*}(\mathbf{r}^2 - \mathbf{r} - \mathbf{i}_1 + \mathbf{i}_2)$

Note diagonal D^E

$D^{E*}_{0_2 0_2}(\mathbf{1}) = 1$

$D^{E*}_{0_2 0_2}(\mathbf{r}) = -\frac{1}{2}$

gives equation for (?)-factor: $\mathbf{P}^{E}_{0_2 1_2}\cdot\mathbf{P}^{E}_{1_2 0_2} = \mathbf{P}^{E}_{0_2 0_2} = (?)^2\cdot(\mathbf{r}^2 - \mathbf{r} - \mathbf{i}_1 + \mathbf{i}_2)(\mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 + \mathbf{i}_2)$

$$= \tfrac{1}{6}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 - \mathbf{i}_2 + 2\mathbf{i}_3) = \left(\tfrac{\ell^E}{{}^{\circ}O} = \tfrac{1}{3}\right)\left(D^{E*}_{0_2 0_2}(1)\mathbf{1} + D^{E*}_{0_2 0_2}(r)\mathbf{r} + \ldots\right)$$

$(?)^2 \cdot 4 = \frac{1}{3}$

$\mathbf{P}^{E}_{0_2 0_2} = (?)^2\cdot$

	$+\mathbf{r}$	$-\mathbf{r}^2$	$-\mathbf{i}_1$	$+\mathbf{i}_2$
$+\mathbf{r}^2$	$+\mathbf{1}$	$-\mathbf{r}$	$-\mathbf{i}_2$	$+\mathbf{i}_3$
$-\mathbf{r}$	$-\mathbf{r}^2$	$+\mathbf{1}$	$+\mathbf{i}_3$	$-\mathbf{i}_1$
$-\mathbf{i}_1$	$-\mathbf{i}_2$	$+\mathbf{i}_3$	$+\mathbf{1}$	$-\mathbf{r}$
$+\mathbf{i}_2$	$+\mathbf{i}_3$	$-\mathbf{i}_1$	$-\mathbf{r}^2$	$+\mathbf{1}$

$= (?)^2\cdot(+4\mathbf{1} - 2\mathbf{r} - 2\mathbf{r}^2 - 2\mathbf{i}_1 - 2\mathbf{i}_2 + 4\mathbf{i}_3)$

Solving gives unknown (?)-factor: (?)=±√3/6

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

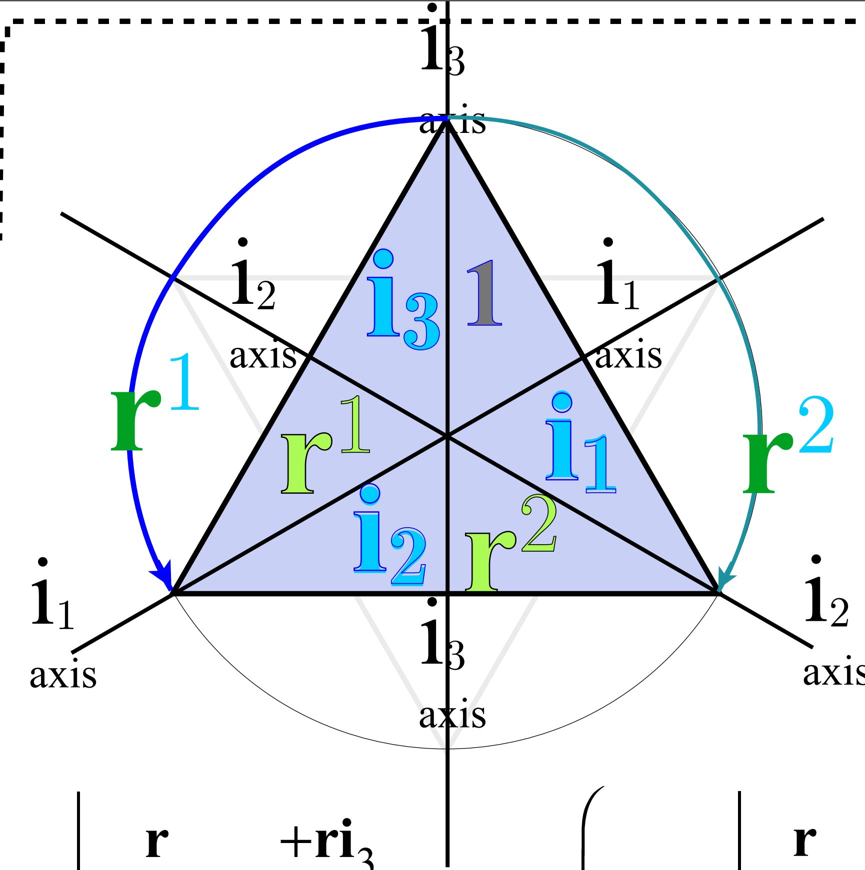
$$\mathbf{P}^{\mu}_{mn} = \frac{\ell^{\mu}}{{}^{\circ}G} \sum_{\mathbf{g}}^{{}^{\circ}G} D^{\mu *}_{mn}(\mathbf{g})\mathbf{g}$$

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

$D_3 : \chi^{\alpha}_{k}$	χ^{α}_{1}	χ^{α}_{r}	χ^{α}_{i}
$\alpha = A_1$	1	1	1
$\alpha = A_2$	1	1	−1
$\alpha = E$	2	−1	0

Given: $\mathbf{P}^{E} = \frac{1}{3}(2\mathbf{c}_1 - \mathbf{c}_r + 0)$

$= \frac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)$



First do $C_2 = \{\mathbf{1}, \mathbf{i}_3\}$ splitting:

$\mathbf{P}^{E}_{0_2 0_2} = \mathbf{P}^{E}\mathbf{p}_{0_2} = \frac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)\frac{1}{2}(\mathbf{1} + \mathbf{i}_3) = \frac{1}{6}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 - \mathbf{i}_2 + 2\mathbf{i}_3)$

$\mathbf{P}^{E}_{1_2 1_2} = \mathbf{P}^{E}\mathbf{p}_{1_2} = \frac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)\frac{1}{2}(\mathbf{1} - \mathbf{i}_3) = \frac{1}{6}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 + \mathbf{i}_1 + \mathbf{i}_2 - 2\mathbf{i}_3)$

Then find nilpotent proportional to: $\mathbf{P}^{E}_{1_2 0_2} = \mathbf{P}^{E}\mathbf{p}_{1_2}\mathbf{r}\mathbf{p}_{0_2} = \mathbf{P}^{E}\,\frac{1}{2}\cdot\frac{1}{2}$

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

$= \frac{1}{4}\,\mathbf{P}^{E}$

	$\mathbf{r}$	$+\mathbf{r}\mathbf{i}_3$
$\mathbf{1}$	$\mathbf{r}$	$+\mathbf{i}_2$
$-\mathbf{i}_3$	$-\mathbf{i}_1$	$-\mathbf{r}^2$

or: $\mathbf{P}^{E}_{1_2 0_2} = (?)\cdot(\mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 + \mathbf{i}_2)$

† conjugation: $(\mathbf{r}^{\dagger} = \mathbf{r}^2, \mathbf{r}^{2\dagger} = \mathbf{r}, \mathbf{i}_1^{\dagger} = \mathbf{i}_1, \mathbf{i}_2^{\dagger} = \mathbf{i}_2)$

so: $\mathbf{P}^{E\dagger}_{1_2 0_2} = \mathbf{P}^{E}_{0_2 1_2} = (?)^{*}(\mathbf{r}^2 - \mathbf{r} - \mathbf{i}_1 + \mathbf{i}_2)$

Note diagonal D^E

$D^{E*}_{0_2 0_2}(\mathbf{1}) = 1$

$D^{E*}_{0_2 0_2}(\mathbf{r}) = -\frac{1}{2}$

gives equation for (?)-factor: $\mathbf{P}^{E}_{0_2 1_2}\cdot\mathbf{P}^{E}_{1_2 0_2} = \mathbf{P}^{E}_{0_2 0_2} = (?)^2\cdot(\mathbf{r}^2 - \mathbf{r} - \mathbf{i}_1 + \mathbf{i}_2)(\mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 + \mathbf{i}_2)$

$= \frac{1}{6}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 - \mathbf{i}_2 + 2\mathbf{i}_3) = (\frac{\ell^E}{{}^{\circ}G} = \frac{1}{3})(D^{E*}_{0_2 0_2}(1)\mathbf{1} + D^{E*}_{0_2 0_2}(r)\mathbf{r} + \ldots)$

$(?)^2\cdot 4 = \frac{1}{3}$

$\mathbf{P}^{E}_{0_2 0_2} = (?)^2\cdot$

	$+\mathbf{r}$	$-\mathbf{r}^2$	$-\mathbf{i}_1$	$+\mathbf{i}_2$
$+\mathbf{r}^2$	$+\mathbf{1}$	$-\mathbf{r}$	$-\mathbf{i}_2$	$+\mathbf{i}_3$
$-\mathbf{r}$	$-\mathbf{r}^2$	$+\mathbf{1}$	$+\mathbf{i}_3$	$-\mathbf{i}_1$
$-\mathbf{i}_1$	$-\mathbf{i}_2$	$+\mathbf{i}_3$	$+\mathbf{1}$	$-\mathbf{r}$
$+\mathbf{i}_2$	$+\mathbf{i}_3$	$-\mathbf{i}_1$	$-\mathbf{r}^2$	$+\mathbf{1}$

$= (?)^2\cdot(+4\mathbf{1} - 2\mathbf{r} - 2\mathbf{r}^2 - 2\mathbf{i}_1 - 2\mathbf{i}_2 + 4\mathbf{i}_3)$

Solving gives unknown (?)-factor: $(?) = \pm\sqrt{3}/6$

$(?)^2\cdot 4 = \frac{1}{3} = \frac{1}{3}D^{E*}_{0_2 0_2}(1)$

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

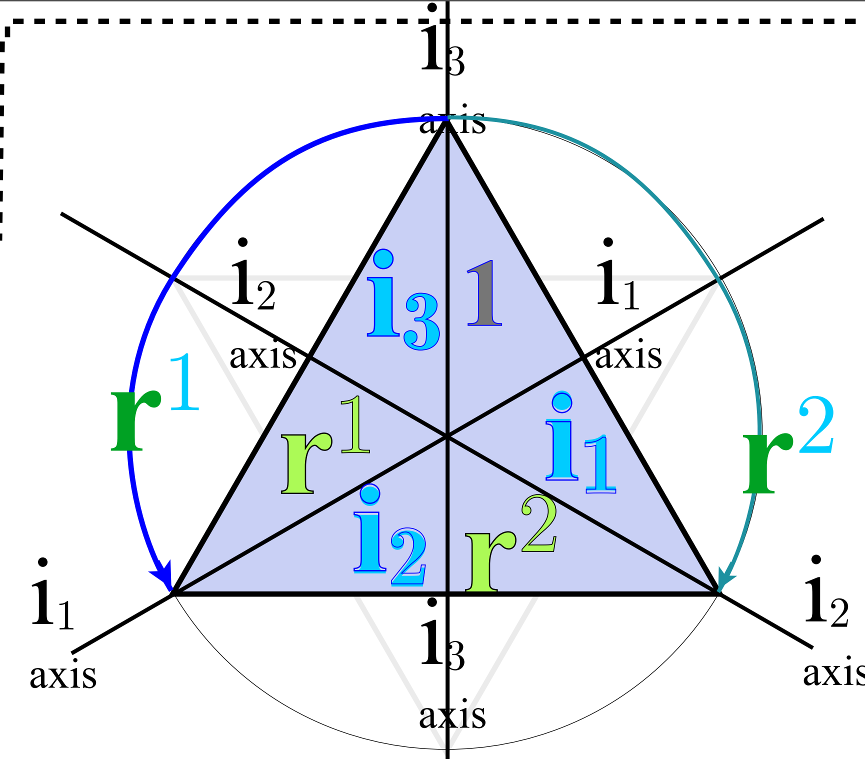
$$\mathbf{P}^{\mu}_{mn} = \frac{\ell^{\mu}}{{}^{\circ}G}\sum_{\mathbf{g}}^{{}^{\circ}G} D^{\mu *}_{mn}(\mathbf{g})\mathbf{g}$$

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

$D_3 : \chi^{\alpha}_{k}$	χ^{α}_{1}	χ^{α}_{r}	χ^{α}_{i}
$\alpha = A_1$	1	1	1
$\alpha = A_2$	1	1	−1
$\alpha = E$	2	−1	0

Given: $\mathbf{P}^{E} = \frac{1}{3}(2\mathbf{c}_1 - \mathbf{c}_r + 0)$

$= \frac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)$



First do $C_2 = \{\mathbf{1}, \mathbf{i}_3\}$ splitting:

$$\mathbf{P}^{E}_{0_2 0_2} = \mathbf{P}^{E}\mathbf{p}_{0_2} = \tfrac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)\tfrac{1}{2}(\mathbf{1} + \mathbf{i}_3) = \tfrac{1}{6}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 - \mathbf{i}_2 + 2\mathbf{i}_3)$$

$$\mathbf{P}^{E}_{1_2 1_2} = \mathbf{P}^{E}\mathbf{p}_{1_2} = \tfrac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)\tfrac{1}{2}(\mathbf{1} - \mathbf{i}_3) = \tfrac{1}{6}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 + \mathbf{i}_1 + \mathbf{i}_2 - 2\mathbf{i}_3)$$

Then find nilpotent proportional to: $\mathbf{P}^{E}_{1_2 0_2} = \mathbf{P}^{E}\mathbf{p}_{1_2}\mathbf{r}\mathbf{p}_{0_2} = \mathbf{P}^{E}\,\frac{1}{2}\cdot\frac{1}{2}\left(\begin{array}{c|cc} & \mathbf{r} & +\mathbf{r}\mathbf{i}_3 \\ \hline \mathbf{1} & \mathbf{r} & +\mathbf{r}\mathbf{i}_3 \\ -\mathbf{i}_3 & -\mathbf{i}_3\mathbf{r} & -\mathbf{i}_3\mathbf{r}\mathbf{i}_3 \end{array}\right) = \frac{1}{4}\,\mathbf{P}^{E}\left(\begin{array}{c|cc} & \mathbf{r} & +\mathbf{r}\mathbf{i}_3 \\ \hline \mathbf{1} & \mathbf{r} & +\mathbf{i}_2 \\ -\mathbf{i}_3 & -\mathbf{i}_1 & -\mathbf{r}^2 \end{array}\right)$

or: $\mathbf{P}^{E}_{1_2 0_2} = (?)\cdot(\mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 + \mathbf{i}_2)$

† conjugation: $(\mathbf{r}^{\dagger} = \mathbf{r}^2, \mathbf{r}^{2\dagger} = \mathbf{r}, \mathbf{i}_1^{\dagger} = \mathbf{i}_1, \mathbf{i}_2^{\dagger} = \mathbf{i}_2)$

so: $\mathbf{P}^{E\dagger}_{1_2 0_2} = \mathbf{P}^{E}_{0_2 1_2} = (?)^{*}(\mathbf{r}^2 - \mathbf{r} - \mathbf{i}_1 + \mathbf{i}_2)$

Note diagonal D^E

$D^{E*}_{0_2 0_2}(\mathbf{1}) = 1$

$D^{E*}_{0_2 0_2}(\mathbf{r}) = -\frac{1}{2}$

gives equation for (?)-factor: $\mathbf{P}^{E}_{0_2 1_2}\cdot\mathbf{P}^{E}_{1_2 0_2} = \mathbf{P}^{E}_{0_2 0_2} = (?)^2\cdot(\mathbf{r}^2 - \mathbf{r} - \mathbf{i}_1 + \mathbf{i}_2)(\mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 + \mathbf{i}_2)$

$$= \tfrac{1}{6}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 - \mathbf{i}_2 + 2\mathbf{i}_3) = \left(\tfrac{\ell^E}{{}^{\circ}O} = \tfrac{1}{3}\right)\left(D^{E*}_{0_2 0_2}(1)\mathbf{1} + D^{E*}_{0_2 0_2}(r)\mathbf{r} + \ldots\right)$$

$(?)^2\cdot 4 = \frac{1}{3}$ This gives off-diagonal $\mathbf{P}^{E}_{xy}$...

$$\pm\mathbf{P}^{E}_{0_2 1_2} = \tfrac{1}{3}\left(-\tfrac{\sqrt{3}}{2}\mathbf{r} + \tfrac{\sqrt{3}}{2}\mathbf{r}^2 - \tfrac{\sqrt{3}}{2}\mathbf{i}_1 + \tfrac{\sqrt{3}}{2}\mathbf{i}_2\right)$$

$$\mathbf{P}^{E}_{0_2 0_2} = (?)^2\cdot\left(\begin{array}{c|cccc} & +\mathbf{r} & -\mathbf{r}^2 & -\mathbf{i}_1 & +\mathbf{i}_2 \\ \hline +\mathbf{r}^2 & +\mathbf{1} & -\mathbf{r} & -\mathbf{i}_2 & +\mathbf{i}_3 \\ -\mathbf{r} & -\mathbf{r}^2 & +\mathbf{1} & +\mathbf{i}_3 & -\mathbf{i}_1 \\ -\mathbf{i}_1 & -\mathbf{i}_2 & +\mathbf{i}_3 & +\mathbf{1} & -\mathbf{r} \\ +\mathbf{i}_2 & +\mathbf{i}_3 & -\mathbf{i}_1 & -\mathbf{r}^2 & +\mathbf{1} \end{array}\right) = (?)^2\cdot(+4\mathbf{1} - 2\mathbf{r} - 2\mathbf{r}^2 - 2\mathbf{i}_1 - 2\mathbf{i}_2 + 4\mathbf{i}_3)$$

Solving gives unknown (?)-factor: $(?) = \pm\sqrt{3}/6$

$(?)^2\cdot 4 = \frac{1}{3} = \frac{1}{3}D^{E*}_{0_2 0_2}(1)$

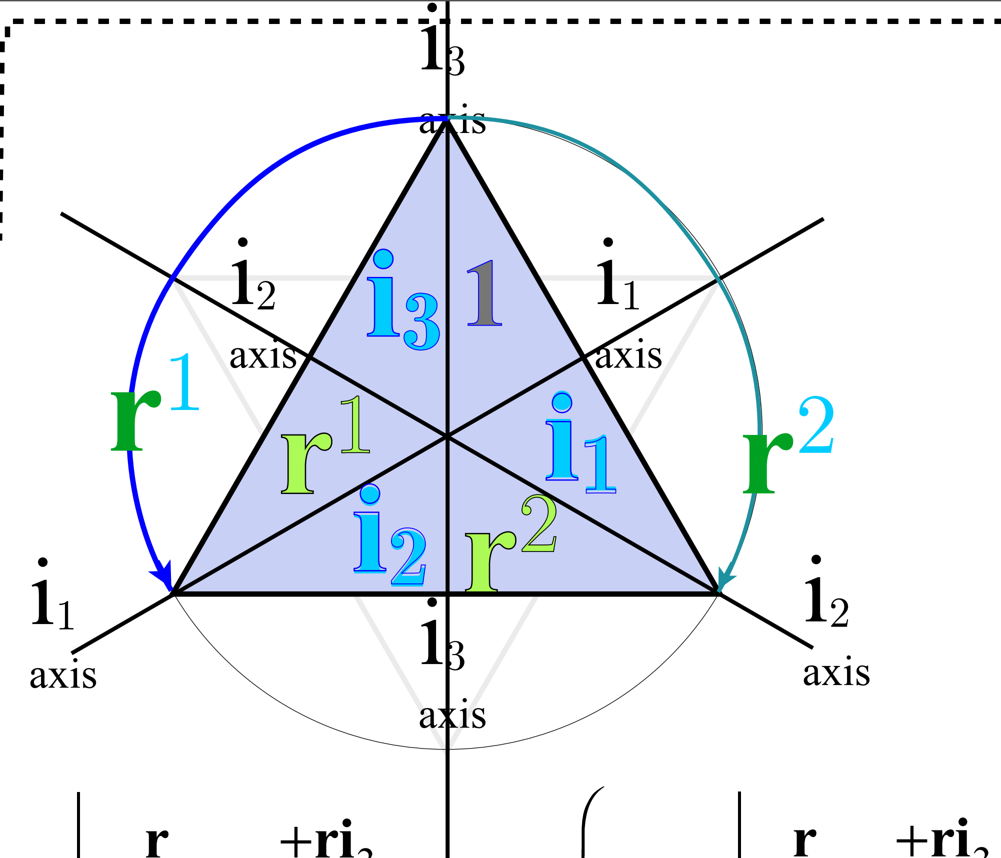
Irreducible nilpotent projectors $\mathbf{P}^{\mu}_{m,n}$ *(m≠n)*

$$\mathbf{P}^{\mu}_{mn} = \frac{\ell^{\mu}}{{}^{\circ}G}\sum_{\mathbf{g}}^{{}^{\circ}G} D^{\mu *}_{mn}(\mathbf{g})\mathbf{g}$$

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

$D_3 : \chi^{\alpha}_{k}$	χ^{α}_{1}	χ^{α}_{r}	χ^{α}_{i}
$\alpha = A_1$	1	1	1
$\alpha = A_2$	1	1	−1
$\alpha = E$	2	−1	0

Given: $\mathbf{P}^{E} = \frac{1}{3}(2\mathbf{c}_1 - \mathbf{c}_r + 0)$
$= \frac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)$



First do $C_2 = \{\mathbf{1}, \mathbf{i}_3\}$ splitting:

$$\mathbf{P}^{E}_{0_2 0_2} = \mathbf{P}^{E}\mathbf{p}_{0_2} = \tfrac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)\tfrac{1}{2}(\mathbf{1} + \mathbf{i}_3) = \tfrac{1}{6}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 - \mathbf{i}_2 + 2\mathbf{i}_3)$$

$$\mathbf{P}^{E}_{1_2 1_2} = \mathbf{P}^{E}\mathbf{p}_{1_2} = \tfrac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)\tfrac{1}{2}(\mathbf{1} - \mathbf{i}_3) = \tfrac{1}{6}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 + \mathbf{i}_1 + \mathbf{i}_2 - 2\mathbf{i}_3)$$

Then find nilpotent proportional to: $\mathbf{P}^{E}_{1_2 0_2} = \mathbf{P}^{E}\mathbf{p}_{1_2}\mathbf{r}\mathbf{p}_{0_2} = \mathbf{P}^{E}\,\frac{1}{2}\cdot\frac{1}{2}$

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

$= \frac{1}{4}\mathbf{P}^{E}$

	$\mathbf{r}$	$+\mathbf{r}\mathbf{i}_3$
$\mathbf{1}$	$\mathbf{r}$	$+\mathbf{i}_2$
$-\mathbf{i}_3$	$-\mathbf{i}_1$	$-\mathbf{r}^2$

or: $\mathbf{P}^{E}_{1_2 0_2} = (?)\cdot(\mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 + \mathbf{i}_2)$

† conjugation: $(\mathbf{r}^{\dagger} = \mathbf{r}^2, \mathbf{r}^{2\dagger} = \mathbf{r}, \mathbf{i}_1^{\dagger} = \mathbf{i}_1, \mathbf{i}_2^{\dagger} = \mathbf{i}_2)$

so: $\mathbf{P}^{E\dagger}_{1_2 0_2} = \mathbf{P}^{E}_{0_2 1_2} = (?)^{*}(\mathbf{r}^2 - \mathbf{r} - \mathbf{i}_1 + \mathbf{i}_2)$

Note diagonal D^E

$D^{E*}_{0_2 0_2}(\mathbf{1}) = 1$

$D^{E*}_{0_2 0_2}(\mathbf{r}) = -\frac{1}{2}$

gives equation for (?)-factor: $\mathbf{P}^{E}_{0_2 1_2}\cdot\mathbf{P}^{E}_{1_2 0_2} = \mathbf{P}^{E}_{0_2 0_2} = (?)^2\cdot(\mathbf{r}^2 - \mathbf{r} - \mathbf{i}_1 + \mathbf{i}_2)(\mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 + \mathbf{i}_2)$

$= \frac{1}{6}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 - \mathbf{i}_2 + 2\mathbf{i}_3) = (\frac{\ell^{E}}{{}^{\circ}D_3} = \frac{1}{3})(D^{E*}_{0_2 0_2}(1)\mathbf{1} + D^{E*}_{0_2 0_2}(r)\mathbf{r} + \ldots$

$(?)^2\cdot 4 = \frac{1}{3}$ This gives off-diagonal $\mathbf{P}^{E}_{xy}$...

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

$\mathbf{P}^{E}_{0_2 0_2} = (?)^2\cdot$

	$+\mathbf{r}$	$-\mathbf{r}^2$	$-\mathbf{i}_1$	$+\mathbf{i}_2$
$+\mathbf{r}^2$	$+\mathbf{1}$	$-\mathbf{r}$	$-\mathbf{i}_2$	$+\mathbf{i}_3$
$-\mathbf{r}$	$-\mathbf{r}^2$	$+\mathbf{1}$	$+\mathbf{i}_3$	$-\mathbf{i}_1$
$-\mathbf{i}_1$	$-\mathbf{i}_2$	$+\mathbf{i}_3$	$+\mathbf{1}$	$-\mathbf{r}$
$+\mathbf{i}_2$	$+\mathbf{i}_3$	$-\mathbf{i}_1$	$-\mathbf{r}^2$	$+\mathbf{1}$

$= (?)^2\cdot(+4\mathbf{1} - 2\mathbf{r} - 2\mathbf{r}^2 - 2\mathbf{i}_1 - 2\mathbf{i}_2 + 4\mathbf{i}_3)$

Solving gives unknown (?)-factor: $(?) = \pm\sqrt{3}/6$

$(?)^2\cdot 4 = \frac{1}{3} = \frac{1}{3}D^{E*}_{0_2 0_2}(1)$ ...and off-diagonal: $\pm D^{E*}_{0_2 1_2}(r) = -\frac{\sqrt{3}}{2}$, *etc.*

Finally, must set ± signs of off-diagonal components...

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

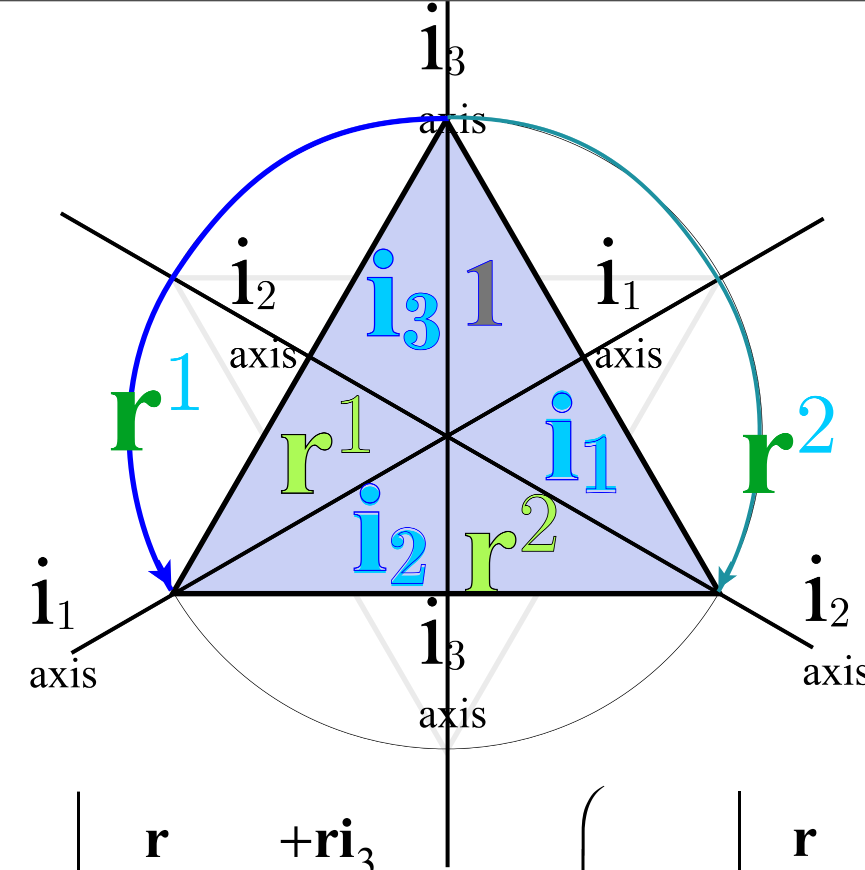
$$\pm D^{E^*}_{0_2 1_2}(r) = \frac{\sqrt{3}}{2}, etc.$$

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

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

$D_3:\chi^{\alpha}_{k}$	χ^{α}_{1}	χ^{α}_{r}	χ^{α}_{i}
$\alpha=A_1$	1	1	1
$\alpha=A_2$	1	1	-1
$\alpha=E$	2	-1	0

Given: $\mathbf{P}^{E}=\frac{1}{3}(2\mathbf{c}_1-\mathbf{c}_r+0)$
$=\frac{1}{3}(2\mathbf{1}-\mathbf{r}-\mathbf{r}^2)$



First do $C_2=\{\mathbf{1},\mathbf{i}_3\}$ splitting:

$$\mathbf{P}^{E}_{0_2 0_2}=\mathbf{P}^{E}\mathbf{p}_{0_2}=\frac{1}{3}(2\mathbf{1}-\mathbf{r}-\mathbf{r}^2)\frac{1}{2}(\mathbf{1}+\mathbf{i}_3)=\frac{1}{6}(2\mathbf{1}-\mathbf{r}-\mathbf{r}^2-\mathbf{i}_1-\mathbf{i}_2+2\mathbf{i}_3)$$

$$\mathbf{P}^{E}_{1_2 1_2}=\mathbf{P}^{E}\mathbf{p}_{1_2}=\frac{1}{3}(2\mathbf{1}-\mathbf{r}-\mathbf{r}^2)\frac{1}{2}(\mathbf{1}-\mathbf{i}_3)=\frac{1}{6}(2\mathbf{1}-\mathbf{r}-\mathbf{r}^2+\mathbf{i}_1+\mathbf{i}_2-2\mathbf{i}_3)$$

Then find nilpotent proportional to: $\mathbf{P}^{E}_{1_2 0_2}=\mathbf{P}^{E}\mathbf{p}_{1_2}\mathbf{r}\mathbf{p}_{0_2}=\mathbf{P}^{E}\,\frac{1}{2}\cdot\frac{1}{2}$

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

$=\frac{1}{4}\,\mathbf{P}^{E}$

	$\mathbf{r}$	$+\mathbf{r}\mathbf{i}_3$
$\mathbf{1}$	$\mathbf{r}$	$+\mathbf{i}_2$
$-\mathbf{i}_3$	$-\mathbf{i}_1$	$-\mathbf{r}^2$

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

Make group space vectors:

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

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

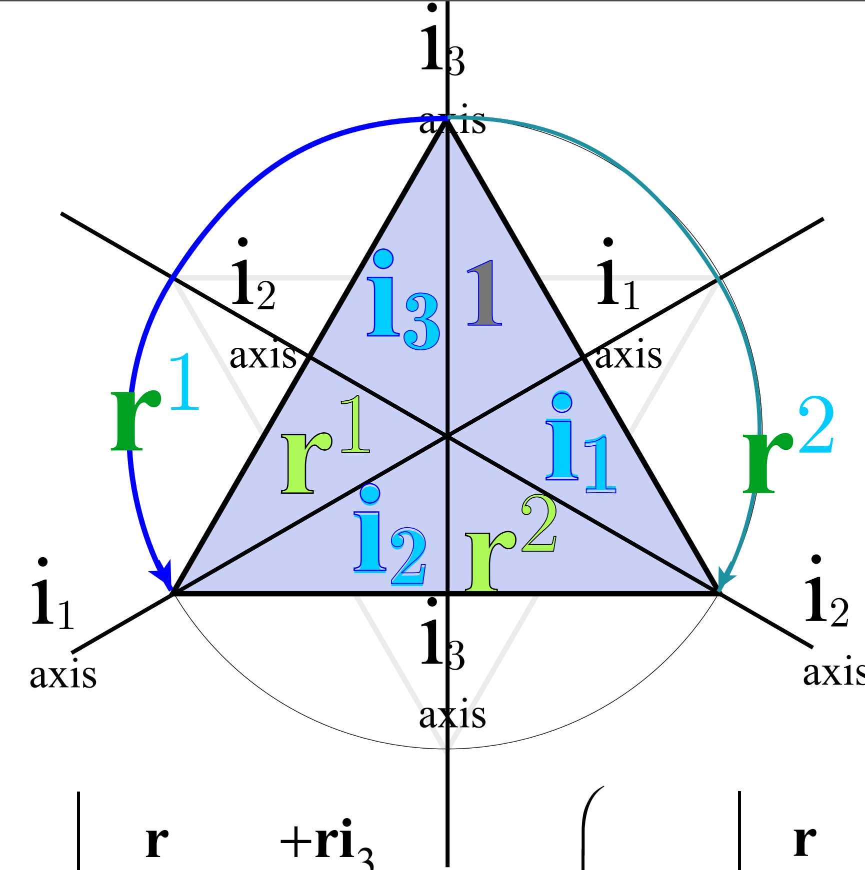
Irreducible nilpotent projectors $\mathbf{P}^{\mu}_{m,n}(m\neq n)$

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

$D_3 : \chi^{\alpha}_{k}$	χ^{α}_{1}	χ^{α}_{r}	χ^{α}_{i}
$\alpha = A_1$	1	1	1
$\alpha = A_2$	1	1	−1
$\alpha = E$	2	−1	0

Given: $\mathbf{P}^{E} = \frac{1}{3}(2\mathbf{c}_1 - \mathbf{c}_r + 0)$

$= \frac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)$



First do $C_2 = \{\mathbf{1}, \mathbf{i}_3\}$ splitting:

$$\mathbf{P}^{E}_{0_2 0_2} = \mathbf{P}^{E}\mathbf{p}_{0_2} = \frac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)\frac{1}{2}(\mathbf{1} + \mathbf{i}_3) = \frac{1}{6}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 - \mathbf{i}_2 + 2\mathbf{i}_3)$$

$$\mathbf{P}^{E}_{1_2 1_2} = \mathbf{P}^{E}\mathbf{p}_{1_2} = \frac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)\frac{1}{2}(\mathbf{1} - \mathbf{i}_3) = \frac{1}{6}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 + \mathbf{i}_1 + \mathbf{i}_2 - 2\mathbf{i}_3)$$

Then find nilpotent proportional to: $\mathbf{P}^{E}_{1_2 0_2} = \mathbf{P}^{E}\mathbf{p}_{1_2}\mathbf{r}\mathbf{p}_{0_2} = \mathbf{P}^{E}\frac{1}{2}\cdot\frac{1}{2}\left(\begin{array}{c|cc} & \mathbf{r} & +\mathbf{r}\mathbf{i}_3 \\ \hline \mathbf{1} & \mathbf{r} & +\mathbf{r}\mathbf{i}_3 \\ -\mathbf{i}_3 & -\mathbf{i}_3\mathbf{r} & -\mathbf{i}_3\mathbf{r}\mathbf{i}_3 \end{array}\right) = \frac{1}{4}\mathbf{P}^{E}\left(\begin{array}{c|cc} & \mathbf{r} & +\mathbf{r}\mathbf{i}_3 \\ \hline \mathbf{1} & \mathbf{r} & +\mathbf{i}_2 \\ -\mathbf{i}_3 & -\mathbf{i}_1 & -\mathbf{r}^2 \end{array}\right)$

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

Make group space vectors:

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

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

Do desired $\mathbf{g}=\mathbf{r}$ transformation:

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

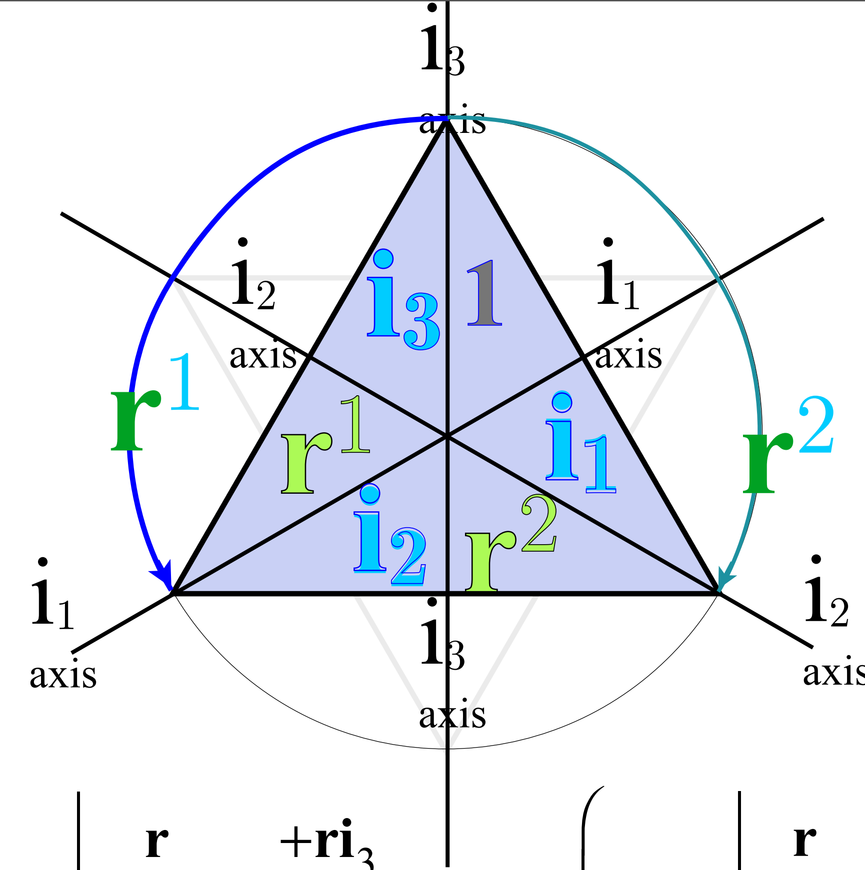
$$\mathbf{r}\left|\mathbf{P}^{E}_{1_2 0_2}\right\rangle = \frac{1}{2}\left(0\left|\mathbf{r}\right\rangle + \left|\mathbf{r}^2\right\rangle - \left|\mathbf{1}\right\rangle - \left|\mathbf{i}_3\right\rangle + \left|\mathbf{i}_1\right\rangle + 0\left|\mathbf{i}_3\right\rangle\right)$$

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

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

$D_3:\chi^{\alpha}_{k}$	χ^{α}_{1}	χ^{α}_{r}	χ^{α}_{i}
$\alpha=A_1$	1	1	1
$\alpha=A_2$	1	1	−1
$\alpha=E$	2	−1	0

Given: $\mathbf{P}^E=\frac{1}{3}(2\mathbf{c}_1-\mathbf{c}_r+0)$
$=\frac{1}{3}(2\mathbf{1}-\mathbf{r}-\mathbf{r}^2)$



First do $C_2=\{\mathbf{1},\mathbf{i}_3\}$ splitting:

$$\mathbf{P}^E_{0_2 0_2}=\mathbf{P}^E\mathbf{p}_{0_2}=\tfrac{1}{3}(2\mathbf{1}-\mathbf{r}-\mathbf{r}^2)\tfrac{1}{2}(\mathbf{1}+\mathbf{i}_3)=\tfrac{1}{6}(2\mathbf{1}-\mathbf{r}-\mathbf{r}^2-\mathbf{i}_1-\mathbf{i}_2+2\mathbf{i}_3)$$

$$\mathbf{P}^E_{1_2 1_2}=\mathbf{P}^E\mathbf{p}_{1_2}=\tfrac{1}{3}(2\mathbf{1}-\mathbf{r}-\mathbf{r}^2)\tfrac{1}{2}(\mathbf{1}-\mathbf{i}_3)=\tfrac{1}{6}(2\mathbf{1}-\mathbf{r}-\mathbf{r}^2+\mathbf{i}_1+\mathbf{i}_2-2\mathbf{i}_3)$$

Then find nilpotent proportional to: $\mathbf{P}^E_{1_2 0_2}=\mathbf{P}^E\mathbf{p}_{1_2}\mathbf{r}\mathbf{p}_{0_2}=\mathbf{P}^E\,\tfrac{1}{2}\cdot\tfrac{1}{2}$

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

$=\tfrac{1}{4}\mathbf{P}^E$

	$\mathbf{r}$	$+\mathbf{r}\mathbf{i}_3$
$\mathbf{1}$	$\mathbf{r}$	$+\mathbf{i}_2$
$-\mathbf{i}_3$	$-\mathbf{i}_1$	$-\mathbf{r}^2$

$\pm\mathbf{P}^E_{0_2 1_2}=\tfrac{1}{3}\left(-\tfrac{\sqrt{3}}{2}\mathbf{r}+\tfrac{\sqrt{3}}{2}\mathbf{r}^2-\tfrac{\sqrt{3}}{2}\mathbf{i}_1+\tfrac{\sqrt{3}}{2}\mathbf{i}_2\right)$ Now, to set ± signs...

Make group space vectors:

$$\left|\mathbf{P}^E_{0_2 0_2}\right\rangle=\tfrac{1}{2\sqrt{3}}(2|\mathbf{1}\rangle-|\mathbf{r}\rangle-|\mathbf{r}^2\rangle-|\mathbf{i}_1\rangle-|\mathbf{i}_2\rangle+2|\mathbf{i}_3\rangle)$$

$$\left|\mathbf{P}^E_{1_2 0_2}\right\rangle=\tfrac{1}{2}(0|\mathbf{1}\rangle+|\mathbf{r}\rangle-|\mathbf{r}^2\rangle-|\mathbf{i}_1\rangle+|\mathbf{i}_2\rangle+0|\mathbf{i}_3\rangle)$$

Do desired $\mathbf{g}=\mathbf{r}$ transformation:

$$\mathbf{r}\left|\mathbf{P}^E_{0_2 0_2}\right\rangle=\tfrac{1}{2\sqrt{3}}(2|\mathbf{r}\rangle-|\mathbf{r}^2\rangle-|\mathbf{1}\rangle-|\mathbf{i}_3\rangle-|\mathbf{i}_1\rangle+2|\mathbf{i}_2\rangle)$$

$$\mathbf{r}\left|\mathbf{P}^E_{1_2 0_2}\right\rangle=\tfrac{1}{2}(0|\mathbf{r}\rangle+|\mathbf{r}^2\rangle-|\mathbf{1}\rangle-|\mathbf{i}_3\rangle+|\mathbf{i}_1\rangle+0|\mathbf{i}_3\rangle)$$

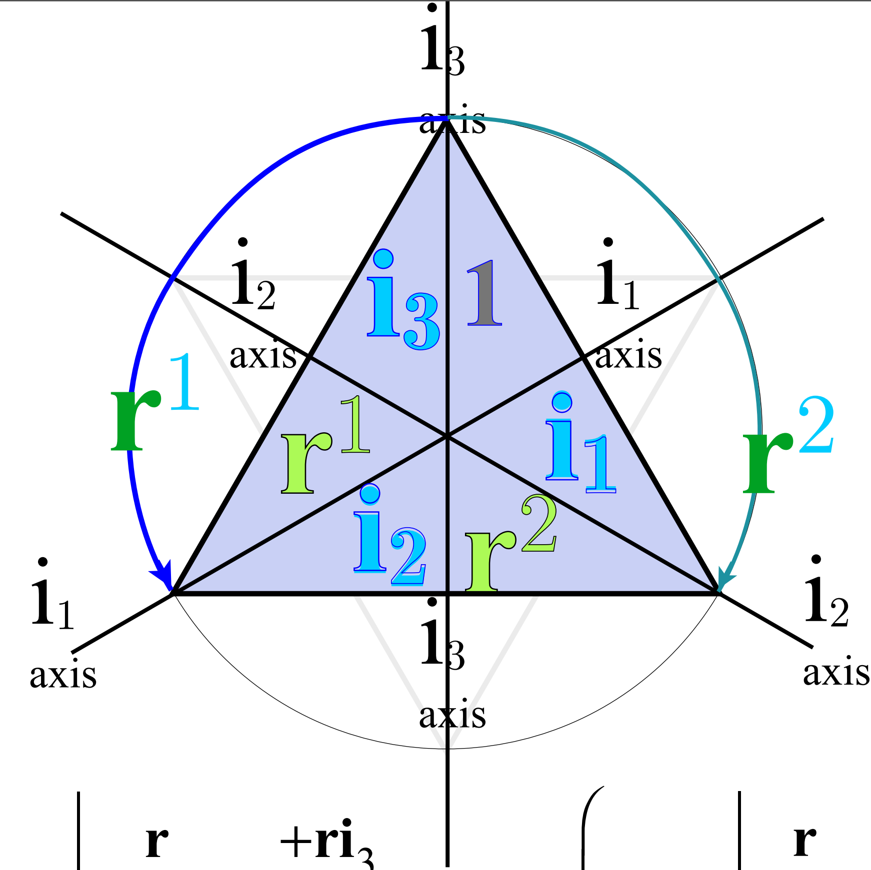
Set up to find matrix of $\mathbf{g}=\mathbf{r}$ transformation:

$$\mathbf{r}\left|\mathbf{P}^E_{0_2 0_2}\right\rangle=\tfrac{1}{2\sqrt{3}}(-|\mathbf{1}\rangle+2|\mathbf{r}\rangle-|\mathbf{r}^2\rangle-|\mathbf{i}_1\rangle+2|\mathbf{i}_2\rangle-|\mathbf{i}_3\rangle)$$

$$\mathbf{r}\left|\mathbf{P}^E_{1_2 0_2}\right\rangle=\tfrac{1}{2}(-|\mathbf{1}\rangle+0|\mathbf{r}\rangle+|\mathbf{r}^2\rangle+|\mathbf{i}_1\rangle+0|\mathbf{i}_3\rangle-|\mathbf{i}_3\rangle)$$

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

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



$D_3:\chi^{\alpha}_{k}$	χ^{α}_{1}	χ^{α}_{r}	χ^{α}_{i}
$\alpha=A_1$	1	1	1
$\alpha=A_2$	1	1	−1
$\alpha=E$	2	−1	0

Given: $\mathbf{P}^E = \frac{1}{3}(2\mathbf{c}_1 - \mathbf{c}_r + 0)$
$= \frac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)$

First do $C_2 = \{\mathbf{1}, \mathbf{i}_3\}$ splitting:

$$\mathbf{P}^E_{0_2 0_2} = \mathbf{P}^E \mathbf{p}_{0_2} = \tfrac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)\tfrac{1}{2}(\mathbf{1} + \mathbf{i}_3) = \tfrac{1}{6}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 - \mathbf{i}_2 + 2\mathbf{i}_3)$$

$$\mathbf{P}^E_{1_2 1_2} = \mathbf{P}^E \mathbf{p}_{1_2} = \tfrac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)\tfrac{1}{2}(\mathbf{1} - \mathbf{i}_3) = \tfrac{1}{6}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 + \mathbf{i}_1 + \mathbf{i}_2 - 2\mathbf{i}_3)$$

Then find nilpotent proportional to: $\mathbf{P}^E_{1_2 0_2} = \mathbf{P}^E \mathbf{p}_{1_2} \mathbf{r} \mathbf{p}_{0_2} = \mathbf{P}^E \frac{1}{2}\cdot\frac{1}{2}\left(\begin{array}{c|cc} & \mathbf{r} & +\mathbf{r}\mathbf{i}_3 \\ \hline \mathbf{1} & \mathbf{r} & +\mathbf{r}\mathbf{i}_3 \\ -\mathbf{i}_3 & -\mathbf{i}_3\mathbf{r} & -\mathbf{i}_3\mathbf{r}\mathbf{i}_3 \end{array}\right) = \frac{1}{4}\mathbf{P}^E \left(\begin{array}{c|cc} & \mathbf{r} & +\mathbf{r}\mathbf{i}_3 \\ \hline \mathbf{1} & \mathbf{r} & +\mathbf{i}_2 \\ -\mathbf{i}_3 & -\mathbf{i}_1 & -\mathbf{r}^2 \end{array}\right)$

$\pm\mathbf{P}^E_{0_2 1_2} = \frac{1}{3}\left(-\frac{\sqrt{3}}{2}\mathbf{r} + \frac{\sqrt{3}}{2}\mathbf{r}^2 - \frac{\sqrt{3}}{2}\mathbf{i}_1 + \frac{\sqrt{3}}{2}\mathbf{i}_2\right)$ Now, to set ± signs...

Make group space vectors:

$$\left|\mathbf{P}^E_{0_2 0_2}\right\rangle = \tfrac{1}{2\sqrt{3}}\left(2|\mathbf{1}\rangle - |\mathbf{r}\rangle - |\mathbf{r}^2\rangle - |\mathbf{i}_1\rangle - |\mathbf{i}_2\rangle + 2|\mathbf{i}_3\rangle\right)$$

$$\left|\mathbf{P}^E_{1_2 0_2}\right\rangle = \tfrac{1}{2}\left(0|\mathbf{1}\rangle + |\mathbf{r}\rangle - |\mathbf{r}^2\rangle - |\mathbf{i}_1\rangle + |\mathbf{i}_2\rangle + 0|\mathbf{i}_3\rangle\right)$$

Do desired $\mathbf{g}=\mathbf{r}$ transformation:

$$\mathbf{r}\left|\mathbf{P}^E_{0_2 0_2}\right\rangle = \tfrac{1}{2\sqrt{3}}\left(2|\mathbf{r}\rangle - |\mathbf{r}^2\rangle - |\mathbf{1}\rangle - |\mathbf{i}_3\rangle - |\mathbf{i}_1\rangle + 2|\mathbf{i}_2\rangle\right)$$

$$\mathbf{r}\left|\mathbf{P}^E_{1_2 0_2}\right\rangle = \tfrac{1}{2}\left(0|\mathbf{r}\rangle + |\mathbf{r}^2\rangle - |\mathbf{1}\rangle - |\mathbf{i}_3\rangle + |\mathbf{i}_1\rangle + 0|\mathbf{i}_3\rangle\right)$$

Set up to find matrix of $\mathbf{g}=\mathbf{r}$ transformation:

$$\mathbf{r}\left|\mathbf{P}^E_{0_2 0_2}\right\rangle = \tfrac{1}{2\sqrt{3}}\left(-|\mathbf{1}\rangle + 2|\mathbf{r}\rangle - |\mathbf{r}^2\rangle - |\mathbf{i}_1\rangle + 2|\mathbf{i}_2\rangle - |\mathbf{i}_3\rangle\right)$$

$$\mathbf{r}\left|\mathbf{P}^E_{1_2 0_2}\right\rangle = \tfrac{1}{2}\left(-|\mathbf{1}\rangle + 0|\mathbf{r}\rangle + |\mathbf{r}^2\rangle + |\mathbf{i}_1\rangle + 0|\mathbf{i}_3\rangle - |\mathbf{i}_3\rangle\right)$$

$$\left\langle\mathbf{P}^E_{0_2 0_2}\right|\mathbf{r}\left|\mathbf{P}^E_{0_2 0_2}\right\rangle = \tfrac{1}{2\sqrt{3}}(2-1-1-1-1+2)\cdot\tfrac{1}{2\sqrt{3}}(-1+2-1-1+2-1) = -1/2$$

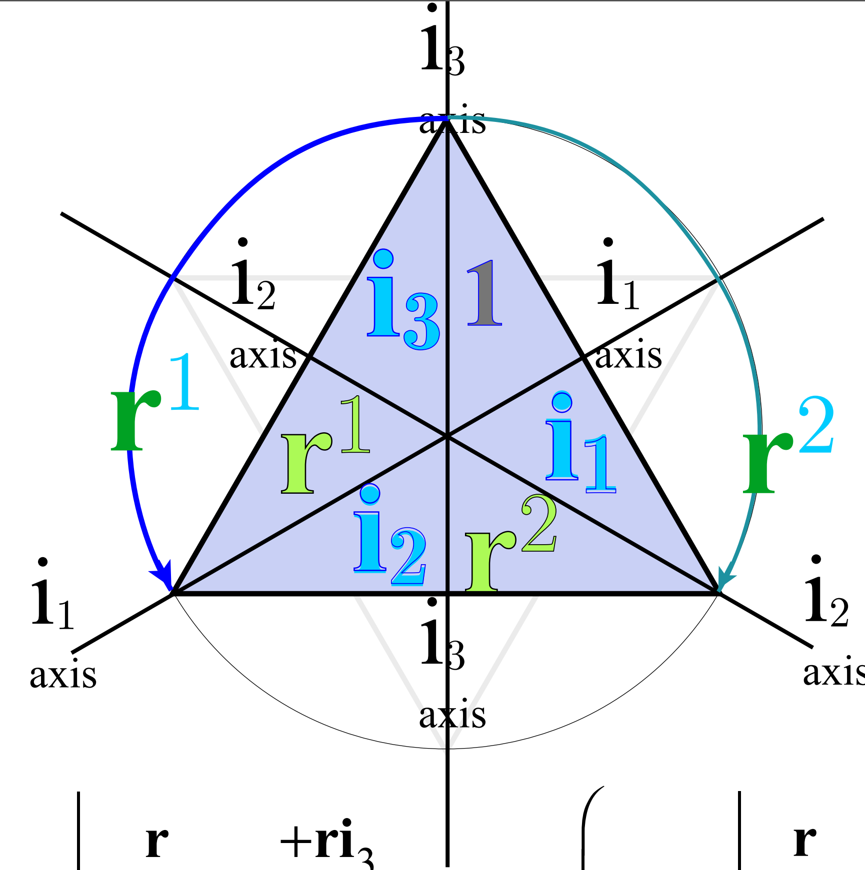
$$\left\langle\mathbf{P}^E_{1_2 0_2}\right|\mathbf{r}\left|\mathbf{P}^E_{0_2 0_2}\right\rangle = \tfrac{1}{2}(0+1-1-1+1+0)\cdot\tfrac{1}{2\sqrt{3}}(-1+2-1-1+2-1) = \sqrt{3}/2$$

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

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}
$\alpha = A_1$	1	1	1
$\alpha = A_2$	1	1	-1
$\alpha = E$	2	-1	0

Given: $\mathbf{P}^E = \frac{1}{3}(2\mathbf{c}_1 - \mathbf{c}_r + 0)$
$= \frac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)$



First do $C_2 = \{\mathbf{1}, \mathbf{i}_3\}$ splitting:

$$\mathbf{P}^E_{0_2 0_2} = \mathbf{P}^E \mathbf{p}_{0_2} = \tfrac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)\tfrac{1}{2}(\mathbf{1} + \mathbf{i}_3) = \tfrac{1}{6}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 - \mathbf{i}_2 + 2\mathbf{i}_3)$$

$$\mathbf{P}^E_{1_2 1_2} = \mathbf{P}^E \mathbf{p}_{1_2} = \tfrac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)\tfrac{1}{2}(\mathbf{1} - \mathbf{i}_3) = \tfrac{1}{6}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 + \mathbf{i}_1 + \mathbf{i}_2 - 2\mathbf{i}_3)$$

Then find nilpotent proportional to: $\mathbf{P}^E_{1_2 0_2} = \mathbf{P}^E \mathbf{p}_{1_2}\mathbf{r}\mathbf{p}_{0_2} = \mathbf{P}^E \frac{1}{2}\cdot\frac{1}{2}\begin{pmatrix} & \mathbf{r} & +\mathbf{r}\mathbf{i}_3 \\ \mathbf{1} & \mathbf{r} & +\mathbf{r}\mathbf{i}_3 \\ -\mathbf{i}_3 & -\mathbf{i}_3\mathbf{r} & -\mathbf{i}_3\mathbf{r}\mathbf{i}_3 \end{pmatrix} = \frac{1}{4}\mathbf{P}^E \begin{pmatrix} & \mathbf{r} & +\mathbf{r}\mathbf{i}_3 \\ \mathbf{1} & \mathbf{r} & +\mathbf{i}_2 \\ -\mathbf{i}_3 & -\mathbf{i}_1 & -\mathbf{r}^2 \end{pmatrix}$

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

Make group space vectors:

$$\left|\mathbf{P}^E_{0_2 0_2}\right\rangle = \tfrac{1}{2\sqrt{3}}\left(2\left|\mathbf{1}\right\rangle - \left|\mathbf{r}\right\rangle - \left|\mathbf{r}^2\right\rangle - \left|\mathbf{i}_1\right\rangle - \left|\mathbf{i}_2\right\rangle + 2\left|\mathbf{i}_3\right\rangle\right)$$

$$\left|\mathbf{P}^E_{1_2 0_2}\right\rangle = \tfrac{1}{2}\left(0\left|\mathbf{1}\right\rangle + \left|\mathbf{r}\right\rangle - \left|\mathbf{r}^2\right\rangle - \left|\mathbf{i}_1\right\rangle + \left|\mathbf{i}_2\right\rangle + 0\left|\mathbf{i}_3\right\rangle\right)$$

Do desired $\mathbf{g}=\mathbf{r}$ transformation:

$$\mathbf{r}\left|\mathbf{P}^E_{0_2 0_2}\right\rangle = \tfrac{1}{2\sqrt{3}}\left(2\left|\mathbf{r}\right\rangle - \left|\mathbf{r}^2\right\rangle - \left|\mathbf{1}\right\rangle - \left|\mathbf{i}_3\right\rangle - \left|\mathbf{i}_1\right\rangle + 2\left|\mathbf{i}_2\right\rangle\right)$$

$$\mathbf{r}\left|\mathbf{P}^E_{1_2 0_2}\right\rangle = \tfrac{1}{2}\left(0\left|\mathbf{r}\right\rangle + \left|\mathbf{r}^2\right\rangle - \left|\mathbf{1}\right\rangle - \left|\mathbf{i}_3\right\rangle + \left|\mathbf{i}_1\right\rangle + 0\left|\mathbf{i}_3\right\rangle\right)$$

Set up to find matrix of $\mathbf{g}=\mathbf{r}$ transformation:

$$\mathbf{r}\left|\mathbf{P}^E_{0_2 0_2}\right\rangle = \tfrac{1}{2\sqrt{3}}\left(-\left|\mathbf{1}\right\rangle + 2\left|\mathbf{r}\right\rangle - \left|\mathbf{r}^2\right\rangle - \left|\mathbf{i}_1\right\rangle + 2\left|\mathbf{i}_2\right\rangle - \left|\mathbf{i}_3\right\rangle\right)$$

$$\mathbf{r}\left|\mathbf{P}^E_{1_2 0_2}\right\rangle = \tfrac{1}{2}\left(-\left|\mathbf{1}\right\rangle + 0\left|\mathbf{r}\right\rangle + \left|\mathbf{r}^2\right\rangle + \left|\mathbf{i}_1\right\rangle + 0\left|\mathbf{i}_3\right\rangle - \left|\mathbf{i}_3\right\rangle\right)$$

$$\left\langle\mathbf{P}^E_{0_2 0_2}\middle|\mathbf{r}\middle|\mathbf{P}^E_{0_2 0_2}\right\rangle = \tfrac{1}{2\sqrt{3}}(2-1-1-1-1+2)\cdot\tfrac{1}{2\sqrt{3}}(-1+2-1-1+2-1) = -1/2 = D^E_{0_2 0_2}(r)$$

$$\left\langle\mathbf{P}^E_{1_2 0_2}\middle|\mathbf{r}\middle|\mathbf{P}^E_{0_2 0_2}\right\rangle = \tfrac{1}{2}(0+1-1-1+1+0)\cdot\tfrac{1}{2\sqrt{3}}(-1+2-1-1+2-1) = \sqrt{3}/2 = D^E_{1_2 0_2}(r)$$

$$\left\langle\mathbf{P}^E_{0_2 0_2}\middle|\mathbf{r}\middle|\mathbf{P}^E_{1_2 0_2}\right\rangle = \tfrac{1}{2\sqrt{3}}(2-1-1-1-1+2)\cdot\tfrac{1}{2}(-1+0+1+1+0-1) = -\sqrt{3}/2 = D^E_{0_2 1_2}(r)$$

$$\left\langle\mathbf{P}^E_{1_2 0_2}\middle|\mathbf{r}\middle|\mathbf{P}^E_{1_2 0_2}\right\rangle = \tfrac{1}{2}(0+1-1-1+1+0)\cdot\tfrac{1}{2}(-1+0+1+1+0-1) = -1/2 = D^E_{1_2 1_2}(r))$$

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

This checks with p. 56

This amounts to the world's most complicated derivation of: cos 120°=-1/2 and: sin 120°=√3/2

$$D^E(\mathbf{r}) = D^E(120°) = \begin{pmatrix} \cos(120°) & -\sin(120°) \\ \sin(120°) & \cos(120°) \end{pmatrix} = \begin{pmatrix} -1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix}$$

$$\mathbf{P}^E_{0_2 1_2} = \tfrac{1}{3}\left(-\tfrac{\sqrt{3}}{2}\mathbf{r} + \tfrac{\sqrt{3}}{2}\mathbf{r}^2 - \tfrac{\sqrt{3}}{2}\mathbf{i}_1 + \tfrac{\sqrt{3}}{2}\mathbf{i}_2\right) = \mathbf{P}^{E\dagger}_{1_2 0_2}$$

Coefficients $D^{(\alpha)}_{i,j}(g)$ *are irreducible representations (ireps) of* **g**

$\mathbf{g} =$	$\mathbf{1}$	$\mathbf{r}^1$	$\mathbf{r}^2$	$\mathbf{i}_1$	$\mathbf{i}_2$	$\mathbf{i}_3$
$D^{A_1}_{xx}(\mathbf{g}) =$	1	1	1	1	1	1
$D^{A_2}_{yy}(\mathbf{g}) =$	1	1	1	−1	−1	−1
$D^{E_1}_{x,y}(\mathbf{g}) =$	$\begin{pmatrix} 1 & \cdot \\ \cdot & 1 \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

Review Calculating idempotent projectors $\mathbf{P}^{\mu}_{m,m}$ *of* $O\supset C_4$ $\mathbf{P}^{E}_{0_4 0_4}$ $\mathbf{P}^{E}_{2_4 2_4}$ $\mathbf{P}^{T_1}_{0_4 0_4}$ $\mathbf{P}^{T_1}_{1_4 1_4}$ $\mathbf{P}^{T_2}_{2_4 2_4}$

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

Review Broken-class-ordered splitting of $O\supset D_4\supset C_4$ *projectors and levels*

Subgroup-defined tunneling parameter modeling

Comparing two diagonal $O\supset C_4$ *parameter sets to* SF_6 *spectra*

Comparing two diagonal $O\supset C_3$ *parameter sets to* SF_6 *spectra*

Why $O\supset C_2$ *parameter sets require off-diagonal nilpotent* $\mathbf{P}^{\mu}_{m,n}$ $(m\neq n)$

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

Using fundamental $\mathbf{g}\rightleftarrows\mathbf{P}^{\mu}_{m,n}$ *relations: (from Lecture 16)*

(a) $\mathbf{P}^{\mu}_{m,m}\,\mathbf{g}\mathbf{P}^{\mu}_{n,n}=D^{\mu}_{m,n}(\mathbf{g})\mathbf{P}^{\mu}_{m,n}$ (b) $\mathbf{g}=\Sigma_{\mu}\Sigma_{m,n}D^{\mu}_{m,n}(\mathbf{g})\mathbf{P}^{\mu}_{m,n}$ (c) $\mathbf{P}^{\mu}_{n,n}=(\ell^{\mu}/{}^{\circ}G)\Sigma_{\mathbf{g}}D^{\mu^*}_{m,n}(\mathbf{g})\mathbf{g}$

Review of $D_3\supset C_2\sim C_{3v}\supset C_v$ *calculations of* $\mathbf{P}^{\mu}_{m,n}$ *and* $D^{\mu}_{m,n}$

➡ *Calculating and Factoring* $\mathbf{P}^{T_1}_{1_4 0_4}$ *and* $\mathbf{P}^{T_1}_{1_4 3_4}$ ⬅

Structure and applications of various subgroup chain irreducible representations

$O_h\supset D_{4h}\supset C_{4v}$, $O_h\supset D_{3h}\supset C_{3v}$, $O_h\supset C_{2v}$

Comparing $O_h\supset D_{4h}\supset D_{2h}$ *and* $O_h\supset D_{3d}\supset C_2$ *representations (*T_1 *vector-type)*

Examples of off-diagonal tunneling coefficients $D^{E}_{0_4 2_4}$

Comparing Local C_4*,* C_3*, and* C_2 *symmetric spectra*

Comparing off-diagonal $O\supset C_2$ *parameter sets to* CH_4 *models with "cluster-crossings"*

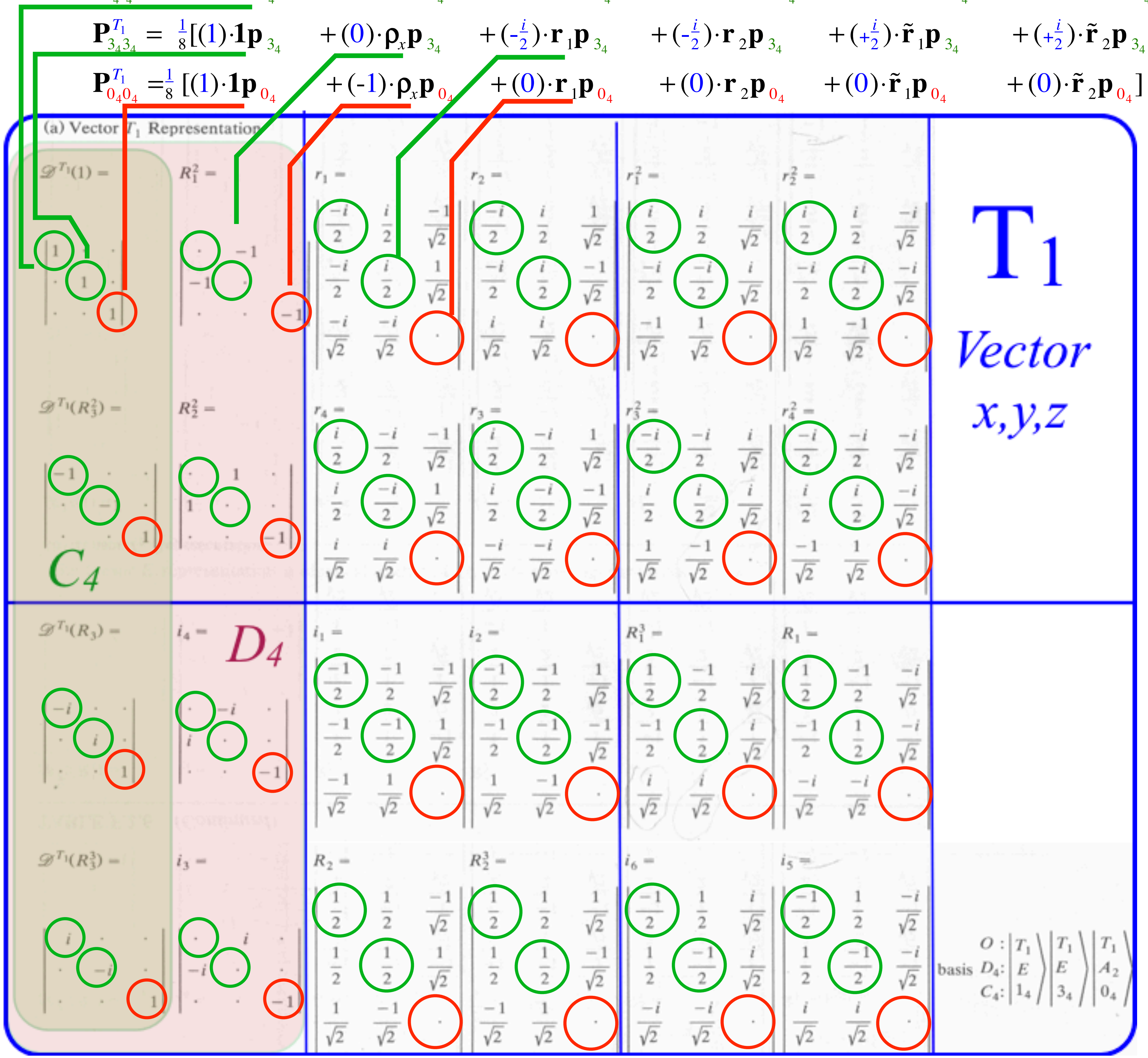
Irreducible nilpotent projectors $\mathbf{P}^{\mu}_{m,n}$

Coset-factored T1*-sum:(First display idempotent projectors* $\mathbf{P}^{T_1}_{kk}$ *and diagonal components* $D^{T_1 *}_{kk}(\mathbf{g})$

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

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

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



$$\mathbf{P}^{T_1}_{mn} = \frac{\ell^{T_1}=3}{{}^\circ G=24}\sum_{\mathbf{g}}^{{}^\circ G} D^{T_1 *}_{mn}(\mathbf{g})\mathbf{g}$$

O⊃C4
left cosets

$\{\mathbf{1},\rho_z,\mathbf{R}_z,\tilde{\mathbf{R}}_z\}$

$\{\rho_x,\rho_y,\mathbf{i}_4,\mathbf{i}_3\}$

$\{\mathbf{r}_1,\mathbf{r}_4,\mathbf{i}_1,\mathbf{R}_y\}$

$\{\mathbf{r}_2,\mathbf{r}_3,\mathbf{i}_2,\tilde{\mathbf{R}}_y\}$

$\{\tilde{\mathbf{r}}_1,\tilde{\mathbf{r}}_3,\tilde{\mathbf{R}}_x,\mathbf{i}_6\}$

$\{\tilde{\mathbf{r}}_2,\tilde{\mathbf{r}}_4,\mathbf{R}_x,\mathbf{i}_5\}$

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

$O \supset C_4$
left cosets

$\{\mathbf{1}, \rho_z, \mathbf{R}_z, \tilde{\mathbf{R}}_z\}$

$\{\rho_x, \rho_y, \mathbf{i}_4, \mathbf{i}_3\}$

$\{\mathbf{r}_1, \mathbf{r}_4, \mathbf{i}_1, \mathbf{R}_y\}$

$\{\mathbf{r}_2, \mathbf{r}_3, \mathbf{i}_2, \tilde{\mathbf{R}}_y\}$

$\{\tilde{\mathbf{r}}_1, \tilde{\mathbf{r}}_3, \tilde{\mathbf{R}}_x, \mathbf{i}_6\}$

$\{\tilde{\mathbf{r}}_2, \tilde{\mathbf{r}}_4, \mathbf{R}_x, \mathbf{i}_5\}$

Coset-factored T1*-sum:(Now find nilpotent projectors* $\mathbf{P}^{T_1}_{jk}$ *and off-diagonal* $D^{T_1 *}_{jk}(\mathbf{g})$

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

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

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

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

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

Consistent with standard: $\mathbf{P}^{\mu}_{m_4 m_4} = \sum_{g}^{\circ O} \frac{\ell^{\mu}}{\circ G} D^{\mu *}_{m_4 m_4}(g)\mathbf{g}$

$O \supset C_4$ left cosets

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

Coset-factored T1*-sum:(Now find nilpotent projectors* $\mathbf{P}^{T_1}_{jk}$ *and off-diagonal* $D^{T_1 *}_{jk}(\mathbf{g})$

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

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

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

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: $\mathbf{p}_{1_4}\mathbf{r}_1\mathbf{p}_{0_4}$

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

Consistent with standard: $\mathbf{P}^{\mu}_{m_4 m_4} = \sum_{g}^{\circ O} \frac{\ell^{\mu}}{\circ G} D^{\mu *}_{m_4 m_4}(g)\mathbf{g}$

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

$O \supset C_4$ left cosets

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

Coset-factored T1-sum: (Now find nilpotent projectors $\mathbf{P}^{T_1}_{jk}$ and off-diagonal $D^{T_1 *}_{jk}(\mathbf{g})$

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

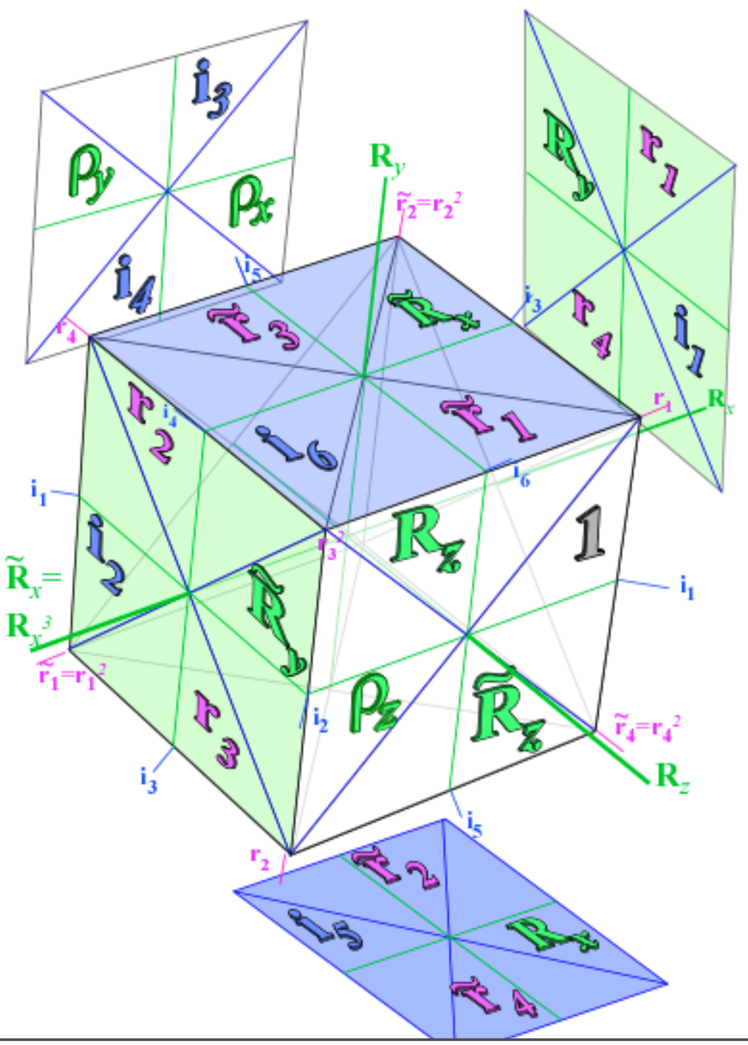
$$\mathbf{P}^{T_1}_{3_4 3_4} = \tfrac{1}{8}[(1)\cdot\mathbf{1p}_{3_4} + (0)\cdot\rho_x\mathbf{p}_{3_4} + (-\tfrac{i}{2})\cdot\mathbf{r}_1\mathbf{p}_{3_4} + (-\tfrac{i}{2})\cdot\mathbf{r}_2\mathbf{p}_{3_4} + (+\tfrac{i}{2})\cdot\tilde{\mathbf{r}}_1\mathbf{p}_{3_4} + (+\tfrac{i}{2})\cdot\tilde{\mathbf{r}}_2\mathbf{p}_{3_4}]$$

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

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

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

Then find nilpotent proportional to: $\mathbf{p}_{1_4}\mathbf{r}_1\mathbf{p}_{0_4} = \frac{1}{16}$



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

Consistent with standard: $\mathbf{P}^{\mu}_{m_4 m_4} = \sum_{g}^{\circ O}\frac{\ell^{\mu}}{\circ G}D^{\mu *}_{m_4 m_4}(g)\mathbf{g}$

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

$O \supset C_4$ left cosets

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

Coset-factored T1-sum: (Now find nilpotent projectors $\mathbf{P}^{T_1}_{jk}$ and off-diagonal $D^{T_1 *}_{jk}(\mathbf{g})$)

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

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

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

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: $\mathbf{p}_{1_4}\mathbf{r}_1\mathbf{p}_{0_4} = \frac{1}{16}$

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

$$=[(\mathbf{r}_1+\mathbf{r}_4+\mathbf{i}_1+\mathbf{R}_y)-(\mathbf{r}_2+\mathbf{r}_3+\mathbf{i}_2+\tilde{\mathbf{R}}_y)-i(\tilde{\mathbf{r}}_1+\tilde{\mathbf{r}}_3+\tilde{\mathbf{R}}_x+\mathbf{i}_6)+i(\tilde{\mathbf{r}}_2+\tilde{\mathbf{r}}_4+\mathbf{R}_x+\mathbf{i}_5)]/16$$

$$=[\mathbf{r}_1\mathbf{p}_{0_4}-\mathbf{r}_2\mathbf{p}_{0_4}-i\tilde{\mathbf{r}}_1\mathbf{p}_{0_4}+i\tilde{\mathbf{r}}_2\mathbf{p}_{0_4}]/4$$

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

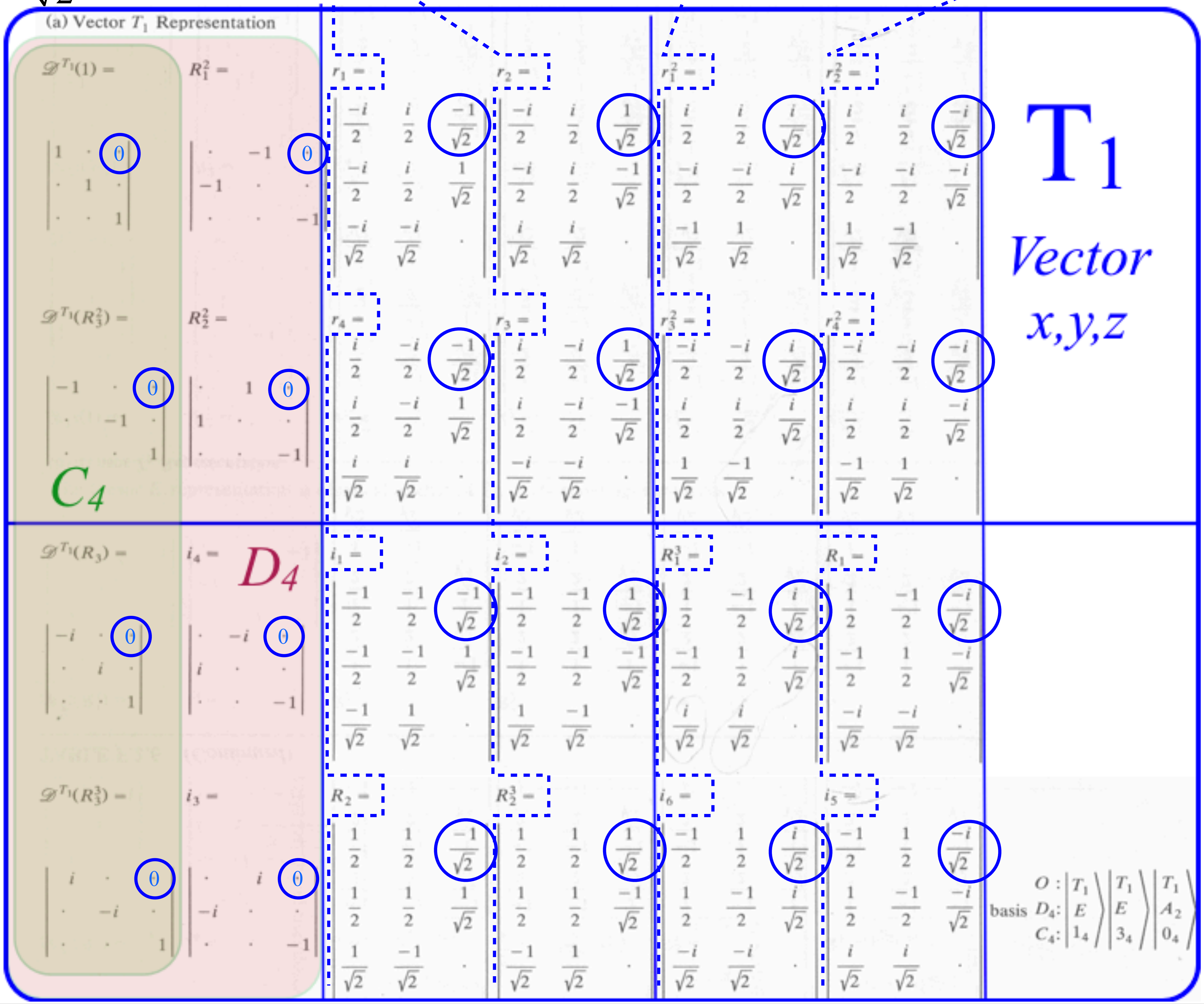
Consistent with standard: $\mathbf{P}^{\mu}_{m_4 m_4}=\sum_{g}^{\circ O}\frac{\ell^{\mu}}{\circ G}D^{\mu *}_{m_4 m_4}(g)\mathbf{g}$

Relating off-diagonal $1_4 0_4$ components $D^{T_1}_{1_4 0_4}(\mathbf{g})$ to coefficients of $\frac{-1}{\sqrt{2}}\mathbf{p}_{1_4}\mathbf{r}_1\mathbf{p}_{0_4}$:

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

$$\frac{-1}{\sqrt{2}}\mathbf{p}_{1_4}\mathbf{r}_1\mathbf{p}_{0_4} = \frac{1}{\sqrt{2}}\left[-\mathbf{r}_1\mathbf{p}_{0_4}+\mathbf{r}_2\mathbf{p}_{0_4}+i\tilde{\mathbf{r}}_1\mathbf{p}_{0_4}-i\tilde{\mathbf{r}}_2\mathbf{p}_{0_4}\right] =$$

$$\frac{1}{\sqrt{2}}\left[-(\mathbf{r}_1+\mathbf{r}_4+\mathbf{i}_1+\mathbf{R}_y)+(\mathbf{r}_2+\mathbf{r}_3+\mathbf{i}_2+\tilde{\mathbf{R}}_y)+i(\tilde{\mathbf{r}}_1+\tilde{\mathbf{r}}_3+\tilde{\mathbf{R}}_x+\mathbf{i}_6)-i(\tilde{\mathbf{r}}_2+\tilde{\mathbf{r}}_4+\mathbf{R}_x+\mathbf{i}_5)\right]$$



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

$O \supset C_4$ left cosets

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

Coset-factored T1-sum: (Now find nilpotent projectors $\mathbf{P}^{T_1}_{jk}$ and off-diagonal $D^{T_1 *}_{jk}(\mathbf{g})$

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

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

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

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

NOTE: These projectors still have phase errors as of 4.12.15
(However final tables OK)

Then find nilpotent proportional to: $\mathbf{p}_{1_4}\mathbf{r}_1\mathbf{p}_{0_4} = \frac{1}{16}$

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

$$=[(\mathbf{r}_1+\mathbf{r}_4+\mathbf{i}_1+\mathbf{R}_y)-(\mathbf{r}_2+\mathbf{r}_3+\mathbf{i}_2+\tilde{\mathbf{R}}_y)+i(\tilde{\mathbf{r}}_1+\tilde{\mathbf{r}}_3+\tilde{\mathbf{R}}_x+\mathbf{i}_6)-i(\tilde{\mathbf{r}}_2+\tilde{\mathbf{r}}_4+\mathbf{R}_x+\mathbf{i}_5)]/16$$

$$=[\mathbf{r}_1\mathbf{p}_{0_4}-\mathbf{r}_2\mathbf{p}_{0_4}+i\tilde{\mathbf{r}}_1\mathbf{p}_{0_4}-i\tilde{\mathbf{r}}_2\mathbf{p}_{0_4}]/4 = (\mathbf{r}_1-\mathbf{r}_2+i\tilde{\mathbf{r}}_1-i\tilde{\mathbf{r}}_2)\mathbf{p}_{0_4}/4$$

Result is nicely factored: $\mathbf{P}^{T_1}_{1_4 0_4}$

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

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

Consistent with standard: $\mathbf{P}^{\mu}_{m_4 m_4}=\sum_{g}^{\circ O}\frac{\ell^{\mu}}{\circ G}D^{\mu *}_{m_4 m_4}(g)\mathbf{g}$

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

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

Coset-factored T1*-sum:*

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

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

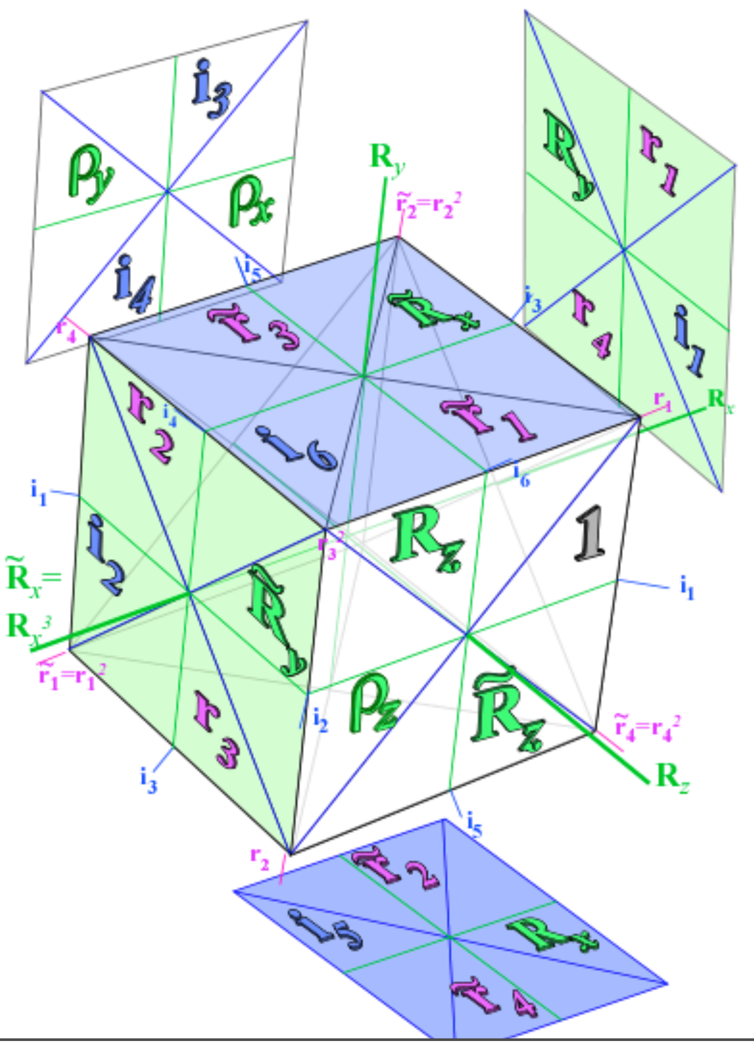
$$\mathbf{P}^{T_1}_{0_4 0_4} = \tfrac{1}{8}[(1)\cdot\mathbf{1}\mathbf{p}_{0_4} + (-1)\cdot\rho_x\mathbf{p}_{0_4} + (0)\cdot\mathbf{r}_1\mathbf{p}_{0_4} + (0)\cdot\mathbf{r}_2\mathbf{p}_{0_4} + (0)\cdot\tilde{\mathbf{r}}_1\mathbf{p}_{0_4} + (0)\cdot\tilde{\mathbf{r}}_2\mathbf{p}_{0_4}]$$

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

NOTE: These projectors
still have phase errors
as of 4.12.15
(However final tables OK)

Then find nilpotent proportional to: $\mathbf{p}_{0_4}\tilde{\mathbf{r}}_1\mathbf{p}_{1_4} = \frac{1}{16}\rho_z$

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



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

Consistent with standard: $\mathbf{P}^{\mu}_{m_4 m_4} = \sum_{g}^{\circ O} \frac{\ell^{\mu}}{\circ G} D^{\mu *}_{m_4 m_4}(g)\mathbf{g}$

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

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

Coset-factored T_1-sum:

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

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

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

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

NOTE: These projectors still have phase errors as of 4.12.15
(However final tables OK)

Then find nilpotent proportional to: $\mathbf{p}_{0_4}\tilde{\mathbf{r}}_1\mathbf{p}_{1_4} = \frac{1}{16}$

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

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

$$= \mathbf{p}_{0_4}\tilde{\mathbf{r}}_1 - \mathbf{p}_{0_4}\tilde{\mathbf{r}}_3 - i\mathbf{p}_{0_4}\tilde{\mathbf{R}}_x + i\mathbf{p}_{0_4}\mathbf{i}_6$$

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

Consistent with standard: $\mathbf{P}^{\mu}_{m_4 m_4} = \sum_{g}^{\circ O} \frac{\ell^{\mu}}{\circ G} D^{\mu *}_{m_4 m_4}(g)\mathbf{g}$

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

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

$O\supset C_4$ left cosets

$\{\mathbf{1},\rho_z,\mathbf{R}_z,\tilde{\mathbf{R}}_z\}$

$\{\rho_x,\rho_y,\mathbf{i}_4,\mathbf{i}_3\}$

$\{\mathbf{r}_1,\mathbf{r}_4,\mathbf{i}_1,\mathbf{R}_y\}$

$\{\mathbf{r}_2,\mathbf{r}_3,\mathbf{i}_2,\tilde{\mathbf{R}}_y\}$

$\{\tilde{\mathbf{r}}_1,\tilde{\mathbf{r}}_3,\tilde{\mathbf{R}}_x,\mathbf{i}_6\}$

$\{\tilde{\mathbf{r}}_2,\tilde{\mathbf{r}}_4,\mathbf{R}_x,\mathbf{i}_5\}$

Coset-factored T_1*-sum:*

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

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

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

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

NOTE: These projectors still have phase errors as of 4.12.15
(However final tables OK)

Then find nilpotent proportional to: $\mathbf{p}_{1_4}\mathbf{r}_1\mathbf{p}_{3_4} = \frac{1}{16}$

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

$$=[(\mathbf{r}_1-\mathbf{r}_4-i\mathbf{i}_1+i\mathbf{R}_y)+(\mathbf{r}_2-\mathbf{r}_3-i\mathbf{i}_2+i\tilde{\mathbf{R}}_y)+(\tilde{\mathbf{r}}_1-\tilde{\mathbf{r}}_3-i\tilde{\mathbf{R}}_x+i\mathbf{i}_6)+(\tilde{\mathbf{r}}_2-\tilde{\mathbf{r}}_4-i\mathbf{R}_x+i\mathbf{i}_5)]/16$$

$$=[\mathbf{r}_1\mathbf{p}_{3_4}+\mathbf{r}_2\mathbf{p}_{3_4}+\tilde{\mathbf{r}}_1\mathbf{p}_{3_4}+\tilde{\mathbf{r}}_2\mathbf{p}_{3_4}]/4$$

Result is nicely factored quite like $\mathbf{P}^{T_1}_{1_4 0_4}$:

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

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

Consistent with standard: $\mathbf{P}^{\mu}_{m_4 m_4}=\sum_{g}^{\circ O}\frac{\ell^{\mu}}{\circ G}D^{\mu *}_{m_4 m_4}(g)\mathbf{g}$

Review Calculating idempotent projectors $\mathbf{P}^{\mu}_{m,m}$ *of* $O\supset C_4$ $\mathbf{P}^{E}_{0_4 0_4}$ $\mathbf{P}^{E}_{2_4 2_4}$ $\mathbf{P}^{T_1}_{0_4 0_4}$ $\mathbf{P}^{T_1}_{1_4 1_4}$ $\mathbf{P}^{T_2}_{2_4 2_4}$

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

Review Broken-class-ordered splitting of $O\supset D_4\supset C_4$ *projectors and levels*

Subgroup-defined tunneling parameter modeling

Comparing two diagonal $O\supset C_4$ *parameter sets to* SF_6 *spectra*

Comparing two diagonal $O\supset C_3$ *parameter sets to* SF_6 *spectra*

Why $O\supset C_2$ *parameter sets require off-diagonal nilpotent* $\mathbf{P}^{\mu}_{m,n}$ $(m\neq n)$

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

Using fundamental $\mathbf{g}\rightleftarrows\mathbf{P}^{\mu}_{m,n}$ *relations: (from Lecture 16)*

(a) $\mathbf{P}^{\mu}_{m,m}\mathbf{g}\mathbf{P}^{\mu}_{n,n}=D^{\mu}_{m,n}(\mathbf{g})\mathbf{P}^{\mu}_{m,n}$ (b) $\mathbf{g}=\Sigma_{\mu}\Sigma_{m,n}D^{\mu}_{m,n}(\mathbf{g})\mathbf{P}^{\mu}_{m,n}$ (c) $\mathbf{P}^{\mu}_{n,n}=(\ell^{\mu}/{}^{\circ}G)\Sigma_{\mathbf{g}}D^{\mu *}_{m,n}(\mathbf{g})\mathbf{g}$

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

Calculating and Factoring $\mathbf{P}^{T_1}_{1_4 0_4}$ *and* $\mathbf{P}^{T_1}_{1_4 3_4}$

Structure and applications of various subgroup chain irreducible representations

➡ $O_h\supset D_{4h}\supset C_{4v}$, $O_h\supset D_{3h}\supset C_{3v}$, $O_h\supset C_{2v}$ ⬅

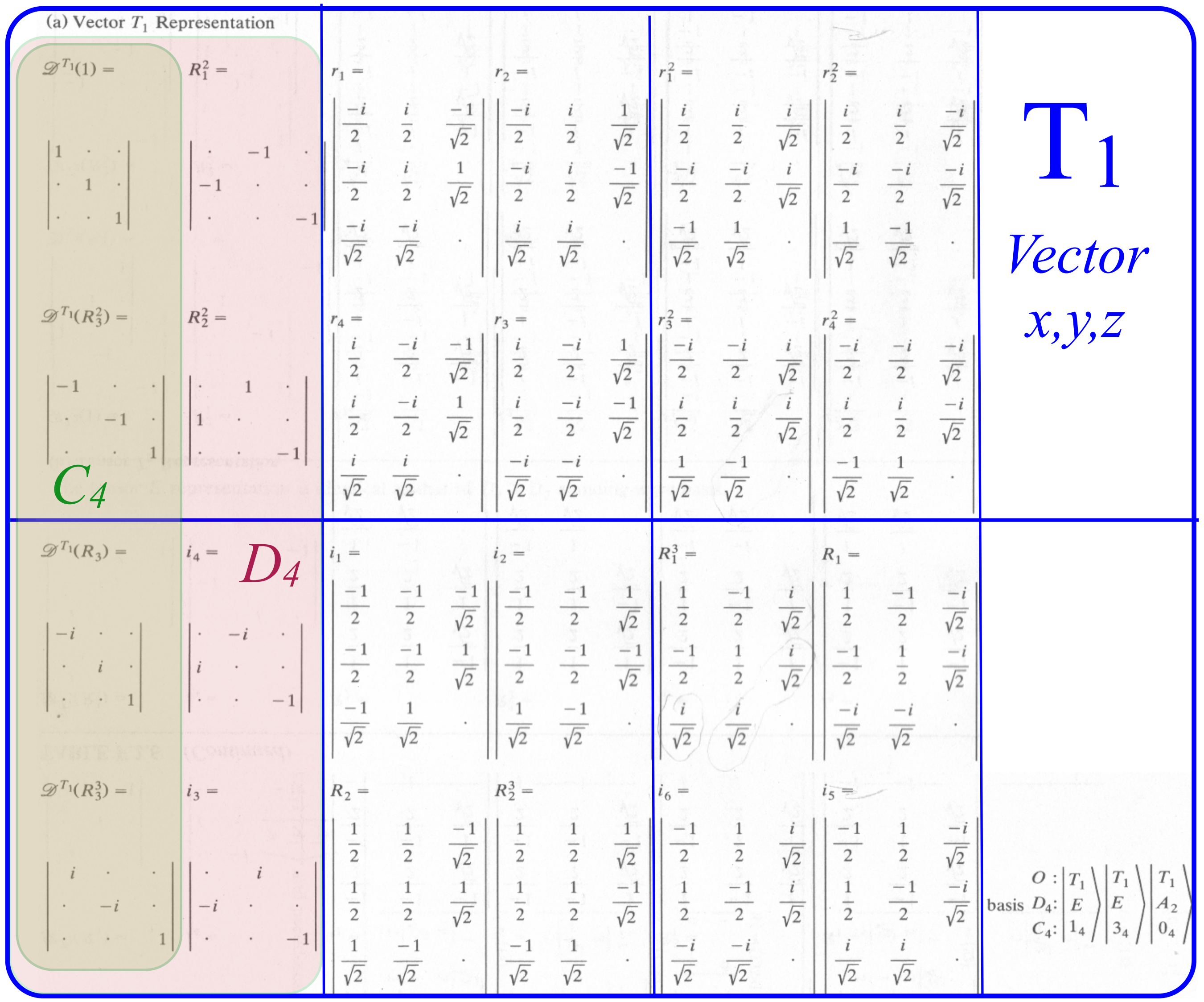
Comparing $O_h\supset D_{4h}\supset D_{2h}$ *and* $O_h\supset D_{3d}\supset C_2$ *representations (*T_1 *vector-type)*

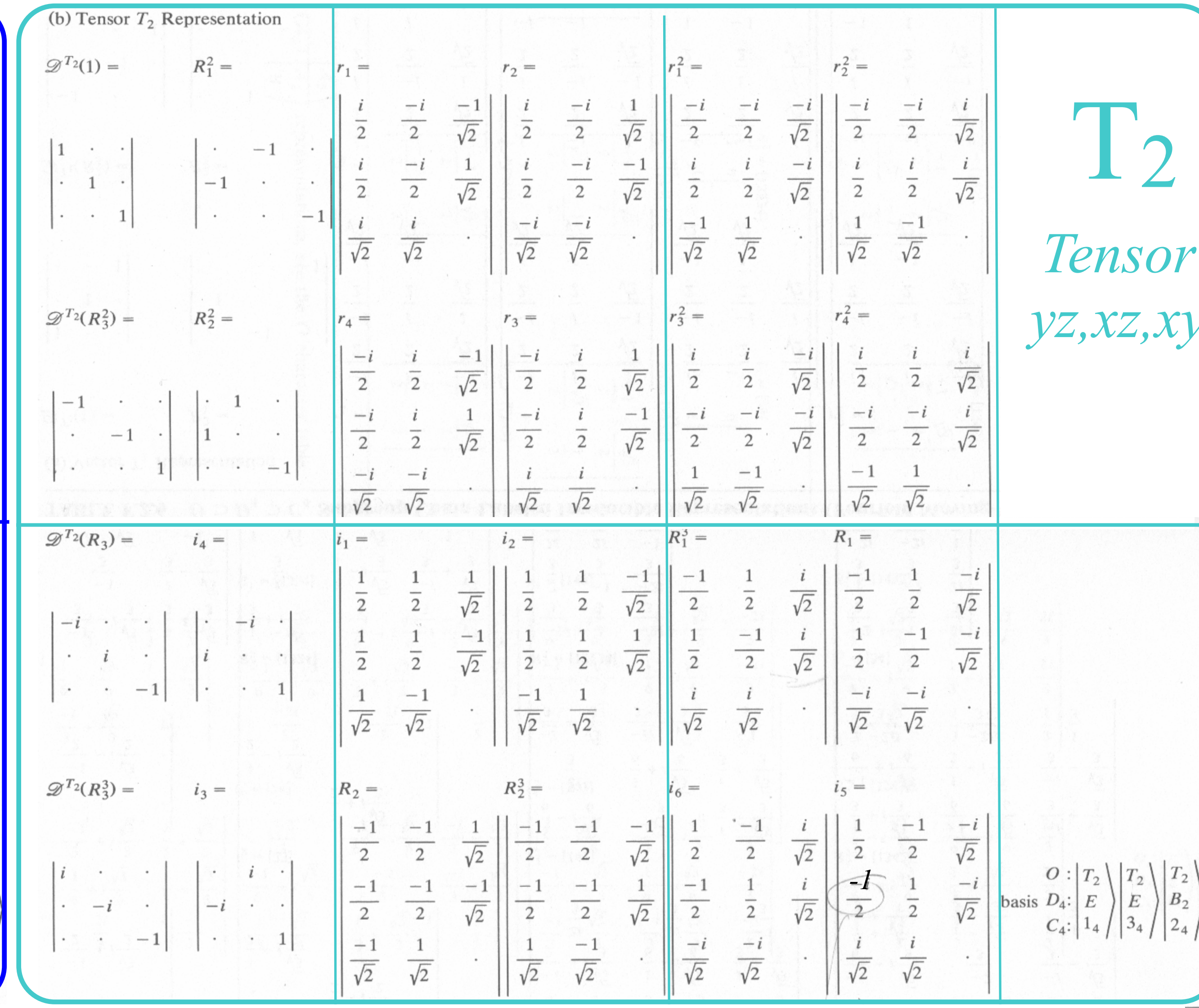
Examples of off-diagonal tunneling coefficients $D^{E}_{0_4 2_4}$

Comparing Local C_4, C_3, *and* C_2 *symmetric spectra*

When Local C_2 *symmetry dominates*

Comparing off-diagonal $O\supset C_2$ *parameter sets to* CH_4 *models with "cluster-crossings"*





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

$1=[1][2][3][4]$: $\begin{pmatrix}1&0\\0&1\end{pmatrix}$ $R_1^2=[13][24]$: $\begin{pmatrix}1&0\\0&1\end{pmatrix}$

$R_3^2=[12][34]$: $\begin{pmatrix}1&0\\0&1\end{pmatrix}$ $R_2^2=[14][23]$: $\begin{pmatrix}1&0\\0&1\end{pmatrix}$

$r_1=[132]$: $\begin{pmatrix}-\frac12&-\frac{\sqrt3}{2}\\+\frac{\sqrt3}{2}&-\frac12\end{pmatrix}$ $r_2=[124]$: $\begin{pmatrix}-\frac12&-\frac{\sqrt3}{2}\\+\frac{\sqrt3}{2}&-\frac12\end{pmatrix}$

$r_4=[234]$: $\begin{pmatrix}-\frac12&-\frac{\sqrt3}{2}\\+\frac{\sqrt3}{2}&-\frac12\end{pmatrix}$ $r_3=[124]$: $\begin{pmatrix}-\frac12&-\frac{\sqrt3}{2}\\+\frac{\sqrt3}{2}&-\frac12\end{pmatrix}$

$r_1^2=[123]$: $\begin{pmatrix}-\frac12&+\frac{\sqrt3}{2}\\-\frac{\sqrt3}{2}&-\frac12\end{pmatrix}$ $r_2^2=[142]$: $\begin{pmatrix}-\frac12&+\frac{\sqrt3}{2}\\-\frac{\sqrt3}{2}&-\frac12\end{pmatrix}$

$r_3^2=[134]$: $\begin{pmatrix}-\frac12&+\frac{\sqrt3}{2}\\-\frac{\sqrt3}{2}&-\frac12\end{pmatrix}$ $r_4^2=[243]$: $\begin{pmatrix}-\frac12&+\frac{\sqrt3}{2}\\-\frac{\sqrt3}{2}&-\frac12\end{pmatrix}$

$R_3=[1423]$: $\begin{pmatrix}1&0\\0&-1\end{pmatrix}$ $i_4=[12]$: $\begin{pmatrix}1&0\\0&-1\end{pmatrix}$

$R_3^3=[1324]$: $\begin{pmatrix}1&0\\0&-1\end{pmatrix}$ $i_3=[34]$: $\begin{pmatrix}1&0\\0&-1\end{pmatrix}$

$i_1=[14]$: $\begin{pmatrix}-\frac12&+\frac{\sqrt3}{2}\\+\frac{\sqrt3}{2}&+\frac12\end{pmatrix}$ $i_2=[23]$: $\begin{pmatrix}-\frac12&+\frac{\sqrt3}{2}\\+\frac{\sqrt3}{2}&+\frac12\end{pmatrix}$

$R_2=[1243]$: $\begin{pmatrix}-\frac12&+\frac{\sqrt3}{2}\\+\frac{\sqrt3}{2}&+\frac12\end{pmatrix}$ $R_2^3=[1342]$: $\begin{pmatrix}-\frac12&+\frac{\sqrt3}{2}\\+\frac{\sqrt3}{2}&+\frac12\end{pmatrix}$

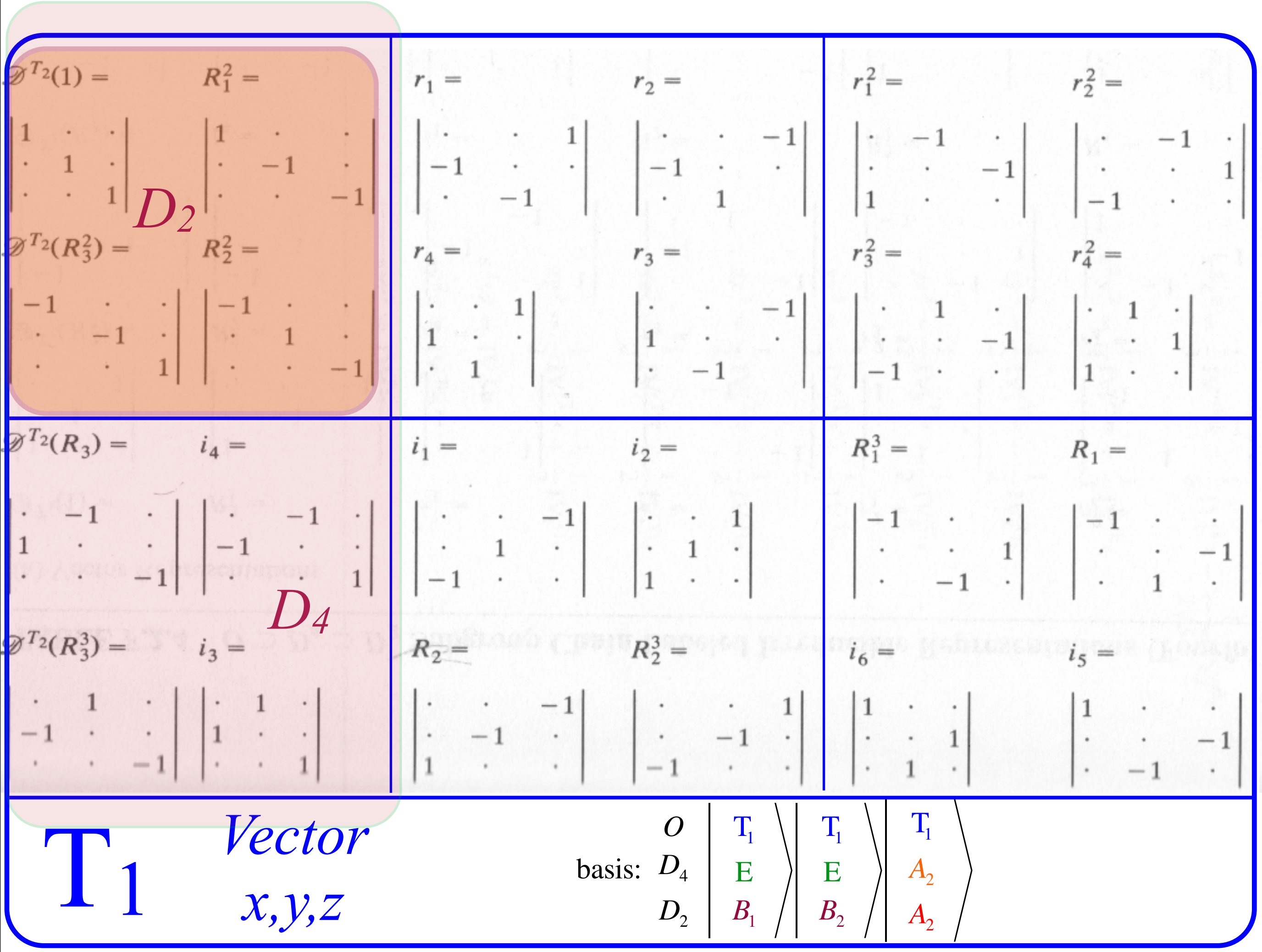
$R_1^3=[1432]$: $\begin{pmatrix}-\frac12&-\frac{\sqrt3}{2}\\-\frac{\sqrt3}{2}&+\frac12\end{pmatrix}$ $R_1=[1234]$: $\begin{pmatrix}-\frac12&-\frac{\sqrt3}{2}\\-\frac{\sqrt3}{2}&+\frac12\end{pmatrix}$

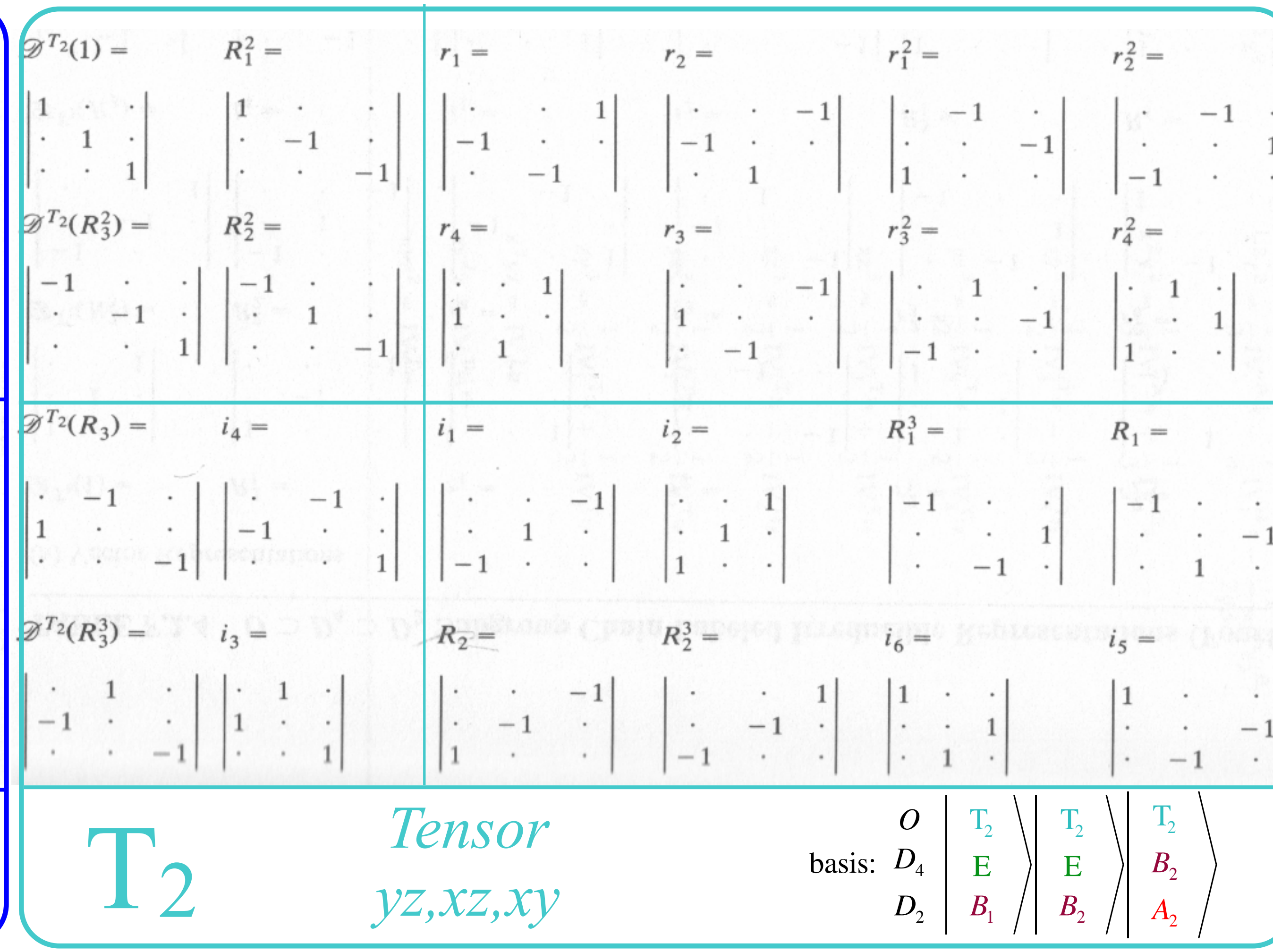
$i_6=[24]$: $\begin{pmatrix}-\frac12&-\frac{\sqrt3}{2}\\-\frac{\sqrt3}{2}&+\frac12\end{pmatrix}$ $i_5=[13]$: $\begin{pmatrix}-\frac12&-\frac{\sqrt3}{2}\\-\frac{\sqrt3}{2}&+\frac12\end{pmatrix}$

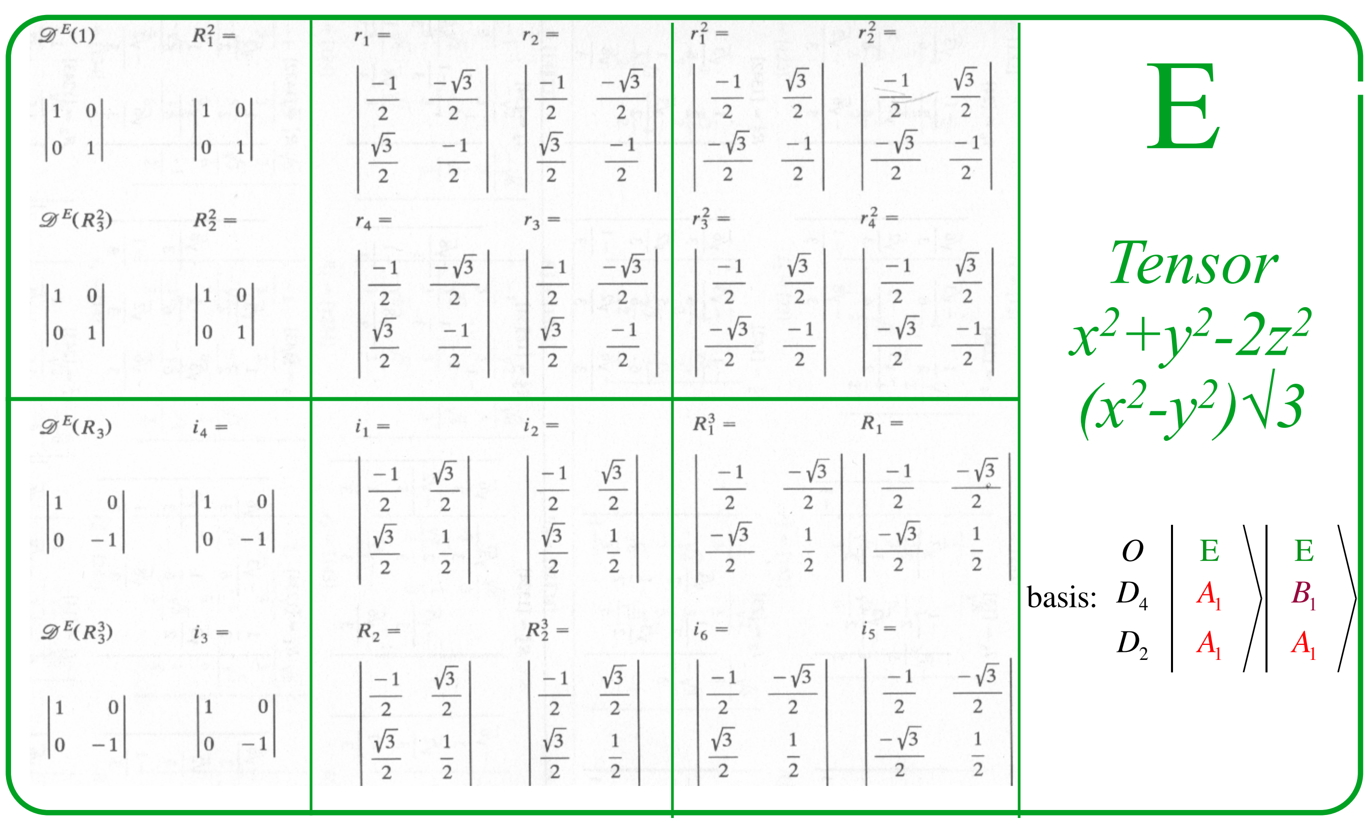
basis: O: $\left|E\right\rangle$, $\left|E\right\rangle$; D_4: A_1, B_1; C_4: 0_4, 2_4

$O: \chi^{\mu}_{\mathbf{g}}$	$\mathbf{g}=1$	$\mathbf{r}_{1-4}$, $\tilde{\mathbf{r}}_{1-4}$	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

Ireps for O⊃D_4⊃D_2 subgroup chain







$O: \chi^{\mu}_{\mathbf{g}}$	$\mathbf{g}$=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

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

T_1 — Vector u, v, w

C_2:

$\mathcal{D}^{T_1}(1) = \begin{vmatrix} 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \end{vmatrix}$ $\quad i_4 = [12]: \begin{vmatrix} 1 & \cdot & \cdot \\ \cdot & -1 & \cdot \\ \cdot & \cdot & -1 \end{vmatrix}$

D_3:

$r_1 = [132]: \begin{vmatrix} \frac{-1}{2} & \frac{-\sqrt3}{2} & \cdot \\ \frac{\sqrt3}{2} & \frac{-1}{2} & \cdot \\ \cdot & \cdot & 1 \end{vmatrix}$ $\quad i_5 = [13]: \begin{vmatrix} \frac{-1}{2} & \frac{-\sqrt3}{2} & \cdot \\ \frac{-\sqrt3}{2} & \frac{1}{2} & \cdot \\ \cdot & \cdot & -1 \end{vmatrix}$

$r_1^2 = [123]: \begin{vmatrix} \frac{-1}{2} & \frac{\sqrt3}{2} & \cdot \\ \frac{-\sqrt3}{2} & \frac{-1}{2} & \cdot \\ \cdot & \cdot & 1 \end{vmatrix}$ $\quad i_2 = [23]: \begin{vmatrix} \frac{-1}{2} & \frac{\sqrt3}{2} & \cdot \\ \frac{\sqrt3}{2} & \frac{1}{2} & \cdot \\ \cdot & \cdot & -1 \end{vmatrix}$

$R_1^2 = [13][24]: \begin{vmatrix} \cdot & \frac{\sqrt3}{3} & \frac{\sqrt6}{3} \\ \frac{\sqrt3}{3} & \frac{-2}{3} & \frac{\sqrt2}{3} \\ \frac{\sqrt6}{3} & \frac{\sqrt2}{3} & \frac{-1}{3} \end{vmatrix}$ $\quad R_3 = [1423]: \begin{vmatrix} \cdot & \frac{-\sqrt3}{3} & \frac{-\sqrt6}{3} \\ \frac{\sqrt3}{3} & \frac{2}{3} & \frac{-\sqrt2}{3} \\ \frac{\sqrt6}{3} & \frac{-\sqrt2}{3} & \frac{1}{3} \end{vmatrix}$

$r_4 = [234]: \begin{vmatrix} \frac{1}{2} & \frac{-\sqrt3}{6} & \frac{\sqrt6}{3} \\ \frac{-\sqrt3}{2} & \frac{-1}{6} & \frac{\sqrt2}{3} \\ \cdot & \frac{-\sqrt8}{3} & \frac{-1}{3} \end{vmatrix}$ $\quad i_6 = [24]: \begin{vmatrix} \frac{-1}{2} & \frac{\sqrt3}{6} & \frac{-\sqrt6}{3} \\ \frac{\sqrt3}{6} & \frac{-5}{6} & \frac{-\sqrt2}{3} \\ \frac{-\sqrt6}{3} & \frac{-\sqrt2}{3} & \frac{1}{3} \end{vmatrix}$

$r_2^2 = [142]: \begin{vmatrix} \frac{-1}{2} & \frac{-\sqrt3}{6} & \frac{\sqrt6}{3} \\ \frac{\sqrt3}{6} & \frac{5}{6} & \frac{\sqrt2}{3} \\ \frac{-\sqrt6}{3} & \frac{\sqrt2}{3} & \frac{-1}{3} \end{vmatrix}$ $\quad R_2^3 = [1342]: \begin{vmatrix} \frac{1}{2} & \frac{\sqrt3}{6} & \frac{-\sqrt6}{3} \\ \frac{-\sqrt3}{2} & \frac{1}{6} & \frac{-\sqrt2}{3} \\ \cdot & \frac{\sqrt8}{3} & \frac{1}{3} \end{vmatrix}$

$R_2^2 = [14][23]: \begin{vmatrix} \cdot & \frac{-\sqrt3}{3} & \frac{-\sqrt6}{3} \\ \frac{-\sqrt3}{3} & \frac{-2}{3} & \frac{\sqrt2}{3} \\ \frac{-\sqrt6}{3} & \frac{\sqrt2}{3} & \frac{-1}{3} \end{vmatrix}$ $\quad R_3^3 = [1324]: \begin{vmatrix} \cdot & \frac{\sqrt3}{3} & \frac{\sqrt6}{3} \\ \frac{-\sqrt3}{3} & \frac{2}{3} & \frac{-\sqrt2}{3} \\ \frac{-\sqrt6}{3} & \frac{-\sqrt2}{3} & \frac{1}{3} \end{vmatrix}$

$R_3^2 = [12][34]: \begin{vmatrix} -1 & \cdot & \cdot \\ \cdot & \frac{1}{3} & \frac{-\sqrt8}{3} \\ \cdot & \frac{-\sqrt8}{3} & \frac{-1}{3} \end{vmatrix}$ $\quad i_3 = [34]: \begin{vmatrix} -1 & \cdot & \cdot \\ \cdot & \frac{-1}{3} & \frac{\sqrt8}{3} \\ \cdot & \frac{\sqrt8}{3} & \frac{1}{3} \end{vmatrix}$

$r_2 = [124]: \begin{vmatrix} \frac{-1}{2} & \frac{\sqrt3}{6} & \frac{-\sqrt6}{3} \\ \frac{-\sqrt3}{6} & \frac{5}{6} & \frac{\sqrt2}{3} \\ \frac{\sqrt6}{3} & \frac{\sqrt2}{3} & \frac{-1}{3} \end{vmatrix}$ $\quad R_1 = [1234]: \begin{vmatrix} \frac{1}{2} & \frac{-\sqrt3}{6} & \frac{\sqrt6}{3} \\ \frac{\sqrt3}{2} & \frac{1}{6} & \frac{-\sqrt2}{3} \\ \cdot & \frac{\sqrt8}{3} & \frac{1}{3} \end{vmatrix}$

$r_3 = [143]: \begin{vmatrix} \frac{1}{2} & \frac{\sqrt3}{2} & \cdot \\ \frac{\sqrt3}{6} & \frac{-1}{6} & \frac{-\sqrt8}{3} \\ \frac{-\sqrt6}{3} & \frac{\sqrt2}{3} & \frac{-1}{3} \end{vmatrix}$ $\quad R_1^3 = [1432]: \begin{vmatrix} \frac{1}{2} & \frac{\sqrt3}{2} & \cdot \\ \frac{-\sqrt3}{6} & \frac{1}{6} & \frac{\sqrt8}{3} \\ \frac{\sqrt6}{3} & \frac{-\sqrt2}{3} & \frac{1}{3} \end{vmatrix}$

$r_3^2 = [134]: \begin{vmatrix} \frac{1}{2} & \frac{\sqrt3}{6} & \frac{-\sqrt6}{3} \\ \frac{\sqrt3}{2} & \frac{-1}{6} & \frac{\sqrt2}{3} \\ \cdot & \frac{-\sqrt8}{3} & \frac{-1}{3} \end{vmatrix}$ $\quad i_1 = [14]: \begin{vmatrix} \frac{-1}{2} & \frac{-\sqrt3}{6} & \frac{\sqrt6}{3} \\ \frac{-\sqrt3}{6} & \frac{-5}{6} & \frac{-\sqrt2}{3} \\ \frac{\sqrt6}{3} & \frac{-\sqrt2}{3} & \frac{1}{3} \end{vmatrix}$

$r_4^2 = [243]: \begin{vmatrix} \frac{1}{2} & \frac{-\sqrt3}{2} & \cdot \\ \frac{-\sqrt3}{6} & \frac{-1}{6} & \frac{-\sqrt8}{3} \\ \frac{\sqrt6}{3} & \frac{\sqrt2}{3} & \frac{-1}{3} \end{vmatrix}$ $\quad R_2 = [1243]: \begin{vmatrix} \frac{1}{2} & \frac{-\sqrt3}{2} & \cdot \\ \frac{\sqrt3}{6} & \frac{1}{6} & \frac{\sqrt8}{3} \\ \frac{-\sqrt6}{3} & \frac{-\sqrt2}{3} & \frac{1}{3} \end{vmatrix}$

T_1 *Vector* *u,v,w*

basis: $\begin{matrix} O \\ D_3 \\ C_2 \end{matrix} \left| \begin{matrix} T_1 \\ E \\ 0_2 \end{matrix} \right\rangle \left| \begin{matrix} T_1 \\ E \\ 1_2 \end{matrix} \right\rangle \left| \begin{matrix} T_1 \\ A_2 \\ 1_2 \end{matrix} \right\rangle$

T_2 — Tensor vw, uw, uv

$\mathcal{D}^{T_2}(1) = \begin{vmatrix} 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \end{vmatrix}$ $\quad i_4 = [12]: \begin{vmatrix} 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & -1 \end{vmatrix}$

$r_1 = [132]: \begin{vmatrix} 1 & \cdot & \cdot \\ \cdot & \frac{-1}{2} & \frac{-\sqrt3}{2} \\ \cdot & \frac{\sqrt3}{2} & \frac{-1}{2} \end{vmatrix}$ $\quad i_5 = [13]: \begin{vmatrix} 1 & \cdot & \cdot \\ \cdot & \frac{-1}{2} & \frac{-\sqrt3}{2} \\ \cdot & \frac{-\sqrt3}{2} & \frac{1}{2} \end{vmatrix}$

$r_1^2 = [123]: \begin{vmatrix} 1 & \cdot & \cdot \\ \cdot & \frac{-1}{2} & \frac{\sqrt3}{2} \\ \cdot & \frac{-\sqrt3}{2} & \frac{-1}{2} \end{vmatrix}$ $\quad i_2 = [23]: \begin{vmatrix} 1 & \cdot & \cdot \\ \cdot & \frac{-1}{2} & \frac{\sqrt3}{2} \\ \cdot & \frac{\sqrt3}{2} & \frac{1}{2} \end{vmatrix}$

$R_1^2 = [13][24]: \begin{vmatrix} \frac{-1}{3} & \frac{-\sqrt2}{3} & \frac{\sqrt6}{3} \\ \frac{-\sqrt2}{3} & \frac{-2}{3} & \frac{-\sqrt3}{3} \\ \frac{\sqrt6}{3} & \frac{-\sqrt3}{3} & \cdot \end{vmatrix}$ $\quad R_3 = [1423]: \begin{vmatrix} \frac{-1}{3} & \frac{-\sqrt2}{3} & \frac{-\sqrt6}{3} \\ \frac{-\sqrt2}{3} & \frac{-2}{3} & \frac{\sqrt3}{3} \\ \frac{\sqrt6}{3} & \frac{-\sqrt3}{3} & \cdot \end{vmatrix}$

$r_4 = [234]: \begin{vmatrix} \frac{-1}{3} & \frac{\sqrt8}{3} & \cdot \\ \frac{-\sqrt2}{3} & \frac{-1}{6} & \frac{\sqrt3}{2} \\ \frac{\sqrt6}{3} & \frac{\sqrt3}{6} & \frac{1}{2} \end{vmatrix}$ $\quad i_6 = [24]: \begin{vmatrix} \frac{-1}{3} & \frac{-\sqrt2}{3} & \frac{\sqrt6}{3} \\ \frac{-\sqrt2}{3} & \frac{5}{6} & \frac{\sqrt3}{6} \\ \frac{\sqrt6}{3} & \frac{\sqrt3}{6} & \frac{1}{2} \end{vmatrix}$

$r_2^2 = [142]: \begin{vmatrix} \frac{-1}{3} & \frac{-\sqrt2}{3} & \frac{-\sqrt6}{3} \\ \frac{-\sqrt2}{3} & \frac{5}{6} & \frac{-\sqrt3}{6} \\ \frac{\sqrt6}{3} & \frac{\sqrt3}{6} & \frac{-1}{2} \end{vmatrix}$ $\quad R_2^3 = [1342]: \begin{vmatrix} \frac{-1}{3} & \frac{\sqrt8}{3} & \cdot \\ \frac{-\sqrt2}{3} & \frac{-1}{6} & \frac{-\sqrt3}{2} \\ \frac{\sqrt6}{3} & \frac{\sqrt3}{6} & \frac{-1}{2} \end{vmatrix}$

$R_2^2 = [14][23]: \begin{vmatrix} \frac{-1}{3} & \frac{-\sqrt2}{3} & \frac{-\sqrt6}{3} \\ \frac{-\sqrt2}{3} & \frac{-2}{3} & \frac{\sqrt3}{3} \\ \frac{-\sqrt6}{3} & \frac{\sqrt3}{3} & \cdot \end{vmatrix}$ $\quad R_3^3 = [1324]: \begin{vmatrix} \frac{-1}{3} & \frac{-\sqrt2}{3} & \frac{\sqrt6}{3} \\ \frac{-\sqrt2}{3} & \frac{-2}{3} & \frac{\sqrt3}{3} \\ \frac{-\sqrt6}{3} & \frac{\sqrt3}{3} & \cdot \end{vmatrix}$

$R_3^2 = [12][34]: \begin{vmatrix} \frac{-1}{3} & \frac{\sqrt8}{3} & \cdot \\ \frac{\sqrt8}{3} & \frac{1}{3} & \cdot \\ \cdot & \cdot & -1 \end{vmatrix}$ $\quad i_3 = [34]: \begin{vmatrix} \frac{-1}{3} & \frac{\sqrt8}{3} & \cdot \\ \frac{\sqrt8}{3} & \frac{1}{3} & \cdot \\ \cdot & \cdot & 1 \end{vmatrix}$

$r_2 = [124]: \begin{vmatrix} \frac{-1}{3} & \frac{-\sqrt2}{3} & \frac{\sqrt6}{3} \\ \frac{-\sqrt2}{3} & \frac{5}{6} & \frac{\sqrt3}{6} \\ \frac{-\sqrt6}{3} & \frac{-\sqrt3}{6} & \frac{-1}{2} \end{vmatrix}$ $\quad R_1 = [1234]: \begin{vmatrix} \frac{-1}{3} & \frac{\sqrt8}{3} & \cdot \\ \frac{-\sqrt2}{3} & \frac{-1}{6} & \frac{\sqrt3}{2} \\ \frac{-\sqrt6}{3} & \frac{-\sqrt3}{6} & \frac{-1}{2} \end{vmatrix}$

$r_3 = [143]: \begin{vmatrix} \frac{-1}{3} & \frac{-\sqrt2}{3} & \frac{-\sqrt6}{3} \\ \frac{\sqrt8}{3} & \frac{-1}{6} & \frac{-\sqrt3}{6} \\ \cdot & \frac{-\sqrt3}{2} & \frac{1}{2} \end{vmatrix}$ $\quad R_1^3 = [1432]: \begin{vmatrix} \frac{-1}{3} & \frac{-\sqrt2}{3} & \frac{-\sqrt6}{3} \\ \frac{\sqrt8}{3} & \frac{-1}{6} & \frac{-\sqrt3}{6} \\ \cdot & \frac{\sqrt3}{2} & \frac{-1}{2} \end{vmatrix}$

$r_3^2 = [134]: \begin{vmatrix} \frac{-1}{3} & \frac{\sqrt8}{3} & \cdot \\ \frac{-\sqrt2}{3} & \frac{-1}{6} & \frac{-\sqrt3}{2} \\ \frac{-\sqrt6}{3} & \frac{-\sqrt3}{6} & \frac{1}{2} \end{vmatrix}$ $\quad i_1 = [14]: \begin{vmatrix} \frac{-1}{3} & \frac{-\sqrt2}{3} & \frac{-\sqrt6}{3} \\ \frac{-\sqrt2}{3} & \frac{5}{6} & \frac{-\sqrt3}{6} \\ \frac{-\sqrt6}{3} & \frac{-\sqrt3}{6} & \frac{1}{2} \end{vmatrix}$

$r_4^2 = [243]: \begin{vmatrix} \frac{-1}{3} & \frac{-\sqrt2}{3} & \frac{\sqrt6}{3} \\ \frac{\sqrt8}{3} & \frac{-1}{6} & \frac{\sqrt3}{6} \\ \cdot & \frac{\sqrt3}{2} & \frac{1}{2} \end{vmatrix}$ $\quad R_2 = [1243]: \begin{vmatrix} \frac{-1}{3} & \frac{-\sqrt2}{3} & \frac{\sqrt6}{3} \\ \frac{\sqrt8}{3} & \frac{-1}{6} & \frac{\sqrt3}{6} \\ \cdot & \frac{-\sqrt3}{2} & \frac{-1}{2} \end{vmatrix}$

T_2 *Tensor* *vw,uw,uv*

basis: $\begin{matrix} O \\ D_3 \\ C_2 \end{matrix} \left| \begin{matrix} T_2 \\ B_2 \\ 0_2 \end{matrix} \right\rangle \left| \begin{matrix} T_2 \\ E \\ 0_2 \end{matrix} \right\rangle \left| \begin{matrix} T_2 \\ E \\ 1_2 \end{matrix} \right\rangle$

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

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

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

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

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

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

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

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

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

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

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

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

E *Tensor*

$u^2+v^2-2w^2$

$(u^2-v^2)\sqrt{3}$

basis: $\begin{matrix} O \\ D_3 \\ C_2 \end{matrix} \left| \begin{matrix} E \\ E \\ 0_2 \end{matrix} \right\rangle \left| \begin{matrix} E \\ E \\ 1_2 \end{matrix} \right\rangle$

$O: \chi_{\mathbf{g}}^{\mu}$	$\mathbf{g}$=1	$\mathbf{r}_{1-4}$ $\tilde{\mathbf{r}}_{1-4}$	$\boldsymbol{\rho}_{xyz}$	$\mathbf{R}_{xyz}$ $\tilde{\mathbf{R}}_{xyz}$	$\mathbf{i}_{1-6}$
$\mu=A_1$	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

Review Calculating idempotent projectors $\mathbf{P}^{\mu}_{m,m}$ *of* $O\supset C_4$ $\mathbf{P}^{E}_{0_4 0_4}$ $\mathbf{P}^{E}_{2_4 2_4}$ $\mathbf{P}^{T_1}_{0_4 0_4}$ $\mathbf{P}^{T_1}_{1_4 1_4}$ $\mathbf{P}^{T_2}_{2_4 2_4}$

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

Review Broken-class-ordered splitting of $O\supset D_4\supset C_4$ *projectors and levels*

Subgroup-defined tunneling parameter modeling

Comparing two diagonal $O\supset C_4$ *parameter sets to* SF_6 *spectra*

Comparing two diagonal $O\supset C_3$ *parameter sets to* SF_6 *spectra*

Why $O\supset C_2$ *parameter sets require off-diagonal nilpotent* $\mathbf{P}^{\mu}_{m,n}$ $(m\neq n)$

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

Using fundamental $\mathbf{g}\rightleftarrows\mathbf{P}^{\mu}_{m,n}$ *relations: (from Lecture 16)*

(a) $\mathbf{P}^{\mu}_{m,m}\mathbf{g}\mathbf{P}^{\mu}_{n,n}=D^{\mu}_{m,n}(\mathbf{g})\mathbf{P}^{\mu}_{m,n}$ (b) $\mathbf{g}=\Sigma_{\mu}\Sigma_{m,n}D^{\mu}_{m,n}(\mathbf{g})\mathbf{P}^{\mu}_{m,n}$ (c) $\mathbf{P}^{\mu}_{n,n}=(\ell^{\mu}/{}^{\circ}G)\Sigma_{\mathbf{g}}D^{\mu *}_{m,n}(\mathbf{g})\mathbf{g}$

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

Calculating and Factoring $\mathbf{P}^{T_1}_{1_4 0_4}$ *and* $\mathbf{P}^{T_1}_{1_4 3_4}$

Structure and applications of various subgroup chain irreducible representations

$O_h\supset D_{4h}\supset C_{4v}$, $O_h\supset D_{3h}\supset C_{3v}$, $O_h\supset C_{2v}$

→ *Comparing* $O_h\supset D_{4h}\supset D_{2h}$ *and* $O_h\supset D_{3d}\supset C_2$ *representations* (T_1 *vector-type*) ←

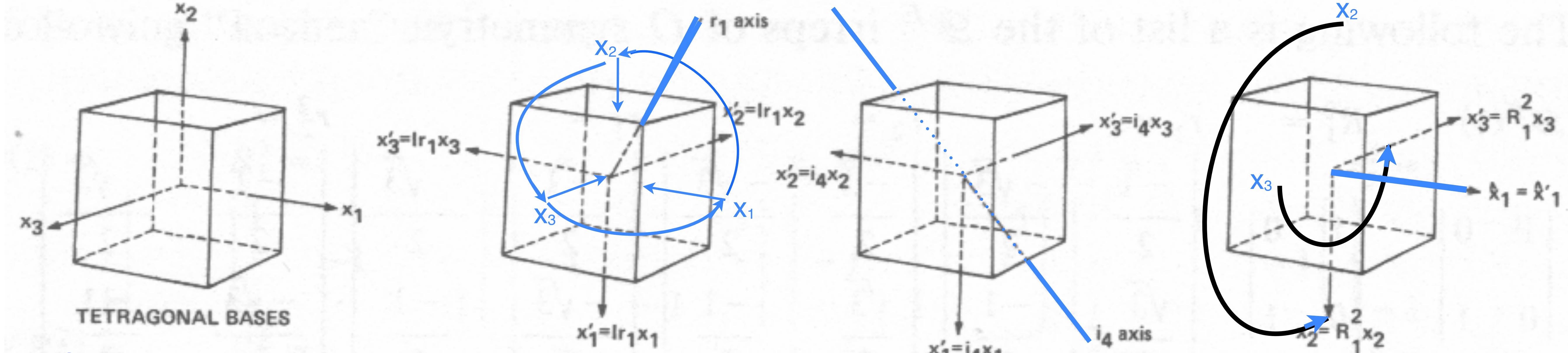
Examples of off-diagonal tunneling coefficients $D^{E}_{0_4 2_4}$

Comparing Local C_4, C_3, *and* C_2 *symmetric spectra*

When Local C_2 *symmetry dominates*

Comparing off-diagonal $O\supset C_2$ *parameter sets to* CH_4 *models with "cluster-crossings"*

Comparing $O_h \supset D_{4h} \supset D_{2h}$ *and* $O_h \supset D_{3d} \supset C_2$ *representations (*T_1 *vector-type)*



$O_h \supset D_{4h} \supset D_{2h}$
x-*representation*

$$D^{T_{1u}}(Ir_1) = \begin{pmatrix} 0 & 0 & -1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix}$$

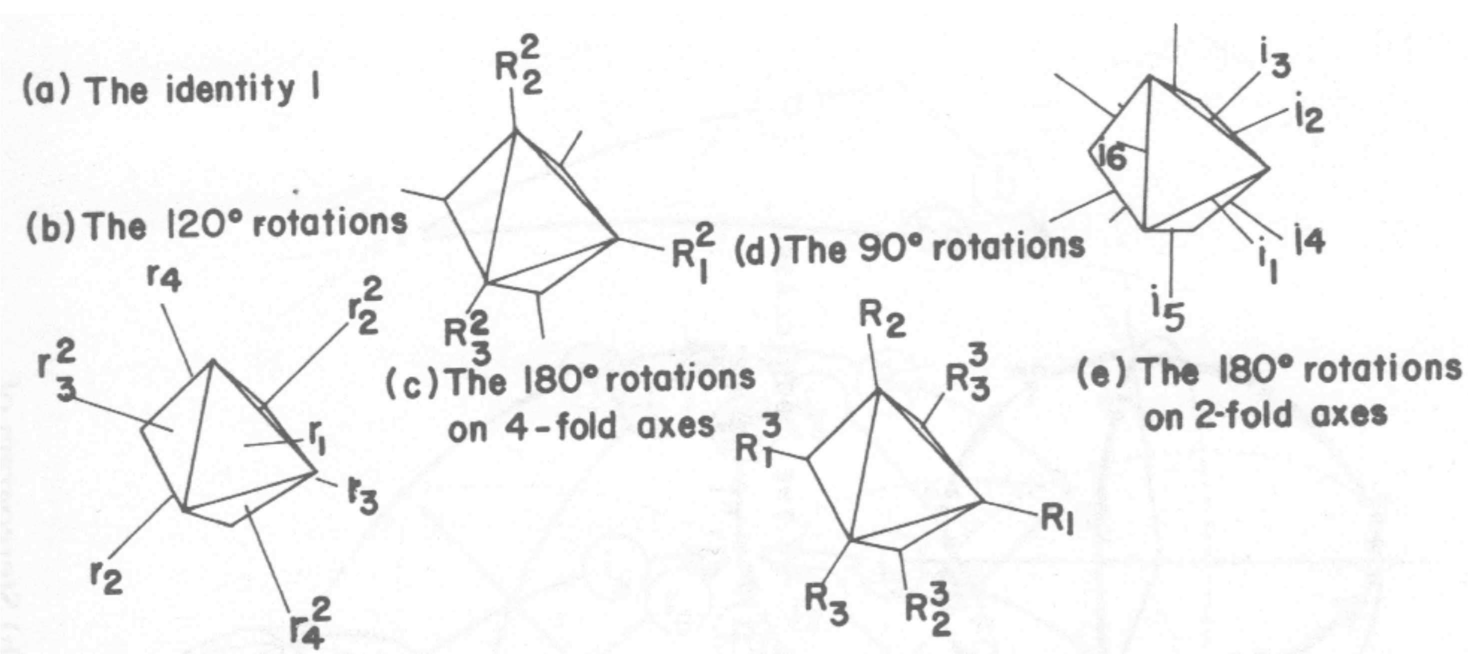
3-by-3 block

$$D^{T_{1u}}(i_4) = \begin{pmatrix} \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix} & \begin{matrix} 0 \\ 0 \end{matrix} \\ \begin{matrix} 0 & 0 \end{matrix} & -1 \end{pmatrix}$$

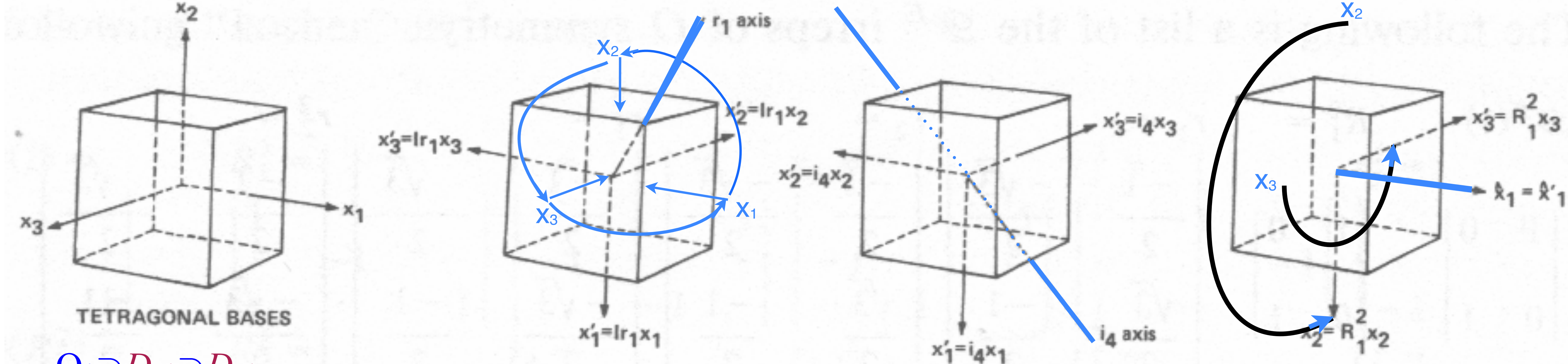
2-by-2 and 1-by-1 blocks

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

diagonal



Comparing $O_h \supset D_{4h} \supset D_{2h}$ and $O_h \supset D_{3d} \supset C_2$ representations (T_1 vector-type)



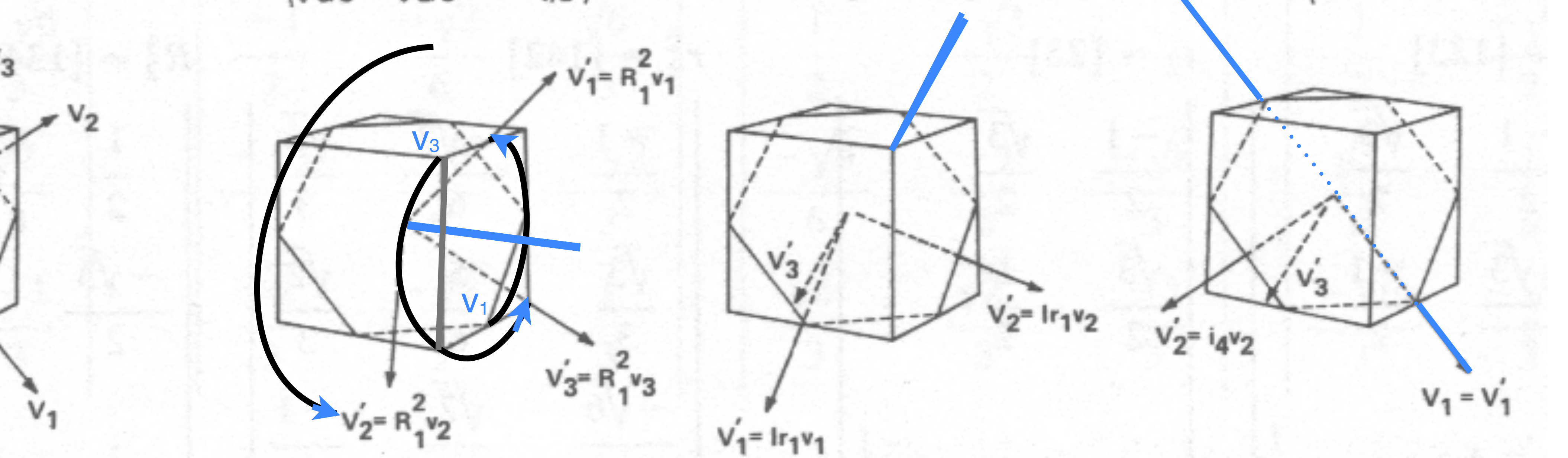
$O_h \supset D_{4h} \supset D_{2h}$
x-*representation*

$$D^{T1u}(Ir_1) = \begin{pmatrix} 0 & 0 & -1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix} \qquad D^{T1u}(i_4) = \begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \qquad D^{T1u}(R_1^2) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

3-by-3 block *2-by-2 and 1-by-1 blocks* *diagonal*

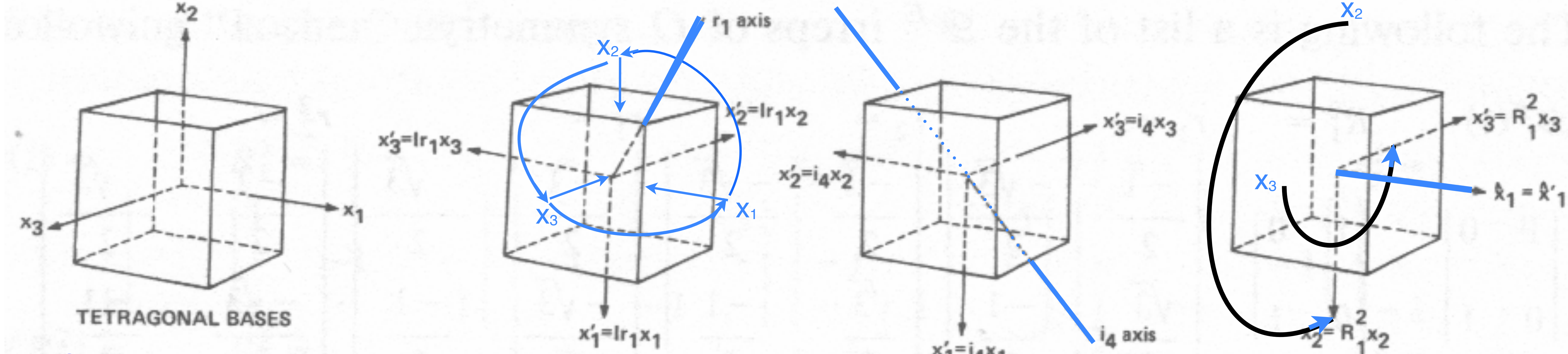
TRIGONAL BASES

$$D^{T1u}(R_1^2) = \begin{pmatrix} 0 & \sqrt{3}/3 & \sqrt{6}/3 \\ \sqrt{3}/3 & -2/3 & \sqrt{2}/3 \\ \sqrt{6}/3 & \sqrt{2}/3 & -1/3 \end{pmatrix} \qquad D^{T1u}(Ir_1) = \begin{pmatrix} 1/2 & \sqrt{3}/2 & 0 \\ -\sqrt{3}/2 & 1/2 & 0 \\ 0 & 0 & -1 \end{pmatrix} \qquad D^{T1u}(i_4) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$



$O_h \supset D_{3d} \supset C_2$
v-*representation*

Comparing $O_h \supset D_{4h} \supset D_{2h}$ and $O_h \supset D_{3d} \supset C_2$ representations (T_1 vector-type)



$O_h \supset D_{4h} \supset D_{2h}$

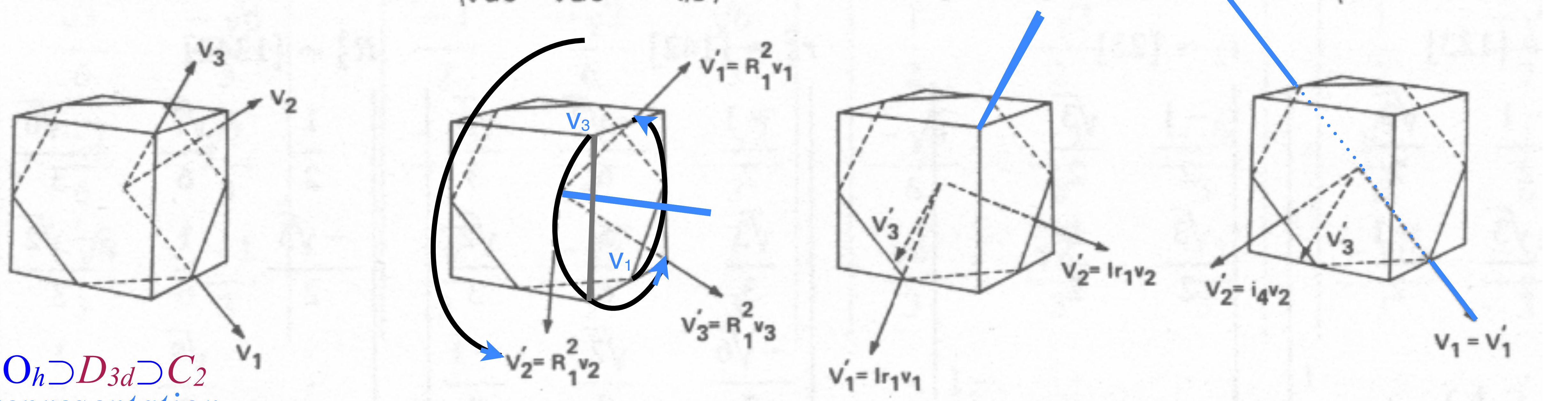
***x**-representation*

$$D^{T_{1u}}(Ir_1) = \begin{pmatrix} 0 & 0 & -1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix} \qquad D^{T_{1u}}(i_4) = \begin{pmatrix} \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix} & \begin{matrix} 0 \\ 0 \end{matrix} \\ \begin{matrix} 0 & 0 \end{matrix} & -1 \end{pmatrix} \qquad D^{T_{1u}}(R_1^2) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

3-by-3 block *2-by-2 and 1-by-1 blocks* *diagonal*

TRIGONAL BASES

$$D^{T_{1u}}(R_1^2) = \begin{pmatrix} 0 & \sqrt{3}/3 & \sqrt{6}/3 \\ \sqrt{3}/3 & -2/3 & \sqrt{2}/3 \\ \sqrt{6}/3 & \sqrt{2}/3 & -1/3 \end{pmatrix} \qquad D^{T_{1u}}(Ir_1) = \begin{pmatrix} \begin{pmatrix} 1/2 & \sqrt{3}/2 \\ -\sqrt{3}/2 & 1/2 \end{pmatrix} & \begin{matrix} 0 \\ 0 \end{matrix} \\ \begin{matrix} 0 & 0 \end{matrix} & -1 \end{pmatrix} \qquad D^{T_{1u}}(i_4) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$



$O_h \supset D_{3d} \supset C_2$

***v**-representation*

Matrix

	$\mathbf{v}_1$	$\mathbf{v}_2$	$\mathbf{v}_3$
$\mathbf{x}_1$	$1/\sqrt{2}$	$1/\sqrt{6}$	$1/\sqrt{3}$
$\mathbf{x}_2$	$-1/\sqrt{2}$	$1/\sqrt{6}$	$1/\sqrt{3}$
$\mathbf{x}_3$	0	$-2/\sqrt{6}$	$1/\sqrt{3}$

*transforms between **x**-and-**v** representations*

Review Calculating idempotent projectors $\mathbf{P}^{\mu}_{m,m}$ *of* $O\supset C_4$ $\mathbf{P}^{E}_{0_4 0_4}$ $\mathbf{P}^{E}_{2_4 2_4}$ $\mathbf{P}^{T_1}_{0_4 0_4}$ $\mathbf{P}^{T_1}_{1_4 1_4}$ $\mathbf{P}^{T_2}_{2_4 2_4}$

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

Review Broken-class-ordered splitting of $O\supset D_4\supset C_4$ *projectors and levels*

Subgroup-defined tunneling parameter modeling

Comparing two diagonal $O\supset C_4$ *parameter sets to* SF_6 *spectra*

Comparing two diagonal $O\supset C_3$ *parameter sets to* SF_6 *spectra*

Why $O\supset C_2$ *parameter sets require off-diagonal nilpotent* $\mathbf{P}^{\mu}_{m,n}$ $(m\neq n)$

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

Using fundamental $\mathbf{g}\rightleftarrows\mathbf{P}^{\mu}_{m,n}$ *relations: (from Lecture 16)*

(a) $\mathbf{P}^{\mu}_{m,m}\mathbf{g}\mathbf{P}^{\mu}_{n,n}=D^{\mu}_{m,n}(\mathbf{g})\mathbf{P}^{\mu}_{m,n}$ (b) $\mathbf{g}=\Sigma_{\mu}\Sigma_{m,n}D^{\mu}_{m,n}(\mathbf{g})\mathbf{P}^{\mu}_{m,n}$ (c) $\mathbf{P}^{\mu}_{n,n}=(\ell^{\mu}/{}^{\circ}G)\Sigma_{\mathbf{g}}D^{\mu *}_{m,n}(\mathbf{g})\mathbf{g}$

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

Calculating and Factoring $\mathbf{P}^{T_1}_{1_4 0_4}$ *and* $\mathbf{P}^{T_1}_{1_4 3_4}$

Structure and applications of various subgroup chain irreducible representations

$O_h\supset D_{4h}\supset C_{4v}$, $O_h\supset D_{3h}\supset C_{3v}$, $O_h\supset C_{2v}$

Comparing $O_h\supset D_{4h}\supset D_{2h}$ *and* $O_h\supset D_{3d}\supset C_2$ *representations (*T_1 *vector-type)*

➡ *Examples of off-diagonal tunneling coefficients* $D^{E}_{0_4 2_4}$ ⬅

Comparing Local C_4, C_3, *and* C_2 *symmetric spectra*

When Local C_2 *symmetry dominates*

Comparing off-diagonal $O\supset C_2$ *parameter sets to* CH_4 *models with "cluster-crossings"*

Examples of off-diagonal tunneling coefficients $D^{E}_{0_4 2_4}$

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

basis: O: $\left|E\right\rangle$, $\left|E\right\rangle$; D_4: A_1, B_1; C_4: 0_4, 2_4

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

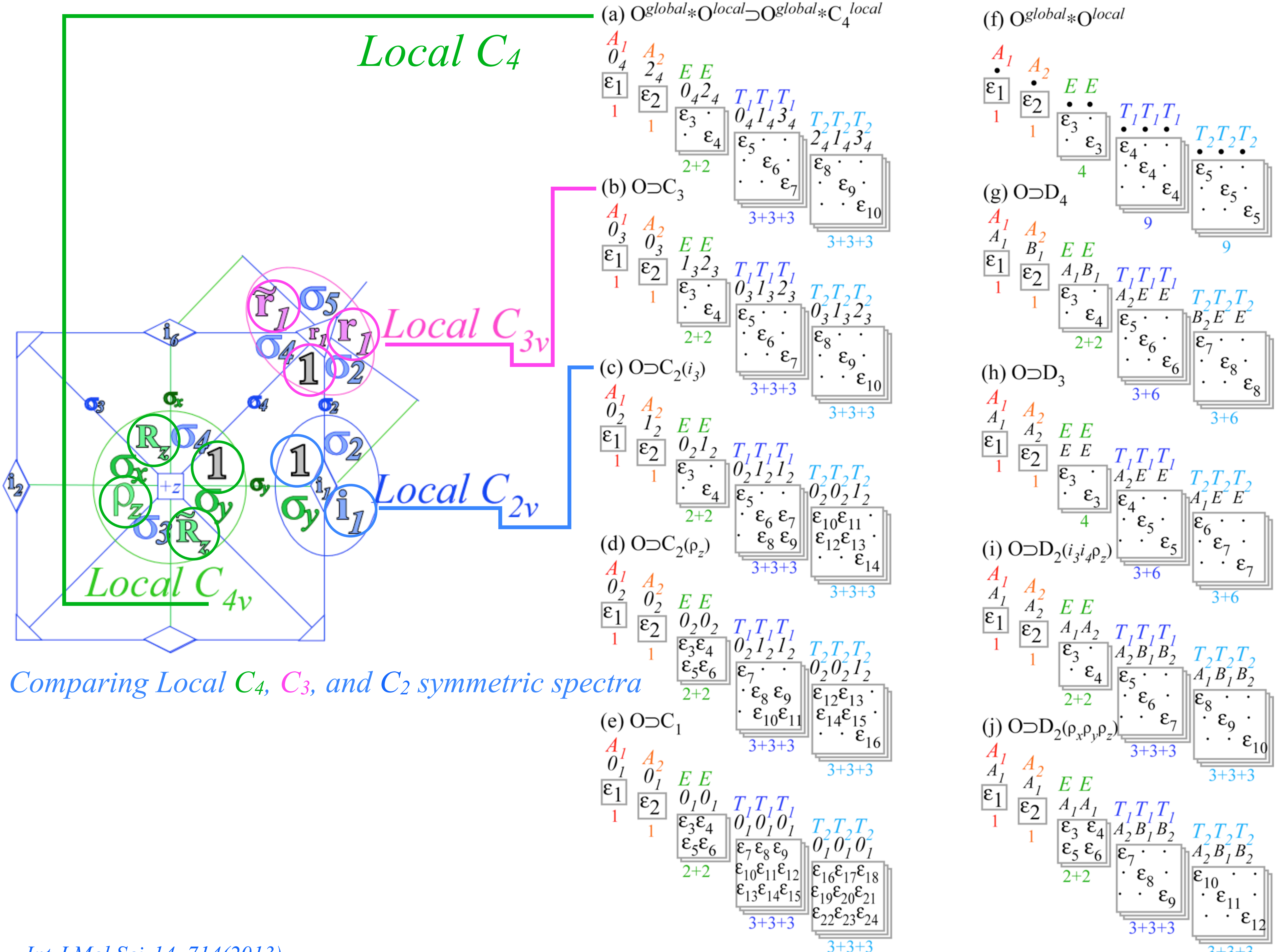
$$D^{A_2}_{2_4 2_4}(i_k\mathbf{i}_k) = -(i_1+i_2+i_3+i_4+i_5+i_6)$$

$D^{E*}(i_k\mathbf{i}_k)$	0_4	2_4
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	$h.c.$	$\frac{1}{2}(i_1+i_2+i_3+i_4+i_5+i_6)-i_3-i_4$

$D^{T_1*}(i_k\mathbf{i}_k)$	1_4	3_4	0_4
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	$h.c.$	$h.c.$	$-(i_3+i_4)$

$D^{T_2*}(i_k\mathbf{i}_k)$	1_4	3_4	2_4
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	$h.c.$	$+\frac{1}{2}(i_1+i_2+i_5+i_6)$	$-\frac{1}{\sqrt{2}}(i_1-i_2)+\frac{i}{\sqrt{2}}(i_5-i_6)$
2_4	$h.c.$	$h.c.$	$+(i_3+i_4)$

Local C_4 symmetry conditions
$i_{1256} = i_1 = i_2 = i_5 = i_6$
and
$i_{34} = i_3 = i_4$
make all off-diagonal coefficients identically ZERO.



Comparing Local C_4, C_3, and C_2 symmetric spectra

Int.J.Mol.Sci, 14, 714(2013)

Review Calculating idempotent projectors $\mathbf{P}^{\mu}_{m,m}$ *of* $O\supset C_4$ $\mathbf{P}^{E}_{0_4 0_4}$ $\mathbf{P}^{E}_{2_4 2_4}$ $\mathbf{P}^{T_1}_{0_4 0_4}$ $\mathbf{P}^{T_1}_{1_4 1_4}$ $\mathbf{P}^{T_2}_{2_4 2_4}$

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

Review Broken-class-ordered splitting of $O\supset D_4\supset C_4$ *projectors and levels*

Subgroup-defined tunneling parameter modeling

Comparing two diagonal $O\supset C_4$ *parameter sets to* SF_6 *spectra*

Comparing two diagonal $O\supset C_3$ *parameter sets to* SF_6 *spectra*

Why $O\supset C_2$ *parameter sets require off-diagonal nilpotent* $\mathbf{P}^{\mu}_{m,n}$ $(m\neq n)$

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

Using fundamental $\mathbf{g}\rightleftarrows\mathbf{P}^{\mu}_{m,n}$ *relations: (from Lecture 16)*

(a) $\mathbf{P}^{\mu}_{m,m}\mathbf{g}\mathbf{P}^{\mu}_{n,n}=D^{\mu}_{m,n}(\mathbf{g})\mathbf{P}^{\mu}_{m,n}$ (b) $\mathbf{g}=\Sigma_{\mu}\Sigma_{m,n}D^{\mu}_{m,n}(\mathbf{g})\mathbf{P}^{\mu}_{m,n}$ (c) $\mathbf{P}^{\mu}_{n,n}=(\ell^{\mu}/{}^{\circ}G)\Sigma_{g}D^{\mu *}_{m,n}(\mathbf{g})\mathbf{g}$

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

Calculating and Factoring $\mathbf{P}^{T_1}_{1_4 0_4}$ *and* $\mathbf{P}^{T_1}_{1_4 3_4}$

Structure and applications of various subgroup chain irreducible representations

$O_h\supset D_{4h}\supset C_{4v}$, $O_h\supset D_{3h}\supset C_{3v}$, $O_h\supset C_{2v}$

Comparing $O_h\supset D_{4h}\supset D_{2h}$ *and* $O_h\supset D_{3d}\supset C_2$ *representations (*T_1 *vector-type)*

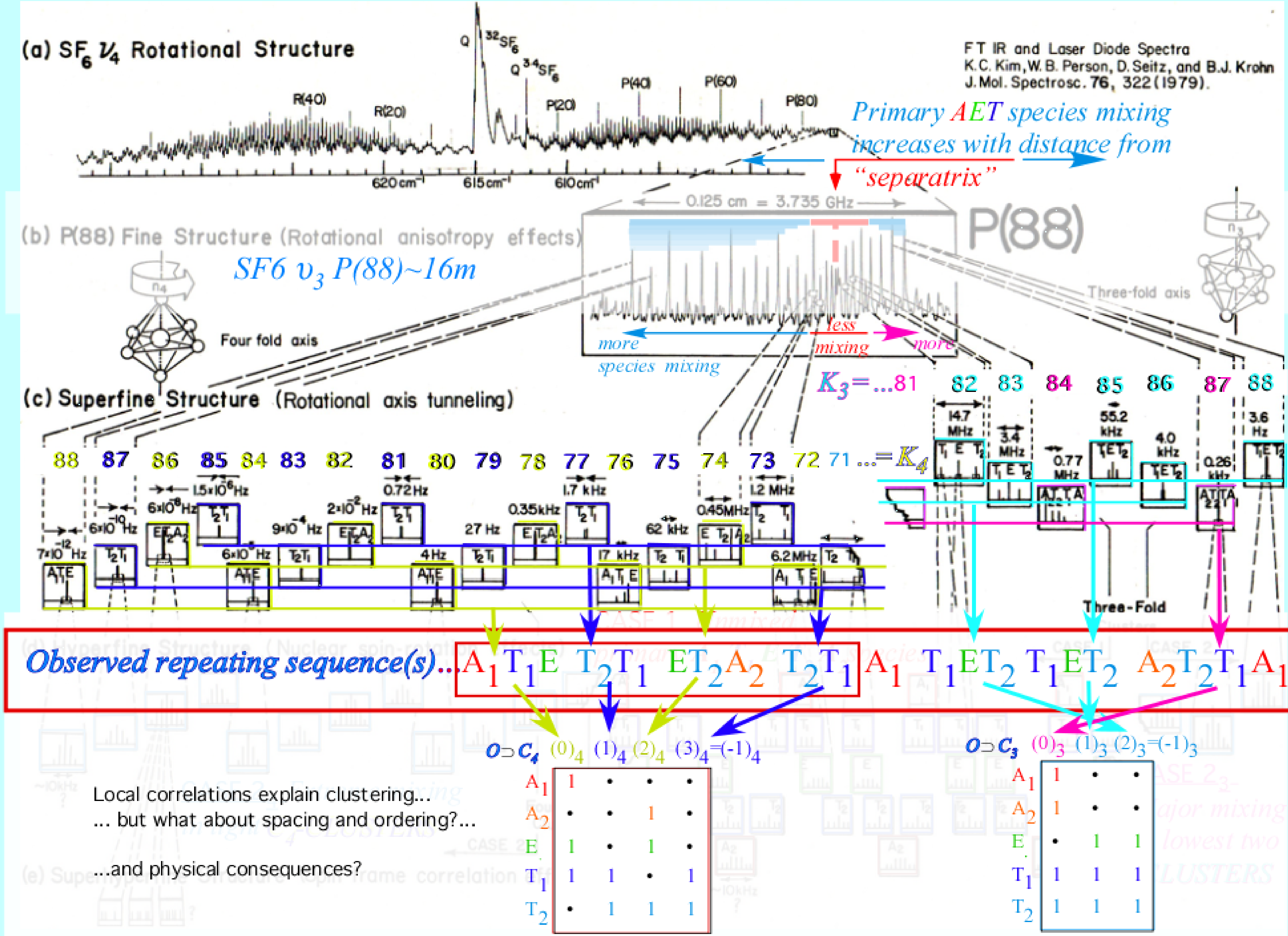
Examples of off-diagonal tunneling coefficients $D^{E}_{0_4 2_4}$

➡ *Comparing Local* C_4, C_3, *and* C_2 *symmetric spectra* ⬅

When Local C_2 *symmetry dominates*

Comparing off-diagonal $O\supset C_2$ *parameter sets to* CH_4 *models with "cluster-crossings"*

Comparing Local C_4, C_3, and C_2 symmetric spectra



	$(0)_4$	$(1)_4$	$(2)_4$	$(3)_4=(-1)_4$
A_1	1	•	•	•
A_2	•	•	1	•
E	1	•	1	•
T_1	1	1	•	1
T_2	•	1	1	1

	$(0)_3$	$(1)_3$	$(2)_3=(-1)_3$
A_1	1	•	•
A_2	1	•	•
E	•	1	1
T_1	1	1	1
T_2	1	1	1

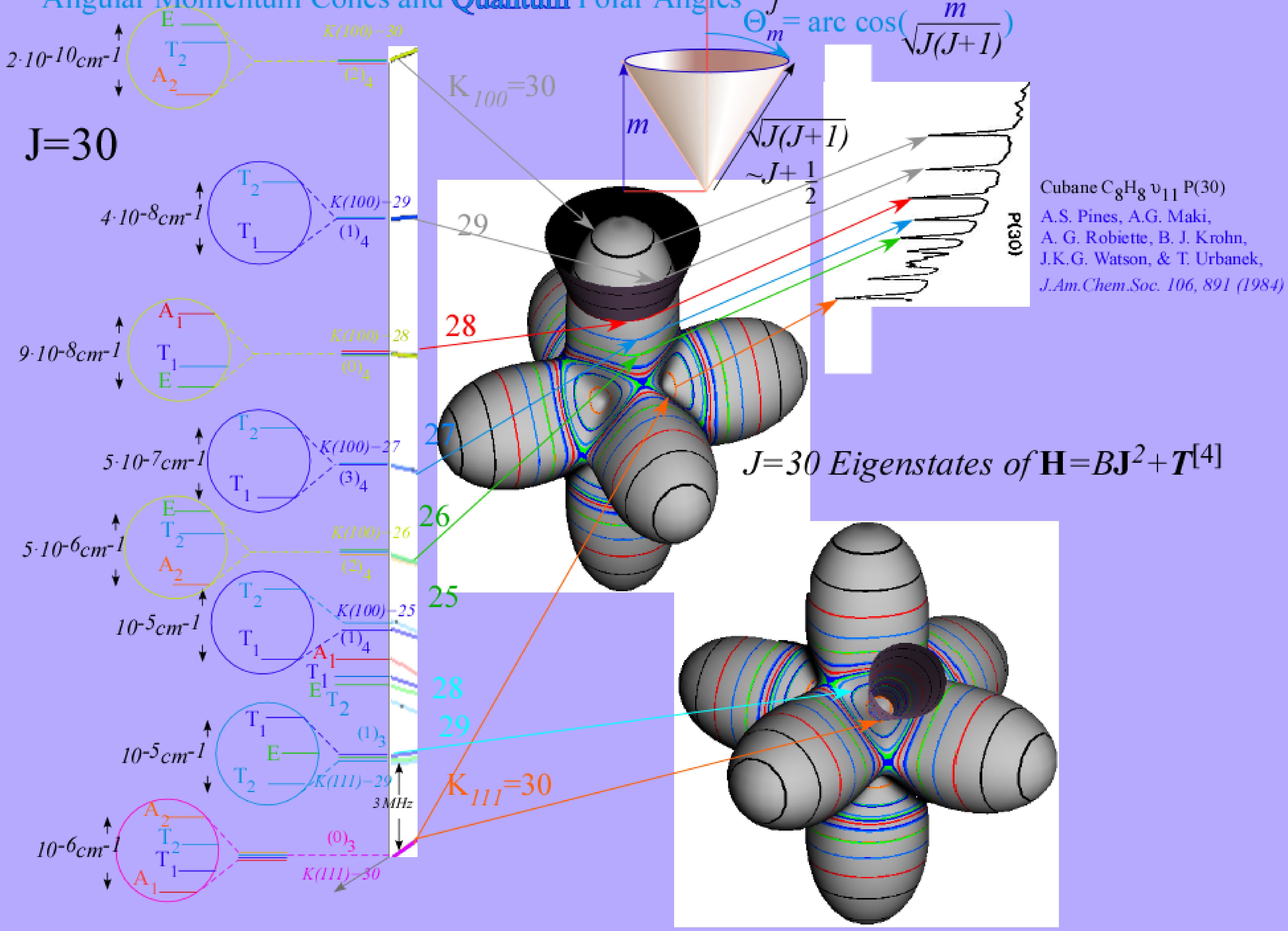
Local correlations explain clustering...
... but what about spacing and ordering?...

...and physical consequences?

Int.J.Mol.Sci, 14, 714(2013)

Comparing Local C_4, C_3, and C_2 symmetric spectra

Angular Momentum Cones and Quantum Polar Angles



Review Calculating idempotent projectors $\mathbf{P}^{\mu}_{m,m}$ *of* $O\supset C_4$ $\mathbf{P}^{E}_{0_4 0_4}$ $\mathbf{P}^{E}_{2_4 2_4}$ $\mathbf{P}^{T_1}_{0_4 0_4}$ $\mathbf{P}^{T_1}_{1_4 1_4}$ $\mathbf{P}^{T_2}_{2_4 2_4}$

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

Review Broken-class-ordered splitting of $O\supset D_4\supset C_4$ *projectors and levels*

Subgroup-defined tunneling parameter modeling

- *Comparing two diagonal* $O\supset C_4$ *parameter sets to* SF_6 *spectra*
- *Comparing two diagonal* $O\supset C_3$ *parameter sets to* SF_6 *spectra*
- *Why* $O\supset C_2$ *parameter sets require off-diagonal nilpotent* $\mathbf{P}^{\mu}_{m,n}$ $(m\neq n)$

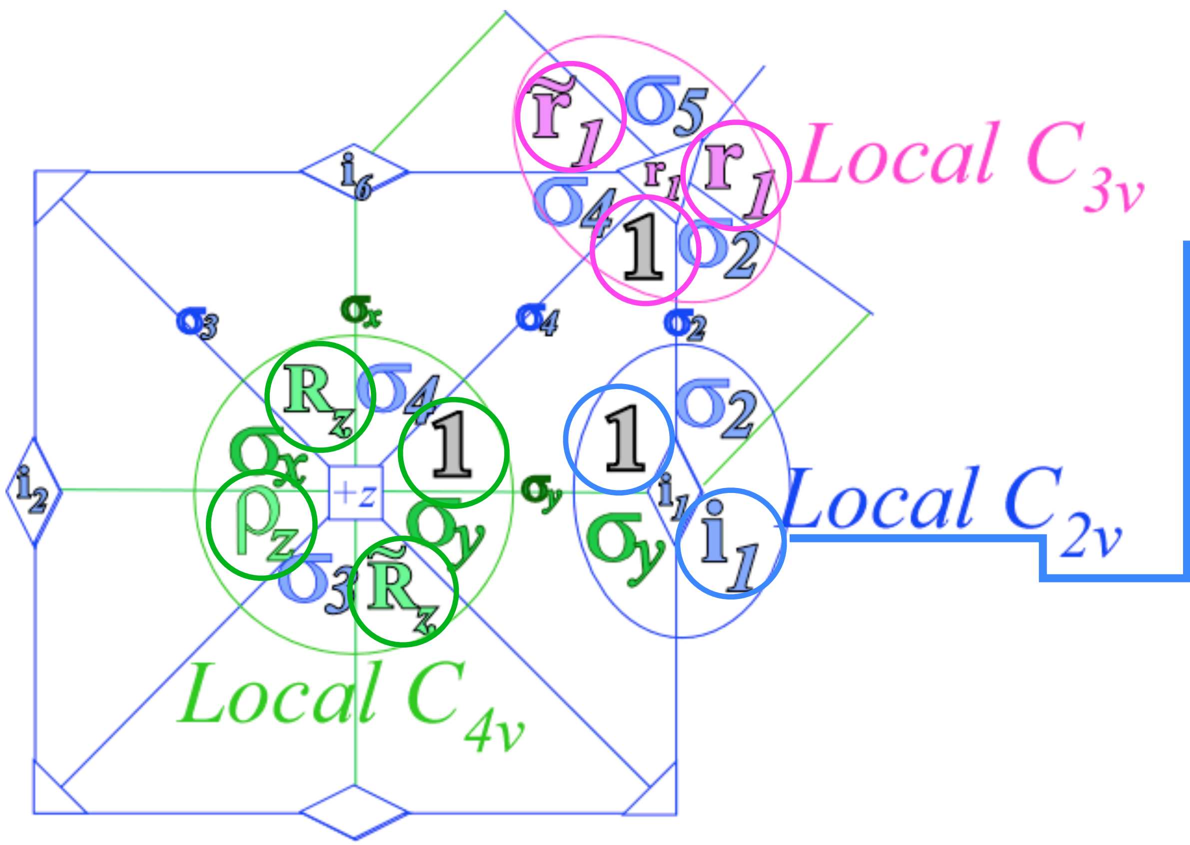
Irreducible nilpotent projectors $\mathbf{P}^{\mu}_{m,n}$ $(m\neq n)$

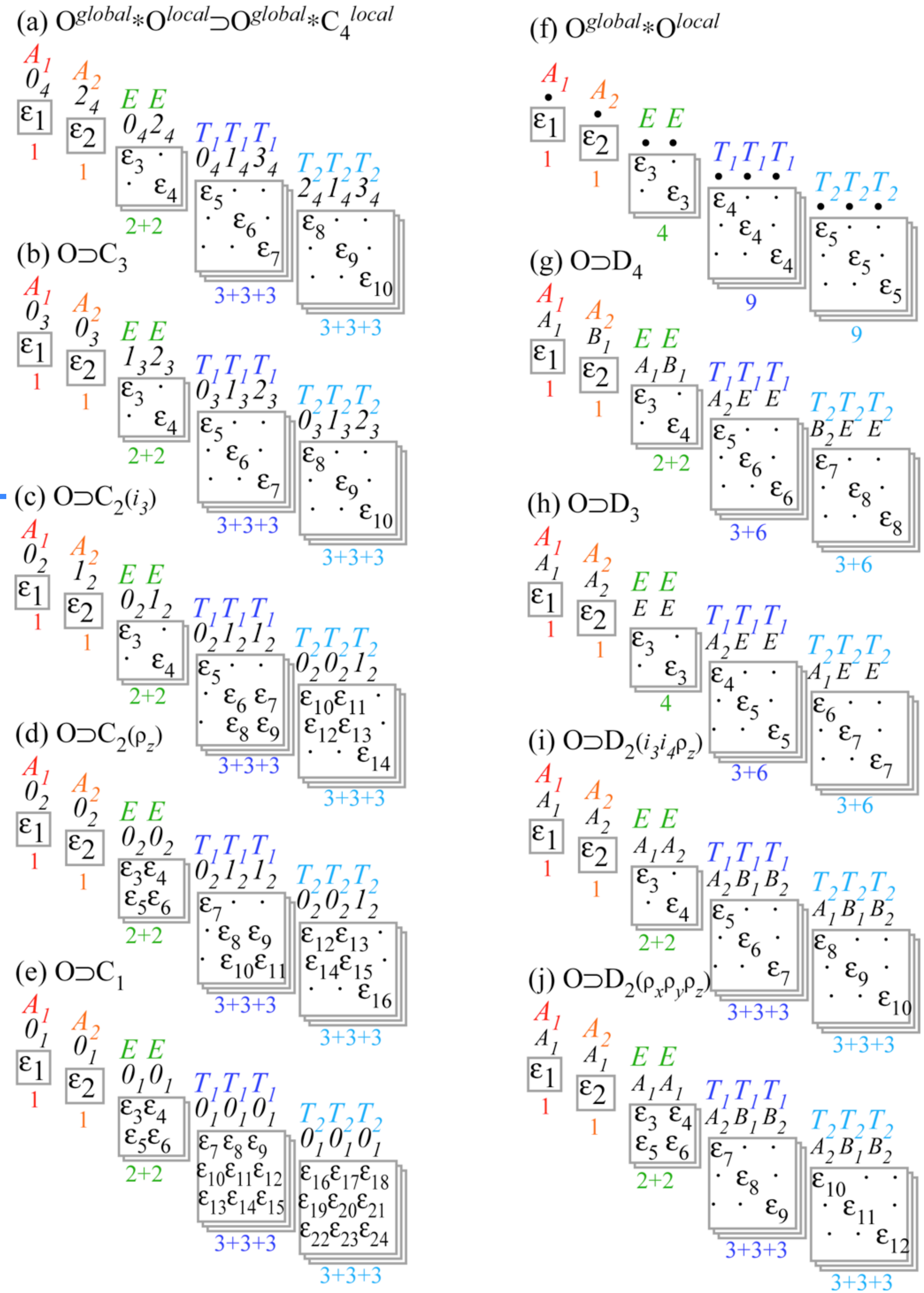
- *Using fundamental* $\mathbf{g}\rightleftarrows\mathbf{P}^{\mu}_{m,n}$ *relations: (from Lecture 16)*
  - (a) $\mathbf{P}^{\mu}_{m,m}\mathbf{g}\mathbf{P}^{\mu}_{n,n}=D^{\mu}_{m,n}(\mathbf{g})\mathbf{P}^{\mu}_{m,n}$ (b) $\mathbf{g}=\Sigma_{\mu}\Sigma_{m,n}D^{\mu}_{m,n}(\mathbf{g})\mathbf{P}^{\mu}_{m,n}$ (c) $\mathbf{P}^{\mu}_{n,n}=(\ell^{\mu}/{}^{\circ}G)\Sigma_{\mathbf{g}}D^{\mu *}_{m,n}(\mathbf{g})\mathbf{g}$
- *Review of* $D_3\supset C_2\sim C_{3v}\supset C_v$
- *Calculating and Factoring* $\mathbf{P}^{T_1}_{1_4 0_4}$ *and* $\mathbf{P}^{T_1}_{1_4 3_4}$

Structure and applications of various subgroup chain irreducible representations

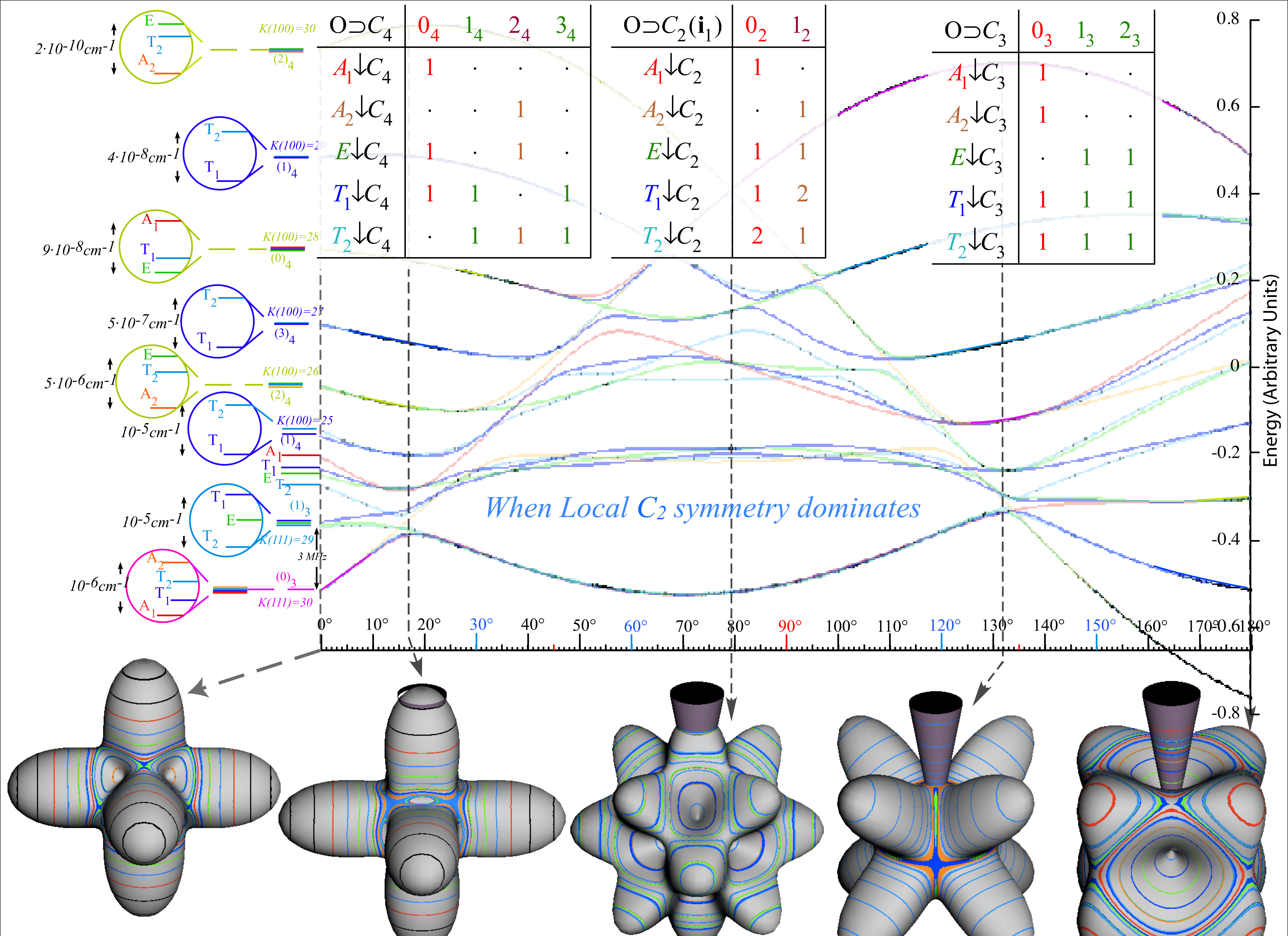
- $O_h\supset D_{4h}\supset C_{4v}$, $O_h\supset D_{3h}\supset C_{3v}$, $O_h\supset C_{2v}$
- *Comparing* $O_h\supset D_{4h}\supset D_{2h}$ *and* $O_h\supset D_{3d}\supset C_2$ *representations* (*T_1* **vector**-*type*)
  - *Examples of off-diagonal tunneling coefficients* $D^{E}_{0_4 2_4}$
- *Comparing Local* C_4, C_3, *and* C_2 *symmetric spectra*
  - ➡ *When Local* C_2 *symmetry dominates* ⬅
- *Comparing off-diagonal* $O\supset C_2$ *parameter sets to* CH_4 *models with "cluster-crossings"*

When Local C_2 symmetry dominates





Int.J.Mol.Sci, 14, 714(2013)



$O\supset C_4$	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

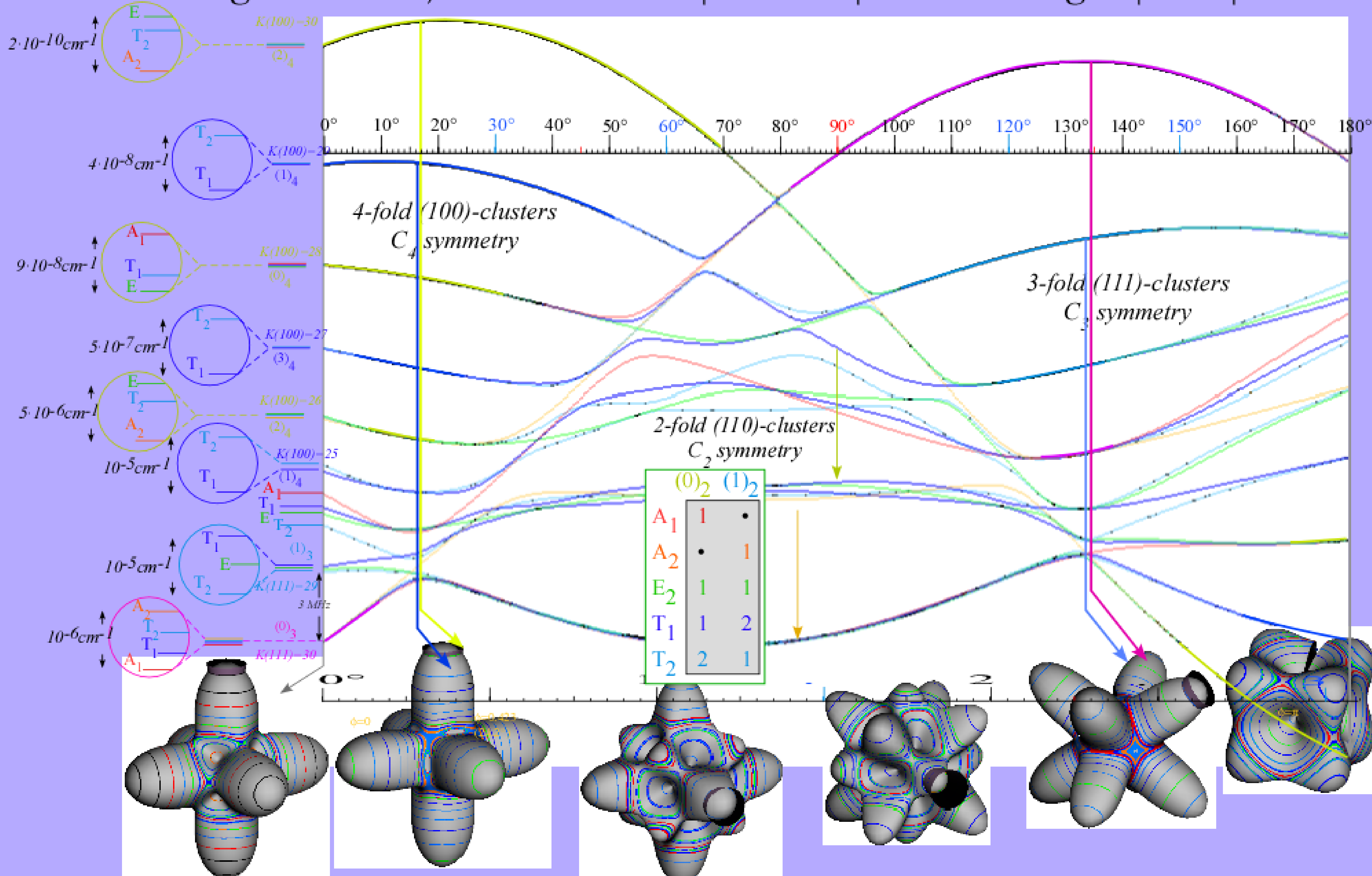
$O\supset C_2(\mathbf{i}_1)$	0_2	1_2
$A_1\downarrow C_2$	1	.
$A_2\downarrow C_2$	.	1
$E\downarrow C_2$	1	1
$T_1\downarrow C_2$	1	2
$T_2\downarrow C_2$	2	1

$O\supset C_3$	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

Int.J.Mol.Sci, 14, 714(2013)

When Local C_2 symmetry dominates

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



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

Int.J.Mol.Sci, 14, 714(2013)

Review Calculating idempotent projectors $\mathbf{P}^{\mu}_{m,m}$ *of* $O\supset C_4$ $\mathbf{P}^{E}_{0_4 0_4}$ $\mathbf{P}^{E}_{2_4 2_4}$ $\mathbf{P}^{T_1}_{0_4 0_4}$ $\mathbf{P}^{T_1}_{1_4 1_4}$ $\mathbf{P}^{T_2}_{2_4 2_4}$

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

Review Broken-class-ordered splitting of $O\supset D_4\supset C_4$ *projectors and levels*

Subgroup-defined tunneling parameter modeling

Comparing two diagonal $O\supset C_4$ *parameter sets to* SF_6 *spectra*

Comparing two diagonal $O\supset C_3$ *parameter sets to* SF_6 *spectra*

Why $O\supset C_2$ *parameter sets require off-diagonal nilpotent* $\mathbf{P}^{\mu}_{m,n}$ $(m\neq n)$

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

Using fundamental $\mathbf{g}\rightleftarrows\mathbf{P}^{\mu}_{m,n}$ *relations: (from Lecture 16)*

(a) $\mathbf{P}^{\mu}_{m,m}\,\mathbf{g}\mathbf{P}^{\mu}_{n,n}=D^{\mu}_{m,n}(\mathbf{g})\mathbf{P}^{\mu}_{m,n}$ (b) $\mathbf{g}=\Sigma_{\mu}\Sigma_{m,n}D^{\mu}_{m,n}(\mathbf{g})\mathbf{P}^{\mu}_{m,n}$ (c) $\mathbf{P}^{\mu}_{n,n}=(\ell^{\mu}/{}^{\circ}G)\Sigma_{\mathbf{g}}D^{\mu *}_{m,n}(\mathbf{g})\mathbf{g}$

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

Calculating and Factoring $\mathbf{P}^{T_1}_{1_4 0_4}$ *and* $\mathbf{P}^{T_1}_{1_4 3_4}$

Structure and applications of various subgroup chain irreducible representations

$O_h\supset D_{4h}\supset C_{4v}$, $O_h\supset D_{3h}\supset C_{3v}$, $O_h\supset C_{2v}$

Comparing $O_h\supset D_{4h}\supset D_{2h}$ *and* $O_h\supset D_{3d}\supset C_2$ *representations (*T_1 *vector-type)*

Examples of off-diagonal tunneling coefficients $D^{E}_{0_4 2_4}$

Comparing Local C_4, C_3, *and* C_2 *symmetric spectra*

When Local C_2 *symmetry dominates*

➡ *Comparing off-diagonal* $O\supset C_2$ *parameter sets to* CH_4 *models with "cluster-crossings"* ⬅

When Local C_2 symmetry dominates

$O \supset C_2(\mathbf{i}_1)$	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

Comparing off-diagonal $O \supset C_2$ parameter sets to CH_4 models with "cluster-crossings"

Table 13. Splittings of $O \supset C_2(i_4)$ given sub-class structure.

$O \supset D_4 \supset C_2(i_4)$	$0°$	$r_n 120°$	$\rho_n 180°$	$R_n 90°$	$i_n 180°$
0_2					
$\varepsilon_{0_2}^{A_1}$	g_0	$4r_{12} + 4r_{34}$	$2\rho_{xy} + \rho_z$	$4R_{xy} + 2R_z$	$4i_{1256} + i_3 + i_4$
$\varepsilon_{0_2}^{E}$	g_0	$-2r_{12} - 2r_{34}$	$2\rho_{xy} + \rho_z$	$-2R_{xy} + 2R_z$	$-2i_{1256} + i_3 + i_4$
$\varepsilon_{0_2}^{T_1}$	g_0	$-2r_{12} + 2r_{34}$	$-\rho_z$	$2R_{xy}$	$-2i_{1256} - i_3 + i_4$
$\varepsilon_{0_2}^{{T_2}_E}$	g_0	$2r_{12} - 2r_{34}$	$-\rho_z$	$-2R_{xy}$	$2i_{1256} - i_3 + i_4$
$\varepsilon_{0_2}^{{T_2}_{A_1}}$	g_0	0	$-2\rho_{xy} + \rho_z$	$-2R_z$	$i_3 + i_4$
1_2					
$\varepsilon_{1_2}^{A_2}$	g_0	$4r_{12} + 4r_{34}$	$2\rho_{xy} + \rho_z$	$-4R_{xy} - 2R_z$	$-4i_{1256} - i_3 - i_4$
$\varepsilon_{1_2}^{E}$	g_0	$-2r_{12} - 2r_{34}$	$2\rho_{xy} + \rho_z$	$2R_{xy} - 2R_z$	$2i_{1256} - i_3 - i_4$
$\varepsilon_{1_2}^{{T_1}_E}$	g_0	$2r_{12} - 2r_{34}$	$-\rho_z$	$2R_z$	$-2i_{1256} + i_3 - i_4$
$\varepsilon_{1_2}^{{T_1}_{A_2}}$	g_0	0	$-2\rho_{xy} + \rho_z$	$-2R_z$	$-i_3 - i_4$
$\varepsilon_{1_2}^{{T_2}_E}$	g_0	$-2r_{12} + 2r_{34}$	$-\rho_z$	$-2R_{xy}$	$2i_{1256} + i_3 - i_4$

Table 14. Matrix that converts tunneling strengths to cluster splitting energi

0_2	$\mathbf{1}$	r_{12}, i_{1256}	r_{34}, R_{xy}	ρ_{xy}, R_z	ρ_z, i_3
$\varepsilon_{0_2}^{A_1}$	1	4	4	2	1
$\varepsilon_{0_2}^{E}$	1	-2	-2	2	1
$\varepsilon_{0_2}^{T_1}$	1	-2	2	0	-1
$\varepsilon_{E,0_2}^{T_2}$	1	2	-2	0	-1
$\varepsilon_{A_1,0_2}^{T_2}$	1	0	0	-2	1

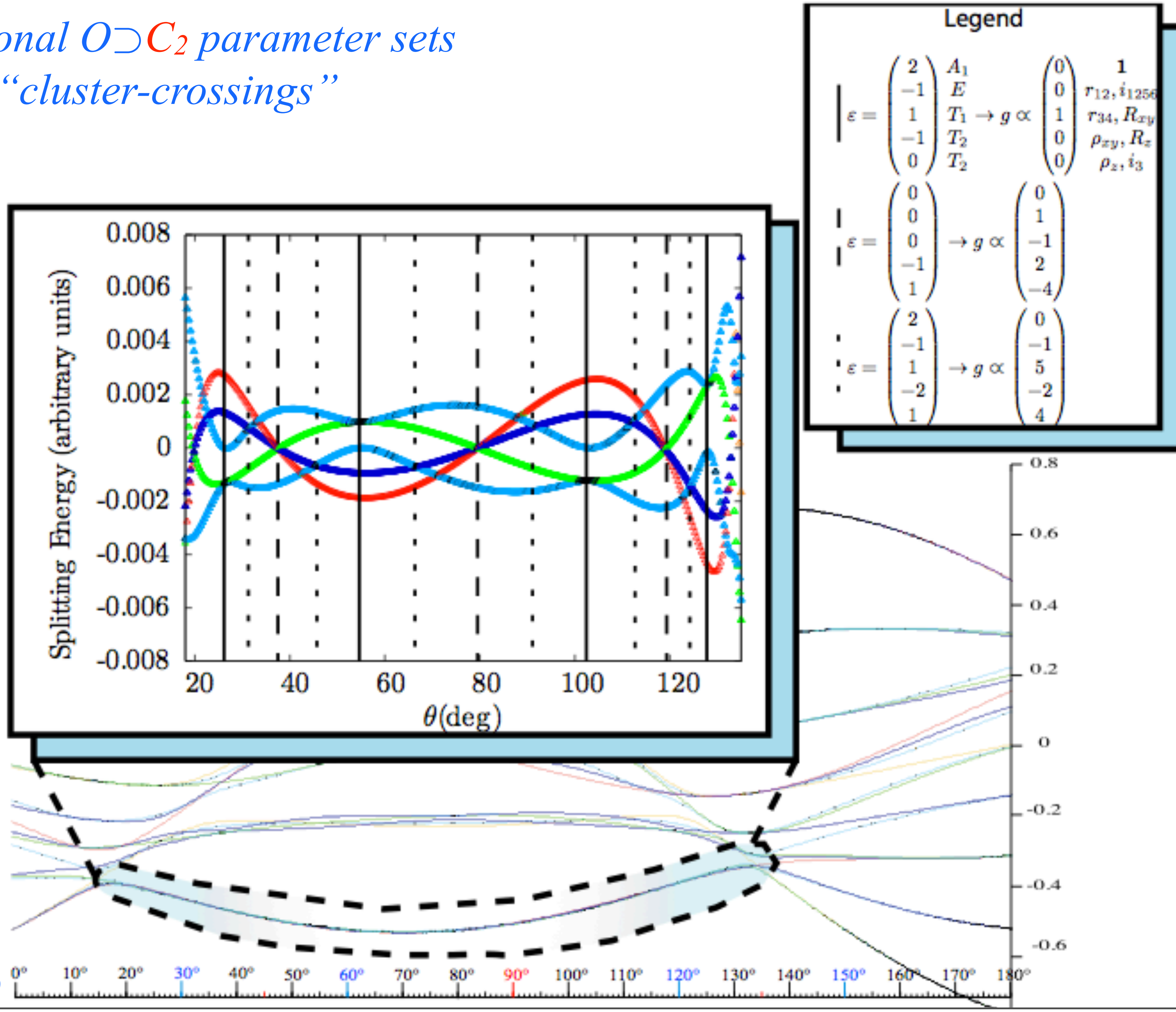
Table 15. Matrix that converts cluster splitting energies to tunneling strength

0_2	$\varepsilon_{0_2}^{A_1}$	$\varepsilon_{0_2}^{E}$	$\varepsilon_{0_2}^{T_1}$	$\varepsilon_{E,0_2}^{T_2}$	$\varepsilon_{A_1,0_2}^{T_2}$
$\mathbf{1}$	$\frac{1}{12}$	$\frac{1}{6}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$
r_{12}, i_{1256}	$\frac{1}{12}$	$-\frac{1}{12}$	$-\frac{1}{8}$	$\frac{1}{8}$	0
r_{34}, R_{xy}	$\frac{1}{12}$	$-\frac{1}{12}$	$\frac{1}{8}$	$-\frac{1}{8}$	0
ρ_{xy}, R_z	$\frac{1}{12}$	$\frac{1}{6}$	0	0	$-\frac{1}{4}$
ρ_z, i_3	$\frac{1}{12}$	$\frac{1}{6}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$

Int.J.Mol.Sci, 14, 714(2013)

Figure 30. The plot focuses on the lowest $0_2(C_2)\uparrow O$ cluster in the previous energy plot (Figure 29) of the $T^{[4,6]}$ Hamiltonian for $J = 30$. The inside plot has been magnified 100 times. The inside diagram also centers the levels around their center-of-energy, showing only the splittings and ignoring the shifts of the cluster. Symmetry species are colored as before: A_1: red, A_2: orange, E_2 : green, T_1: dark blue, and T_2: light blue. The vertical lines on inside plot draw attention to specific clustering patterns described in the text. $1_2(C_2)\uparrow O$ clusters have similar superfine structure but with A_2 replacing A_1 and T_1 switched with T_2.

Comparing off-diagonal $O\supset C_2$ parameter sets to CH_4 models with "cluster-crossings"



Int.J.Mol.Sci, 14, 714(2013)

End of Lecture 21

$O \supset C_4$	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

$O \supset C_2(\mathbf{i}_1)$	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
$A_{1g} \downarrow C_{4v}$	·	·	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

,

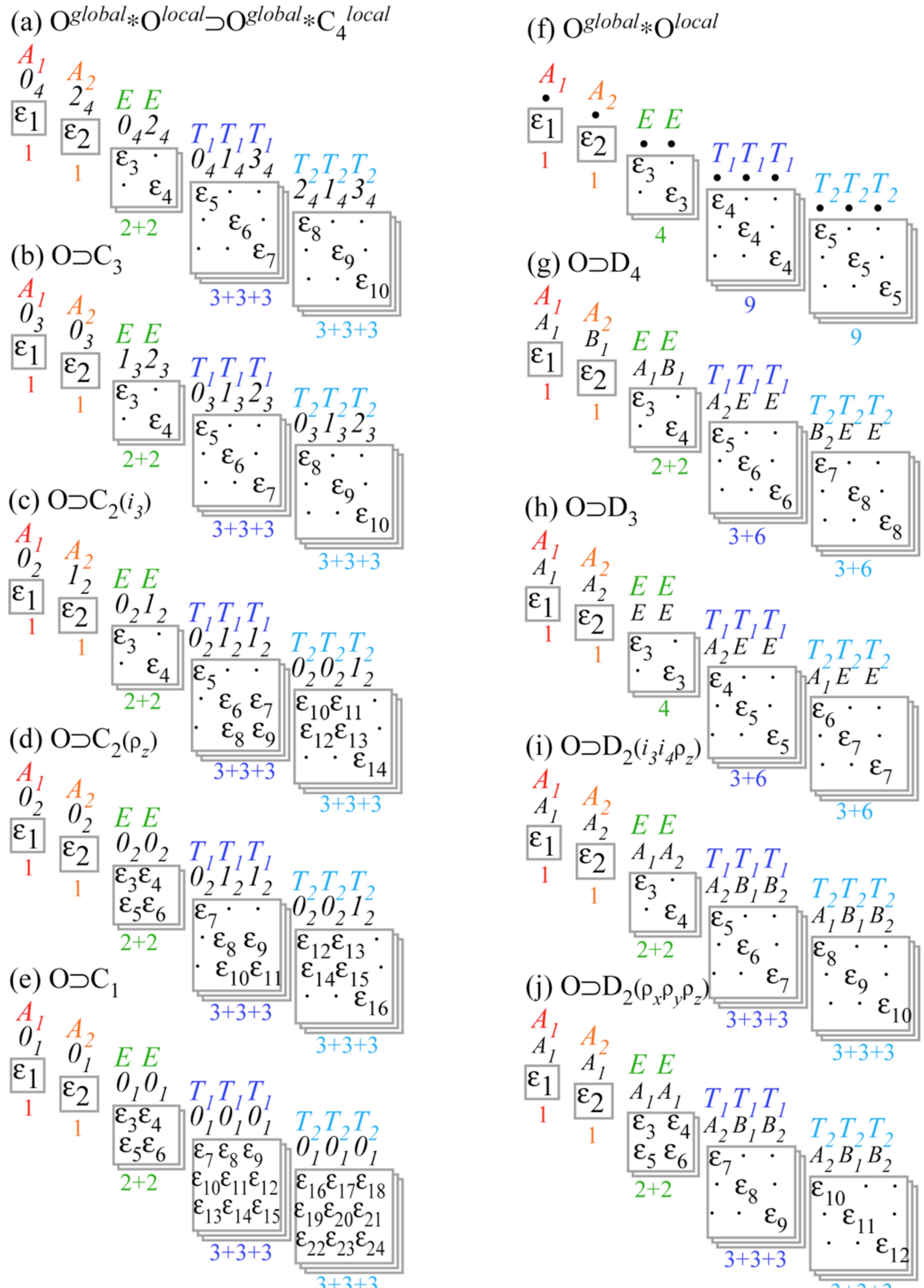
$O_h \supset C_{3v}$	A'	A''	E
$A_{1g} \downarrow C_{3v}$	1	·	·
$A_{2g} \downarrow C_{3v}$	·	1	·
$E_g \downarrow C_{3v}$	·	·	1
$T_{1g} \downarrow C_{3v}$	·	1	1
$T_{2g} \downarrow C_{3v}$	1	·	1
$A_{1g} \downarrow C_{3v}$	·	1	·
$A_{2u} \downarrow C_{3v}$	1	·	·
$E_u \downarrow C_{3v}$	·	·	1
$T_{1u} \downarrow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

,

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

,

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


(a) O^global*O^local⊃O^global*C4^local
(b) O⊃C3
(c) O⊃C2(i3)
(d) O⊃C2(ρz)
(e) O⊃C1
(f) O^global*O^local
(g) O⊃D4
(h) O⊃D3
(i) O⊃D2(i3i4ρz)
(j) O⊃D2(ρxρyρz)

Ireps for O⊃D_4⊃C_4 *subgroup chain*

T_1

Vector
x,y,z

T_2

Tensor
yz,xz,xy

E

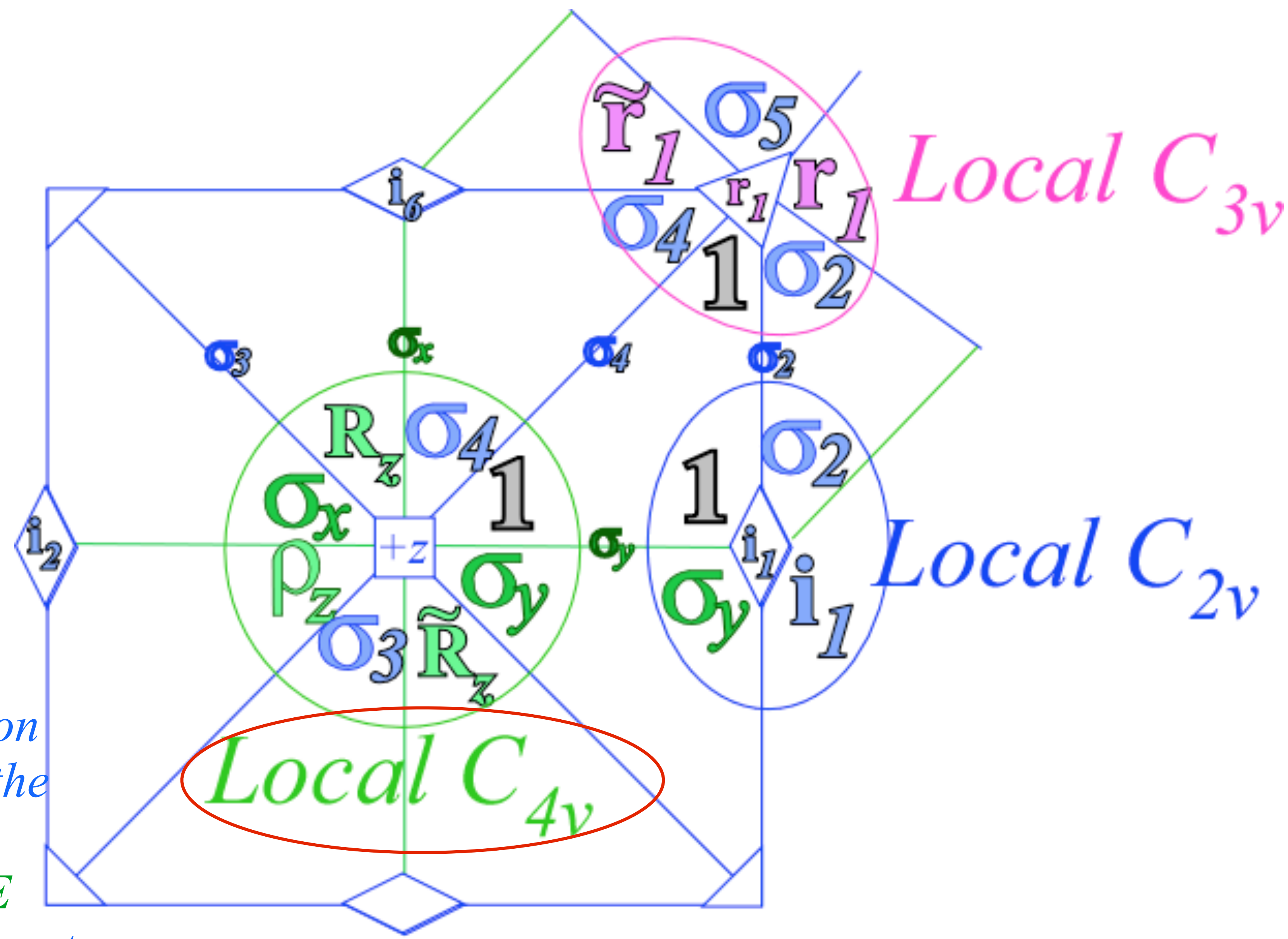
Tensor
$x^2+y^2-2z^2$
$(x^2-y^2)\sqrt{3}$

$O \supset C_4$	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
$A_{1g} \downarrow C_{4v}$	·	·	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

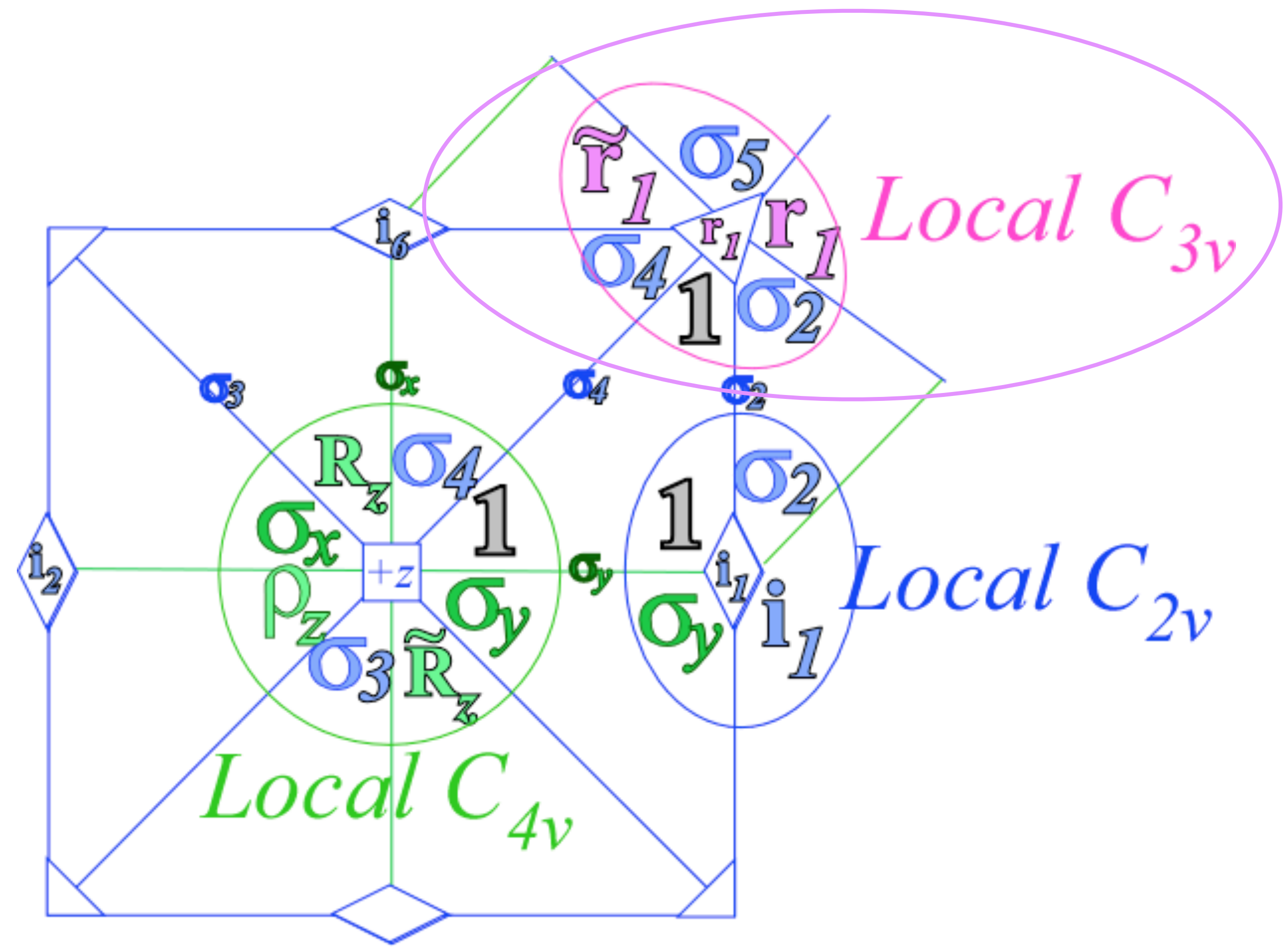
,

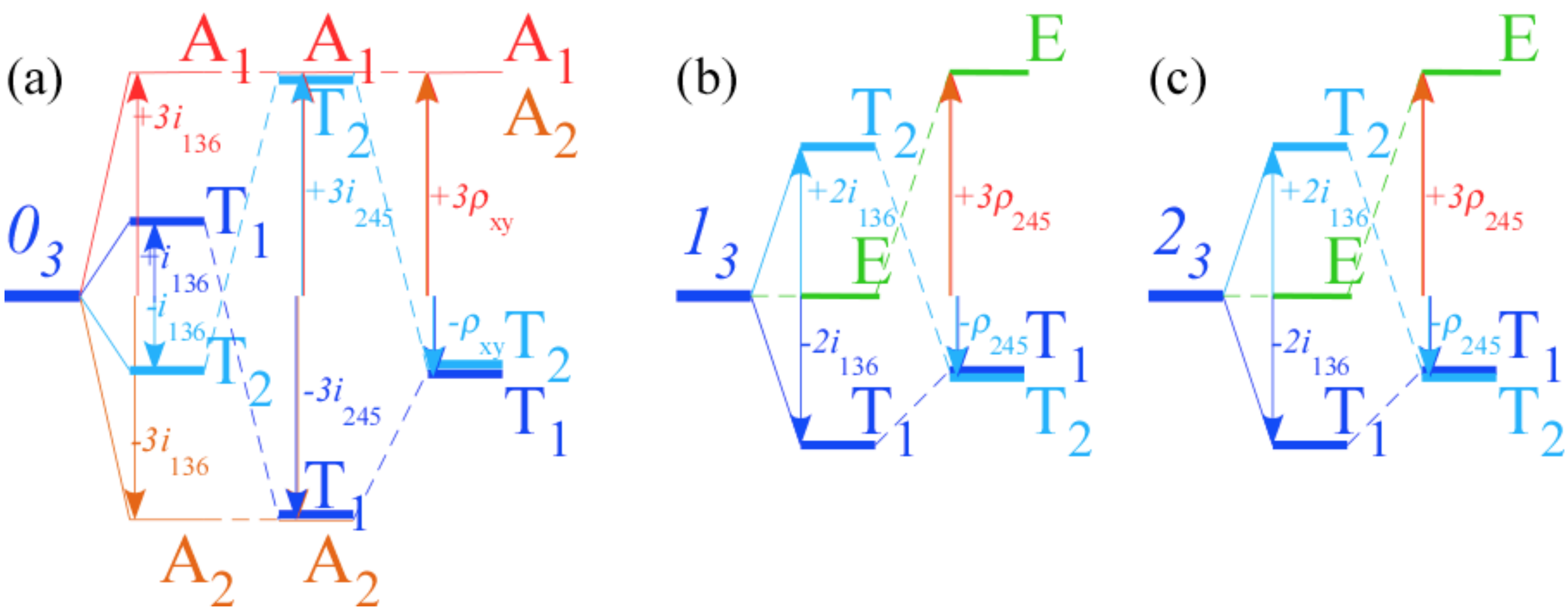
$O_h \supset C_{4v}$ correlation predicts the parity of the A_1T_1E cluster is not uniformly even (g) or odd (u): $A_{1g}T_{1u}E_g$



$O \supset C_3$	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)
(b)
(c)
0_3
1_3
2_3
A_1
A_2
T_1
T_2
E
$+3i_{136}$
$+i_{136}$
$-i_{136}$
$-3i_{136}$
$+3i_{245}$
$-3i_{245}$
$+3\rho_{xy}$
$-\rho_{xy}$
$+2i_{136}$
$-2i_{136}$
$+3\rho_{245}$
$-\rho_{245}$

$\ell^{A_1} = 1$

$\ell^{A_2} = 1$

$\ell^{E} = 2$

$\ell^{T_1} = 3$

$\ell^{T_2} = 3$

Example: $G = O$

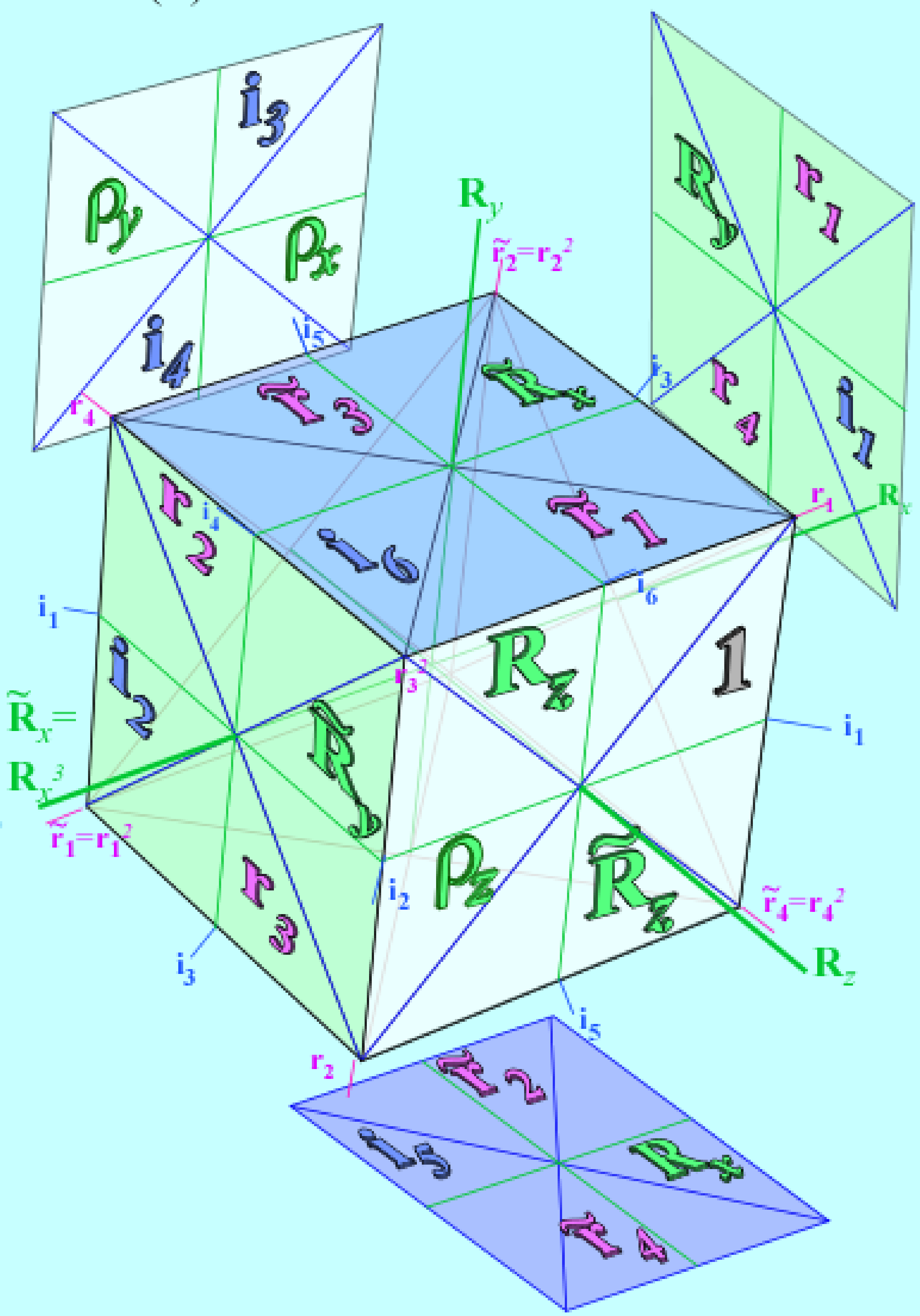
Cubic-Octahedral Group O

Centrum: $\kappa(O) = \Sigma_{(\alpha)} (\ell^{\alpha})^0 = 1^0 + 1^0 + 2^0 + 3^0 + 3^0 = 5$

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

Order: $^o(O) = \Sigma_{(\alpha)} (\ell^{\alpha})^0 = 1^2 + 1^2 + 2^2 + 3^2 + 3^2 = 24$

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

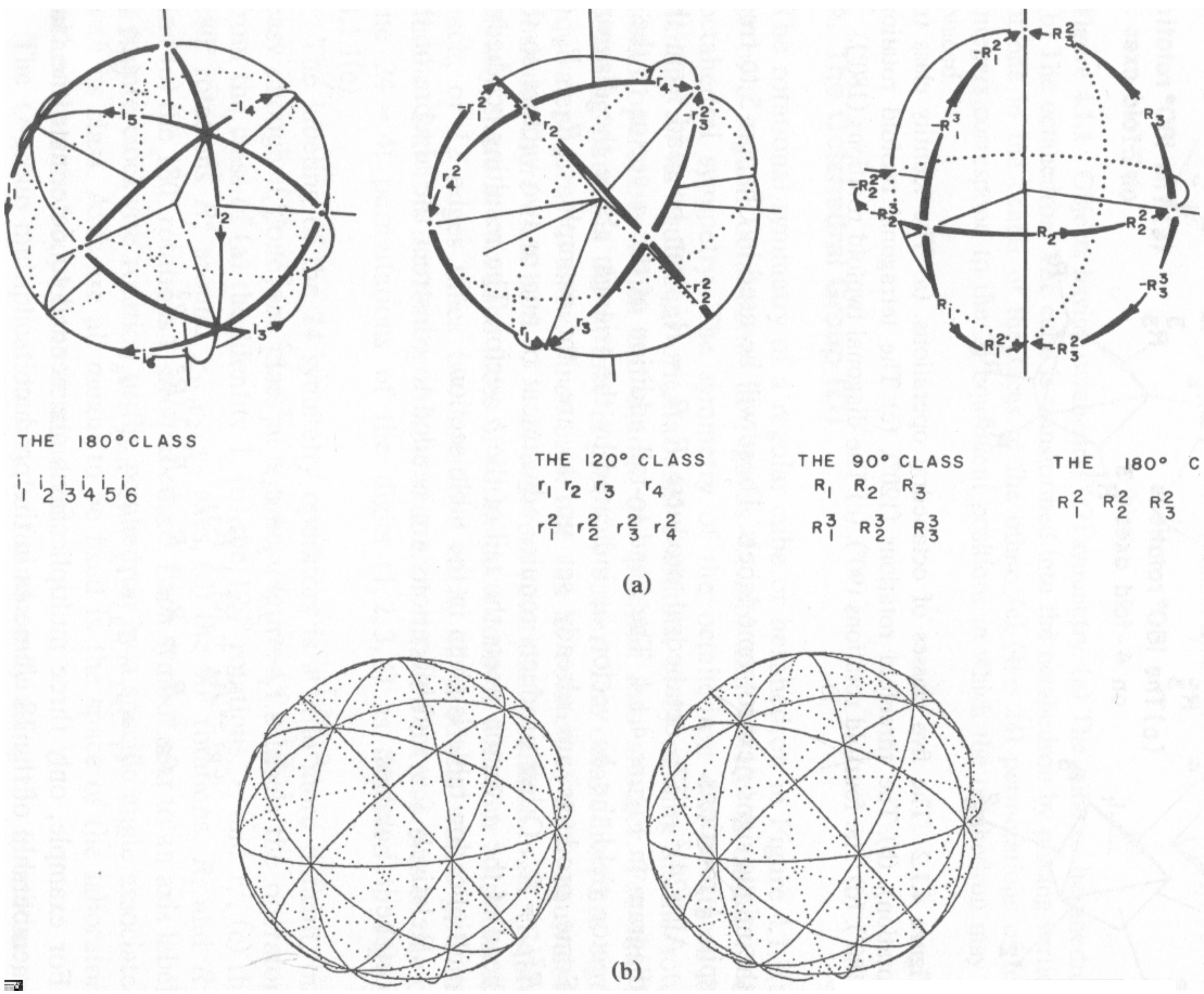


$O \supset C_4$

	$(0)_4$	$(1)_4$	$(2)_4$	$(3)_4 = (-1)_4$
A_1	1	•	•	•
A_2	•	•	1	•
E	1	•	1	•
T_1	1	1	•	1
T_2	•	1	1	1

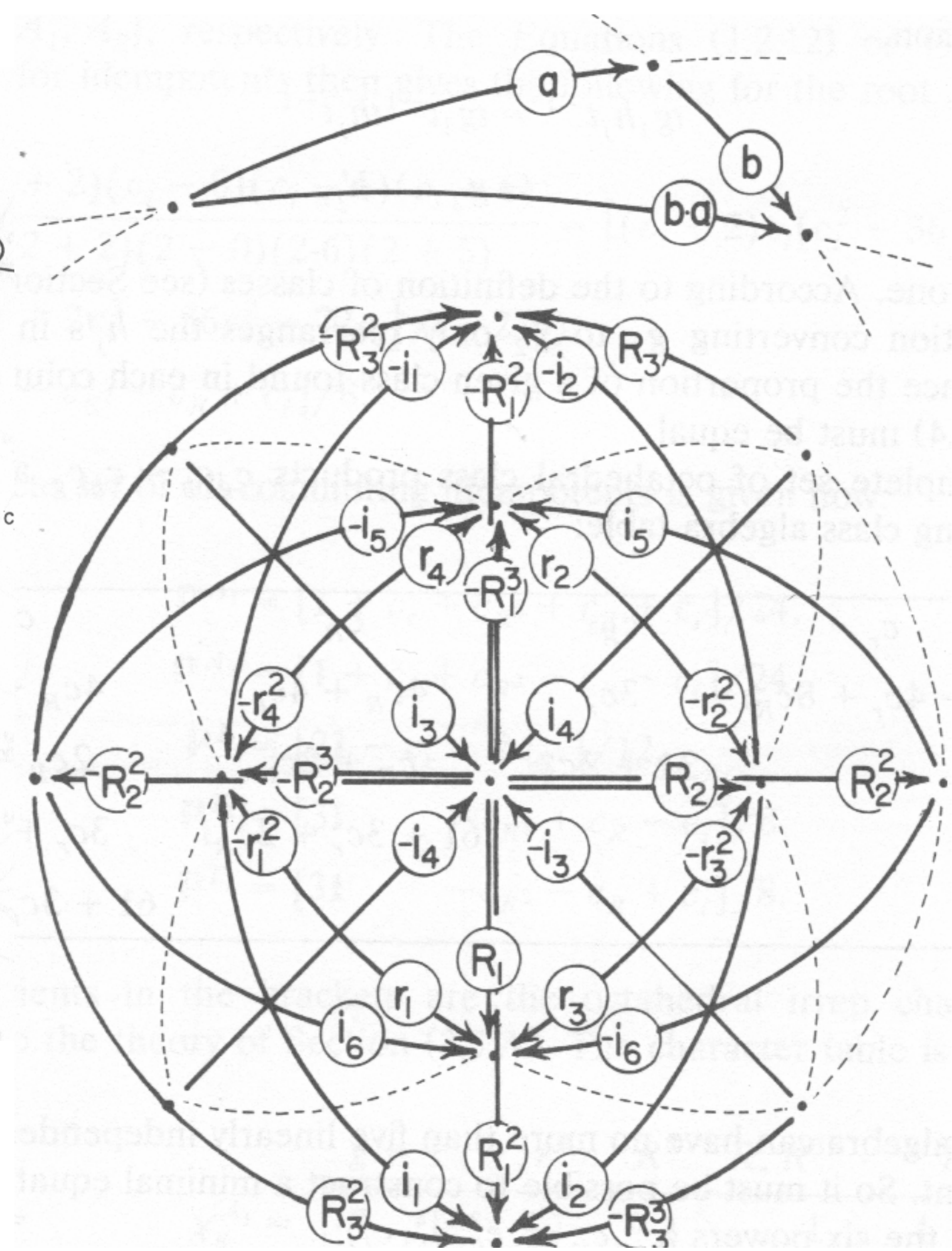
$O \supset C_3$

	$(0)_3$	$(1)_3$	$(2)_3 = (-1)_3$
A_1	1	•	•
A_2	1	•	•
E	•	1	1
T_1	1	1	1
T_2	1	1	1


THE 180° CLASS
i1 i2 i3 i4 i5 i6
THE 120° CLASS
r1 r2 r3 r4
r1² r2² r3² r4²
THE 90° CLASS
R1 R2 R3
R1³ R2³ R3³
THE 180° C
R1² R2² R3²

(a)

(b)


a
b
b·a
R3
-R3²
-R1²
-R1³
R1
R1²
R2
R2²
-R2²
-R2³
R3²
-R3³

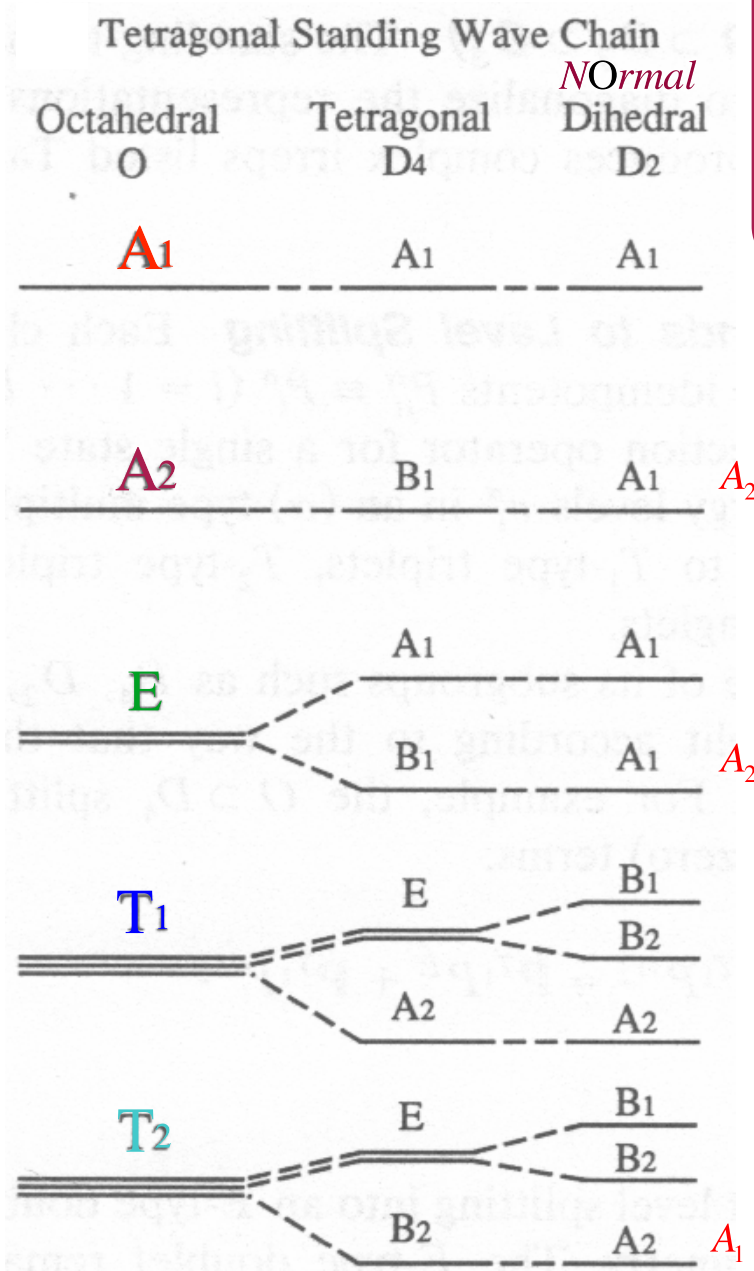
$O_h \supset O \supset D_4 \supset C_4$ subgroup splitting

D_4	**1**	ρ_z	$\mathbf{R}_z$	$\rho_{x,y}$	$\mathbf{i}_{3,4}$
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

$D_2^{Nm}\{\ \mathbf{1},\ \mathbf{R}_z^2,\ \mathbf{R}_x^2,\ \mathbf{R}_y^2\ \}$

$D_2^{Un}\{\ \mathbf{1},\ \mathbf{R}_z^2,\ \mathbf{i}_3,\ \mathbf{i}_4\ \}$

A_1	1	1	1	1
B_1	1	-1	1	-1
A_2	1	1	-1	-1
B_2	1	-1	-1	1

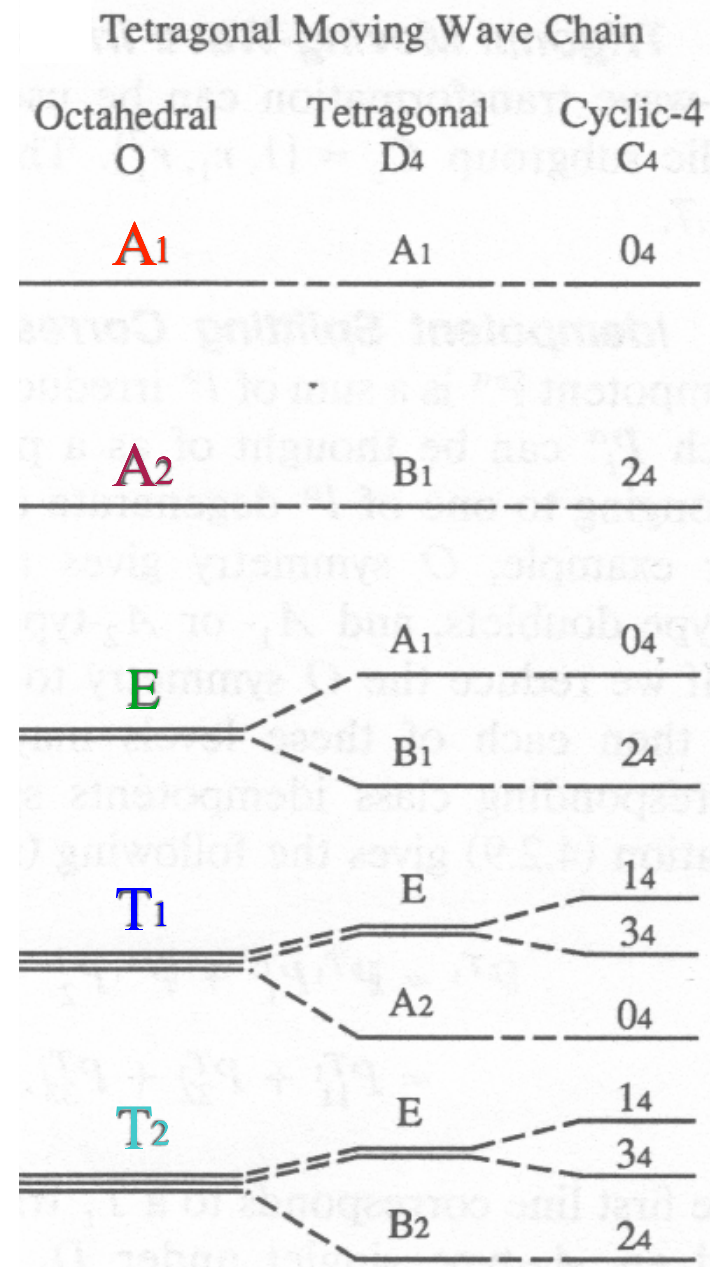


NOrmal $D_2 = \{1, \mathbf{R}_3^2, \mathbf{R}_1^2, \mathbf{R}_2^2\}$

$D_4 \downarrow D_2$	A_1	B_1	A_2	B_2
A_1	1	·	·	·
B_1	1	·	·	·
A_2	·	·	1	·
B_2	·	·	1	·
E	·	1	·	1

*Un*O*rmal* $D_2 = \{1, \mathbf{R}_3^2, \mathbf{i}_3, \mathbf{i}_4\}$

$D_4 \downarrow D_2$	A_1	B_1	A_2	B_2
A_1	1	·	·	·
B_1	·	·	1	·
A_2	·	·	1	·
B_2	1	·	·	·
E	·	1	·	1



$-1_4 =$

$D_4 \downarrow C_4$	0_4	1_4	2_4	3_4
A_1	1	·	·	·
B_1	·	·	1	·
A_2	1	·	·	·
B_2	·	·	1	·
E	·	1	·	1

O	**1**	$\mathbf{r}, \tilde{\mathbf{r}}_i$: **r**	ρ_{xyz}: $\mathbf{R}^2$	$\mathbf{R}, \tilde{\mathbf{R}}_{xyz}$: $\mathbf{R}^3$	$\mathbf{i}_k$
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

NOrmal $D_2 = \{1, \mathbf{R}_3^2, \mathbf{R}_1^2, \mathbf{R}_2^2\}$

$O \downarrow D_2$	A_1	B_1	A_2	B_2
A_1	1	·	·	·
A_2	1	·	·	·
E	2	·	·	·
T_1	·	1	1	1
T_2	·	1	1	1

*Un*O*rmal* $D_2 = \{1, \mathbf{R}_3^2, \mathbf{i}_3, \mathbf{i}_4\}$

$O \downarrow D_2$	A_1	B_1	A_2	B_2
A_1	1	·	·	·
A_2	·	·	1	·
E	1	·	1	·
T_1	·	1	1	1
T_2	1	1	·	1

$O \downarrow D_4$	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

$-1_4 =$

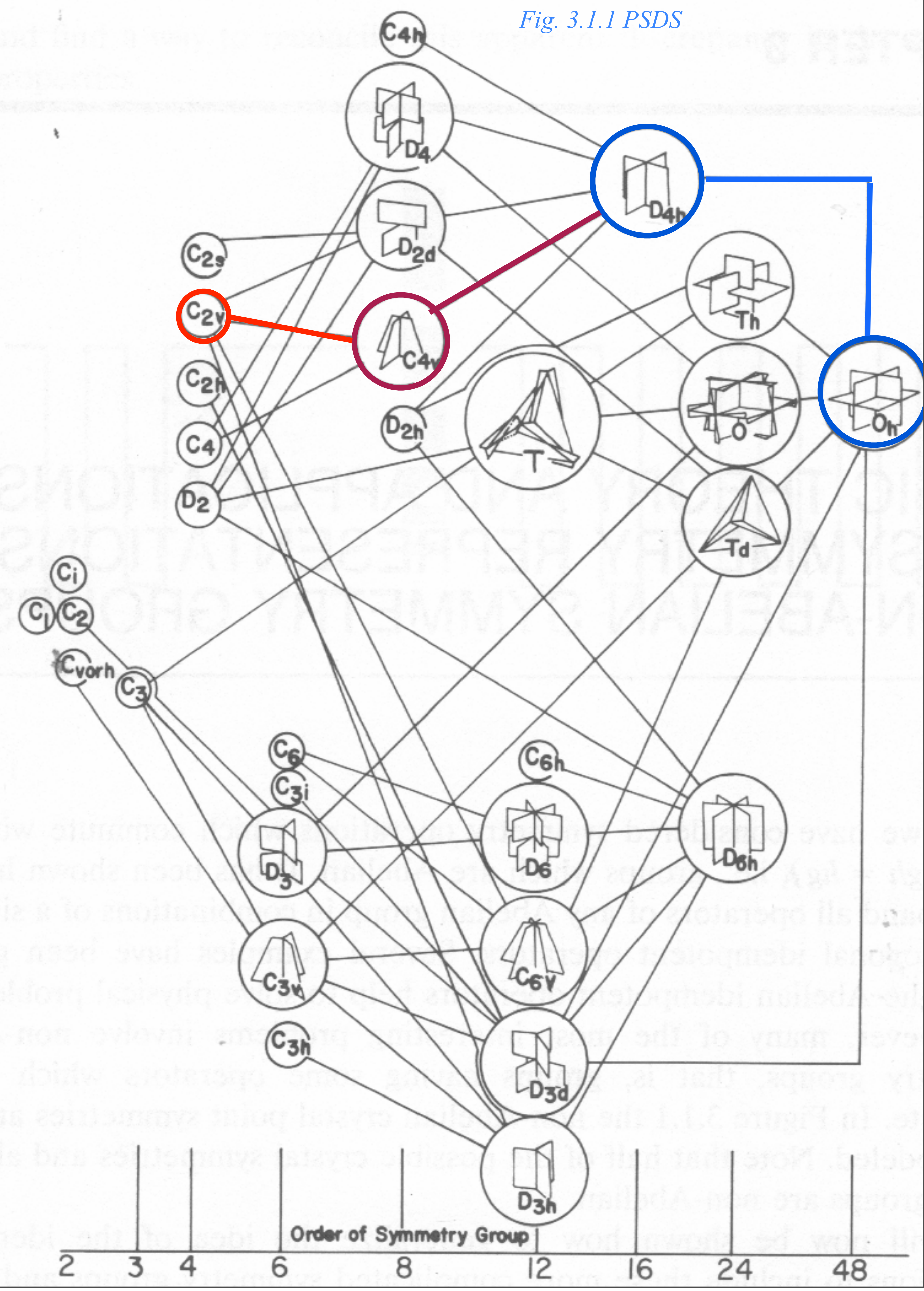
$O \downarrow C_4$	0_4	1_4	2_4	3_4
A_1	1	·	·	·
A_2	·	·	1	·
E	1	·	1	·
T_1	1	1	·	1
T_2	·	1	1	1

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

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

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

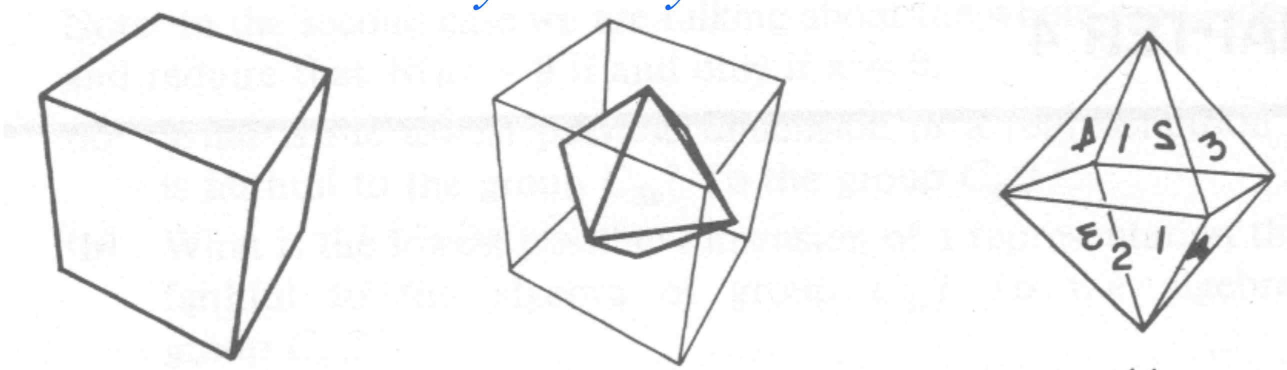
Fig. 3.1.1 PSDS

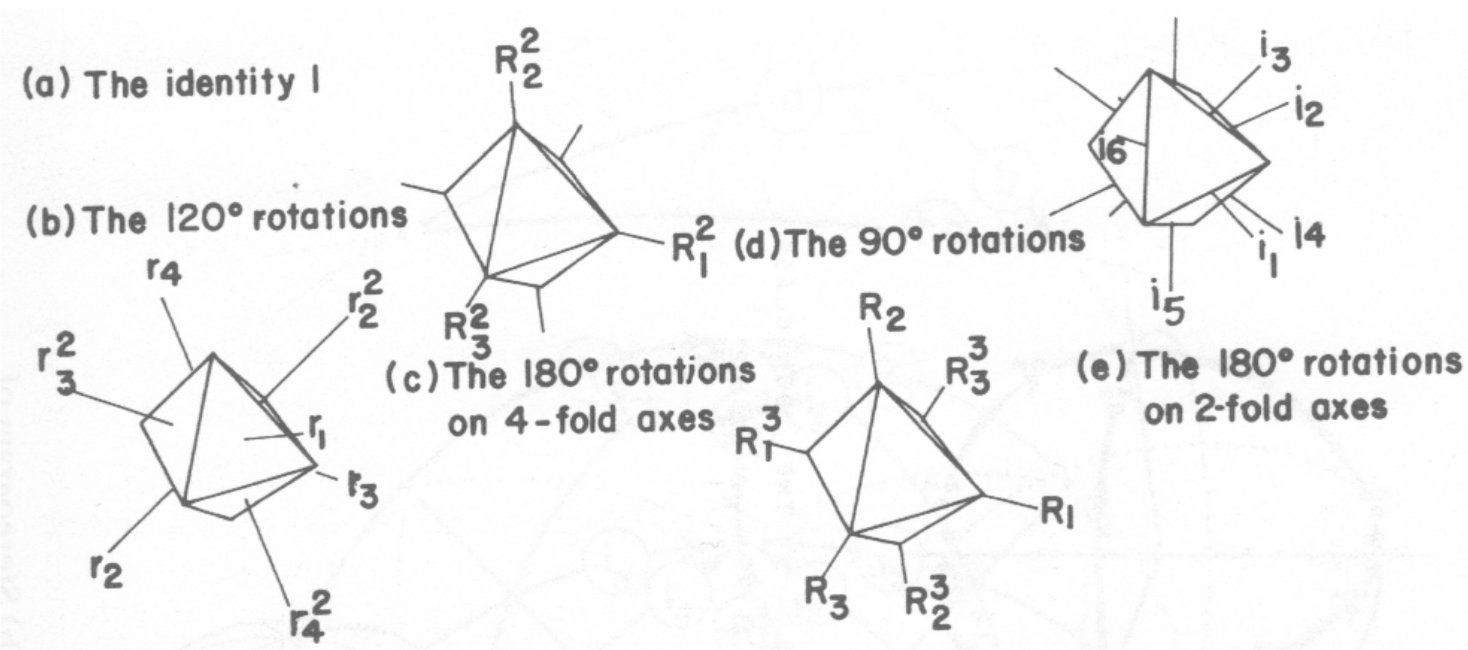


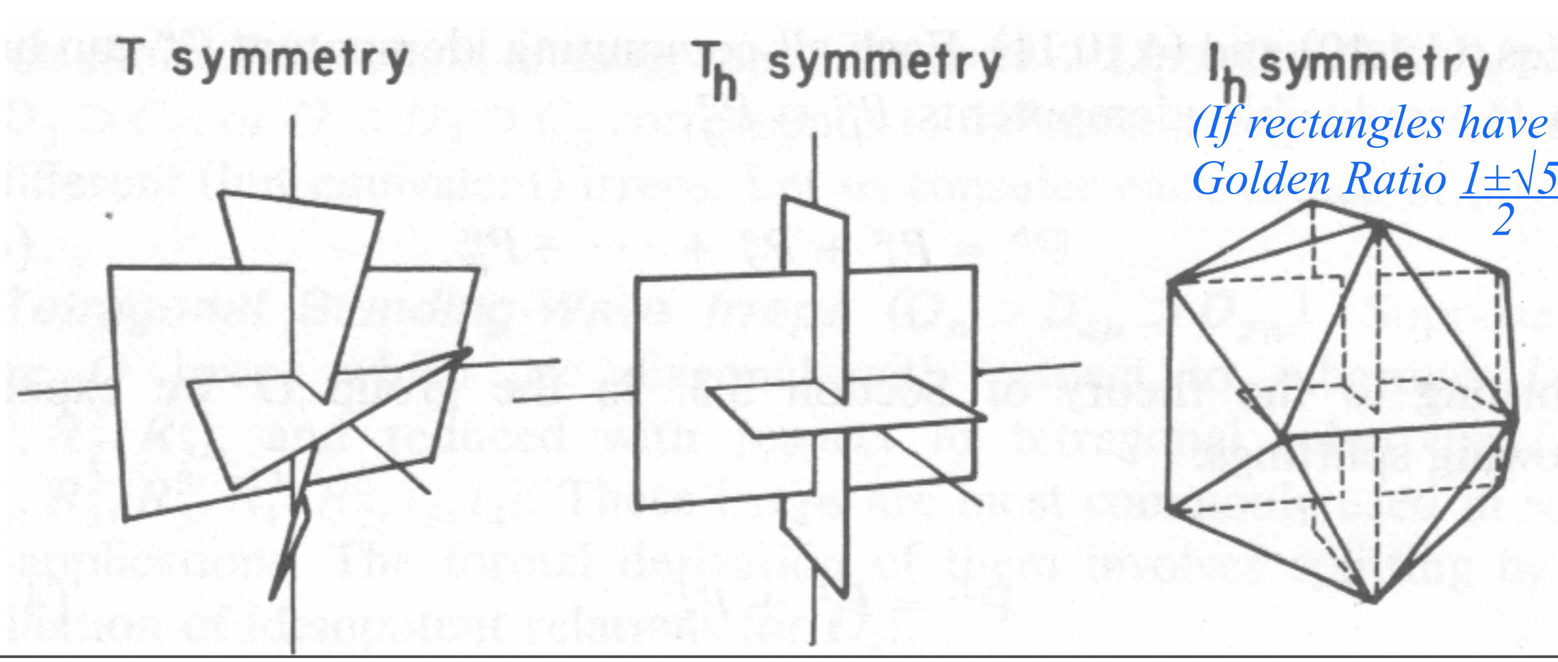
Introduction to octahedral/ tetrahedral symmetry $O_h \supset O \sim T_d \supset T$

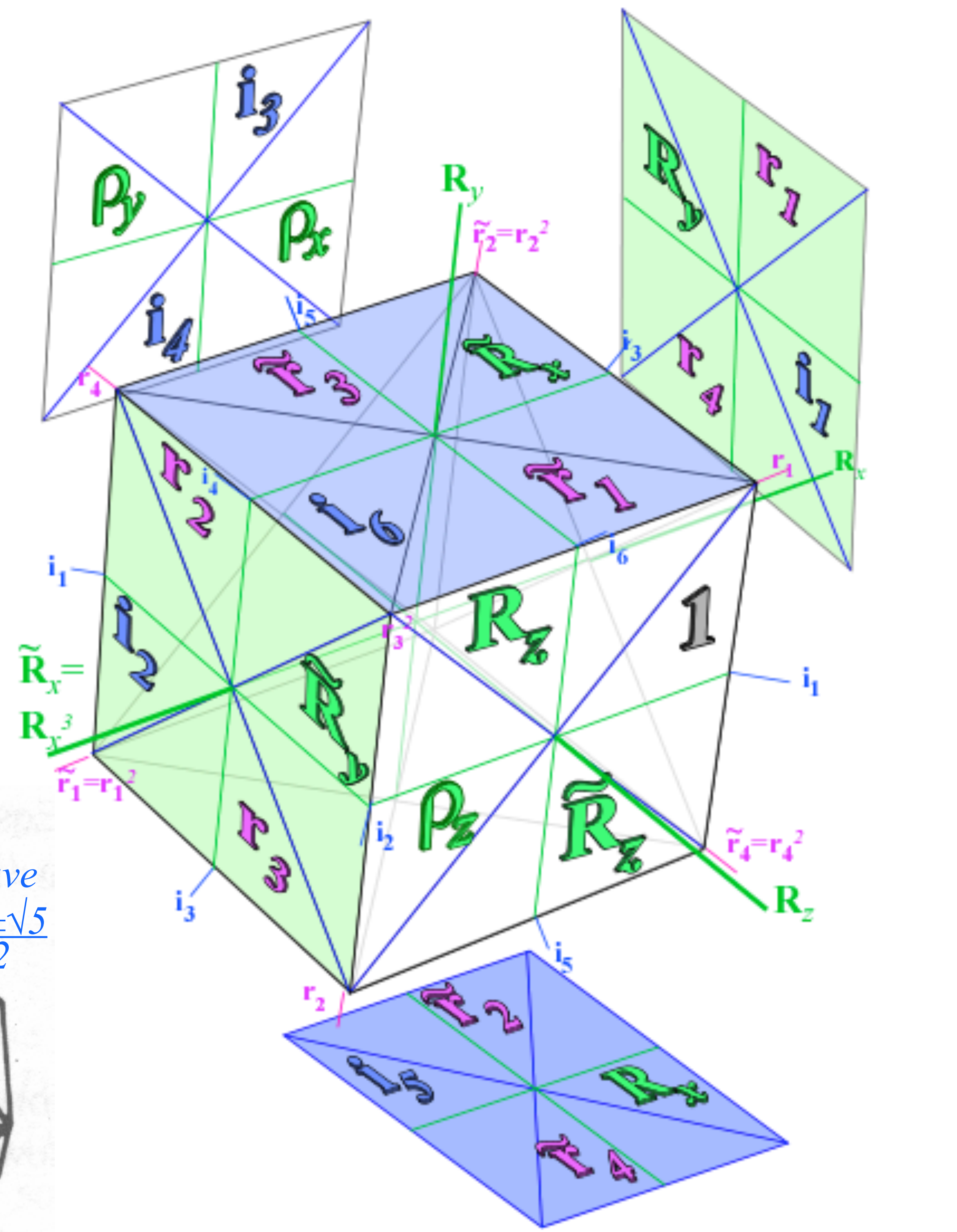
Octahedral-cubic O symmetry

Order °O=6 hexahedron squares · 4 pts =24
=8 octahedron triangles · 3 pts =24
=12 lines · 2 pts =24 positions









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

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

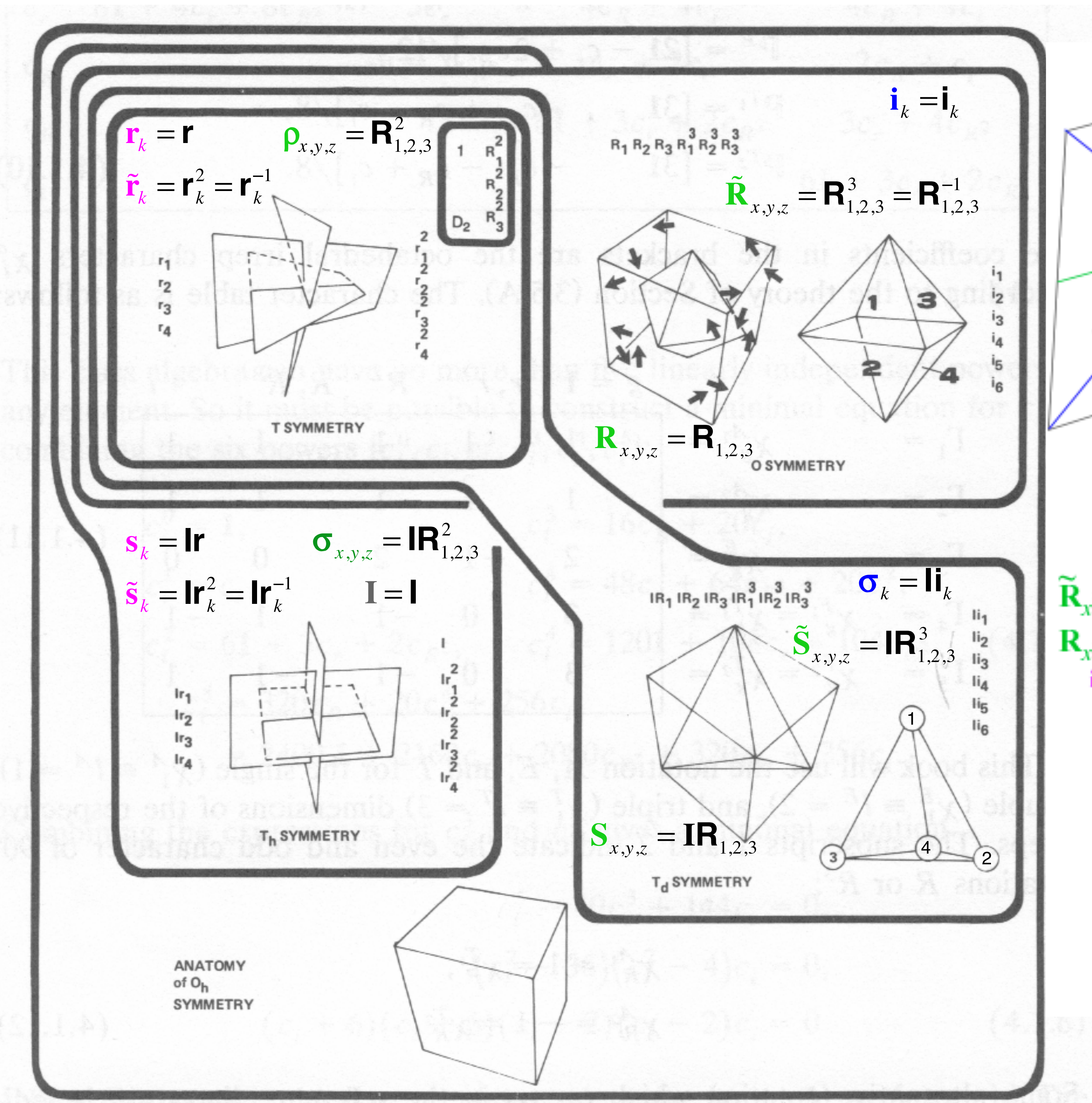


Figure 4.1.5 The full octahedral group (O_h) and four non-Abelian subgroups T, T_h, T_d, and O. The Abelian D_2 subgroup of T is indicated also.

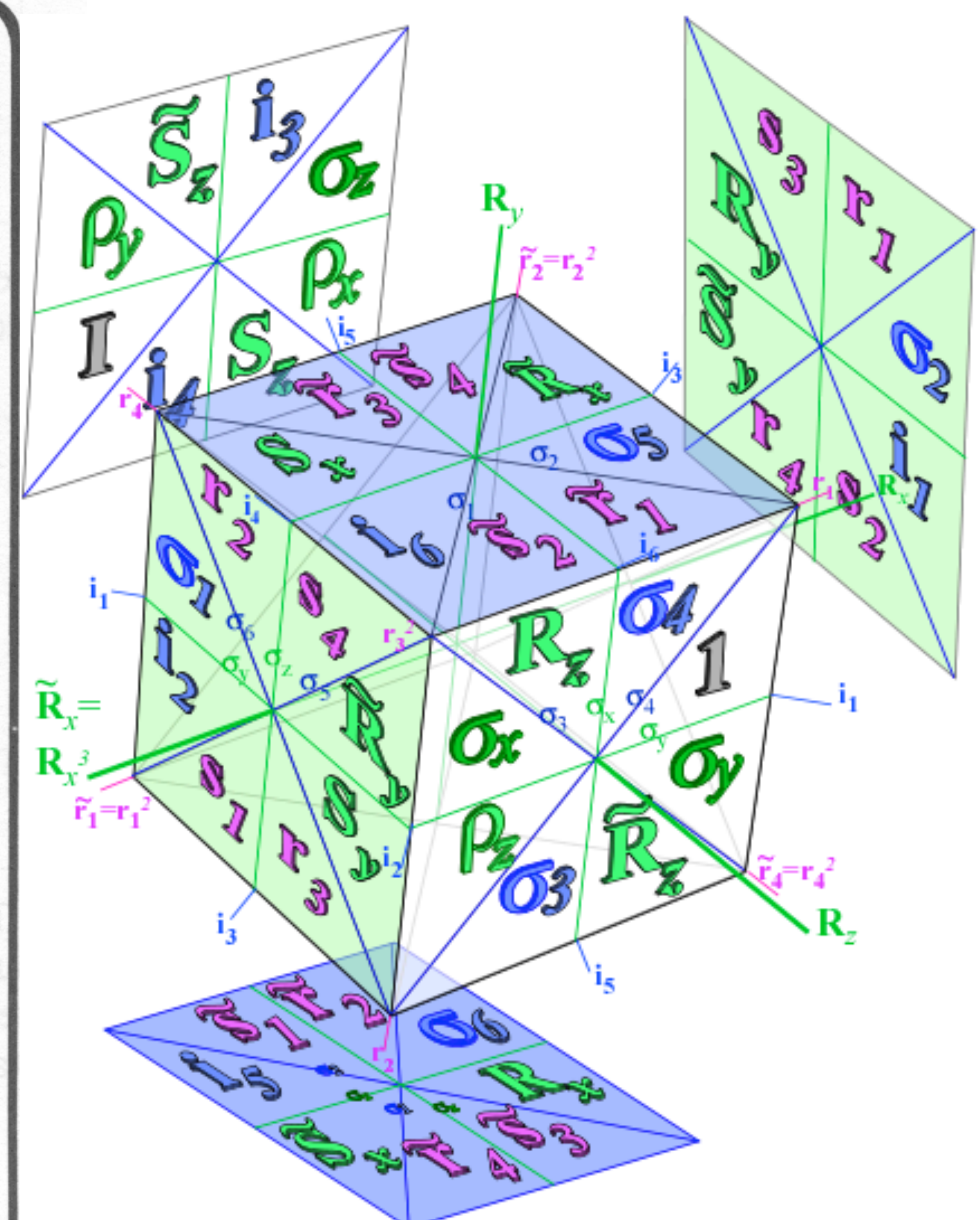
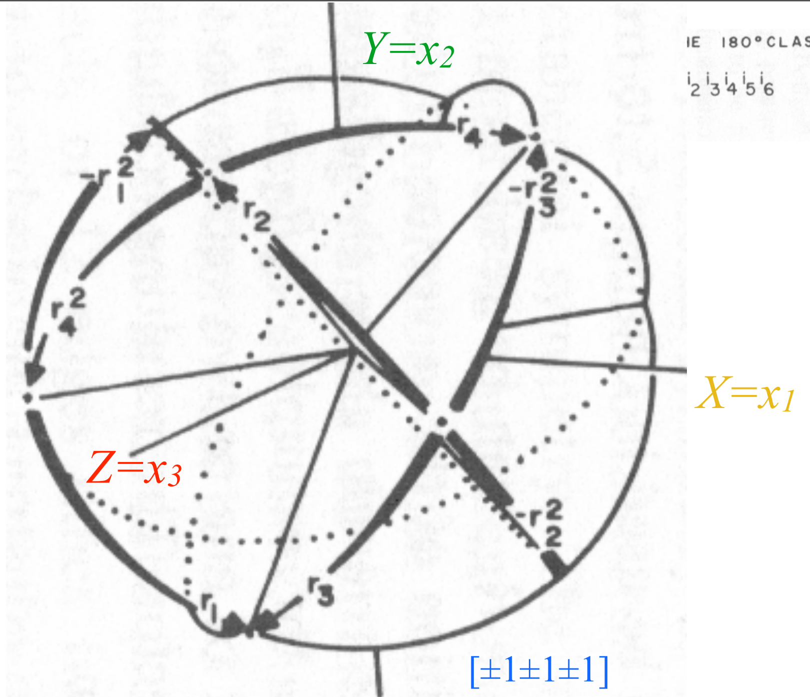
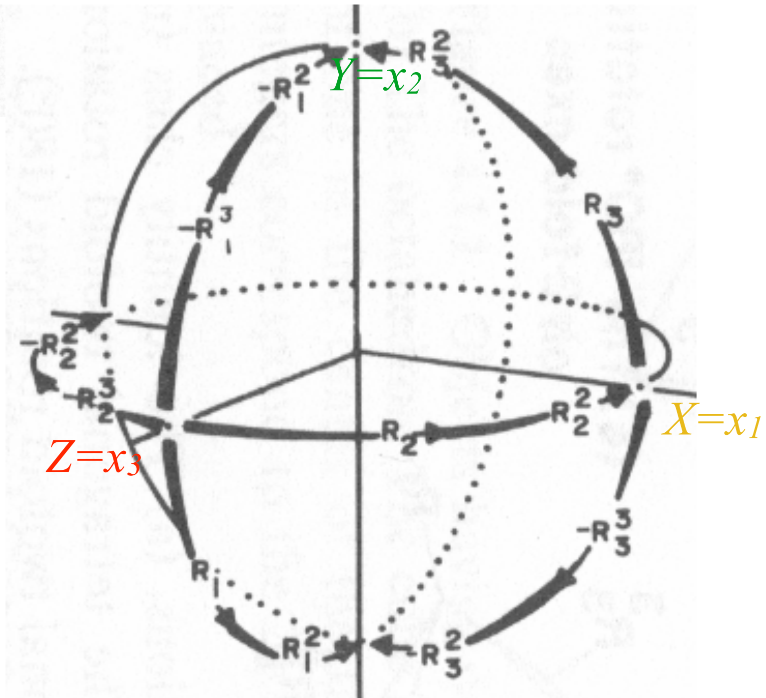
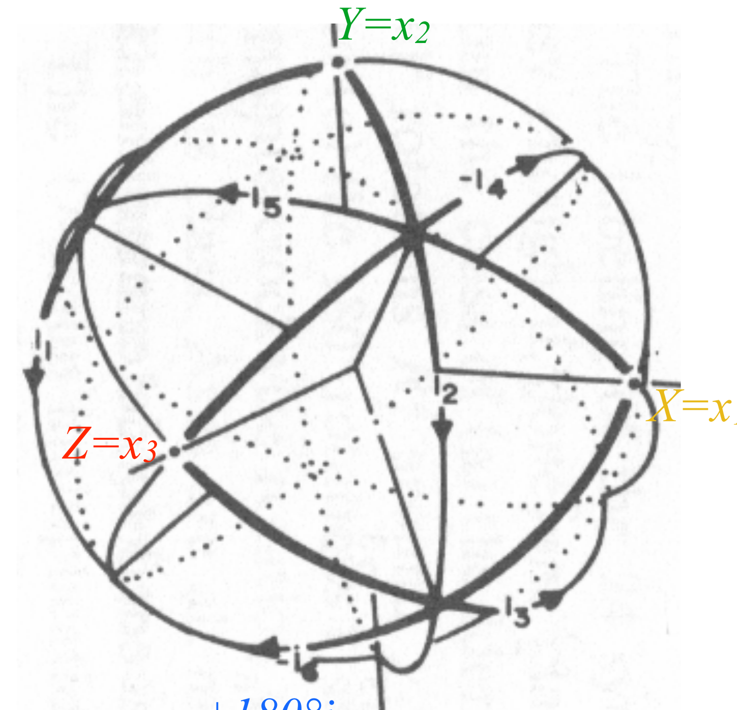


Fig. 4.1.5 from Principles of Symmetry, Dynamics and Spectroscopy







[±1±1±1] +120° -120° ±180° XYZ +90° XYZ -90° XYZ ±180° i_k

$[1\,1\,1][\bar{1}\,\bar{1}\,1][1\,\bar{1}\,\bar{1}][\bar{1}\,1\,\bar{1}]\;[\bar{1}\,\bar{1}\,\bar{1}][1\,1\,\bar{1}][\bar{1}\,1\,1][1\,\bar{1}\,1]\;[1\,0\,0][0\,1\,0][0\,0\,1]\;[1\,0\,0][0\,1\,0][0\,0\,1]\;[\bar{1}\,0\,0][0\,\bar{1}\,0][0\,0\,\bar{1}]\;[1\,0\,1][1\,0\,\bar{1}][1\,1\,0][1\,\bar{1}\,0][0\,1\,\bar{1}][0\,1\,1]$

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_3^2	$-r_2$	$-r_3$	$-r_4^2$	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	$-r_4^2$	$-R_3^2$	$-R_2^2$
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_2^3	$-r_3^2$	$-R_1^2$	$-r_3$	$-r_2^2$	$-R_3^2$	$-r_2$	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	$-R_2^3$	$-R_2$	$-R_3^3$	$-R_3$	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-O⊂U(2) rotation product Table F.2.1 from Principles of Symmetry, Dynamics and Spectroscopy