AMOP
reference links
on following page

3.12.18 class 17.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Discrete symmetry subgroups of $O(3)\supset$(Octahedral $O_h\supset O$): Part II Full $D^{(\alpha)}$-matrices defined by subgroup-chains $O\supset D_4\supset C_4$, D_2, or C_3 applied to eigensolutions of O_h-tensors $\mathbf{T}^{[4]}+\mathbf{T}^{[6]}$

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

Review Coset factored splitting of projectors for $O\supset D_4\supset C_4$ *into split classes and level structure*

Hamiltonian level cluster models with subgroup-defined tunneling parameters

Diagonal idempotent $\mathbf{P}^{\mu}_{m,m}$ *parameter sets for* $O\supset C_4$ *and* $O\supset C_3$ *case of* SF_6 *level clusters*

Off-diagonal nilpotent $\mathbf{P}^{\mu}_{m,n}$ $(m\neq n)$ *parameter sets needed for* $O\supset C_2$ *clusters*

Deriving nilpotent projectors $\mathbf{P}^{\mu}_{m,n}$ *and ireps* $D^{\mu}_{m,n}$ *by fundamental* $\mathbf{g}\rightleftarrows\mathbf{P}^{\mu}_{m,n}$ *relations:*

(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 nilpotent projectors for simple $D_3\supset C_2\sim C_{3v}\supset C_v$ *chains* *(Lect13p95)*

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

Structure and applications of coset tabulated $D^{\mu}_{m,n}$ *irreps for various* O_h *subgroup chains*

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

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 *cluster spectra of* O_h*-symmetric tensors* $\mathbf{T}^{[4]}+\mathbf{T}^{[6]}$

Monster clusters: When local C_2 *symmetry dominates*

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

Are these "accidents" or not?

AMOP reference links *(Updated list given on 2nd page of each class presentation)*

Web Resources - front page
UAF Physics UTube channel

Quantum Theory for the Computer Age
Principles of Symmetry, Dynamics, and Spectroscopy
Classical Mechanics with a Bang!
Modern Physics and its Classical Foundations

2014 AMOP
2017 Group Theory for QM
2018 AMOP

Frame Transformation Relations And Multipole Transitions In Symmetric Polyatomic Molecules - RMP-1978
Rotational energy surfaces and high- J eigenvalue structure of polyatomic molecules - Harter - Patterson - 1984
Galloping waves and their relativistic properties - aip-1985-Harter
Asymptotic eigensolutions of fourth and sixth rank octahedral tensor operators - Harter-Patterson-JMP-1979
Nuclear spin weights and gas phase spectral structure of 12C60 and 13C60 buckminsterfullerene -Harter-Reimer-Cpl-1992 - (Alt1, Alt2 Erratum)

Theory of hyperfine and superfine levels in symmetric polyatomic molecules.

- I) Trigonal and tetrahedral molecules: Elementary spin-1/2 cases in vibronic ground states - PRA-1979-Harter-Patterson (Alt scan)
- II) Elementary cases in octahedral hexafluoride molecules - Harter-PRA-1981 (Alt scan)

Rotation-vibration scalar coupling zeta coefficients and spectroscopic band shapes of buckminsterfullerene - Weeks-Harter-CPL-1991 (Alt scan)
Fullerene symmetry reduction and rotational level fine structure/ the Buckyball isotopomer 12C 13C59 - jcp-Reimer-Harter-1997 (HiRez)
Molecular Eigensolution Symmetry Analysis and Fine Structure - IJMS-harter-mitchell-2013

Rotation–vibration spectra of icosahedral molecules.

- I) Icosahedral symmetry analysis and fine structure - harter-weeks-jcp-1989
- II) Icosahedral symmetry, vibrational eigenfrequencies, and normal modes of buckminsterfullerene - weeks-harter-jcp-1989
- III) Half-integral angular momentum - harter-reimer-jcp-1991

QTCA Unit 10 Ch 30 - 2013
Molecular Symmetry and Dynamics - Ch32-Springer Handbooks of Atomic, Molecular, and Optical Physics - Harter-2006
AMOP Ch 0 Space-Time Symmetry - 2019

RESONANCE AND REVIVALS

- I) QUANTUM ROTOR AND INFINITE-WELL DYNAMICS - ISMSLi2012 (Talk) OSU knowledge Bank
- II) Comparing Half-integer Spin and Integer Spin - Alva-ISMS-Ohio2013-R777 (Talks)
- III) Quantum Resonant Beats and Revivals in the Morse Oscillators and Rotors - (2013-Li-Diss)

Rovibrational Spectral Fine Structure Of Icosahedral Molecules - Cpl 1986 (Alt Scan)
Gas Phase Level Structure of C60 Buckyball and Derivatives Exhibiting Broken Icosahedral Symmetry - reimer-diss-1996
Resonance and Revivals in Quantum Rotors - Comparing Half-integer Spin and Integer Spin - Alva-ISMS-Ohio2013-R777 (Talk)
Quantum Revivals of Morse Oscillators and Farey-Ford Geometry - Li-Harter-cpl-2013
Wave Node Dynamics and Revival Symmetry in Quantum Rotors - harter - jms - 2001

**In development - a web based A.M.O.P. oriented reference page, with thumbnail/previews, greater control over the information display, and eventually full on* Apache-SOLR *Index and search for* nuanced, whole-site content/metadata level *searching. This bad boy will be a sure force multiplier.*

AMOP reference links on page 2

3.12.18 class 17.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Discrete symmetry subgroups of O(3)⊃(Octahedral O_h⊃O): Part II Full $D^{(\alpha)}$-matrices defined by subgroup-chains $O\supset D_4\supset C_4$, D_2, or C_3 applied to eigensolutions of O_h-tensors $\mathbf{T}^{[4]}+\mathbf{T}^{[6]}$

Review *Idempotent projector splits* $\mathbf{P}^{\mu}_{m,m}$ *of* $O\supset C_4$ $\mathbf{P}^{E}_{0404}$ $\mathbf{P}^{E}_{2424}$ $\mathbf{P}^{T_1}_{0404}$ $\mathbf{P}^{T_1}_{1414}$ $\mathbf{P}^{T_2}_{2424}$ $\mathbf{P}^{T_2}_{1414}$

Review *Coset factored splitting of projectors for* $O\supset D_4\supset C_4$ *into split classes and level structure*

Hamiltonian level cluster models with subgroup-defined tunneling parameters

- *Diagonal idempotent* $\mathbf{P}^{\mu}_{m,m}$ *parameter sets for* $O\supset C_4$ *and* $O\supset C_3$ *case of* SF_6 *level clusters*
- *Off-diagonal nilpotent* $\mathbf{P}^{\mu}_{m,n}$ $(m\neq n)$ *parameter sets needed for* $O\supset C_2$ *clusters*

Deriving nilpotent projectors $\mathbf{P}^{\mu}_{m,n}$ *and ireps* $D^{\mu}_{m,n}$ *by fundamental* $\mathbf{g}\rightleftarrows\mathbf{P}^{\mu}_{m,n}$ *relations:*

(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 nilpotent projectors for simple* $D_3\supset C_2\sim C_{3v}\supset C_v$ *chains* (Lect13p95)
- *Calculating and Factoring* $\mathbf{P}^{T_1}_{1404}$ *and* $\mathbf{P}^{T_1}_{1434}$

Structure and applications of coset tabulated $D^{\mu}_{m,n}$ *irreps for various* O_h *subgroup chains*

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

- *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}_{0424}
- *Comparing local* C_4, C_3, *and* C_2 *cluster spectra of* O_h*-symmetric tensors* $\mathbf{T}^{[4]}+\mathbf{T}^{[6]}$
  - *Monster clusters: When local* C_2 *symmetry dominates*

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

Are these "accidents" or not?

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

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

$$= \sum_{g}^{\circ O} \frac{\ell^{E}}{\circ O} (\chi^{E*}_{g}) \cdot \mathbf{g} \cdot \left(\mathbf{p}_{0_4}\right) \longrightarrow$$

$$= \sum_{g}^{\circ O} \frac{2}{96} (\chi^{E*}_{g}) \cdot \mathbf{g} \cdot \left(1 \cdot \mathbf{1} + 1 \cdot \rho_z + 1 \cdot \mathbf{R}_z + 1 \cdot \tilde{\mathbf{R}}_z \right)$$

$O \supset C_4$	0_4	1_4	2_4	3_4
$A_1 \downarrow C_4$	1	·	·	·
$A_2 \downarrow C_4$	·	·	1	·
$E \downarrow C_4$	$\boxed{1}$	·	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

C4 characters

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

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

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

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

1/48(	$4\mathbf{1}$	$4\rho_z$	$4\mathbf{R}_z$	$4\tilde{\mathbf{R}}_z$
2·(	+1	+1	+1	+1)
$\mathbf{1}$	$\mathbf{1}$	ρ_z	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$
2·(	+1	+1	+1	+1)
ρ_z	ρ_z	$\mathbf{1}$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$
0·(	+1	+1	+1	+1)
$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$	$\mathbf{1}$	ρ_z
0·(	+1	+1	+1	+1)
$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$	ρ_z	$\mathbf{1}$

	$4\rho_x$	$4\rho_y$	$4\,\mathbf{i}_4$	$4\,\mathbf{i}_3$
+2·(	+1	+1	+1	+1)
ρ_x	$\mathbf{1}$	ρ_z	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$
+2·(	+1	+1	+1	+1)
ρ_y	ρ_z	$\mathbf{1}$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$
+0·(	+1	+1	+1	+1)
$\mathbf{i}_4$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$	$\mathbf{1}$	ρ_z
+0·(	+1	+1	+1	+1)
$\mathbf{i}_3$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$	ρ_z	$\mathbf{1}$

	$-2\mathbf{r}_1$	$-2\mathbf{r}_4$	$-2\mathbf{i}_1$	$-2\mathbf{R}_y$
-1·(	+1	+1	+1	+1)
$\mathbf{r}_1$	$\mathbf{1}$	ρ_z	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$
-1·(	+1	+1	+1	+1)
$\mathbf{r}_4$	ρ_z	$\mathbf{1}$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$
+0·(	+1	+1	+1	+1)
$\mathbf{i}_1$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$	$\mathbf{1}$	ρ_z
+0·(	+1	+1	+1	+1)
$\mathbf{R}_y$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$	ρ_z	$\mathbf{1}$

	$-2\mathbf{r}_2$	$-2\mathbf{r}_3$	$-2\mathbf{i}_2$	$-2\tilde{\mathbf{R}}_y$
-1·(	+1	+1	+1	+1)
$\mathbf{r}_2$	$\mathbf{1}$	ρ_z	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$
-1·(	+1	+1	+1	+1)
$\mathbf{r}_3$	ρ_z	$\mathbf{1}$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$
+0·(	+1	+1	+1	+1)
$\mathbf{i}_2$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$	$\mathbf{1}$	ρ_z
+0·(	+1	+1	+1	+1)
$\tilde{\mathbf{R}}_y$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$	ρ_z	$\mathbf{1}$

	$-2\tilde{\mathbf{r}}_1$	$-2\tilde{\mathbf{r}}_3$	$-2\tilde{\mathbf{R}}_x$	$-2\,\mathbf{i}_6$
-1·(	+1	+1	+1	+1)
$\tilde{\mathbf{r}}_1$	$\mathbf{1}$	ρ_z	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$
-1·(	+1	+1	+1	+1)
$\tilde{\mathbf{r}}_3$	ρ_z	$\mathbf{1}$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$
+0·(	+1	+1	+1	+1)
$\tilde{\mathbf{R}}_x$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$	$\mathbf{1}$	ρ_z
+0·(	+1	+1	+1	+1)
$\mathbf{i}_6$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$	ρ_z	$\mathbf{1}$

	$-2\tilde{\mathbf{r}}_2$	$-2\tilde{\mathbf{r}}_4$	$-2\mathbf{R}_x$	$-2\,\mathbf{i}_5$)
-1·(	+1	+1	+1	+1)
$\tilde{\mathbf{r}}_2$	$\mathbf{1}$	ρ_z	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$
-1·(	+1	+1	+1	+1)
$\tilde{\mathbf{r}}_4$	ρ_z	$\mathbf{1}$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$
+0·(	+1	+1	+1	+1)
$\mathbf{R}_x$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$	$\mathbf{1}$	ρ_z
+0·(	+1	+1	+1	+1)
$\mathbf{i}_5$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$	ρ_z	$\mathbf{1}$

$\mathbf{i}_5 = \mathbf{g}\mathbf{R}^{p}$-coefficient is its column sum $\sum_{g}^{\circ O} \frac{\ell^{E}}{\circ O}(\chi^{E*}_{g}) \cdot \mathbf{g}\mathbf{R}^{p} \cdot d^{*m_4}_{R^p}$ of products $\frac{\ell^{E}}{\circ O}(\chi^{E*}_{g}) d^{*m_4}_{R^p}$

Coset-factored sum:

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

Split-classes-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 $\mathbf{P}^{E}{}_{2_4 2_4}$

$$\mathbf{P}^{E}_{2_42_4} = \mathbf{p}_{2_4}\mathbf{P}^{E} = \mathbf{P}^{E}\mathbf{p}_{2_4}$$

$$= \sum_{g}^{\circ O} \frac{\ell^{E}}{\circ O}(\chi_g^{E*})\cdot\mathbf{g}\cdot\left(\mathbf{p}_{2_4}\right)$$

$$= \sum_{g}^{\circ O} \frac{2}{96}(\chi_g^{E*})\cdot\mathbf{g}\cdot\left(1\cdot\mathbf{1}+1\cdot\boldsymbol{\rho}_z-1\cdot\mathbf{R}_z-1\cdot\tilde{\mathbf{R}}_z\right)$$

$O\supset C_4$	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	$\mathbf{r}^{p}_{1-4}$	$\boldsymbol{\rho}_{xyz}$	$\mathbf{R}^{p}_{xyz}$	$\mathbf{i}_{1-6}$
$\mu=A_1$	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

C_4 characters

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

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

$$\mathbf{P}^{E}_{2_42_4}=$$

$$\tfrac{1}{12}(1\mathbf{1}+1\boldsymbol{\rho}_z\text{-}1\mathbf{R}_z\text{-}1\tilde{\mathbf{R}}_z \quad +1\boldsymbol{\rho}_x+1\boldsymbol{\rho}_y\text{-}1\mathbf{i}_4\text{-}1\mathbf{i}_3 \quad \text{-}\tfrac{1}{2}\mathbf{r}_1\text{-}\tfrac{1}{2}\mathbf{r}_4+\tfrac{1}{2}\mathbf{i}_1+\tfrac{1}{2}\mathbf{R}_y \quad \text{-}\tfrac{1}{2}\mathbf{r}_2\text{-}\tfrac{1}{2}\mathbf{r}_3+\tfrac{1}{2}\mathbf{i}_2+\tfrac{1}{2}\tilde{\mathbf{R}}_y \quad \text{-}\tfrac{1}{2}\tilde{\mathbf{r}}_1\text{-}\tfrac{1}{2}\tilde{\mathbf{r}}_3+\tfrac{1}{2}\tilde{\mathbf{R}}_x+\tfrac{1}{2}\mathbf{i}_6 \quad \text{-}\tfrac{1}{2}\tilde{\mathbf{r}}_2\text{-}\tfrac{1}{2}\tilde{\mathbf{r}}_4+\tfrac{1}{2}\mathbf{R}_x+\tfrac{1}{2}\mathbf{i}_5)$$

1/48(	$4\mathbf{1}$	$4\boldsymbol{\rho}_z$	$4\mathbf{R}_z$	$4\tilde{\mathbf{R}}_z$
2·(	+1	+1	-1	-1)
$\mathbf{1}$	$\mathbf{1}$	$\boldsymbol{\rho}_z$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$
2·(	+1	+1	-1	-1)
$\boldsymbol{\rho}_z$	$\boldsymbol{\rho}_z$	$\mathbf{1}$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$
0·(	-1	-1	+1	+1)
$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$	$\mathbf{1}$	$\boldsymbol{\rho}_z$
0·(	-1	-1	+1	+1)
$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$	$\boldsymbol{\rho}_z$	$\mathbf{1}$

	$4\boldsymbol{\rho}_x$	$4\boldsymbol{\rho}_y$	$-4\,\mathbf{i}_4$	$-4\mathbf{i}_3$
+2· (	+1	+1	-1	-1)
$\boldsymbol{\rho}_x$	$\mathbf{1}$	$\boldsymbol{\rho}_z$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$
+2· (	+1	+1	-1	-1)
$\boldsymbol{\rho}_y$	$\boldsymbol{\rho}_z$	$\mathbf{1}$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$
+0· (	-1	-1	+1	+1)
$\mathbf{i}_4$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$	$\mathbf{1}$	$\boldsymbol{\rho}_z$
+0· (	-1	-1	+1	+1)
$\mathbf{i}_3$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$	$\boldsymbol{\rho}_z$	$\mathbf{1}$

	$-2\mathbf{r}_1$	$-2\mathbf{r}_4$	$+2\mathbf{i}_1$	$+2.\mathbf{R}_y$
-1· (	+1	+1	-1	-1)
$\mathbf{r}_1$	$\mathbf{1}$	$\boldsymbol{\rho}_z$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$
-1· (	+1	+1	-1	-1)
$\mathbf{r}_4$	$\boldsymbol{\rho}_z$	$\mathbf{1}$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$
+0· (	-1	-1	+1	+1)
$\mathbf{i}_1$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$	$\mathbf{1}$	$\boldsymbol{\rho}_z$
+0· (	-1	-1	+1	+1)
$\mathbf{R}_y$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$	$\boldsymbol{\rho}_z$	$\mathbf{1}$

	$-2.\mathbf{r}_2$	$-2.\mathbf{r}_3$	$+2.\mathbf{i}_2$	$+2.\tilde{\mathbf{R}}_y$
-1· (	+1	+1	-1	-1)
$\mathbf{r}_2$	$\mathbf{1}$	$\boldsymbol{\rho}_z$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$
-1· (	+1	+1	-1	-1)
$\mathbf{r}_3$	$\boldsymbol{\rho}_z$	$\mathbf{1}$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$
+0· (	-1	-1	+1	+1)
$\mathbf{i}_2$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$	$\mathbf{1}$	$\boldsymbol{\rho}_z$
+0· (	-1	-1	+1	+1)
$\tilde{\mathbf{R}}_y$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$	$\boldsymbol{\rho}_z$	$\mathbf{1}$

	$-2.\tilde{\mathbf{r}}_1$	$-2.\tilde{\mathbf{r}}_3$	$+2\tilde{\mathbf{R}}_x$	$+2\mathbf{i}_6$
-1· (	+1	+1	-1	-1)
$\tilde{\mathbf{r}}_1$	$\mathbf{1}$	$\boldsymbol{\rho}_z$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$
-1· (	+1	+1	-1	-1)
$\tilde{\mathbf{r}}_3$	$\boldsymbol{\rho}_z$	$\mathbf{1}$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$
+0· (	-1	-1	+1	+1)
$\tilde{\mathbf{R}}_x$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$	$\mathbf{1}$	$\boldsymbol{\rho}_z$
+0· (	-1	-1	+1	+1)
$\mathbf{i}_6$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$	$\boldsymbol{\rho}_z$	$\mathbf{1}$

	$-2.\tilde{\mathbf{r}}_2$	$-2.\tilde{\mathbf{r}}_4$	$+2\mathbf{R}_x$	$+2\,\mathbf{i}_5$)
-1· (	+1	+1	-1	-1)
$\tilde{\mathbf{r}}_2$	$\mathbf{1}$	$\boldsymbol{\rho}_z$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$
-1· (	+1	+1	-1	-1)
$\tilde{\mathbf{r}}_4$	$\boldsymbol{\rho}_z$	$\mathbf{1}$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$
+0· (	-1	-1	+1	+1)
$\mathbf{R}_x$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$	$\mathbf{1}$	$\boldsymbol{\rho}_z$
+0· (	-1	-1	+1	+1)
$\mathbf{i}_5$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$	$\boldsymbol{\rho}_z$	$\mathbf{1}$

Coset-factored sum:

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

Split-classes-ordered sum:

$$\mathbf{P}^{E}_{2_42_4}=\tfrac{1}{12}(1\cdot\mathbf{1} \quad \text{-}\tfrac{1}{2}\mathbf{r}_1\text{-}\tfrac{1}{2}\mathbf{r}_2 \quad \text{-}\tfrac{1}{2}\mathbf{r}_3\text{-}\tfrac{1}{2}\mathbf{r}_4 \quad \text{-}\tfrac{1}{2}\tilde{\mathbf{r}}_1\text{-}\tfrac{1}{2}\tilde{\mathbf{r}}_2 \quad \text{-}\tfrac{1}{2}\tilde{\mathbf{r}}_3\text{-}\tfrac{1}{2}\tilde{\mathbf{r}}_4 \quad +1\boldsymbol{\rho}_x+1\boldsymbol{\rho}_y+1\boldsymbol{\rho}_z \quad +\tfrac{1}{2}\mathbf{R}_x+\tfrac{1}{2}\mathbf{R}_y-1\mathbf{R}_z \quad +\tfrac{1}{2}\tilde{\mathbf{R}}_x+\tfrac{1}{2}\tilde{\mathbf{R}}_y-1\tilde{\mathbf{R}}_z \quad +\tfrac{1}{2}\mathbf{i}_1+\tfrac{1}{2}\mathbf{i}_2 \quad -1\mathbf{i}_3-1\mathbf{i}_4 \quad +\tfrac{1}{2}\mathbf{i}_5+\tfrac{1}{2}\mathbf{i}_6)$$

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

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

$$= \sum_{g}^{°O} \frac{\ell^{T_1^*}}{°O} (\chi_g^{T_1^*}) \cdot \mathbf{g} \cdot \left(\mathbf{p}_{2_4}\right) \longrightarrow$$

$$= \sum_{g}^{°O} \frac{3}{96} (\chi_g^{T_1^*}) \cdot \mathbf{g} \cdot \left(1 \cdot \mathbf{1} + 1 \cdot \boldsymbol{\rho}_z + 1 \cdot \mathbf{R}_z + 1 \cdot \tilde{\mathbf{R}}_z \right)$$

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

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

O characters

$$\underbrace{C_4 \textit{ characters}}$$

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

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

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

$$\tfrac{1}{8}\big(1 \cdot \mathbf{1} + 1 \cdot \boldsymbol{\rho}_z + 1 \cdot \mathbf{R}_z + 1 \cdot \tilde{\mathbf{R}}_z \quad - 1 \cdot \boldsymbol{\rho}_x - 1 \cdot \boldsymbol{\rho}_y - 1 \cdot \mathbf{i}_4 - 1 \cdot \mathbf{i}_3 \quad + 0 \cdot \mathbf{r}_1 + 0 \cdot \mathbf{r}_4 + 0 \cdot \mathbf{i}_1 + 0 \cdot \mathbf{R}_y \quad + 0 \cdot \mathbf{r}_2 + 0 \cdot \mathbf{r}_3 + 0 \cdot \mathbf{i}_2 + 0 \cdot \tilde{\mathbf{R}}_y \quad + 0 \cdot \tilde{\mathbf{r}}_1 + 0 \cdot \tilde{\mathbf{r}}_3 + 0 \cdot \tilde{\mathbf{R}}_x + 0 \cdot \mathbf{i}_6 \quad + 0 \cdot \tilde{\mathbf{r}}_2 + 0 \cdot \tilde{\mathbf{r}}_4 + 0 \cdot \mathbf{R}_x + 0 \cdot \mathbf{i}_5\big)$$

1/32(	+4 $\mathbf{1}$	+4 $\boldsymbol{\rho}_z$	+4 $\mathbf{R}_z$	+4 $\tilde{\mathbf{R}}_z$
+3·(	+1	+1	+1	+1)
$\mathbf{1}$	$\mathbf{1}$	$\boldsymbol{\rho}_z$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$
-1·(	+1	+1	+1	+1)
$\boldsymbol{\rho}_z$	$\boldsymbol{\rho}_z$	$\mathbf{1}$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$
+1·(	+1	+1	+1	+1)
$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$	$\mathbf{1}$	$\boldsymbol{\rho}_z$
+1·(	+1	+1	+1	+1)
$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$	$\boldsymbol{\rho}_z$	$\mathbf{1}$

	-4 $\boldsymbol{\rho}_x$	-4 $\boldsymbol{\rho}_y$	-4 $\mathbf{i}_4$	-4 $\mathbf{i}_3$
-1·(	+1	+1	+1	+1)
$\boldsymbol{\rho}_x$	$\mathbf{1}$	$\boldsymbol{\rho}_z$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$
-1·(	+1	+1	+1	+1)
$\boldsymbol{\rho}_y$	$\boldsymbol{\rho}_z$	$\mathbf{1}$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$
-1·(	+1	+1	+1	+1)
$\mathbf{i}_4$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$	$\mathbf{1}$	$\boldsymbol{\rho}_z$
-1·(	+1	+1	+1	+1)
$\mathbf{i}_3$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$	$\boldsymbol{\rho}_z$	$\mathbf{1}$

	0 $\mathbf{r}_1$	0 $\mathbf{r}_4$	0 $\mathbf{i}_1$	0.$\mathbf{R}_y$
0 (	+1	+1	+1	+1)
$\mathbf{r}_1$	$\mathbf{1}$	$\boldsymbol{\rho}_z$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$
0 (	+1	+1	+1	+1)
$\mathbf{r}_4$	$\boldsymbol{\rho}_z$	$\mathbf{1}$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$
-1·(	+1	+1	+1	+1)
$\mathbf{i}_1$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$	$\mathbf{1}$	$\boldsymbol{\rho}_z$
+1·(	+1	+1	+1	+1)
$\mathbf{R}_y$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$	$\boldsymbol{\rho}_z$	$\mathbf{1}$

	0 $\mathbf{r}_2$	0 $\mathbf{r}_3$	0 $\mathbf{i}_2$	0 $\tilde{\mathbf{R}}_y$
0 (	+1	+1	+1	+1)
$\mathbf{r}_2$	$\mathbf{1}$	$\boldsymbol{\rho}_z$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$
0 (	+1	+1	+1	+1)
$\mathbf{r}_3$	$\boldsymbol{\rho}_z$	$\mathbf{1}$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$
-1·(	+1	+1	+1	+1)
$\mathbf{i}_2$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$	$\mathbf{1}$	$\boldsymbol{\rho}_z$
+1·(	+1	+1	+1	+1)
$\tilde{\mathbf{R}}_y$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$	$\boldsymbol{\rho}_z$	$\mathbf{1}$

	0 $\tilde{\mathbf{r}}_1$	0 $\tilde{\mathbf{r}}_3$	0.$\tilde{\mathbf{R}}_x$	0 $\mathbf{i}_6$
0 (	+1	+1	+1	+1)
$\tilde{\mathbf{r}}_1$	$\mathbf{1}$	$\boldsymbol{\rho}_z$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$
0 (	+1	+1	+1	+1)
$\tilde{\mathbf{r}}_3$	$\boldsymbol{\rho}_z$	$\mathbf{1}$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$
+1·(	+1	+1	+1	+1)
$\tilde{\mathbf{R}}_x$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$	$\mathbf{1}$	$\boldsymbol{\rho}_z$
-1·(	+1	+1	+1	+1)
$\mathbf{i}_6$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$	$\boldsymbol{\rho}_z$	$\mathbf{1}$

	0 $\tilde{\mathbf{r}}_2$	0 $\tilde{\mathbf{r}}_4$	0 $\mathbf{R}_x$	0 $\mathbf{i}_5$)
0 (	+1	+1	+1	+1)
$\tilde{\mathbf{r}}_2$	$\mathbf{1}$	$\boldsymbol{\rho}_z$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$
0 (	+1	+1	+1	+1)
$\tilde{\mathbf{r}}_4$	$\boldsymbol{\rho}_z$	$\mathbf{1}$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$
+1·(	+1	+1	+1	+1)
$\mathbf{R}_x$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$	$\mathbf{1}$	$\boldsymbol{\rho}_z$
-1·(	+1	+1	+1	+1)
$\mathbf{i}_5$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$	$\boldsymbol{\rho}_z$	$\mathbf{1}$

Coset-factored sum:

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

Split-classes-ordered sum:

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

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

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

$$= \sum_g^{\circ O} \frac{\ell^{T_1^*}}{\circ O}(\chi_g^{T_1^*})\cdot\mathbf{g}\cdot\left(\mathbf{p}_{1_4}\right) \longrightarrow$$

$$= \sum_g^{\circ O} \frac{3}{96}(\chi_g^{T_1^*})\cdot\mathbf{g}\cdot\left(1\cdot\mathbf{1} - i\cdot\boldsymbol{\rho}_z - 1\cdot\mathbf{R}_z + i\cdot\tilde{\mathbf{R}}_z \right)$$

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

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

O characters

C4 characters

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

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

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

$\frac{1}{8}(1\cdot\mathbf{1} - 1\cdot\boldsymbol{\rho}_z - i\cdot\mathbf{R}_z + i\cdot\tilde{\mathbf{R}}_z$

1/32(	$+4\,\mathbf{1}$	$-4\,\boldsymbol{\rho}_z$	$-4i\,\mathbf{R}_z$	$+4i\,\tilde{\mathbf{R}}_z$
+3·(	+1	-1	$-i$	$+i$)
$\mathbf{1}$	$\mathbf{1}$	$\boldsymbol{\rho}_z$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$
-1·(	-1	+1	$+i$	$-i$)
$\boldsymbol{\rho}_z$	$\boldsymbol{\rho}_z$	$\mathbf{1}$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$
+1·(	$+i$	$-i$	+1	-1)
$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$	$\mathbf{1}$	$\boldsymbol{\rho}_z$
+1·(	$-i$	$+i$	-1	+1)
$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$	$\boldsymbol{\rho}_z$	$\mathbf{1}$

$-0\boldsymbol{\rho}_x - 0\boldsymbol{\rho}_y - 0\mathbf{i}_4 - 0\mathbf{i}_3$

	$-0\boldsymbol{\rho}_x$	$-0\boldsymbol{\rho}_y$	$-0\,\mathbf{i}_4$	$-0\,\mathbf{i}_3$
-1·(	+1	-1	$-i$	$+i$)
$\boldsymbol{\rho}_x$	$\mathbf{1}$	$\boldsymbol{\rho}_z$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$
-1·(	-1	+1	$+i$	$-i$)
$\boldsymbol{\rho}_y$	$\boldsymbol{\rho}_z$	$\mathbf{1}$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$
-1·(	$+i$	$-i$	+1	-1)
$\mathbf{i}_4$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$	$\mathbf{1}$	$\boldsymbol{\rho}_z$
-1·(	$-i$	$+i$	-1	+1)
$\mathbf{i}_3$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$	$\boldsymbol{\rho}_z$	$\mathbf{1}$

$-\frac{i}{2}\cdot\mathbf{r}_1 + \frac{i}{2}\cdot\mathbf{r}_4 - \frac{1}{2}\cdot\mathbf{i}_1 + \frac{1}{2}\cdot\mathbf{R}_y$

	$-2i\,\mathbf{r}_1$	$+2i\,\mathbf{r}_4$	$-2\,\mathbf{i}_1$	$+2\,\mathbf{R}_y$
0 (	+1	-1	$-i$	$+i$)
$\mathbf{r}_1$	$\mathbf{1}$	$\boldsymbol{\rho}_z$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$
0 (	-1	+1	$+i$	$-i$)
$\mathbf{r}_4$	$\boldsymbol{\rho}_z$	$\mathbf{1}$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$
-1 · (	$+i$	$-i$	+1	-1)
$\mathbf{i}_1$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$	$\mathbf{1}$	$\boldsymbol{\rho}_z$
+1·(	$-i$	$+i$	-1	+1)
$\mathbf{R}_y$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$	$\boldsymbol{\rho}_z$	$\mathbf{1}$

$-\frac{i}{2}\cdot\mathbf{r}_2 + \frac{i}{2}\cdot\mathbf{r}_3 - \frac{1}{2}\cdot\mathbf{i}_2 + \frac{1}{2}\cdot\tilde{\mathbf{R}}_y$

	$-2i\,\mathbf{r}_2$	$+2i\,\mathbf{r}_3$	$-2\,\mathbf{i}_2$	$+2\,\tilde{\mathbf{R}}_y$
0 (	+1	-1	$-i$	$+i$)
$\mathbf{r}_2$	$\mathbf{1}$	$\boldsymbol{\rho}_z$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$
0 (	-1	+1	$+i$	$-i$)
$\mathbf{r}_3$	$\boldsymbol{\rho}_z$	$\mathbf{1}$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$
-1 · (	$+i$	$-i$	+1	-1)
$\mathbf{i}_2$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$	$\mathbf{1}$	$\boldsymbol{\rho}_z$
+1·(	$-i$	$+i$	-1	+1)
$\tilde{\mathbf{R}}_y$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$	$\boldsymbol{\rho}_z$	$\mathbf{1}$

$+\frac{i}{2}\cdot\tilde{\mathbf{r}}_1 - \frac{i}{2}\cdot\tilde{\mathbf{r}}_3 + \frac{1}{2}\cdot\tilde{\mathbf{R}}_x - \frac{1}{2}\cdot\mathbf{i}_6$

	$+2i\,\tilde{\mathbf{r}}_1$	$-2i\,\tilde{\mathbf{r}}_3$	$+2\,\tilde{\mathbf{R}}_x$	$-2\,\mathbf{i}_6$
0 (	+1	-1.	$-i$	$+i$)
$\tilde{\mathbf{r}}_1$	$\mathbf{1}$	$\boldsymbol{\rho}_z$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$
0 (	-1	+1	$+i$	$-i$)
$\tilde{\mathbf{r}}_3$	$\boldsymbol{\rho}_z$	$\mathbf{1}$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$
+1·(	$+i$	$-i$	+1	-1)
$\tilde{\mathbf{R}}_x$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$	$\mathbf{1}$	$\boldsymbol{\rho}_z$
-1 · (	$-i$	$+i$	-1	+1)
$\mathbf{i}_6$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$	$\boldsymbol{\rho}_z$	$\mathbf{1}$

$+\frac{i}{2}\cdot\tilde{\mathbf{r}}_2 - \frac{i}{2}\cdot\tilde{\mathbf{r}}_4 + \frac{1}{2}\cdot\mathbf{R}_x - \frac{1}{2}\cdot\mathbf{i}_5)$

	$+2i\,\tilde{\mathbf{r}}_2$	$-2i\,\tilde{\mathbf{r}}_4$	$+2\,\mathbf{R}_x$	$-2\,\mathbf{i}_5$)
0 (	+1	-1	$-i$	$+i$)
$\tilde{\mathbf{r}}_2$	$\mathbf{1}$	$\boldsymbol{\rho}_z$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$
0 (	-1	+1	$+i$	$-i$)
$\tilde{\mathbf{r}}_4$	$\boldsymbol{\rho}_z$	$\mathbf{1}$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$
+1·(	$+i$	$-i$	+1	-1)
$\mathbf{R}_x$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$	$\mathbf{1}$	$\boldsymbol{\rho}_z$
-1 · (	$-i$	$+i$	-1	+1)
$\mathbf{i}_5$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$	$\boldsymbol{\rho}_z$	$\mathbf{1}$

Coset-factored sum:

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

Split-classes-ordered sum:

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

Calculating $\mathbf{P}^{T_2}{}_{2_42_4}$

$$\mathbf{P}^{T_2}_{2_42_4}=\mathbf{p}_{2_4}\mathbf{P}^{T_2}=\mathbf{P}^{T_2}\mathbf{p}_{2_4}$$

$$=\sum_g^{\circ O}\frac{\ell^{T_2}}{{}^\circ O}(\chi_g^{T_2^*})\cdot\mathbf{g}\cdot\left(\mathbf{p}_{2_4}\right)$$

$$=\sum_g^{\circ O}\frac{3}{96}(\chi_g^{T_2^*})\cdot\mathbf{g}\cdot\left(1\cdot\mathbf{1}+1\cdot\boldsymbol{\rho}_z-1\cdot\mathbf{R}_z-1\cdot\tilde{\mathbf{R}}_z\right)$$

$O\supset C_4$	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

$O:\chi_{\mathbf{g}}^{\mu}$	$\mathbf{g}$=**1**	$\mathbf{r}_{1-4}^{p}$	$\boldsymbol{\rho}_{xyz}$	$\mathbf{R}_{xyz}^{p}$	$\mathbf{i}_{1-6}$
μ=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

C4 characters

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

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

$$\mathbf{P}^{T_2}_{2_42_4}=$$

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

1/32(	$4\mathbf{1}$	$4\boldsymbol{\rho}_z$	$-4\mathbf{R}_z$	$-4\tilde{\mathbf{R}}_z$
3·(	+1	+1	-1	-1)
1	**1**	$\boldsymbol{\rho}_z$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$
-1·(	+1	+1	-1	-1)
$\boldsymbol{\rho}_z$	$\boldsymbol{\rho}_z$	**1**	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$
-1·(	-1	-1	+1	+1)
$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$	**1**	$\boldsymbol{\rho}_z$
-1·(	-1	-1	+1	+1)
$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$	$\boldsymbol{\rho}_z$	**1**

	$-4\boldsymbol{\rho}_x$	$-4\boldsymbol{\rho}_y$	$+4\mathbf{i}_4$	$+4\mathbf{i}_3$
-1·(	+1	+1	-1	-1)
$\boldsymbol{\rho}_x$	**1**	$\boldsymbol{\rho}_z$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$
-1·(	+1	+1	-1	-1)
$\boldsymbol{\rho}_y$	$\boldsymbol{\rho}_z$	**1**	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$
+1·(	-1	-1	+1	+1)
$\mathbf{i}_4$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$	**1**	$\boldsymbol{\rho}_z$
+1·(	-1	-1	+1	+1)
$\mathbf{i}_3$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$	$\boldsymbol{\rho}_z$	**1**

	$0\,\mathbf{r}_1$	$0\,\mathbf{r}_4$	$0\,\mathbf{i}_1$	$0\,\mathbf{R}_y$
-1·(	+1	+1	-1	-1)
$\mathbf{r}_1$	**1**	$\boldsymbol{\rho}_z$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$
-1·(	+1	+1	-1	-1)
$\mathbf{r}_4$	$\boldsymbol{\rho}_z$	**1**	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$
+0·(	-1	-1	+1	+1)
$\mathbf{i}_1$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$	**1**	$\boldsymbol{\rho}_z$
+0·(	-1	-1	+1	+1)
$\mathbf{R}_y$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$	$\boldsymbol{\rho}_z$	**1**

	$0\,\mathbf{r}_2$	$0\,\mathbf{r}_3$	$0\,\mathbf{i}_2$	$0\,\tilde{\mathbf{R}}_y$
-1·(	+1	+1	-1	-1)
$\mathbf{r}_2$	**1**	$\boldsymbol{\rho}_z$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$
-1·(	+1	+1	-1	-1)
$\mathbf{r}_3$	$\boldsymbol{\rho}_z$	**1**	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$
+0·(	-1	-1	+1	+1)
$\mathbf{i}_2$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$	**1**	$\boldsymbol{\rho}_z$
+0·(	-1	-1	+1	+1)
$\tilde{\mathbf{R}}_y$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$	$\boldsymbol{\rho}_z$	**1**

	$0\tilde{\mathbf{r}}_1$	$0\tilde{\mathbf{r}}_3$	$0\tilde{\mathbf{R}}_x$	$0\,\mathbf{i}_6$
-1·(	+1	+1	-1	-1)
$\tilde{\mathbf{r}}_1$	**1**	$\boldsymbol{\rho}_z$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$
-1·(	+1	+1	-1	-1)
$\tilde{\mathbf{r}}_3$	$\boldsymbol{\rho}_z$	**1**	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$
+0·(	-1	-1	+1	+1)
$\tilde{\mathbf{R}}_x$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$	**1**	$\boldsymbol{\rho}_z$
+0·(	-1	-1	+1	+1)
$\mathbf{i}_6$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$	$\boldsymbol{\rho}_z$	**1**

	$0\tilde{\mathbf{r}}_2$	$0\tilde{\mathbf{r}}_4$	$0\mathbf{R}_x$	$0\mathbf{i}_5$)
-1·(	+1	+1	-1	-1)
$\tilde{\mathbf{r}}_2$	**1**	$\boldsymbol{\rho}_z$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$
-1·(	+1	+1	-1	-1)
$\tilde{\mathbf{r}}_4$	$\boldsymbol{\rho}_z$	**1**	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$
+0·(	-1	-1	+1	+1)
$\mathbf{R}_x$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$	**1**	$\boldsymbol{\rho}_z$
+0·(	-1	-1	+1	+1)
$\mathbf{i}_5$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$	$\boldsymbol{\rho}_z$	**1**

Coset-factored sum:

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

Split-classes-ordered sum:

$$\mathbf{P}^{T_2}_{2_42_4}=\tfrac{1}{8}(1\cdot\mathbf{1}\quad+0+0+0+0+0+0+0+0\quad-1\boldsymbol{\rho}_x-1\boldsymbol{\rho}_y+1\boldsymbol{\rho}_z\quad+0+0-1\mathbf{R}_z+0+0-1\tilde{\mathbf{R}}_z\quad+0+0+1\mathbf{i}_4+1\mathbf{i}_3+0+0\,)$$

Calculating $\mathbf{P}^{T_2}{}_{1_4 1_4}$

$$\mathbf{P}^{T_2}_{1_4 1_4} = \mathbf{p}_{1_4}\mathbf{P}^{T_2} = \mathbf{P}^{T_2}\mathbf{p}_{1_4}$$

$$= \sum_{g}^{\circ O} \frac{\ell^{T_2^*}}{\circ O}(\chi_g^{T_2^*})\cdot \mathbf{g}\cdot\left(\mathbf{p}_{1_4}\right)$$

$$= \sum_{g}^{\circ O} \frac{3}{96}(\chi_g^{T_2^*})\cdot \mathbf{g}\cdot\left(\, 1\cdot\mathbf{1} - i\cdot\boldsymbol{\rho}_z - 1\cdot\mathbf{R}_z + i\cdot\tilde{\mathbf{R}}_z\right)$$

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

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

O characters

C4 characters

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

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

$$\mathbf{P}^{T_2}_{1_4 1_4} =$$

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

1/32(	+4 $\mathbf{1}$	-4 $\boldsymbol{\rho}_z$	-4i $\mathbf{R}_z$	+4i $\tilde{\mathbf{R}}_z$
+3·(	+1	-1	$-i$	$+i$)
$\mathbf{1}$	$\mathbf{1}$	$\boldsymbol{\rho}_z$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$
-1·(	-1	+1	$+i$	$-i$)
$\boldsymbol{\rho}_z$	$\boldsymbol{\rho}_z$	$\mathbf{1}$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$
+1·(	$+i$	$-i$	+1	-1)
$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$	$\mathbf{1}$	$\boldsymbol{\rho}_z$
+1·(	$-i$	$+i$	-1	+1)
$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$	$\boldsymbol{\rho}_z$	$\mathbf{1}$

	-0 $\boldsymbol{\rho}_x$	-0 $\boldsymbol{\rho}_y$	-0 $\mathbf{i}_4$	-0 $\mathbf{i}_3$
-1·(	+1	-1	$-i$	$+i$)
$\boldsymbol{\rho}_x$	$\mathbf{1}$	$\boldsymbol{\rho}_z$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$
-1·(	-1	+1	$+i$	$-i$)
$\boldsymbol{\rho}_y$	$\boldsymbol{\rho}_z$	$\mathbf{1}$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$
+1·(	$+i$	$-i$	+1	-1)
$\mathbf{i}_4$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$	$\mathbf{1}$	$\boldsymbol{\rho}_z$
+1·(	$-i$	$+i$	-1	+1)
$\mathbf{i}_3$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$	$\boldsymbol{\rho}_z$	$\mathbf{1}$

	+2i $\mathbf{r}_1$	-2i $\mathbf{r}_4$	+2 $\mathbf{i}_1$	-2 $\mathbf{R}_y$
0 (	+1	-1	$-i$	$+i$)
$\mathbf{r}_1$	$\mathbf{1}$	$\boldsymbol{\rho}_z$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$
0 (	-1	+1	$+i$	$-i$)
$\mathbf{r}_4$	$\boldsymbol{\rho}_z$	$\mathbf{1}$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$
+1·(	$+i$	$-i$	+1	-1)
$\mathbf{i}_1$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$	$\mathbf{1}$	$\boldsymbol{\rho}_z$
-1·(	$-i$	$+i$	-1	+1)
$\mathbf{R}_y$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$	$\boldsymbol{\rho}_z$	$\mathbf{1}$

	+2i $\mathbf{r}_2$	-2i $\mathbf{r}_3$	+2 $\mathbf{i}_2$	-2 $\tilde{\mathbf{R}}_y$
0 (	+1	-1	$-i$	$+i$)
$\mathbf{r}_2$	$\mathbf{1}$	$\boldsymbol{\rho}_z$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$
0 (	-1	+1	$+i$	$-i$)
$\mathbf{r}_3$	$\boldsymbol{\rho}_z$	$\mathbf{1}$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$
+1·(	$+i$	$-i$	+1	-1)
$\mathbf{i}_2$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$	$\mathbf{1}$	$\boldsymbol{\rho}_z$
-1·(	$-i$	$+i$	-1	+1)
$\tilde{\mathbf{R}}_y$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$	$\boldsymbol{\rho}_z$	$\mathbf{1}$

	-2i $\tilde{\mathbf{r}}_1$	+2i $\tilde{\mathbf{r}}_3$	-2 $\tilde{\mathbf{R}}_x$	+2 $\mathbf{i}_6$
0 (	+1	-1.	$-i$	$+i$)
$\tilde{\mathbf{r}}_1$	$\mathbf{1}$	$\boldsymbol{\rho}_z$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$
0 (	-1	+1	$+i$	$-i$)
$\tilde{\mathbf{r}}_3$	$\boldsymbol{\rho}_z$	$\mathbf{1}$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$
-1·(	$+i$	$-i$	+1	-1)
$\tilde{\mathbf{R}}_x$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$	$\mathbf{1}$	$\boldsymbol{\rho}_z$
+1·(	$-i$	$+i$	-1	+1)
$\mathbf{i}_6$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$	$\boldsymbol{\rho}_z$	$\mathbf{1}$

	-2i $\tilde{\mathbf{r}}_2$	+2i $\tilde{\mathbf{r}}_4$	-2 $\mathbf{R}_x$	+2 $\mathbf{i}_5$)
0 (	+1	-1	$-i$	$+i$)
$\tilde{\mathbf{r}}_2$	$\mathbf{1}$	$\boldsymbol{\rho}_z$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$
0 (	-1	+1	$+i$	$-i$)
$\tilde{\mathbf{r}}_4$	$\boldsymbol{\rho}_z$	$\mathbf{1}$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$
-1·(	$+i$	$-i$	+1	-1)
$\mathbf{R}_x$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$	$\mathbf{1}$	$\boldsymbol{\rho}_z$
+1·(	$-i$	$+i$	-1	+1)
$\mathbf{i}_5$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$	$\boldsymbol{\rho}_z$	$\mathbf{1}$

Coset-factored sum:

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

Split-classes-ordered sum:

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

AMOP
reference links
on page 2

3.12.18 class 17.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Discrete symmetry subgroups of O(3)⊃(Octahedral O_h⊃O): Part II Full $D^{(\alpha)}$-matrices defined by subgroup-chains $O\supset D_4\supset C_4$, D_2, or C_3 applied to eigensolutions of O_h-tensors $\mathbf{T}^{[4]}+\mathbf{T}^{[6]}$

Review *Idempotent projector splits* $\mathbf{P}^{\mu}_{m,m}$ *of* $O\supset C_4$ $\mathbf{P}^{E}_{0404}$ $\mathbf{P}^{E}_{2424}$ $\mathbf{P}^{T_1}_{0404}$ $\mathbf{P}^{T_1}_{1414}$ $\mathbf{P}^{T_2}_{2424}$ $\mathbf{P}^{T_2}_{1414}$

Review *Coset factored splitting of projectors for* $O\supset D_4\supset C_4$ *into split classes and level structure*

Hamiltonian level cluster models with subgroup-defined tunneling parameters

Diagonal idempotent $\mathbf{P}^{\mu}_{m,m}$ *parameter sets for* $O\supset C_4$ *and* $O\supset C_3$ *case of* SF_6 *level clusters*

Off-diagonal nilpotent $\mathbf{P}^{\mu}_{m,n}$ $(m\neq n)$ *parameter sets needed for* $O\supset C_2$ *clusters*

Deriving nilpotent projectors $\mathbf{P}^{\mu}_{m,n}$ *and ireps* $D^{\mu}_{m,n}$ *by fundamental* $\mathbf{g}\rightleftarrows\mathbf{P}^{\mu}_{m,n}$ *relations:*

(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 nilpotent projectors for simple $D_3\supset C_2\sim C_{3v}\supset C_v$ *chains* (Lect13p95)

Calculating and Factoring $\mathbf{P}^{T_1}_{1404}$ *and* $\mathbf{P}^{T_1}_{1434}$

Structure and applications of coset tabulated $D^{\mu}_{m,n}$ *irreps for various* O_h *subgroup chains*

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

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}_{0424}

Comparing local C_4, C_3, *and* C_2 *cluster spectra of* O_h*-symmetric tensors* $\mathbf{T}^{[4]}+\mathbf{T}^{[6]}$

Monster clusters: When local C_2 *symmetry dominates*

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

Are these "accidents" or not?

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:*

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

Coset-factored A₁-sum:

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

Coset-factored A₂-sum:

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

Coset-factored E-sum:

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

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

Coset-factored T₁-sum:

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

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

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

Coset-factored T₂-sum:

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

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

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

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

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

$C_4:\chi^{\mu}_{\mathbf{g}}$	$\mathbf{g}=\mathbf{1}$	$\mathbf{R}_z$	$\boldsymbol{\rho}_z$	$\tilde{\mathbf{R}}_z$
$\mu=0_4$	1	1	1	1
1_4	1	$-i$	-1	i
2_4	1	-1	1	-1
3_4	1	$-i$	-1	$-i$

10 split projectors in terms of 6 coset sums

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

Split-class-ordered A1-sum:

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

Split-class-ordered A2-sum:

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

Split-class-ordered E-sum:

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

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

Split-class-ordered T1-sum:

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

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

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

Split-class-ordered T2-sum:

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

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

$$\mathbf{P}^{T_2}_{2_4 2_4}=\tfrac{1}{8}(1\cdot\mathbf{1}\quad +0+0\quad +0+0\quad +0+0\quad +0+0\quad -1\rho_x-1\rho_y+1\rho_z\quad +0+0\quad -1\mathbf{R}_z\quad +0+0\quad -1\tilde{\mathbf{R}}_z\quad +0+0\quad +1\mathbf{i}_4+1\mathbf{i}_3\quad +0+0\ )$$

10 split projectors in terms of 10 split class sums

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

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

$$\underbrace{C_4\ \text{characters}}$$

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

AMOP
reference links
on page 2

3.12.18 class 17.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Discrete symmetry subgroups of O(3)⊃(Octahedral O_h⊃O): Part II Full $D^{(\alpha)}$-matrices defined by subgroup-chains $O\supset D_4\supset C_4$, D_2, or C_3 applied to eigensolutions of O_h-tensors $\mathbf{T}^{[4]}+\mathbf{T}^{[6]}$

Review *Idempotent projector splits* $\mathbf{P}^{\mu}_{m,m}$ *of* $O\supset C_4$ $\mathbf{P}^{E}_{0404}$ $\mathbf{P}^{E}_{2424}$ $\mathbf{P}^{T_1}_{0404}$ $\mathbf{P}^{T_1}_{1414}$ $\mathbf{P}^{T_2}_{2424}$ $\mathbf{P}^{T_2}_{1414}$

Review *Coset factored splitting of projectors for* $O\supset D_4\supset C_4$ *into split classes and level structure*

Hamiltonian level cluster models with subgroup-defined tunneling parameters

Diagonal idempotent $\mathbf{P}^{\mu}_{m,m}$ *parameter sets for* $O\supset C_4$ *and* $O\supset C_3$ *case of* SF_6 *level clusters*

Off-diagonal nilpotent $\mathbf{P}^{\mu}_{m,n}$ $(m\neq n)$ *parameter sets needed for* $O\supset C_2$ *clusters*

Deriving nilpotent projectors $\mathbf{P}^{\mu}_{m,n}$ *and ireps* $D^{\mu}_{m,n}$ *by fundamental* $\mathbf{g}\rightleftarrows\mathbf{P}^{\mu}_{m,n}$ *relations:*

(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 nilpotent projectors for simple $D_3\supset C_2\sim C_{3v}\supset C_v$ *chains* (Lect13p95)

Calculating and Factoring $\mathbf{P}^{T_1}_{1404}$ *and* $\mathbf{P}^{T_1}_{1434}$

Structure and applications of coset tabulated $D^{\mu}_{m,n}$ *irreps for various* O_h *subgroup chains*

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

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}_{0424}

Comparing local C_4, C_3, *and* C_2 *cluster spectra of* O_h*-symmetric tensors* $\mathbf{T}^{[4]}+\mathbf{T}^{[6]}$

Monster clusters: When local C_2 *symmetry dominates*

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

Are these "accidents" or not?

$O\supset C_4$	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

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

$$\mathbf{1}\cdot\mathbf{P}^{A_1} = \mathbf{P}^{A_1}_{0_4 0_4} + 0 + 0 + 0$$

$$\mathbf{1}\cdot\mathbf{P}^{A_2} = 0 + 0 + \mathbf{P}^{A_2}_{2_4 2_4} + 0$$

$$\mathbf{1}\cdot\mathbf{P}^{E} = \mathbf{P}^{E}_{0_4 0_4} + 0 + \mathbf{P}^{E}_{2_4 2_4} + 0$$

$$\mathbf{1}\cdot\mathbf{P}^{T_1} = \mathbf{P}^{T_1}_{0_4 0_4} + \mathbf{P}^{T_1}_{1_4 1_4} + 0 + \mathbf{P}^{T_1}_{3_4 3_4}$$

$$\mathbf{1}\cdot\mathbf{P}^{T_2} = 0 + \mathbf{P}^{T_2}_{1_4 1_4} + \mathbf{P}^{T_2}_{2_4 2_4} + \mathbf{P}^{T_2}_{3_4 3_4}$$

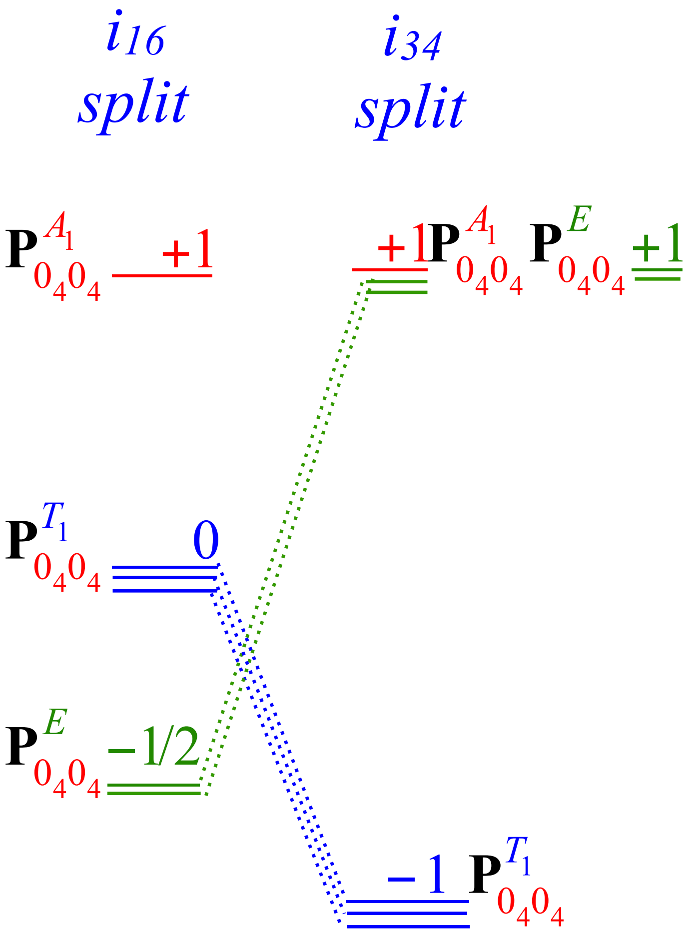
Summary of $O\supset C_4$ diagonal (idempotent) projectors $\mathbf{P}^{\mu}_{jj}$

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

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

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

The $0_4\uparrow$ cluster



Int.J.Mol.Sci, 14, 714(2013)pdf p67

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

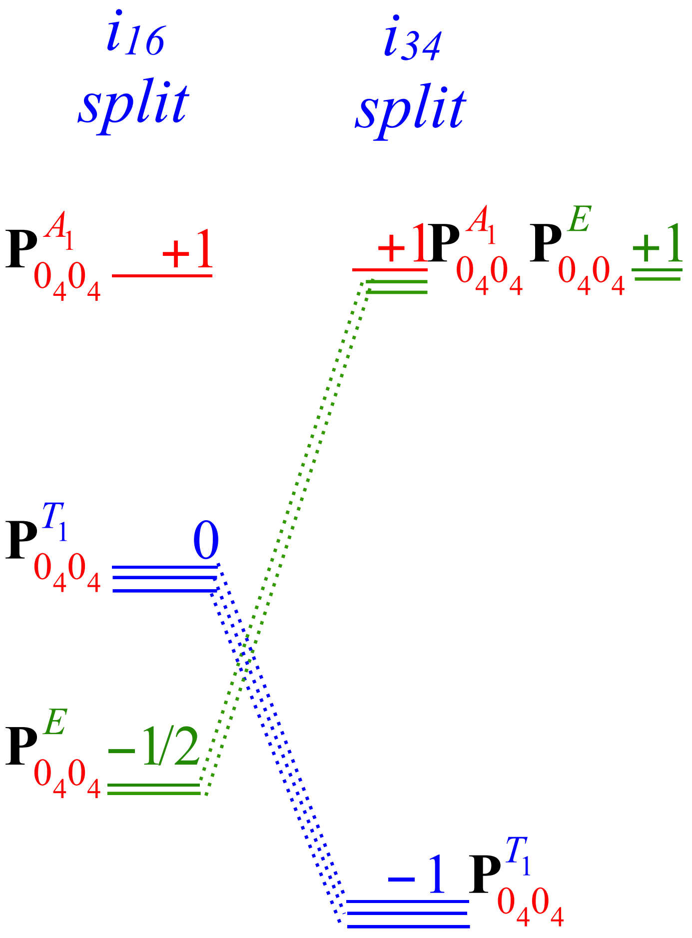
$$\mathbf{p}_{m_4} = \begin{cases} \mathbf{p}_{0_4} = (\mathbf{1} + \mathbf{R}_z + \rho_z + \tilde{\mathbf{R}}_z)/4 \\ \mathbf{p}_{1_4} = (\mathbf{1} + i\mathbf{R}_z - \rho_z - i\tilde{\mathbf{R}}_z)/4 \\ \mathbf{p}_{2_4} = (\mathbf{1} - \mathbf{R}_z + \rho_z - \tilde{\mathbf{R}}_z)/4 \\ \mathbf{p}_{3_4}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

10 split-class sums (Each commutes only with all 4 operators in C₄)

10 $\mathbf{P}^\mu_{kk}$ projectors

$\mathbf{P}^{(\alpha)}_{n_4n_4}(O\supset C_4)$		$\mathbf{1}$	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	⓵ $+1$
$24\cdot\mathbf{P}^{A_2}_{2_42_4}$	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	$-\frac{1}{2}$	$\boxed{+1}$
$12\cdot\mathbf{P}^{E}_{2_42_4}$	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	$\boxed{-1}$
$8\cdot\mathbf{P}^{T_2}_{1_41_4}$	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

The $0_4\uparrow$cluster



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	$\mathbf{r}_{1-4}$ $\tilde{\mathbf{r}}_{1-4}$	$\boldsymbol{\rho}_{xyz}$	$\mathbf{R}_{xyz}$ $\tilde{\mathbf{R}}_{xyz}$	$\mathbf{i}_{1-6}$
$\mu=A_1$	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

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 only with all 4 operators in C_4)

10 $\mathbf{P}^\mu_{kk}$ projectors

$\mathbf{P}^{(\alpha)}_{n_4n_4}(O\supset C_4)$			$\mathbf{1}$	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	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	−1	−1	−1	1	−1
$12\cdot\mathbf{P}^{E}_{0_40_4}$	3	2	1	$-\frac{1}{2}$	-1	$-\frac{1}{2}$	1	2	1	$-\frac{1}{2}$	0	1	1	$-\frac{1}{2}$	0	+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	3	1	$+\frac{i}{2}$	0	$-\frac{i}{2}$	0	-1	−1	$+\frac{1}{2}$	1	$+i$	$-i$	$-\frac{1}{2}$	-1	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	3	1	$-\frac{i}{2}$	0	$+\frac{i}{2}$	0	-1	−1	$-\frac{1}{2}$	-1	$+i$	$-i$	$+\frac{1}{2}$	1	0
$8\cdot\mathbf{P}^{T_2}_{2_42_4}$	10		1	0		0	−1		1	0		−1	−1	0		1

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

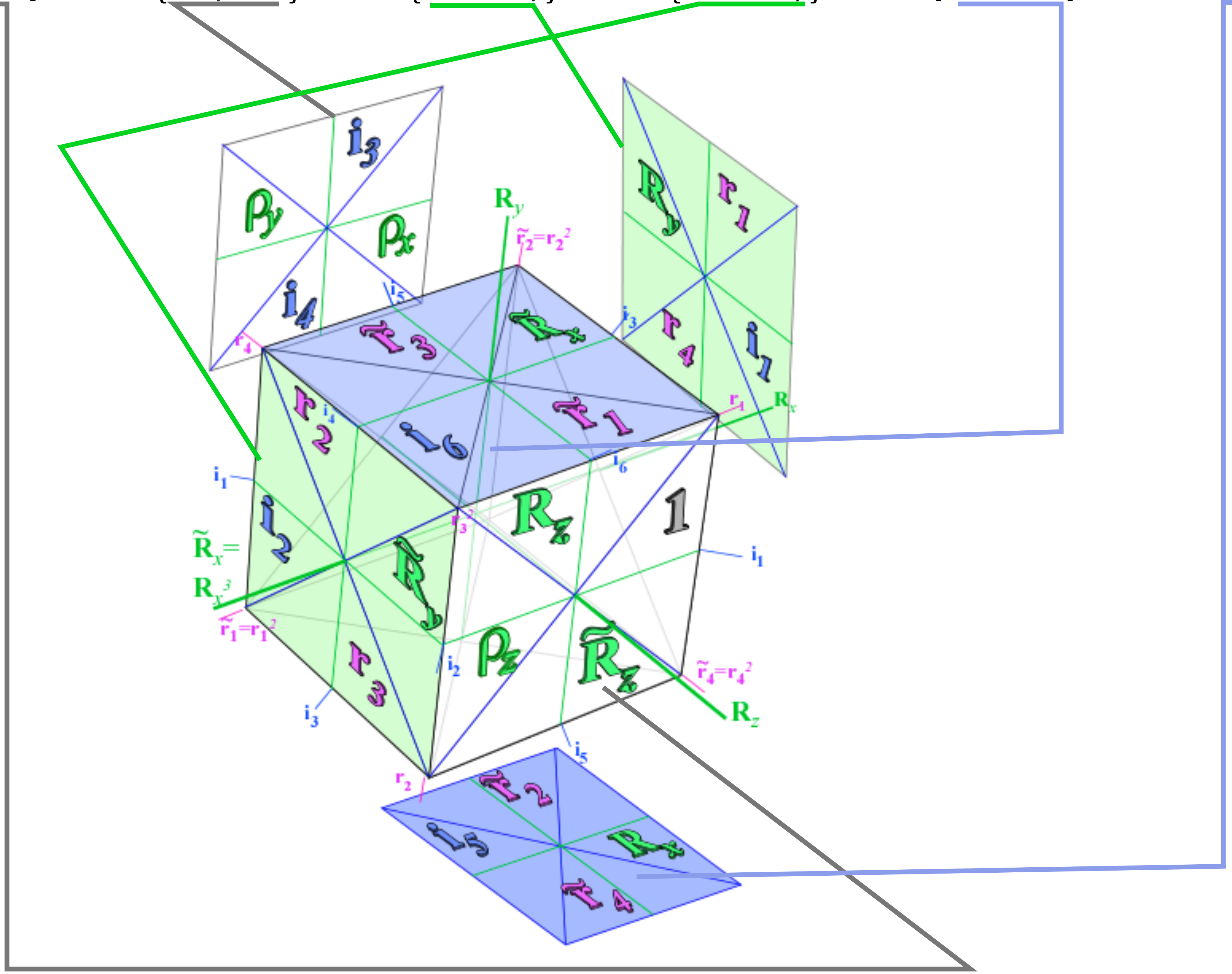
Int.J.Mol.Sci, 14, 714(2013)pdf p67

Preceding development of irreducible C4-projectors and split sub-classes:

$$\mathbf{P}^{\mu}_{m_4 m_4} \equiv \mathbf{p}_{m_4}\mathbf{P}^{\mu} = \mathbf{P}^{\mu}\mathbf{p}_{m_4}$$

...uses left-coset combinations... *...and projector "factoring"...*

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



Preceding development of irreducible C₄-projectors and split sub-classes:

$$\mathbf{P}^{\mu}_{m_4 m_4} \equiv \mathbf{p}_{m_4}\mathbf{P}^{\mu} = \mathbf{P}^{\mu}\mathbf{p}_{m_4}$$

...uses left-coset combinations...

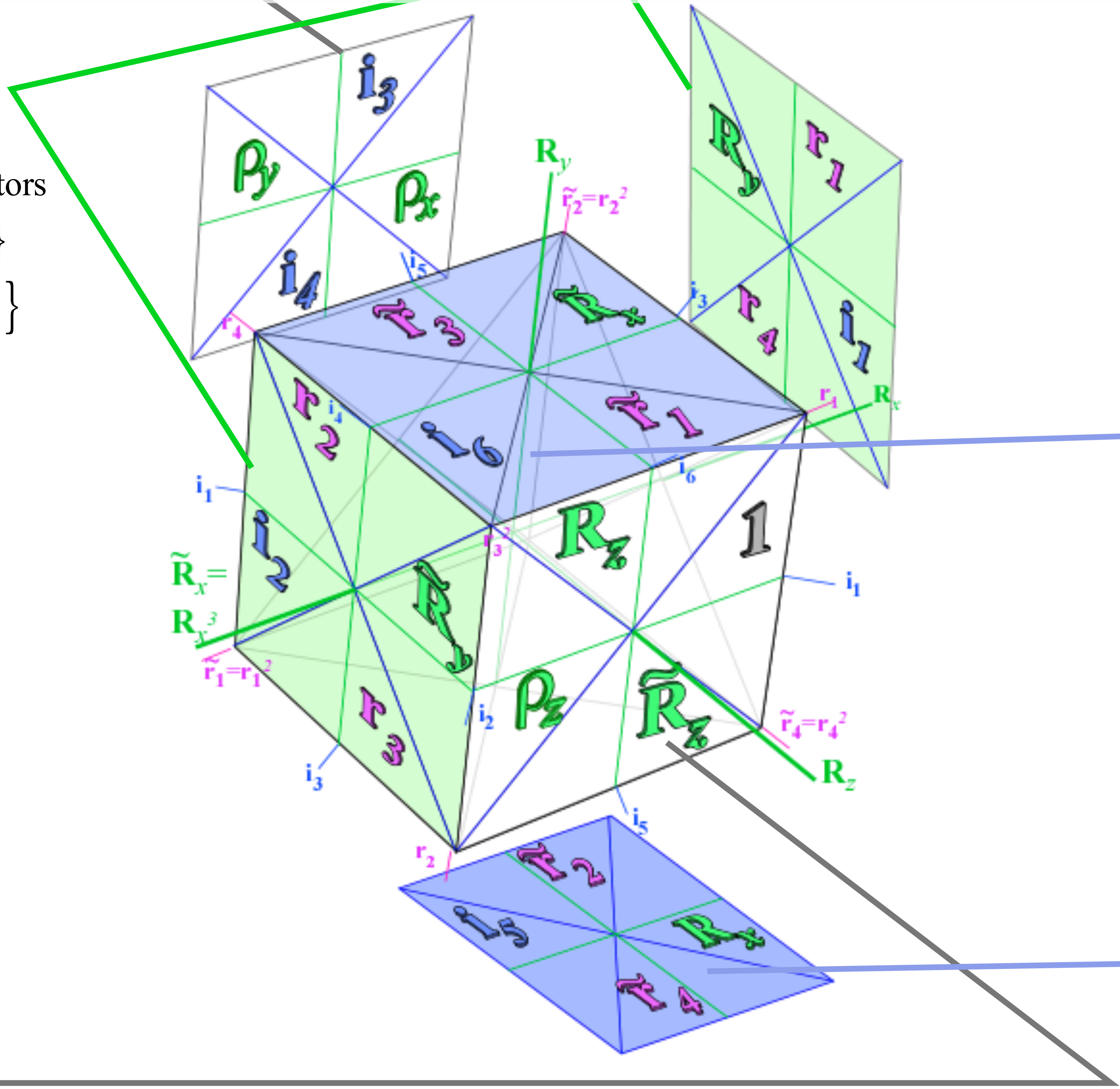
...and projector "factoring"...

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

$$C_4\text{-Split subclasses}: [\mathbf{1}],[\{\mathbf{r}_1,\mathbf{r}_2,\tilde{\mathbf{r}}_3,\tilde{\mathbf{r}}_4\},\{\tilde{\mathbf{r}}_1,\tilde{\mathbf{r}}_2,\mathbf{r}_3,\mathbf{r}_4\}],[\{\boldsymbol{\rho}_x,\boldsymbol{\rho}_y\},\{\boldsymbol{\rho}_z\}],[\{\mathbf{R}_x,\tilde{\mathbf{R}}_x,\mathbf{R}_y,\tilde{\mathbf{R}}_y\},\{\mathbf{R}_z\},\{\tilde{\mathbf{R}}_z\}],[\{\mathbf{i}_1,\mathbf{i}_2,\mathbf{i}_5,\mathbf{i}_6\}\{\mathbf{i}_3,\mathbf{i}_4\}]$$

O-subgroup operators

$$C_4 = \{\mathbf{1},\boldsymbol{\rho}_z,\mathbf{R}_z,\tilde{\mathbf{R}}_z\}$$
$$= \{\mathbf{1},\mathbf{R}_z^2,\mathbf{R}_z,\mathbf{R}_z^3\}$$



Preceding development of irreducible C₄-projectors and split sub-classes:

$$\mathbf{P}^{\mu}_{m_4 m_4} \equiv \mathbf{p}_{m_4}\mathbf{P}^{\mu} = \mathbf{P}^{\mu}\mathbf{p}_{m_4}$$

...uses left-coset combinations... *...and projector "factoring"...*

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

C_4*-Split subclasses* : $[\mathbf{1}],[\{\mathbf{r}_1,\mathbf{r}_2,\tilde{\mathbf{r}}_3,\tilde{\mathbf{r}}_4\},\{\tilde{\mathbf{r}}_1,\tilde{\mathbf{r}}_2,\mathbf{r}_3,\mathbf{r}_4\}],[\{\boldsymbol{\rho}_x,\boldsymbol{\rho}_y\},\{\boldsymbol{\rho}_z\}],[\{\mathbf{R}_x,\tilde{\mathbf{R}}_x,\mathbf{R}_y,\tilde{\mathbf{R}}_y\},\{\mathbf{R}_z\},\{\tilde{\mathbf{R}}_z\}],[\{\mathbf{i}_1,\mathbf{i}_2,\mathbf{i}_5,\mathbf{i}_6\}\{\mathbf{i}_3,\mathbf{i}_4\}]$

O-subgroup operators

$C_4 = \{\mathbf{1},\boldsymbol{\rho}_z,\mathbf{R}_z,\tilde{\mathbf{R}}_z\}$

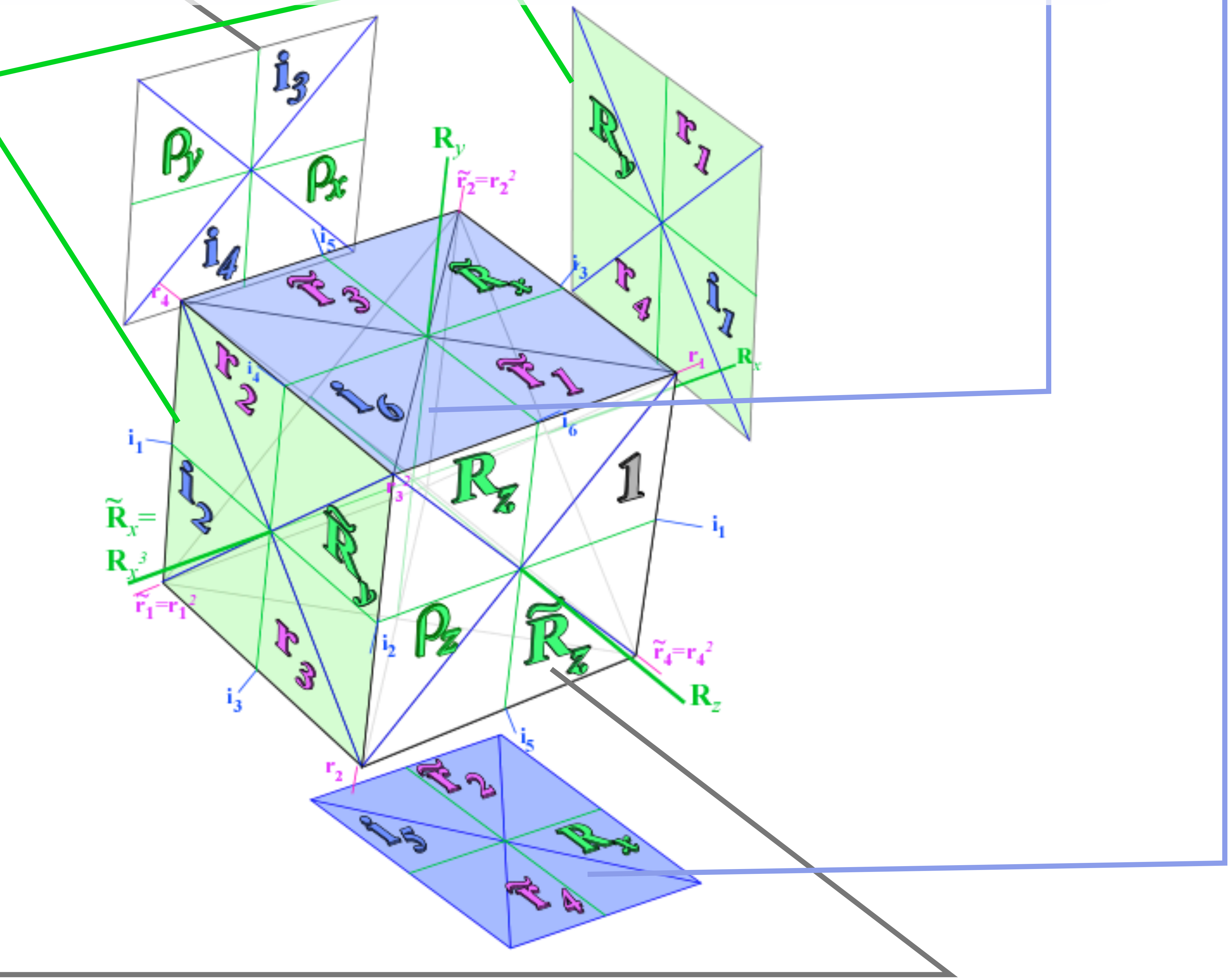
$= \{\mathbf{1},\mathbf{R}_z^2,\mathbf{R}_z,\mathbf{R}_z^3\}$

cannot transform

sub-class operators

$\{\mathbf{r}_1,\mathbf{r}_2,\tilde{\mathbf{r}}_3,\tilde{\mathbf{r}}_4\}$ into

$\{\tilde{\mathbf{r}}_1,\tilde{\mathbf{r}}_2,\mathbf{r}_3,\mathbf{r}_4\}$



Preceding development of irreducible C_4-projectors and split sub-classes:

$$\mathbf{P}^{\mu}_{m_4 m_4} \equiv \mathbf{p}_{m_4}\mathbf{P}^{\mu} = \mathbf{P}^{\mu}\mathbf{p}_{m_4}$$

...uses left-coset combinations... *...and projector "factoring"...*

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

C_4-*Split subclasses* : $[\mathbf{1}],[\{\mathbf{r}_1,\mathbf{r}_2,\tilde{\mathbf{r}}_3,\tilde{\mathbf{r}}_4\},\{\tilde{\mathbf{r}}_1,\tilde{\mathbf{r}}_2,\mathbf{r}_3,\mathbf{r}_4\}],[\{\rho_x,\rho_y\},\{\rho_z\}],[\{\mathbf{R}_x,\tilde{\mathbf{R}}_x,\mathbf{R}_y,\tilde{\mathbf{R}}_y\},\{\mathbf{R}_z\},\{\tilde{\mathbf{R}}_z\}],[\{\mathbf{i}_1,\mathbf{i}_2,\mathbf{i}_5,\mathbf{i}_6\}\{\mathbf{i}_3,\mathbf{i}_4\}]$

O-subgroup operators

$C_4 = \{\mathbf{1},\rho_z,\mathbf{R}_z,\tilde{\mathbf{R}}_z\}$

$= \{\mathbf{1},\mathbf{R}_z^2,\mathbf{R}_z,\mathbf{R}_z^3\}$

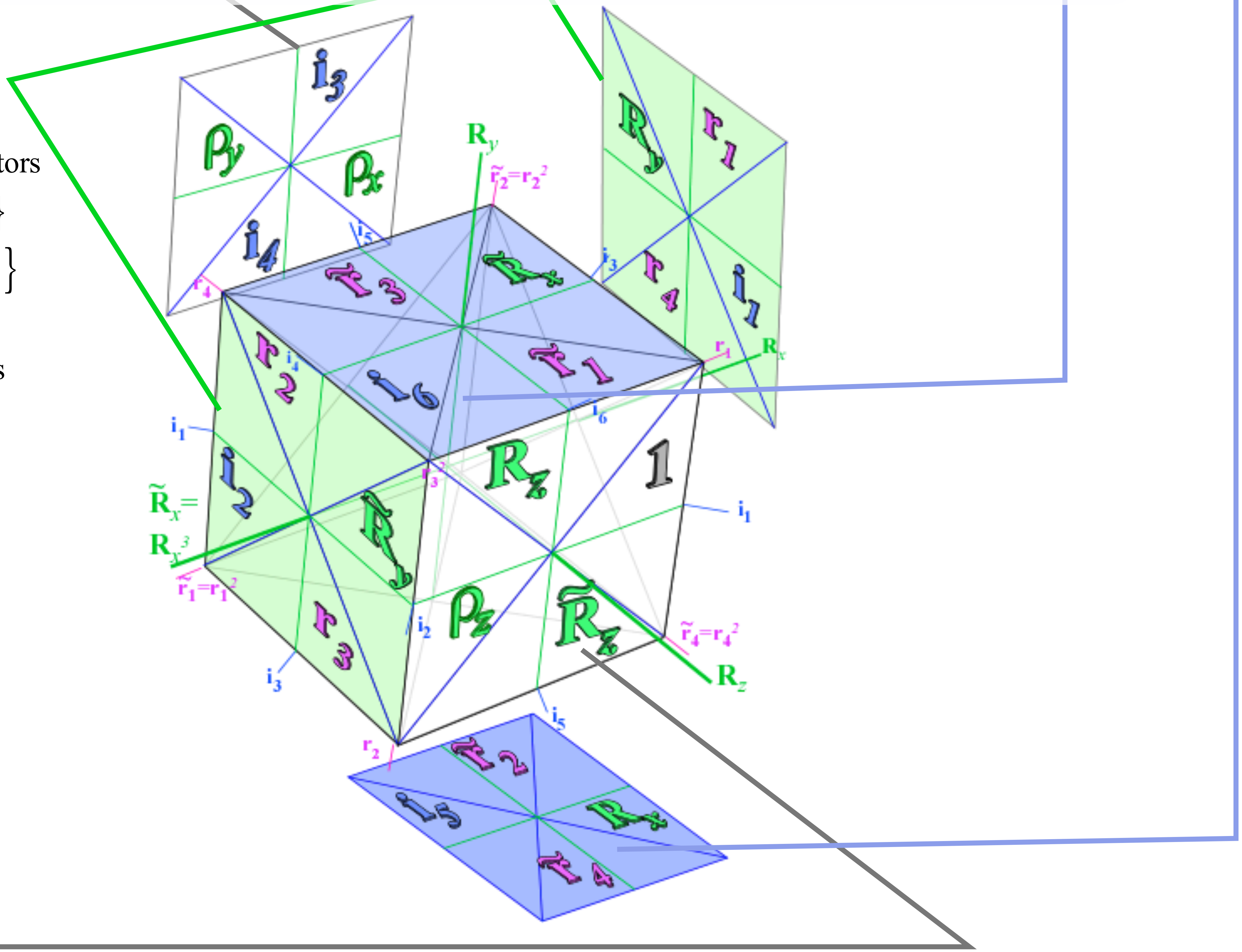
cannot transform

sub-class operators

$\{\mathbf{r}_1,\mathbf{r}_2,\tilde{\mathbf{r}}_3,\tilde{\mathbf{r}}_4\}$ into

$\{\tilde{\mathbf{r}}_1,\tilde{\mathbf{r}}_2,\mathbf{r}_3,\mathbf{r}_4\}$ or

$\{\rho_x,\rho_y\}$ into $\{\rho_z\}$



Preceding development of irreducible C4-projectors and split sub-classes:

$$\mathbf{P}^{\mu}_{m_4 m_4} \equiv \mathbf{p}_{m_4}\mathbf{P}^{\mu} = \mathbf{P}^{\mu}\mathbf{p}_{m_4}$$

...uses left-coset combinations... *...and projector "factoring"...*

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

$$C_4\text{-Split subclasses}: \left[\mathbf{1}\right],\left[\{\mathbf{r}_1,\mathbf{r}_2,\tilde{\mathbf{r}}_3,\tilde{\mathbf{r}}_4\},\{\tilde{\mathbf{r}}_1,\tilde{\mathbf{r}}_2,\mathbf{r}_3,\mathbf{r}_4\}\right],\left[\{\boldsymbol{\rho}_x,\boldsymbol{\rho}_y\},\{\boldsymbol{\rho}_z\}\right],\left[\{\mathbf{R}_x,\tilde{\mathbf{R}}_x,\mathbf{R}_y,\tilde{\mathbf{R}}_y\},\{\mathbf{R}_z\},\{\tilde{\mathbf{R}}_z\}\right],\left[\{\mathbf{i}_1,\mathbf{i}_2,\mathbf{i}_5,\mathbf{i}_6\}\{\mathbf{i}_3,\mathbf{i}_4\}\right]$$

O-subgroup operators

$$C_4 = \left\{\mathbf{1},\boldsymbol{\rho}_z,\mathbf{R}_z,\tilde{\mathbf{R}}_z\right\}$$
$$= \left\{\mathbf{1},\mathbf{R}_z^2,\mathbf{R}_z,\mathbf{R}_z^3\right\}$$

cannot transform

sub-class operators

$\{\mathbf{r}_1,\mathbf{r}_2,\tilde{\mathbf{r}}_3,\tilde{\mathbf{r}}_4\}$ into

$\{\tilde{\mathbf{r}}_1,\tilde{\mathbf{r}}_2,\mathbf{r}_3,\mathbf{r}_4\}$ or

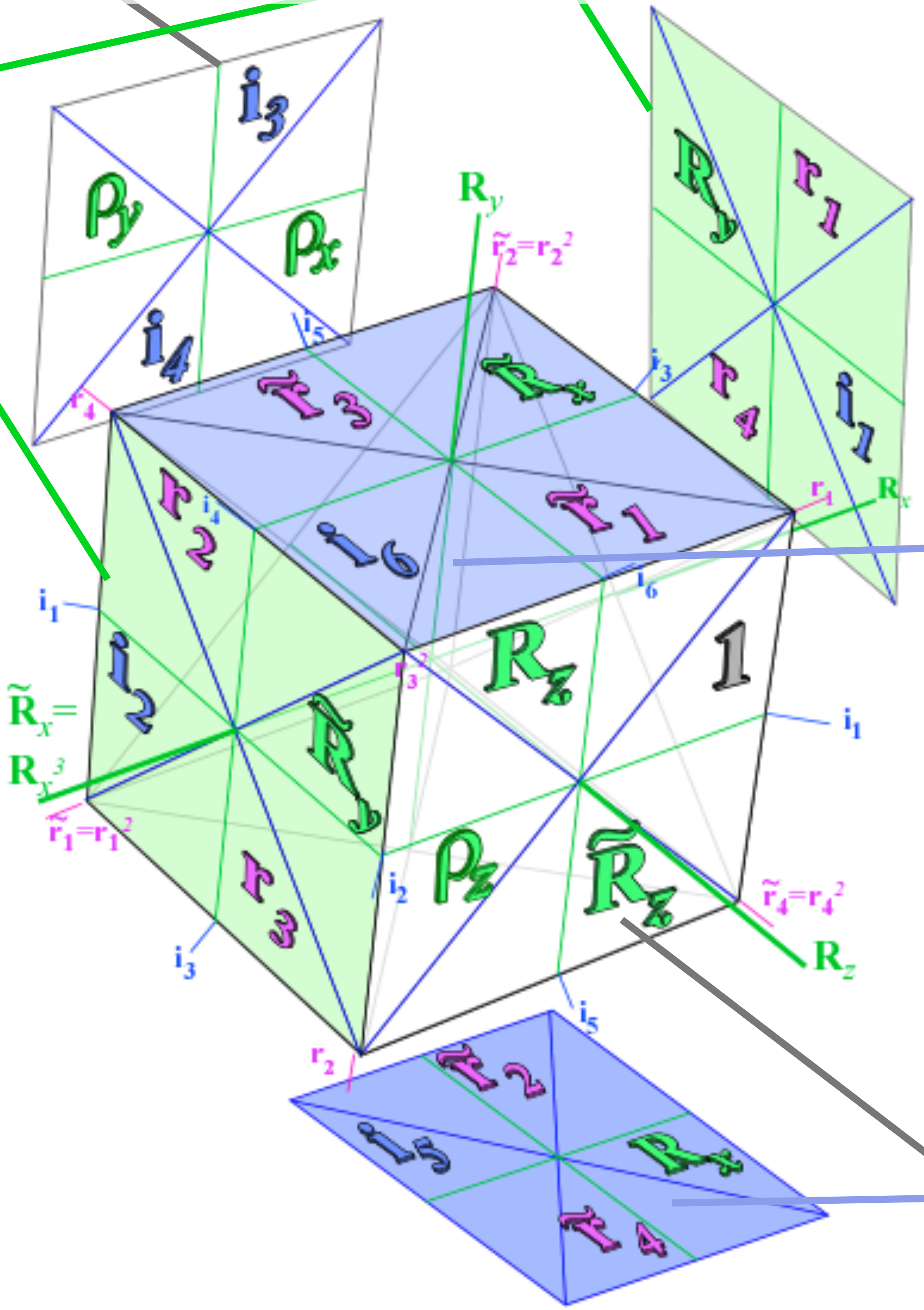
$\{\boldsymbol{\rho}_x,\boldsymbol{\rho}_y\}$ into $\{\boldsymbol{\rho}_z\}$

or $\{\mathbf{R}_x..\}$ into $\{\mathbf{R}_z\}$

or $\{\mathbf{i}_1,\mathbf{i}_2...\}$ into $\{\mathbf{i}_3\}$

etc....

(*O* does all that easily!)



AMOP
reference links
on page 2

3.12.18 class 17.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Discrete symmetry subgroups of O(3)⊃(Octahedral O_h⊃O): Part II Full $D^{(\alpha)}$-matrices defined by subgroup-chains $O\supset D_4\supset C_4$, D_2, or C_3 applied to eigensolutions of O_h-tensors $\mathbf{T}^{[4]}+\mathbf{T}^{[6]}$

Review Idempotent projector splits $\mathbf{P}^{\mu}_{m,m}$ *of* $O\supset C_4$ $\mathbf{P}^{E}_{0_40_4}$ $\mathbf{P}^{E}_{2_42_4}$ $\mathbf{P}^{T_1}_{0_40_4}$ $\mathbf{P}^{T_1}_{1_41_4}$ $\mathbf{P}^{T_2}_{2_42_4}$ $\mathbf{P}^{T_2}_{1_41_4}$

Review Coset factored splitting of projectors for $O\supset D_4\supset C_4$ *into split classes and level structure*

Hamiltonian level cluster models with subgroup-defined tunneling parameters

Diagonal idempotent $\mathbf{P}^{\mu}_{m,m}$ *parameter sets for* $O\supset C_4$ *and* $O\supset C_3$ *case of* SF_6 *level clusters*

Off-diagonal nilpotent $\mathbf{P}^{\mu}_{m,n}$ $(m\neq n)$ *parameter sets needed for* $O\supset C_2$ *clusters*

Deriving nilpotent projectors $\mathbf{P}^{\mu}_{m,n}$ *and ireps* $D^{\mu}_{m,n}$ *by fundamental* $\mathbf{g}\rightleftarrows\mathbf{P}^{\mu}_{m,n}$ *relations:*

(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 nilpotent projectors for simple $D_3\supset C_2\sim C_{3v}\supset C_v$ *chains* (Lect13p95)

Calculating and Factoring $\mathbf{P}^{T_1}_{1_40_4}$ *and* $\mathbf{P}^{T_1}_{1_43_4}$

Structure and applications of coset tabulated $D^{\mu}_{m,n}$ *irreps for various* O_h *subgroup chains*

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

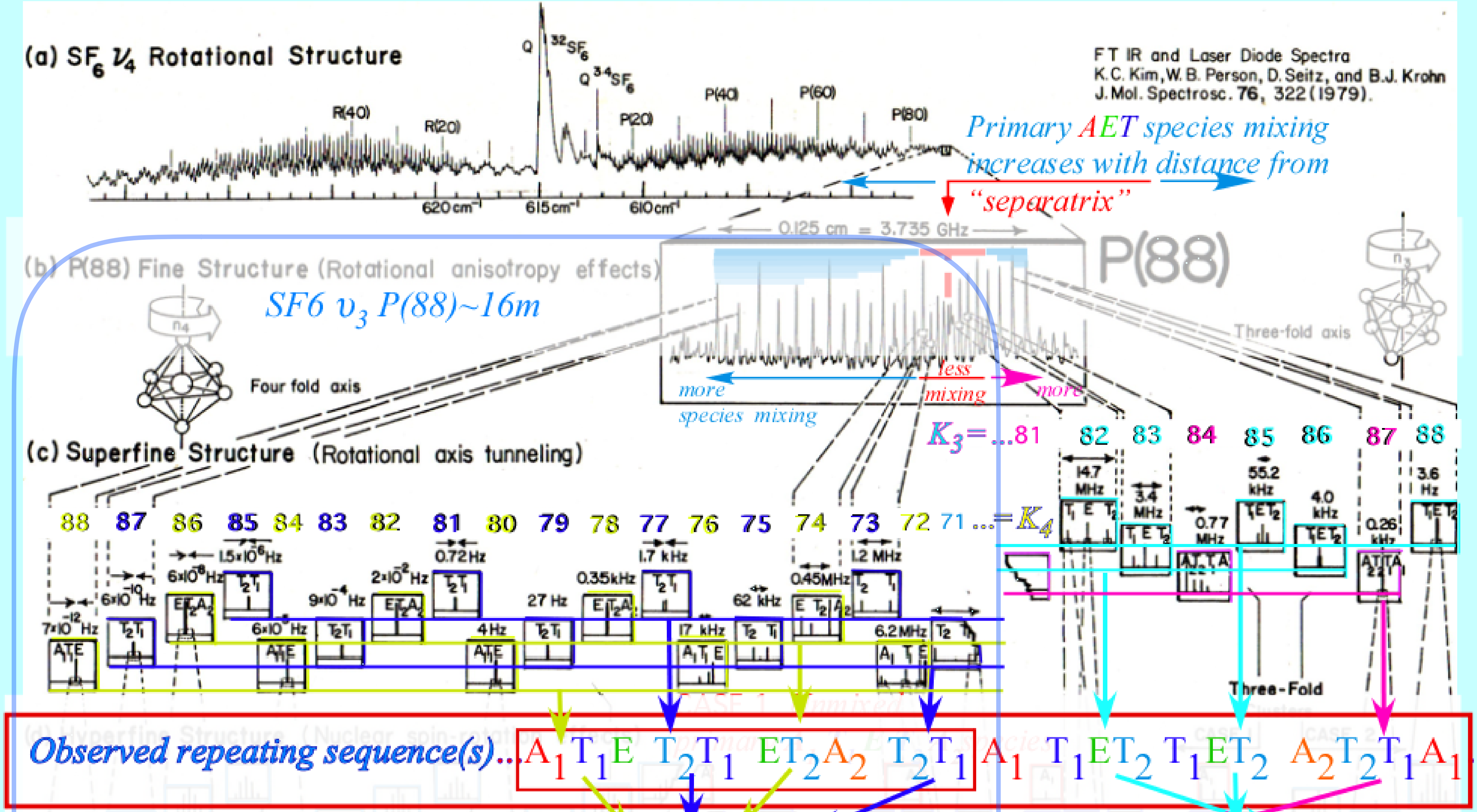
Comparing $O_h\supset D_{4h}\supset D_{2h}$ *and* $O_h\supset D_{3d}\supset C_2$ *representations (*T_1 *vector-type)*

Examples of off-diagonal tunneling coefficients $D^{E}_{0_42_4}$

Comparing local C_4, C_3, *and* C_2 *cluster spectra of* O_h*-symmetric tensors* $\mathbf{T}^{[4]}+\mathbf{T}^{[6]}$

Monster clusters: When local C_2 *symmetry dominates*

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



Primary *AET* species mixing increases with distance from "separatrix"

SF6 υ_3 P(88)~16m

Observed repeating sequence(s)...$A_1 T_1 E\ T_2 T_1\ E T_2 A_2\ T_2 T_1\ A_1\ T_1 E T_2\ T_1 E T_2\ A_2 T_2 T_1 A_1$...

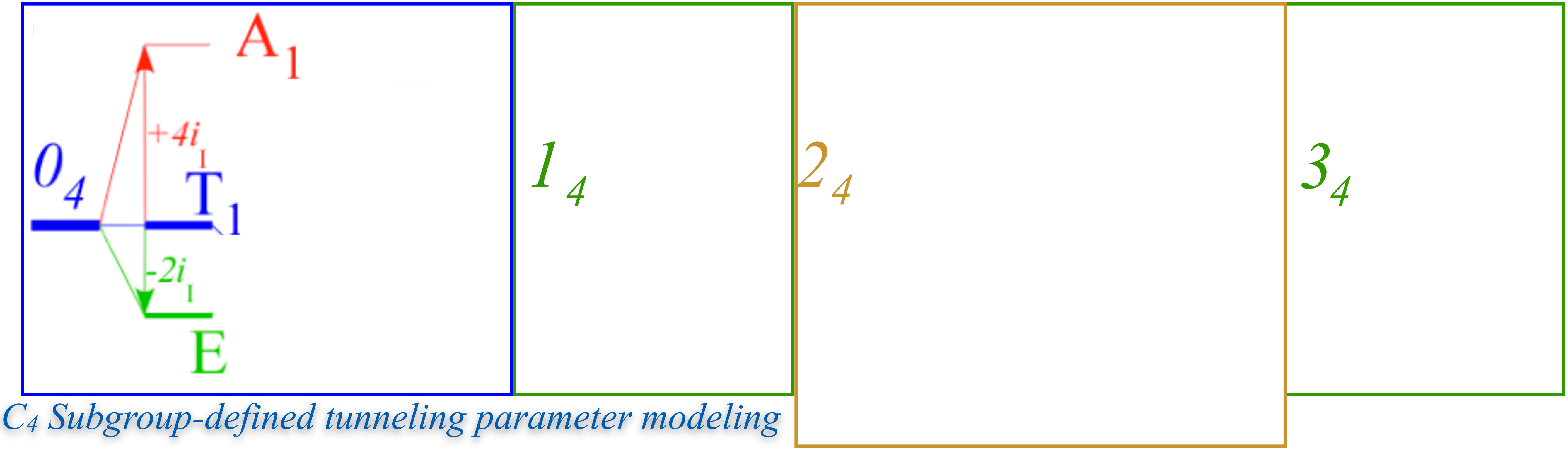
$O \supset C_4$	$(0)_4$	$(1)_4$	$(2)_4$	$(3)_4=(-1)_4$
A_1	1	·	·	·
A_2	·	·	1	·
E	1	·	1	·
T_1	1	1	·	1
T_2	·	1	1	1

$O \supset C_3$	$(0)_3$	$(1)_3$	$(2)_3=(-1)_3$
A_1	1	·	·
A_2	1	·	·
E	·	1	1
T_1	1	1	1
T_2	1	1	1

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

...and physical consequences?

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

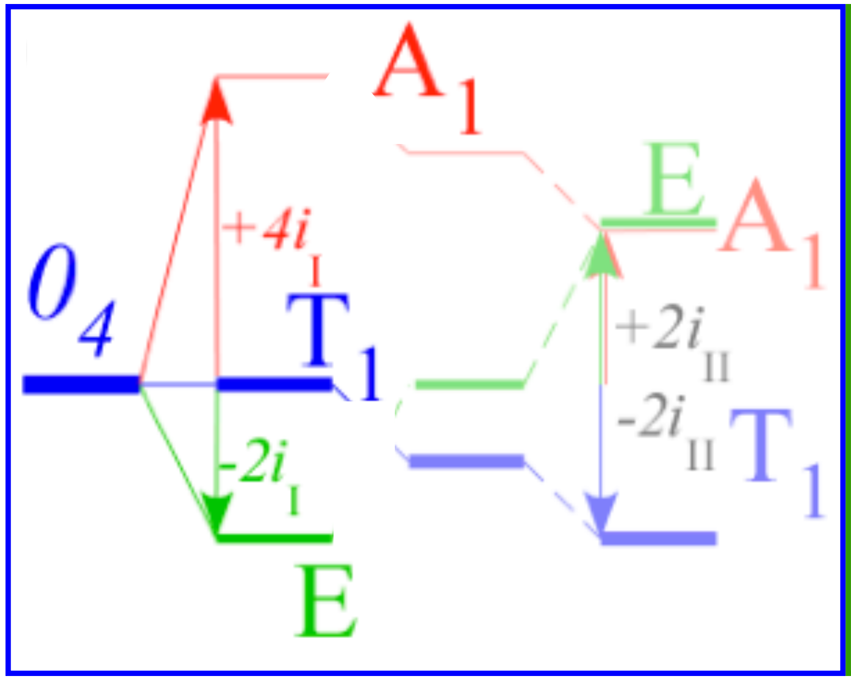


C_4 Subgroup-defined tunneling parameter modeling

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	$\cdot$	$r_{\mathrm{I}} = \mathrm{Re}\, r_{1234}$ $m_{\mathrm{I}} = \mathrm{Im}\, r_{1234}$	$\cdot$	$R_z = \mathrm{Re} R_z$ $I_z = \mathrm{Im} R_z$	$i_{\mathrm{I}} = i_{1256}$ $i_{\mathrm{II}} = i_{34}$
$\varepsilon_{0_4}^{A_1} =$	g_0	$+8r_{\mathrm{I}}$	$+2\rho_{xy} + \rho_z$	$+4R_{xy} + 2R_z$	$\boxed{+4i_{\mathrm{I}}} + 2i_{\mathrm{II}}$
$\varepsilon_{0_4}^{T_1}$	g_0	0	$-2\rho_{xy} + \rho_z$	$+2R_z$	$-2i_{\mathrm{II}}$
$\varepsilon_{0_4}^{E}$	g_0	$-2r_{\mathrm{I}}$	$+2\rho_{xy} + \rho_z$	$-2R_{xy} - R_z$	$\boxed{-2i_{\mathrm{I}}} + 2i_{\mathrm{II}}$
1_4	$\cdot$	$\cdot$	$\cdot$	$\cdot$	$\cdot$
$\varepsilon_{1_4}^{T_2}$	g_0	$+2m_{\mathrm{I}}$	$-\rho_z$	$-R_{xy} - 2I_z$	$+2i_{\mathrm{I}}$
$\varepsilon_{1_4}^{T_1}$	g_0	$-2m_{\mathrm{I}}$	$-\rho_z$	$+R_{xy} - 2I_z$	$-2i_{\mathrm{I}}$
2_4	$\cdot$	$\cdot$	$\cdot$	$\cdot$	$\cdot$
$\varepsilon_{2_4}^{E}$	g_0	$-2r_{\mathrm{I}}$	$+2\rho_{xy} + \rho_z$	$+2R_{xy} - R_z$	$+2i_{\mathrm{I}} - 2i_{\mathrm{II}}$
$\varepsilon_{2_4}^{T_2}$	g_0	0	$-2\rho_{xy} + \rho_z$	$-2R_z$	$+2i_{\mathrm{II}}$
$\varepsilon_{2_4}^{A_2}$	g_0	$+8r_{\mathrm{I}}$	$+2\rho_{xy} + \rho_z$	$-4R_{xy} - 2R_z$	$-4i_{\mathrm{I}} - 2i_{\mathrm{II}}$
3_4	$\cdot$	$\cdot$	$\cdot$	$\cdot$	$\cdot$
$\varepsilon_{3_4}^{T_2}$	g_0	$-2m_{\mathrm{I}}$	$-\rho_z$	$-R_{xy} + 2I_z$	$+2i_{\mathrm{I}}$
$\varepsilon_{3_4}^{T_1}$	g_0	$+2m_{\mathrm{I}}$	$-\rho_z$	$+R_{xy} + 2I_z$	$-2i_{\mathrm{I}}$

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



1_4

2_4

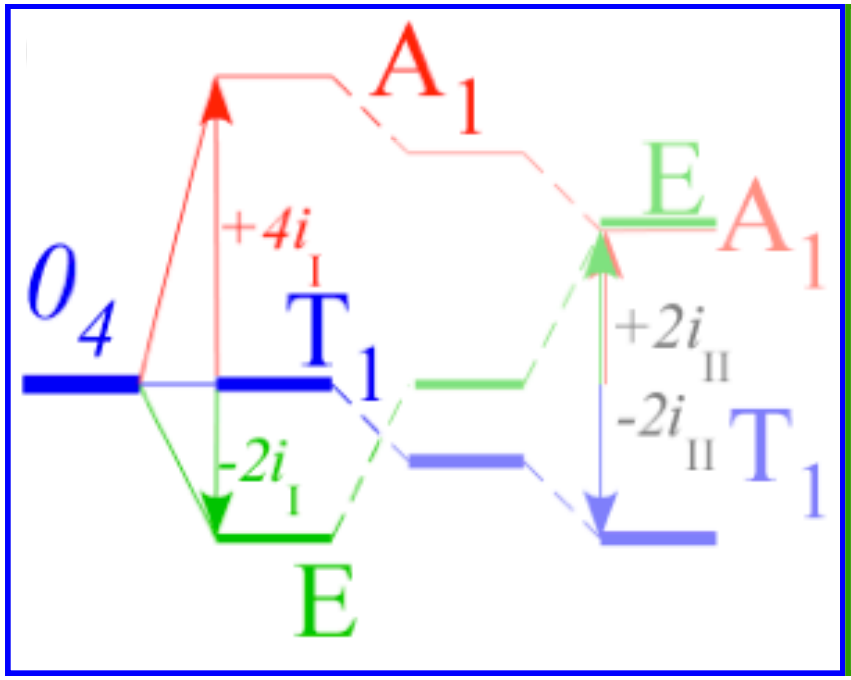
3_4

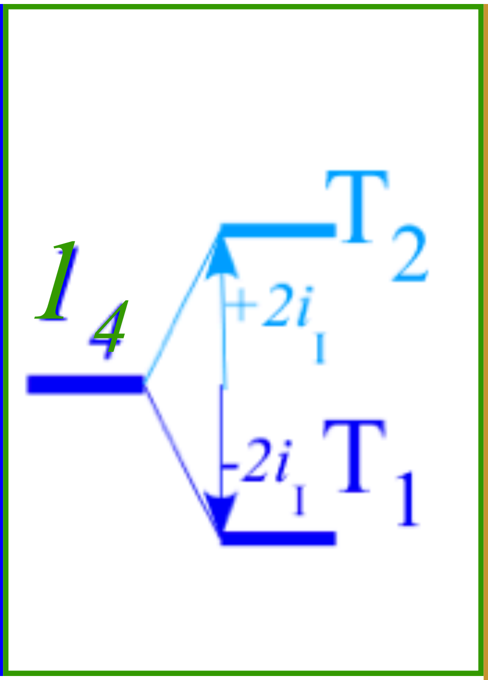
C_4 Subgroup-defined tunneling parameter modeling

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	$\cdot$	$r_{\mathrm{I}} = \mathrm{Re}\, r_{1234}$ $m_{\mathrm{I}} = \mathrm{Im}\, r_{1234}$	$\cdot$	$R_z = \mathrm{Re} R_z$ $I_z = \mathrm{Im} R_z$	$i_{\mathrm{I}} = i_{1256}$ $i_{\mathrm{II}} = i_{34}$
$\varepsilon_{0_4}^{A_1} =$	g_0	$+8r_{\mathrm{I}}$	$+2\rho_{xy} + \rho_z$	$+4R_{xy} + 2R_z$	$+4i_{\mathrm{I}} + 2i_{\mathrm{II}}$
$\varepsilon_{0_4}^{T_1}$	g_0	0	$-2\rho_{xy} + \rho_z$	$+2R_z$	$-2i_{\mathrm{II}}$
$\varepsilon_{0_4}^{E}$	g_0	$-2r_{\mathrm{I}}$	$+2\rho_{xy} + \rho_z$	$-2R_{xy} - R_z$	$-2i_{\mathrm{I}} + 2i_{\mathrm{II}}$
1_4	$\cdot$	$\cdot$	$\cdot$	$\cdot$	$\cdot$
$\varepsilon_{1_4}^{T_2}$	g_0	$+2m_{\mathrm{I}}$	$-\rho_z$	$-R_{xy} - 2I_z$	$+2i_{\mathrm{I}}$
$\varepsilon_{1_4}^{T_1}$	g_0	$-2m_{\mathrm{I}}$	$-\rho_z$	$+R_{xy} - 2I_z$	$-2i_{\mathrm{I}}$
2_4	$\cdot$	$\cdot$	$\cdot$	$\cdot$	$\cdot$
$\varepsilon_{2_4}^{E}$	g_0	$-2r_{\mathrm{I}}$	$+2\rho_{xy} + \rho_z$	$+2R_{xy} - R_z$	$+2i_{\mathrm{I}} - 2i_{\mathrm{II}}$
$\varepsilon_{2_4}^{T_2}$	g_0	0	$-2\rho_{xy} + \rho_z$	$-2R_z$	$+2i_{\mathrm{II}}$
$\varepsilon_{2_4}^{A_2}$	g_0	$+8r_{\mathrm{I}}$	$+2\rho_{xy} + \rho_z$	$-4R_{xy} - 2R_z$	$-4i_{\mathrm{I}} - 2i_{\mathrm{II}}$
3_4	$\cdot$	$\cdot$	$\cdot$	$\cdot$	$\cdot$
$\varepsilon_{3_4}^{T_2}$	g_0	$-2m_{\mathrm{I}}$	$-\rho_z$	$-R_{xy} + 2I_z$	$+2i_{\mathrm{I}}$
$\varepsilon_{3_4}^{T_1}$	g_0	$+2m_{\mathrm{I}}$	$-\rho_z$	$+R_{xy} + 2I_z$	$-2i_{\mathrm{I}}$

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





2_4

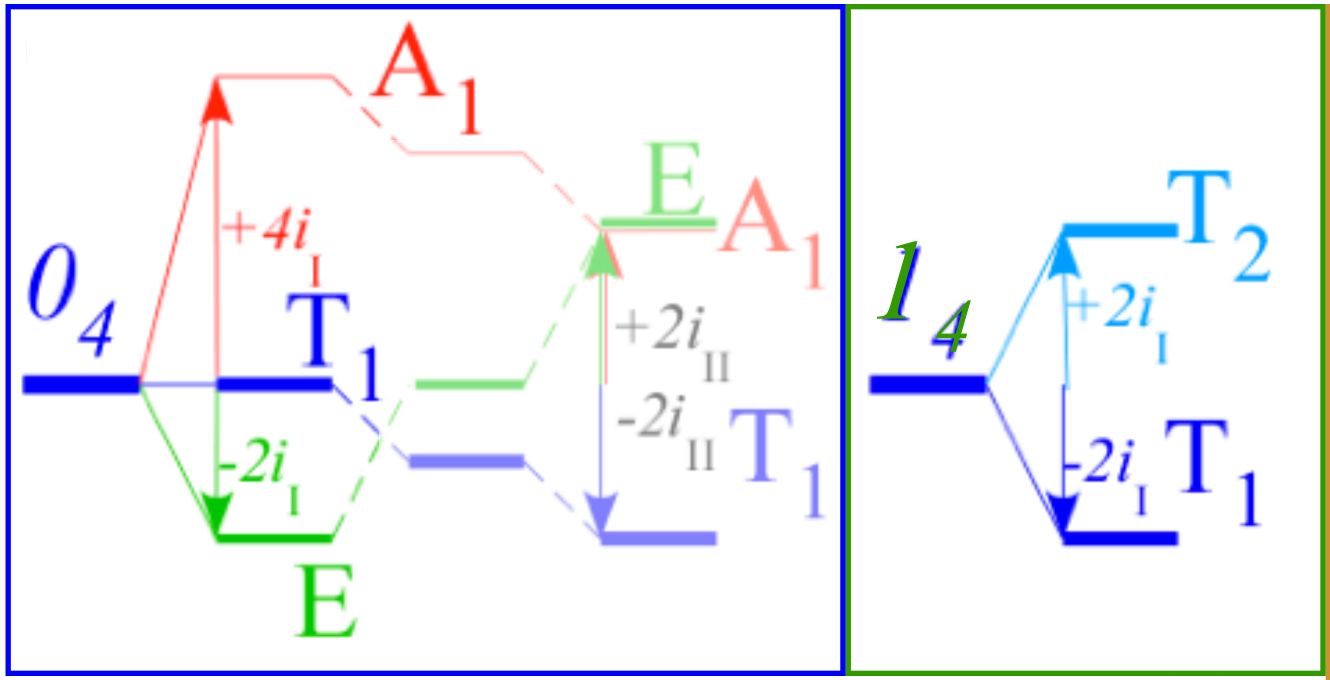
3_4

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	$\cdot$	$r_{\text{I}} = \text{Re}\, r_{1234}$ $m_{\text{I}} = \text{Im}\, r_{1234}$	$\cdot$	$R_z = \text{Re} R_z$ $I_z = \text{Im} R_z$	$i_{\text{I}} = i_{1256}$ $i_{\text{II}} = i_{34}$
$\varepsilon^{A_1}_{0_4} =$	g_0	$+8r_{\text{I}}$	$+2\rho_{xy} + \rho_z$	$+4R_{xy} + 2R_z$	$+4i_{\text{I}} + 2i_{\text{II}}$
$\varepsilon^{T_1}_{0_4}$	g_0	0	$-2\rho_{xy} + \rho_z$	$+2R_z$	$-2i_{\text{II}}$
$\varepsilon^{E}_{0_4}$	g_0	$-2r_{\text{I}}$	$+2\rho_{xy} + \rho_z$	$-2R_{xy} - R_z$	$-2i_{\text{I}} + 2i_{\text{II}}$
1_4	$\cdot$	$\cdot$	$\cdot$	$\cdot$	$\cdot$
$\varepsilon^{T_2}_{1_4}$	g_0	$+2m_{\text{I}}$	$-\rho_z$	$-R_{xy} - 2I_z$	$+2i_{\text{I}}$
$\varepsilon^{T_1}_{1_4}$	g_0	$-2m_{\text{I}}$	$-\rho_z$	$+R_{xy} - 2I_z$	$-2i_{\text{I}}$
2_4	$\cdot$	$\cdot$	$\cdot$	$\cdot$	$\cdot$
$\varepsilon^{E}_{2_4}$	g_0	$-2r_{\text{I}}$	$+2\rho_{xy} + \rho_z$	$+2R_{xy} - R_z$	$+2i_{\text{I}} - 2i_{\text{II}}$
$\varepsilon^{T_2}_{2_4}$	g_0	0	$-2\rho_{xy} + \rho_z$	$-2R_z$	$+2i_{\text{II}}$
$\varepsilon^{A_2}_{2_4}$	g_0	$+8r_{\text{I}}$	$+2\rho_{xy} + \rho_z$	$-4R_{xy} - 2R_z$	$-4i_{\text{I}} - 2i_{\text{II}}$
3_4	$\cdot$	$\cdot$	$\cdot$	$\cdot$	$\cdot$
$\varepsilon^{T_2}_{3_4}$	g_0	$-2m_{\text{I}}$	$-\rho_z$	$-R_{xy} + 2I_z$	$+2i_{\text{I}}$
$\varepsilon^{T_1}_{3_4}$	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

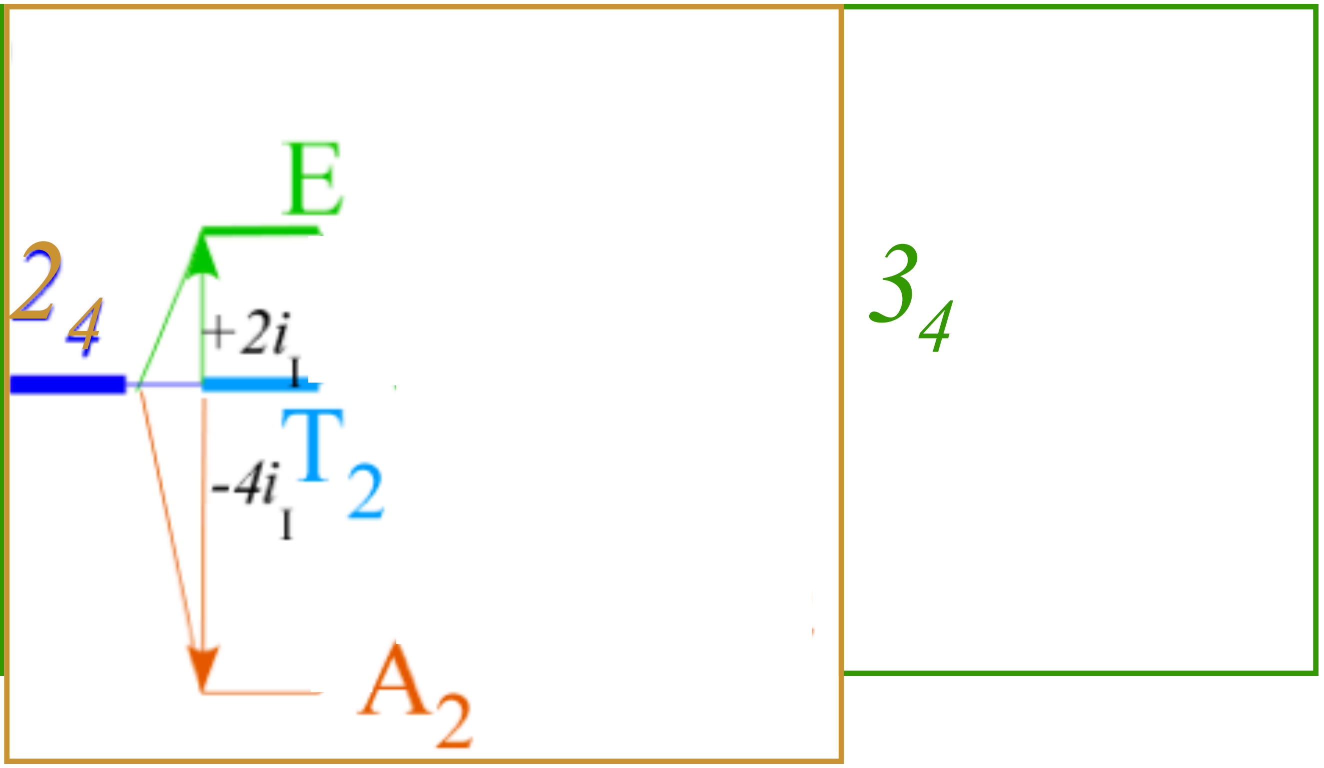
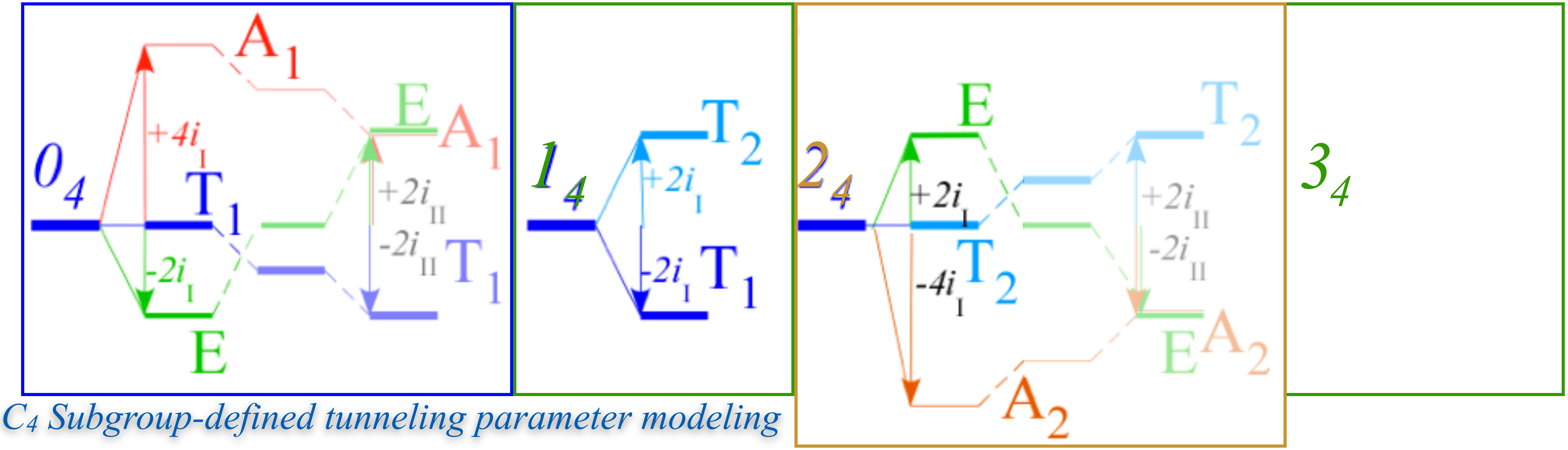


Table 11. Splittings of $O \supset C_4$ given sub-class structure.

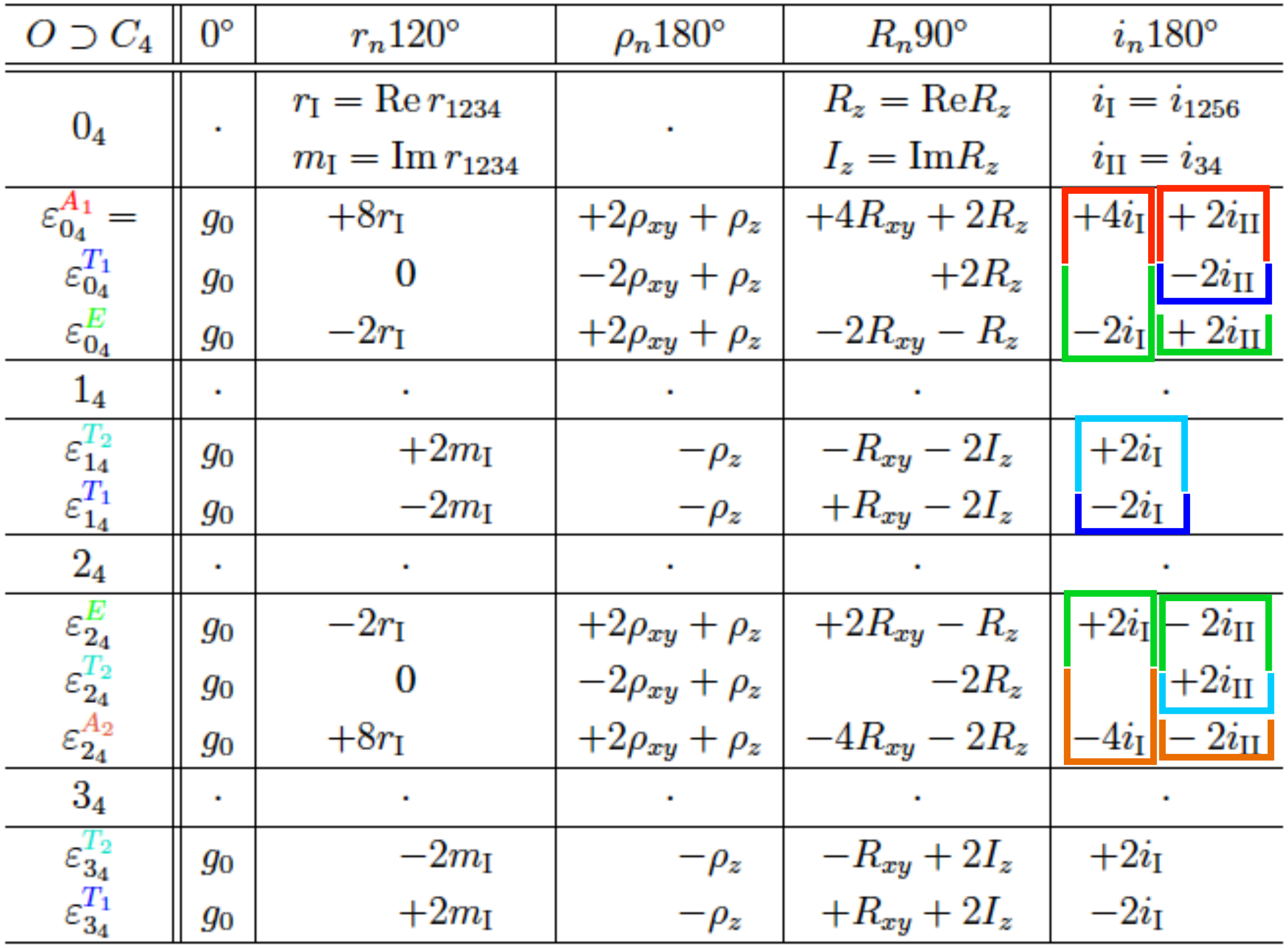
$O \supset C_4$	$0°$	$r_n 120°$	$\rho_n 180°$	$R_n 90°$	$i_n 180°$
0_4	$\cdot$	$r_{\mathrm{I}} = \mathrm{Re}\, r_{1234}$ $m_{\mathrm{I}} = \mathrm{Im}\, r_{1234}$	$\cdot$	$R_z = \mathrm{Re} R_z$ $I_z = \mathrm{Im} R_z$	$i_{\mathrm{I}} = i_{1256}$ $i_{\mathrm{II}} = i_{34}$
$\varepsilon_{0_4}^{A_1} =$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

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



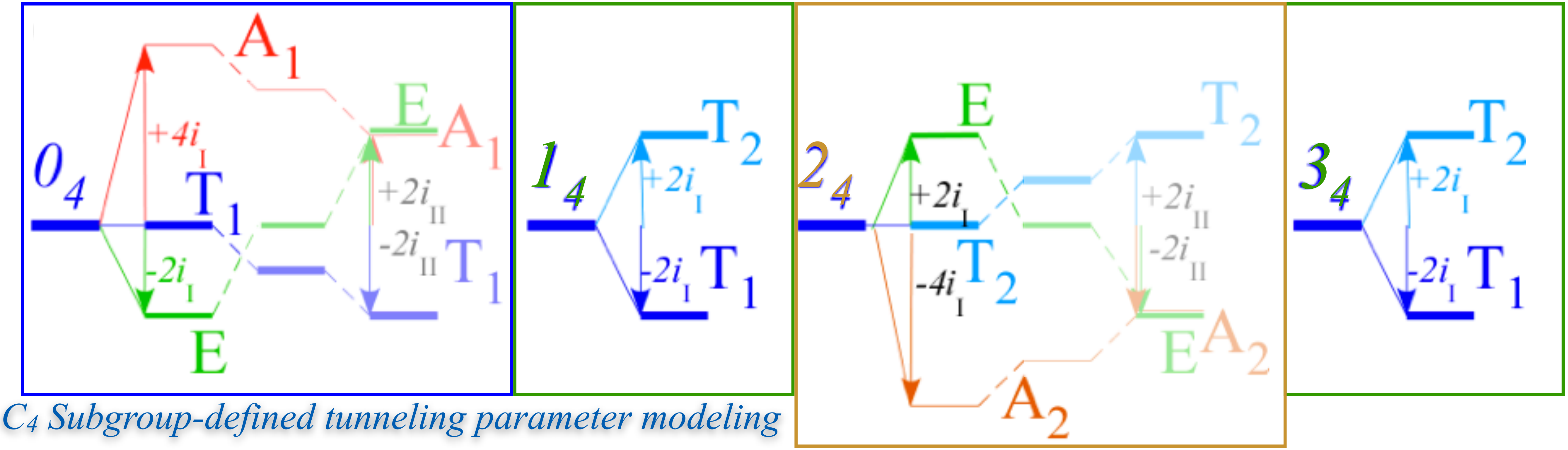
C_4 Subgroup-defined tunneling parameter modeling

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	$\cdot$	$r_{\mathrm{I}} = \mathrm{Re}\, r_{1234}$ $m_{\mathrm{I}} = \mathrm{Im}\, r_{1234}$	$\cdot$	$R_z = \mathrm{Re} R_z$ $I_z = \mathrm{Im} R_z$	$i_{\mathrm{I}} = i_{1256}$ $i_{\mathrm{II}} = i_{34}$
$\varepsilon_{0_4}^{A_1} =$	g_0	$+8r_{\mathrm{I}}$	$+2\rho_{xy} + \rho_z$	$+4R_{xy} + 2R_z$	$+4i_{\mathrm{I}}$ $+ 2i_{\mathrm{II}}$
$\varepsilon_{0_4}^{T_1}$	g_0	0	$-2\rho_{xy} + \rho_z$	$+2R_z$	$-2i_{\mathrm{II}}$
$\varepsilon_{0_4}^{E}$	g_0	$-2r_{\mathrm{I}}$	$+2\rho_{xy} + \rho_z$	$-2R_{xy} - R_z$	$-2i_{\mathrm{I}}$ $+ 2i_{\mathrm{II}}$
1_4	$\cdot$	$\cdot$	$\cdot$	$\cdot$	$\cdot$
$\varepsilon_{1_4}^{T_2}$	g_0	$+2m_{\mathrm{I}}$	$-\rho_z$	$-R_{xy} - 2I_z$	$+2i_{\mathrm{I}}$
$\varepsilon_{1_4}^{T_1}$	g_0	$-2m_{\mathrm{I}}$	$-\rho_z$	$+R_{xy} - 2I_z$	$-2i_{\mathrm{I}}$
2_4	$\cdot$	$\cdot$	$\cdot$	$\cdot$	$\cdot$
$\varepsilon_{2_4}^{E}$	g_0	$-2r_{\mathrm{I}}$	$+2\rho_{xy} + \rho_z$	$+2R_{xy} - R_z$	$+2i_{\mathrm{I}}$ $- 2i_{\mathrm{II}}$
$\varepsilon_{2_4}^{T_2}$	g_0	0	$-2\rho_{xy} + \rho_z$	$-2R_z$	$+2i_{\mathrm{II}}$
$\varepsilon_{2_4}^{A_2}$	g_0	$+8r_{\mathrm{I}}$	$+2\rho_{xy} + \rho_z$	$-4R_{xy} - 2R_z$	$-4i_{\mathrm{I}}$ $- 2i_{\mathrm{II}}$
3_4	$\cdot$	$\cdot$	$\cdot$	$\cdot$	$\cdot$
$\varepsilon_{3_4}^{T_2}$	g_0	$-2m_{\mathrm{I}}$	$-\rho_z$	$-R_{xy} + 2I_z$	$+2i_{\mathrm{I}}$
$\varepsilon_{3_4}^{T_1}$	g_0	$+2m_{\mathrm{I}}$	$-\rho_z$	$+R_{xy} + 2I_z$	$-2i_{\mathrm{I}}$

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

AMOP reference links on page 2

3.12.18 class 17.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Discrete symmetry subgroups of O(3)⊃(Octahedral $O_h \supset O$): Part II Full $D^{(\alpha)}$-matrices defined by subgroup-chains $O\supset D_4 \supset C_4$, D_2, or C_3 applied to eigensolutions of O_h-tensors $\mathbf{T}^{[4]}+\mathbf{T}^{[6]}$

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

Review *Coset factored splitting of projectors for* $O\supset D_4 \supset C_4$ *into split classes and level structure*

Hamiltonian level cluster models with subgroup-defined tunneling parameters

Diagonal idempotent $\mathbf{P}^{\mu}_{m,m}$ *parameter sets for* $O\supset C_4$ *and* $O\supset C_3$ *case of* SF_6 *level clusters*

Off-diagonal nilpotent $\mathbf{P}^{\mu}_{m,n}$ $(m\neq n)$ *parameter sets needed for* $O\supset C_2$ *clusters*

Deriving nilpotent projectors $\mathbf{P}^{\mu}_{m,n}$ *and ireps* $D^{\mu}_{m,n}$ *by fundamental* $\mathbf{g}\rightleftarrows\mathbf{P}^{\mu}_{m,n}$ *relations:*

(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 nilpotent projectors for simple $D_3\supset C_2 \sim C_{3v}\supset C_v$ *chains* (Lect13p95)

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

Structure and applications of coset tabulated $D^{\mu}_{m,n}$ *irreps for various* O_h *subgroup chains*

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

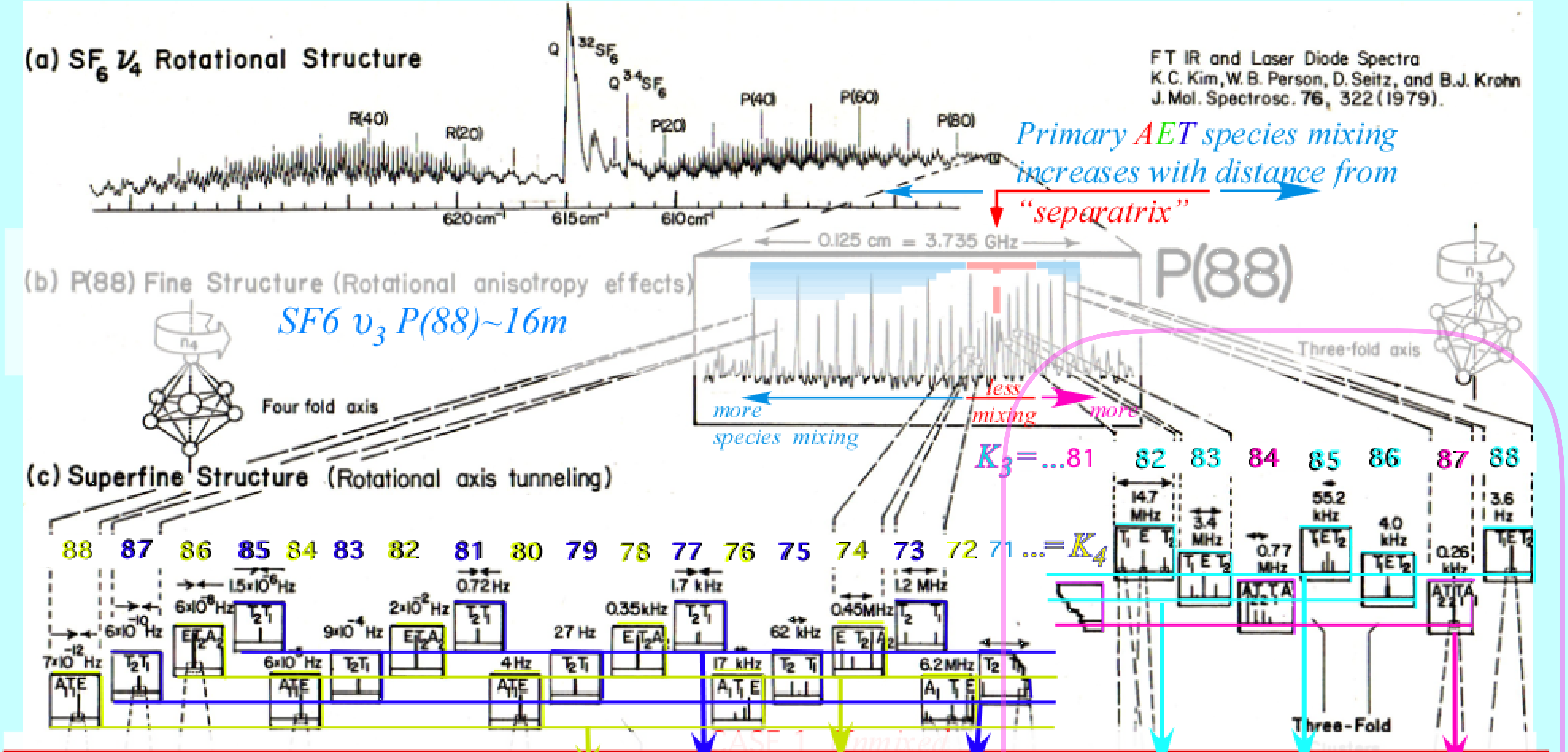
Comparing $O_h\supset D_{4h}\supset D_{2h}$ *and* $O_h\supset D_{3d}\supset C_2$ *representations (*T_1 *vector-type)*

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

Comparing local C_4, C_3, *and* C_2 *cluster spectra of* O_h*-symmetric tensors* $\mathbf{T}^{[4]}+\mathbf{T}^{[6]}$

Monster clusters: When local C_2 *symmetry dominates*

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



Primary AET species mixing increases with distance from "separatrix"

SF6 υ_3 P(88)~16m

Observed repeating sequence(s)...$A_1\ T_1E\ \ T_2T_1\ \ ET_2A_2\ \ T_2T_1\ A_1\ \ T_1ET_2\ T_1ET_2\ \ A_2T_2T_1A_1$...

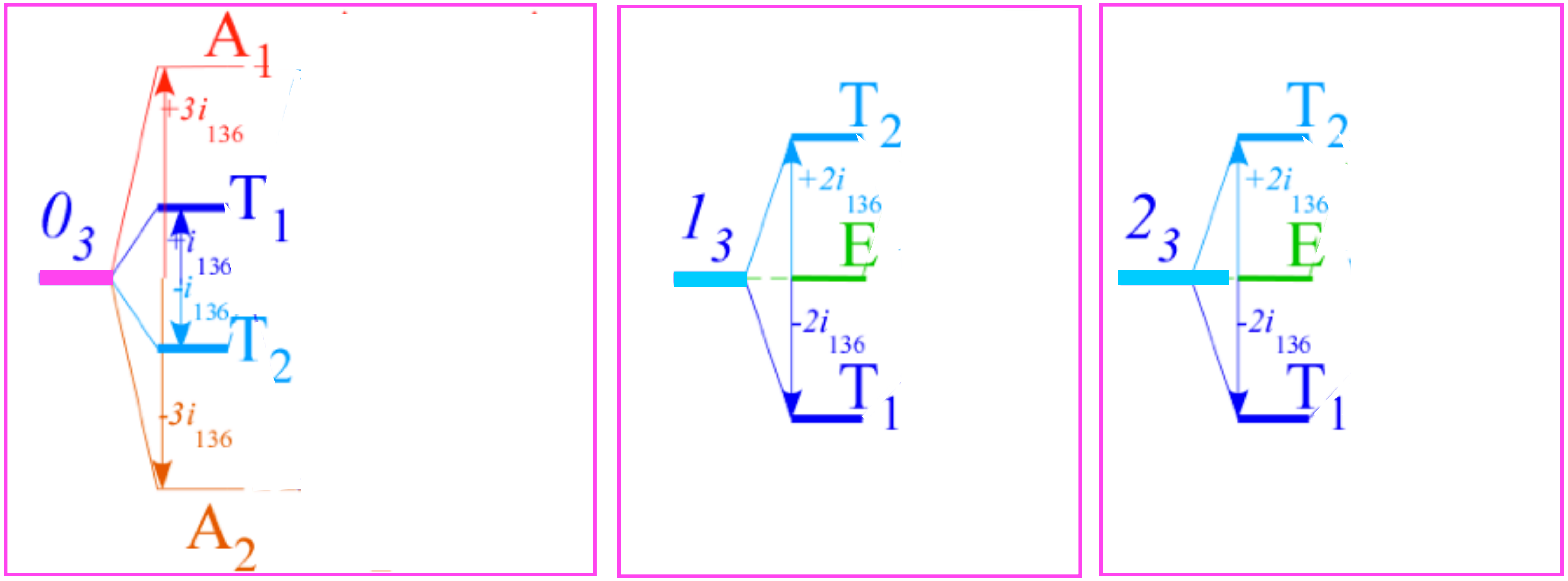
$O \supset C_4$	$(0)_4$	$(1)_4$	$(2)_4$	$(3)_4$=$(-1)_4$
A_1	1	•	•	•
A_2	•	•	1	•
E	1	•	1	•
T_1	1	1	•	1
T_2	•	1	1	1

$O \supset C_3$	$(0)_3$	$(1)_3$	$(2)_3$=$(-1)_3$
A_1	1	•	•
A_2	1	•	•
E	•	1	1
T_1	1	1	1
T_2	1	1	1

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

...and physical consequences?

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

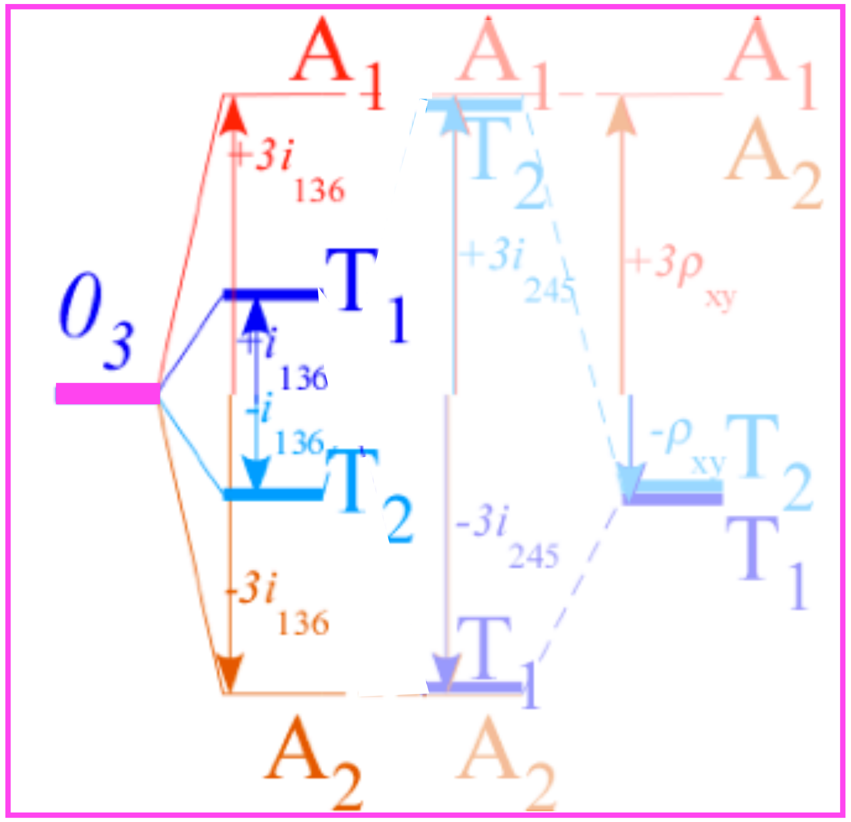


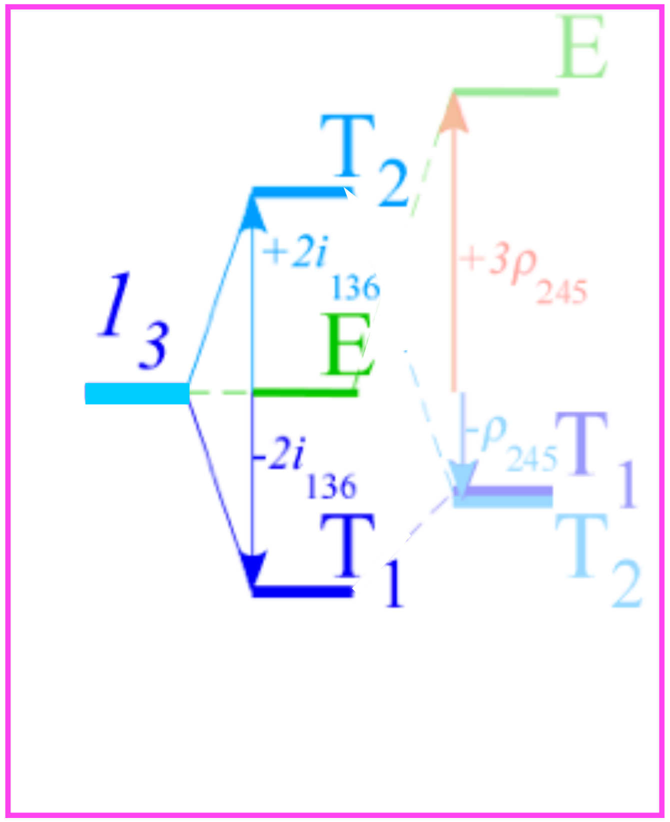
C_3 Subgroup-defined tunneling parameter modeling

Int.J.Mol.Sci, 14, 714(2013)pdf p73

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

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





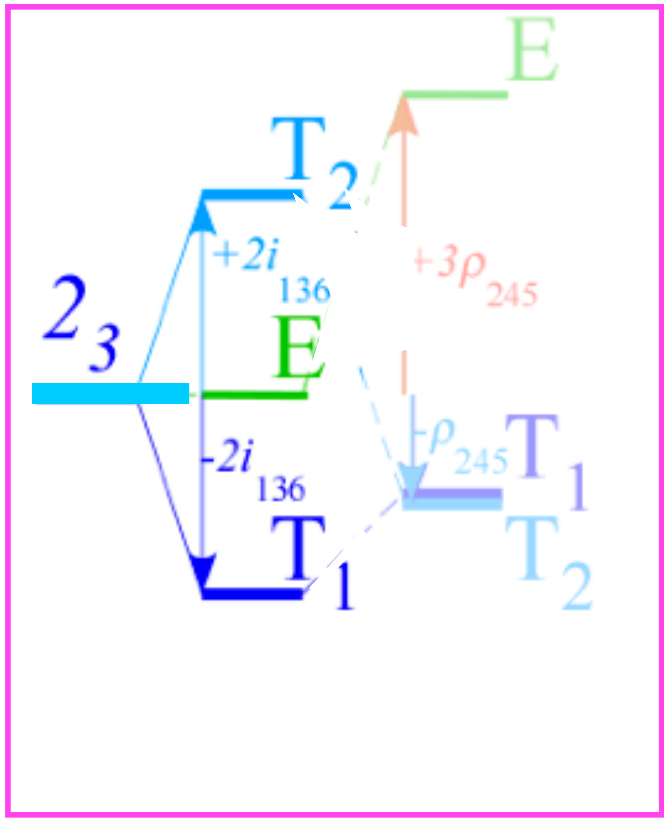


Table 12. Splittings of $O \supset C_3$ given sub-class structure.

Int.J.Mol.Sci, 14, 714(2013)pdf p73

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	$\cdot$	$r_{\mathrm{I}} = Re(r_1) \quad i_{\mathrm{I}} = Im(r_1)$ $r_{\mathrm{II}} = Re(r_{234}) \quad i_{\mathrm{I}} = Im(r_{234})$	$\rho = \rho_{xyz}$	$R_n = Re(R_{xyz})$ $I_n = Im(R_{xyz})$	$i_{\mathrm{I}} = i_{136}$ $i_{\mathrm{II}} = i_{245}$
$\varepsilon_{0_3}^{A_1}$	g_0	$2r_{\mathrm{I}} \quad + 6r_{\mathrm{II}}$	3ρ	$6R_n$	$3i_{\mathrm{I}} + 3i_{\mathrm{I}}$
$\varepsilon_{0_3}^{A_2}$	g_0	$2r_{\mathrm{I}} \quad + 6r_{\mathrm{II}}$	3ρ	$-6R_n$	$-3i_{\mathrm{I}} - 3i_{\mathrm{II}}$
$\varepsilon_{0_3}^{T_1}$	g_0	$2r_{\mathrm{I}} \quad - 2r_{\mathrm{II}}$	$-\rho$	$2R_n$	$i_{\mathrm{I}} + 3i_{\mathrm{II}}$
$\varepsilon_{0_3}^{T_2}$	g_0	$2r_{\mathrm{I}} \quad - 2r_{\mathrm{II}}$	$-\rho$	$-2R_n$	$-i_{\mathrm{I}} + 3i_{\mathrm{II}}$
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)

AMOP reference links on page 2

3.12.18 class 17.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Discrete symmetry subgroups of O(3)⊃(Octahedral O_h⊃O): Part II Full $D^{(\alpha)}$-matrices defined by subgroup-chains $O\supset D_4\supset C_4$, D_2, or C_3 applied to eigensolutions of O_h-tensors $\mathbf{T}^{[4]}+\mathbf{T}^{[6]}$

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

Review Coset factored splitting of projectors for $O\supset D_4\supset C_4$ *into split classes and level structure*

Hamiltonian level cluster models with subgroup-defined tunneling parameters

Diagonal idempotent $\mathbf{P}^{\mu}_{m,m}$ *parameter sets for* $O\supset C_4$ *and* $O\supset C_3$ *case of* SF_6 *level clusters*

Off-diagonal nilpotent $\mathbf{P}^{\mu}_{m,n}$ $(m\neq n)$ *parameter sets needed for* $O\supset C_2$ *clusters*

Deriving nilpotent projectors $\mathbf{P}^{\mu}_{m,n}$ *and ireps* $D^{\mu}_{m,n}$ *by fundamental* $\mathbf{g}\rightleftarrows\mathbf{P}^{\mu}_{m,n}$ *relations:*

(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 nilpotent projectors for simple $D_3\supset C_2\sim C_{3v}\supset C_v$ *chains* (Lect13p95)

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

Structure and applications of coset tabulated $D^{\mu}_{m,n}$ *irreps for various* O_h *subgroup chains*

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

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 *cluster spectra of* O_h*-symmetric tensors* $\mathbf{T}^{[4]}+\mathbf{T}^{[6]}$

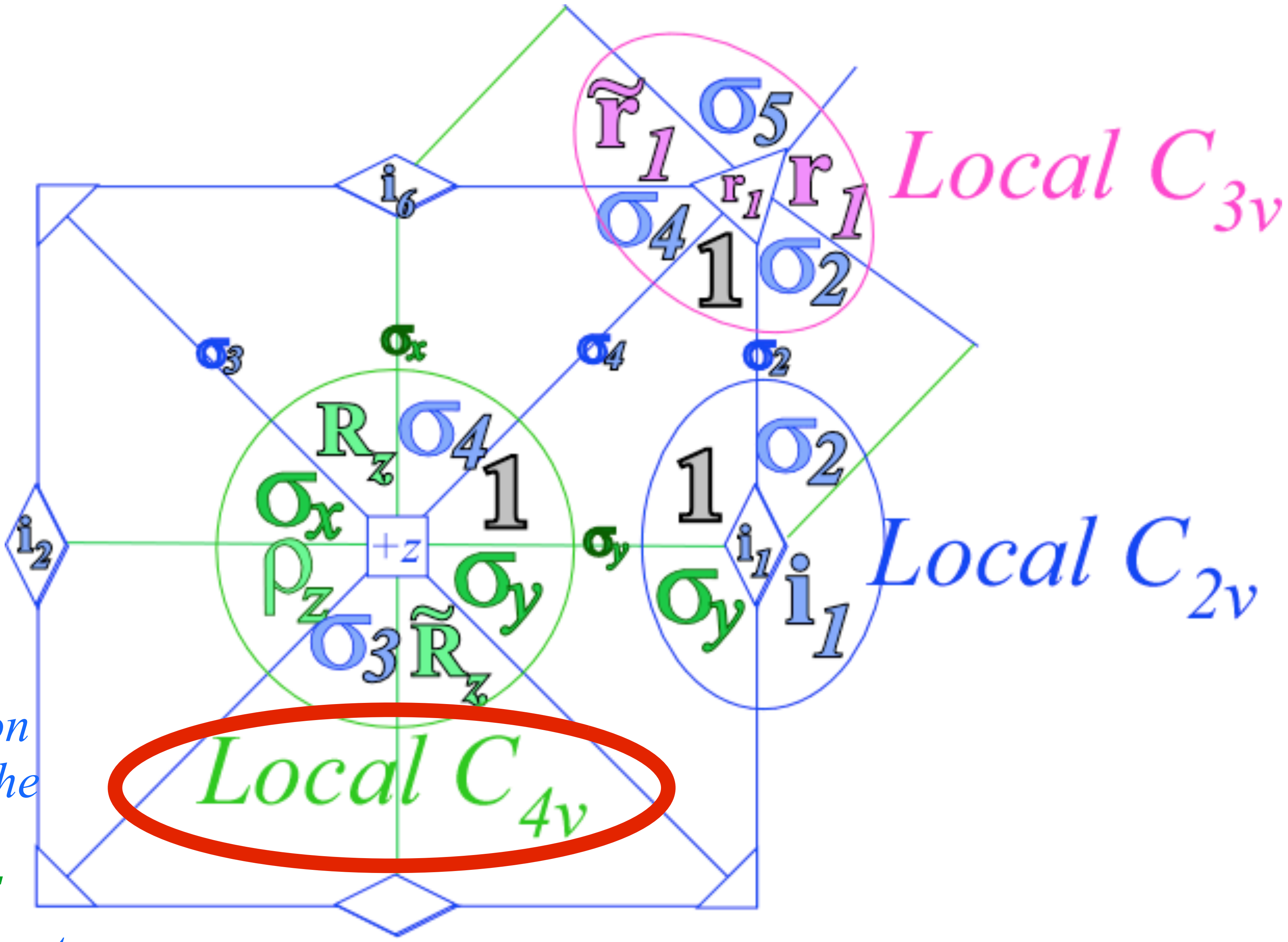
Monster clusters: When local C_2 *symmetry dominates*

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

Correlations for local $O_h \supset C_{4v}$ symmetry

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

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



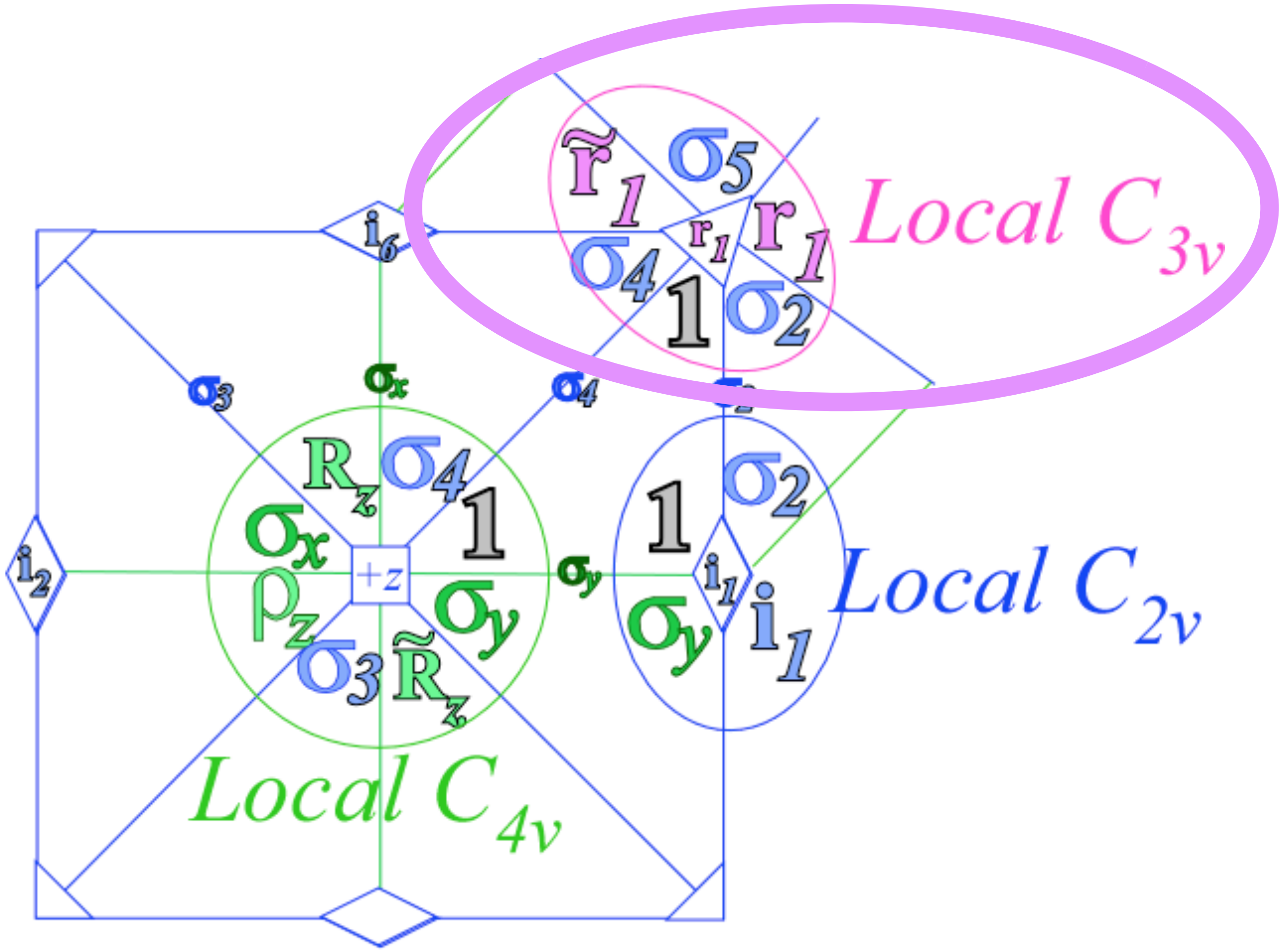
$O_h \supset C_{4v}$ correlation predicts the parity of the A_1T_1E cluster is not uniformly even (g) or odd (u): $A_{1g}T_{1u}E_g$

Int.J.Mol.Sci, 14, 714(2013)pdf p64

Correlations for local $O_h \supset C_{3v}$ symmetry

$O \supset C_3$	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
$A_{1u} \downarrow C_{3v}$	·	1	·
$A_{2u} \downarrow C_{3v}$	1	·	·
$E_u \downarrow C_{3v}$	·	·	1
$T_{1u} \downarrow C_{3v}$	1	·	1
$T_{2u} \downarrow C_{3v}$	·	1	1



Int.J.Mol.Sci, 14, 714(2013)pdf p64

Correlations for local $O_h \supset C_{2v}$ symmetry

$O \supset C_2(\mathbf{i}_1)$	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

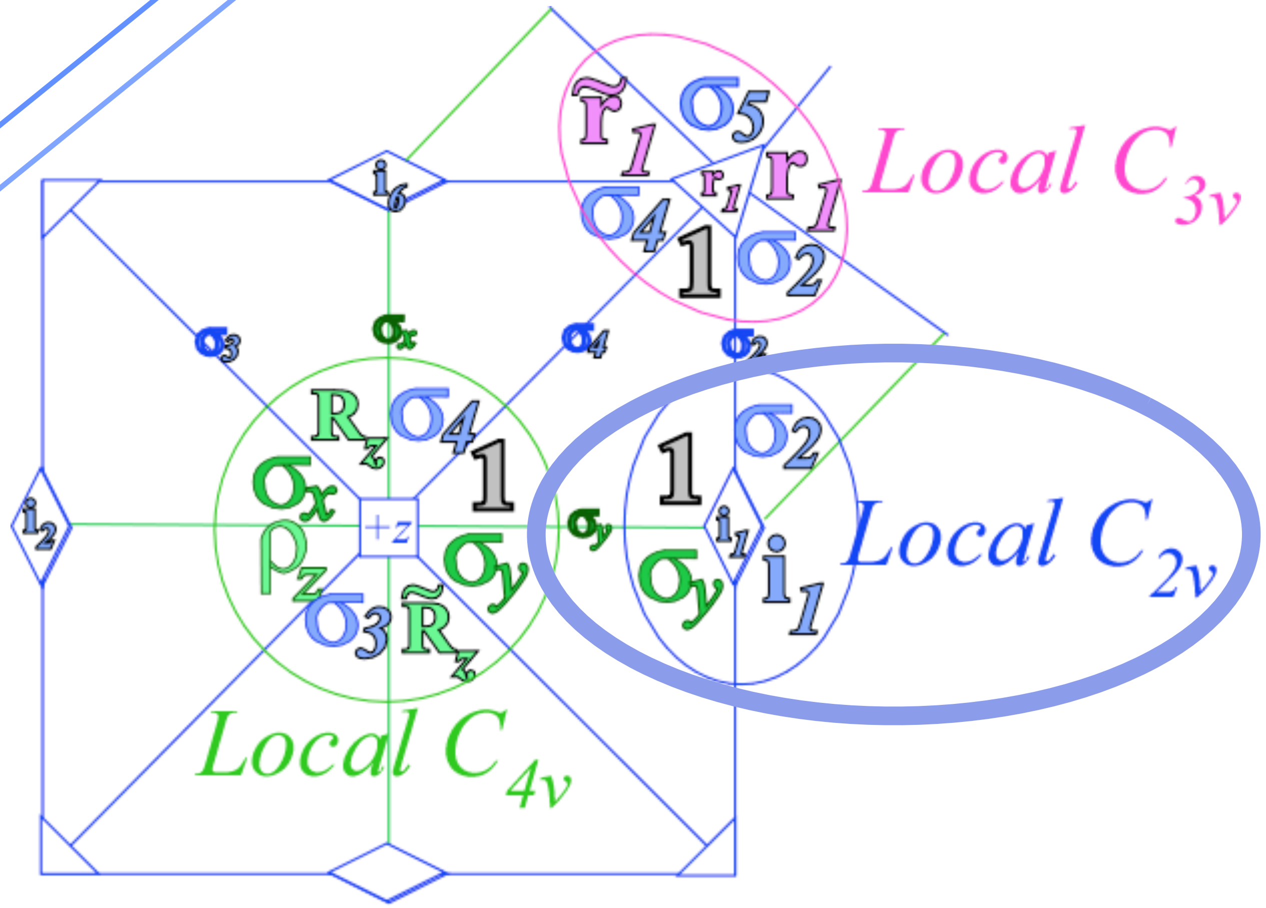
$O \supset C_2(\rho_z)$	0_2	1_2
$A_1 \downarrow C_2$	1	·
$A_2 \downarrow C_2$	1	·
$E \downarrow C_2$	2	·
$T_1 \downarrow C_2$	1	2
$T_2 \downarrow C_2$	1	2

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

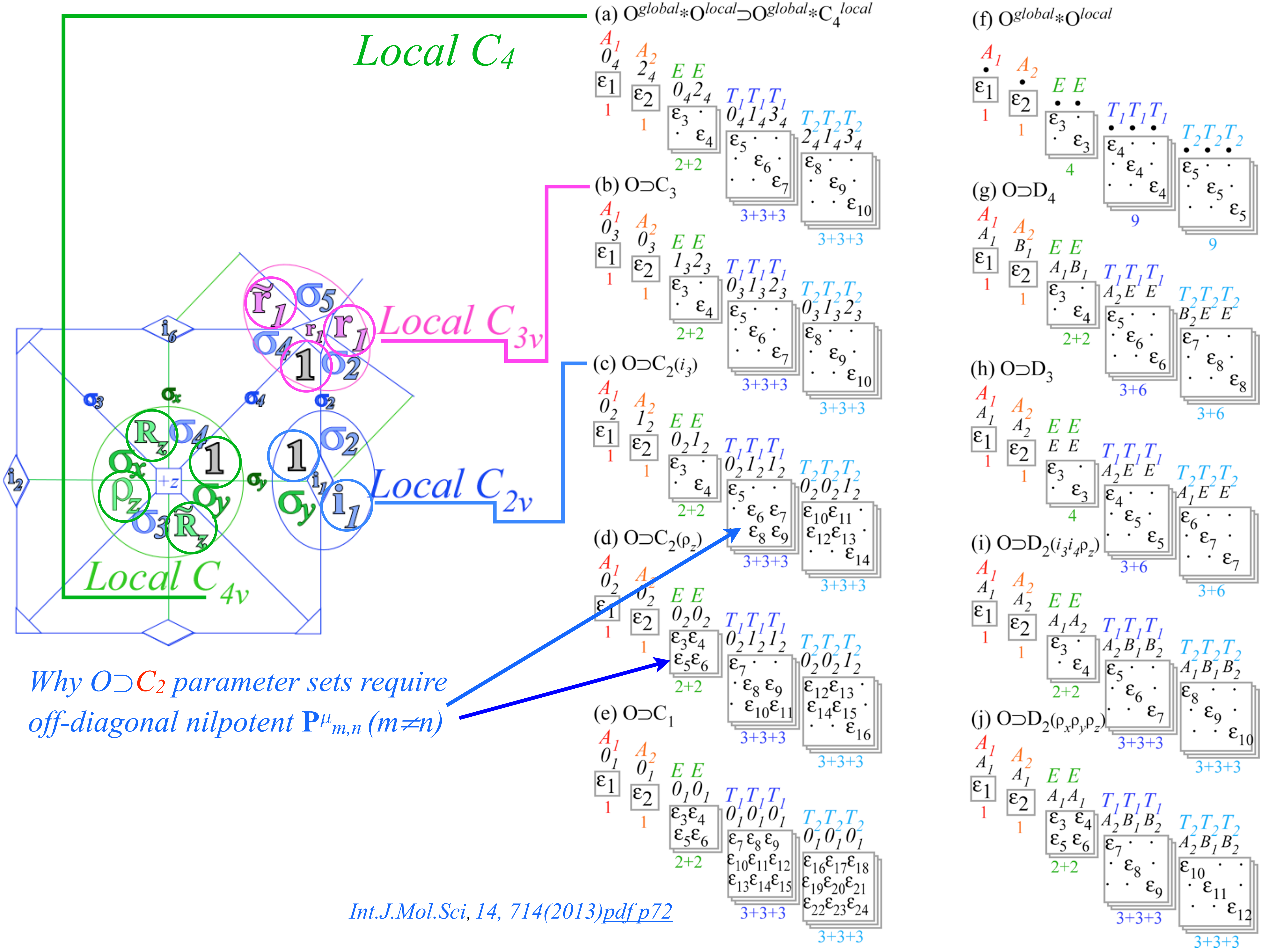
$O_h \supset C^i_{2v}$	A'	B'	A''	B''
$A_{1g} \downarrow C^i_{2v}$	1	·	·	·
$A_{2g} \downarrow C^i_{2v}$	·	1	·	·
$E_g \downarrow C^i_{2v}$	1	1	·	·
$T_{1g} \downarrow C^i_{2v}$	·	1	1	1
$T_{2g} \downarrow C^i_{2v}$	1	·	1	1
$A_{1u} \downarrow C^i_{2v}$	·	·	1	·
$A_{2u} \downarrow C^i_{2v}$	·	·	·	1
$E_u \downarrow C^i_{2v}$	·	·	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
$A_{1u} \downarrow C^z_{2v}$	·	·	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)pdf p64



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

Int.J.Mol.Sci, 14, 714(2013)pdf p72

AMOP reference links on page 2

3.12.18 class 17.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Discrete symmetry subgroups of O(3)⊃(Octahedral O_h⊃O): Part II Full $D^{(\alpha)}$-matrices defined by subgroup-chains $O\supset D_4\supset C_4$, D_2, or C_3 applied to eigensolutions of O_h-tensors $\mathbf{T}^{[4]}+\mathbf{T}^{[6]}$

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

Review *Coset factored splitting of projectors for* $O\supset D_4\supset C_4$ *into split classes and level structure*

Hamiltonian level cluster models with subgroup-defined tunneling parameters

- *Diagonal idempotent* $\mathbf{P}^{\mu}_{m,m}$ *parameter sets for* $O\supset C_4$ *and* $O\supset C_3$ *case of* SF_6 *level clusters*
- *Off-diagonal nilpotent* $\mathbf{P}^{\mu}_{m,n}$ $(m\neq n)$ *parameter sets needed for* $O\supset C_2$ *clusters*

Deriving nilpotent projectors $\mathbf{P}^{\mu}_{m,n}$ *and ireps* $D^{\mu}_{m,n}$ *by fundamental* $\mathbf{g}\rightleftarrows\mathbf{P}^{\mu}_{m,n}$ *relations:*

(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 nilpotent projectors for simple* $D_3\supset C_2\sim C_{3v}\supset C_v$ *chains* (Lect13p95)
- *Calculating and Factoring* $\mathbf{P}^{T_1}_{1_4 0_4}$ *and* $\mathbf{P}^{T_1}_{1_4 3_4}$

Structure and applications of coset tabulated $D^{\mu}_{m,n}$ *irreps for various* O_h *subgroup chains*

- $O_h\supset D_{4h}\supset C_{4v}$, $O_h\supset D_{3h}\supset C_{3v}$, $O_h\supset C_{2v}$
- *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 *cluster spectra of* O_h*-symmetric tensors* $\mathbf{T}^{[4]}+\mathbf{T}^{[6]}$
  - *Monster clusters: When local* C_2 *symmetry dominates*

Comparing off-diagonal $O\supset C_2$ *parameter sets to* CH_4 *models with triple point 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) $\mathbf{P}^{\mu}_{mn} = \frac{\ell^{\mu}}{°G}\sum_{\mathbf{g}}^{°G} D^{\mu*}_{mn}(\mathbf{g})\mathbf{g}$

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* $D^{\mu}{}_{m,n}$(g) for unequal *($m\neq n$)* values.

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

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 *($m \neq n$)* values.

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

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

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:

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

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

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 *($m\neq n$)* 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 normalization: $\mathbf{P}^{\mu}_{mn}\mathbf{P}^{\mu\dagger}_{mn} = \mathbf{P}^{\mu}_{mn}\mathbf{P}^{\mu}_{nm} = \mathbf{P}^{\mu}_{mm}$

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* $D^{\mu}_{m,n}(\mathrm{g})$ 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 $D^{\mu}_{m,n}(\mathrm{g})$ 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 normalization: $\mathbf{P}^{\mu}_{mn}\mathbf{P}^{\mu\dagger}_{mn} = \mathbf{P}^{\mu}_{mn}\mathbf{P}^{\mu}_{nm} = \mathbf{P}^{\mu}_{mm}$

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: $\left\langle\mathbf{P}^{\mu}_{kn}\middle|\mathbf{g}\middle|\mathbf{P}^{\mu}_{mn}\right\rangle = D^{\mu}_{km}(\mathbf{g})$

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

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

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

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 normalization: $\mathbf{P}^{\mu}_{mn}\mathbf{P}^{\mu\dagger}_{mn} = \mathbf{P}^{\mu}_{mn}\mathbf{P}^{\mu}_{nm} = \mathbf{P}^{\mu}_{mm}$

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

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* $D^{\mu}_{m,n}(\mathrm{g})$ for unequal *$(m \neq n)$* 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 $D^{\mu}_{m,n}(\mathrm{g})$ 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 normalization: $\mathbf{P}^{\mu}_{mn}\mathbf{P}^{\mu\dagger}_{mn} = \mathbf{P}^{\mu}_{mn}\mathbf{P}^{\mu}_{nm} = \mathbf{P}^{\mu}_{mm}$

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: $\left\langle\mathbf{P}^{\mu}_{kn}\middle|\mathbf{g}\middle|\mathbf{P}^{\mu}_{mn}\right\rangle = D^{\mu}_{km}(\mathbf{g})$

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: $\mathbf{P}^{\mu}_{m_4 m_4}\mathbf{g}\mathbf{P}^{\mu}_{n_4 n_4} = \mathbf{P}^{\mu}\mathbf{p}_{m_4}\mathbf{g}\mathbf{p}_{n_4}$

AMOP reference links on page 2

3.12.18 class 17.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Discrete symmetry subgroups of O(3)⊃(Octahedral O_h⊃O): Part II Full $D^{(\alpha)}$-matrices defined by subgroup-chains $O\supset D_4\supset C_4$, D_2, or C_3 applied to eigensolutions of O_h-tensors $\mathbf{T}^{[4]}+\mathbf{T}^{[6]}$

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

Review Coset factored splitting of projectors for $O\supset D_4\supset C_4$ *into split classes and level structure*

Hamiltonian level cluster models with subgroup-defined tunneling parameters

- *Diagonal idempotent* $\mathbf{P}^{\mu}_{m,m}$ *parameter sets for* $O\supset C_4$ *and* $O\supset C_3$ *case of* SF_6 *level clusters*
- *Off-diagonal nilpotent* $\mathbf{P}^{\mu}_{m,n}$ *(m≠n) parameter sets needed for* $O\supset C_2$ *clusters*

Deriving nilpotent projectors $\mathbf{P}^{\mu}_{m,n}$ *and ireps* $D^{\mu}_{m,n}$ *by fundamental* $\mathbf{g}\rightleftarrows\mathbf{P}^{\mu}_{m,n}$ *relations:*

(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 nilpotent projectors for simple $D_3\supset C_2\sim C_{3v}\supset C_v$ *chains* (Lect13p95)

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

Structure and applications of coset tabulated $D^{\mu}_{m,n}$ *irreps for various* O_h *subgroup chains*

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

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 *cluster spectra of* O_h*-symmetric tensors* $\mathbf{T}^{[4]}+\mathbf{T}^{[6]}$

Monster clusters: When local C_2 *symmetry dominates*

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

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

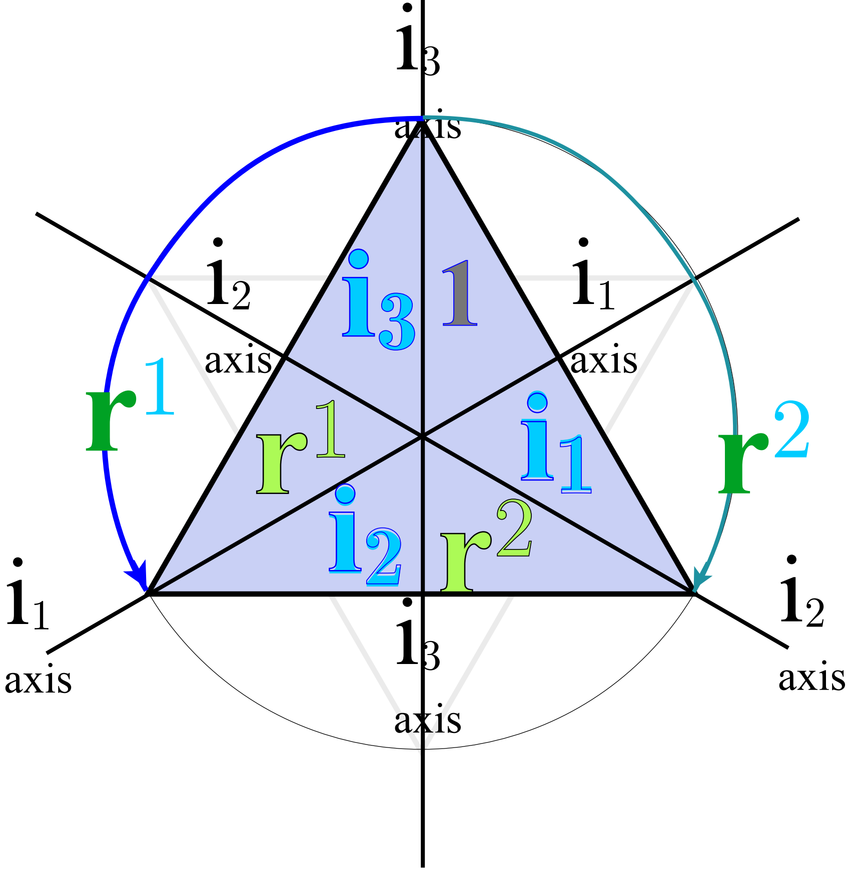
$= \frac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)$

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

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

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

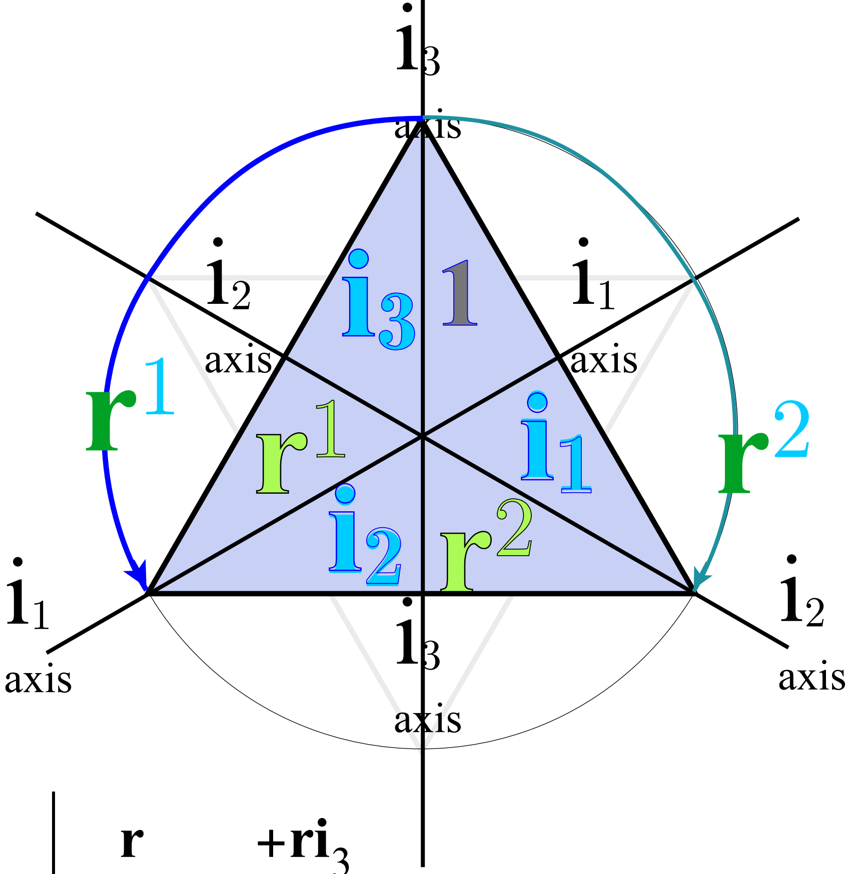
Then find nilpotent proportional to: $\mathbf{P}^{E}_{1_2 0_2} = \mathbf{P}^{E}\mathbf{p}_{1_2}\mathbf{r}\mathbf{p}_{0_2}$



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: $\mathbf{P}^{E}_{1_2 0_2} = \mathbf{P}^{E}\mathbf{p}_{1_2}\mathbf{r}\mathbf{p}_{0_2} = \mathbf{P}^{E}\,\frac{1}{2}\cdot\frac{1}{2}\left(\begin{array}{c|cc} & \mathbf{r} & +\mathbf{r}\mathbf{i}_3 \\ \hline \mathbf{1} & \mathbf{r} & +\mathbf{r}\mathbf{i}_3 \\ -\mathbf{i}_3 & -\mathbf{i}_3\mathbf{r} & -\mathbf{i}_3\mathbf{r}\mathbf{i}_3 \end{array}\right.$

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

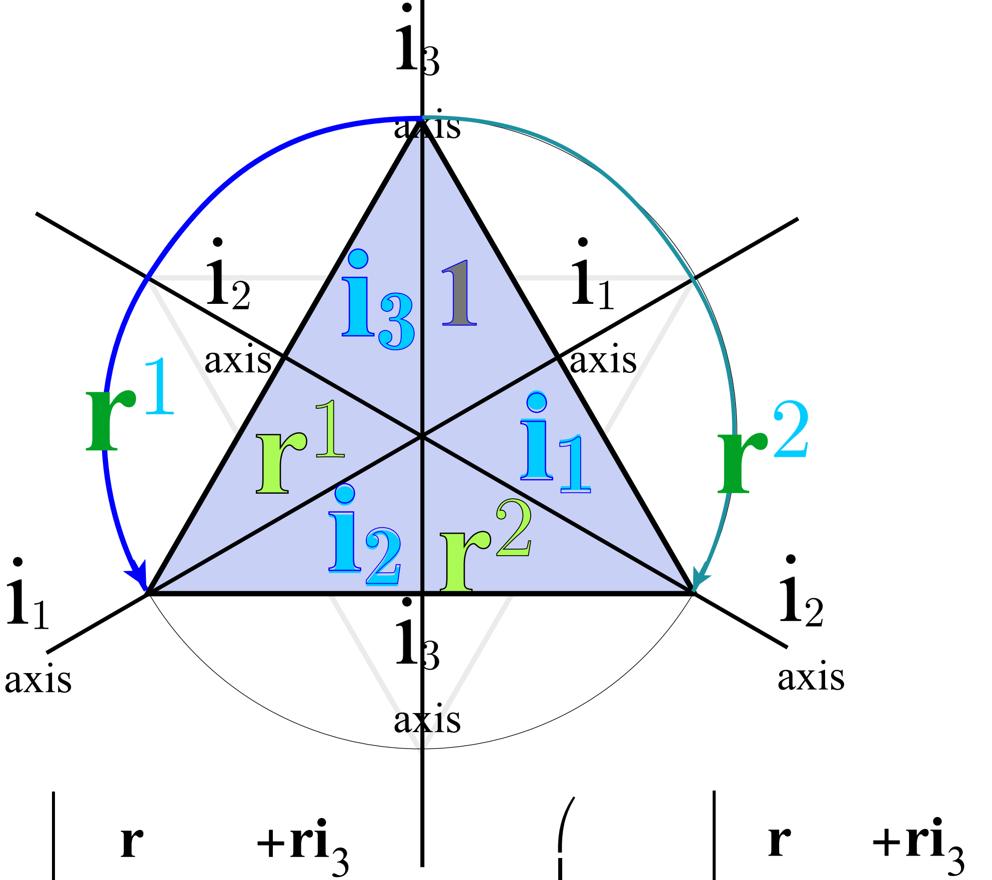
Review of $D_3 \supset C_2 \sim C_{3v} \supset C_v$

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

$D_3 : \chi^{\alpha}_{k}$	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: $\mathbf{P}^{E}_{1_2 0_2} = \mathbf{P}^{E}\mathbf{p}_{1_2}\mathbf{r}\mathbf{p}_{0_2} = \mathbf{P}^{E}\,\frac{1}{2}\cdot\frac{1}{2}\left(\begin{array}{c|cc} & \mathbf{r} & +\mathbf{r}\mathbf{i}_3 \\ \hline \mathbf{1} & \mathbf{r} & +\mathbf{r}\mathbf{i}_3 \\ -\mathbf{i}_3 & -\mathbf{i}_3\mathbf{r} & -\mathbf{i}_3\mathbf{r}\mathbf{i}_3 \end{array}\right) = \frac{1}{4}\,\mathbf{P}^{E}\left(\begin{array}{c|cc} & \mathbf{r} & +\mathbf{r}\mathbf{i}_3 \\ \hline \mathbf{1} & \mathbf{r} & +\mathbf{i}_2 \\ -\mathbf{i}_3 & -\mathbf{i}_1 & -\mathbf{r}^2 \end{array}\right)$

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

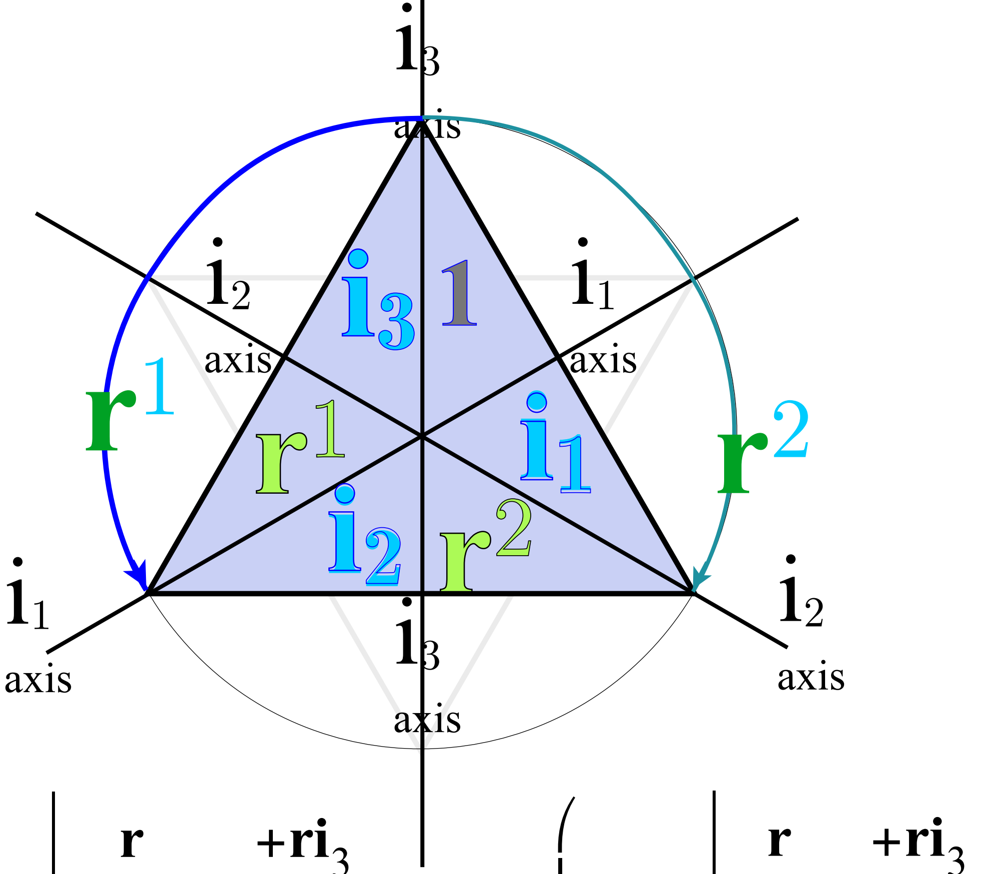
Review of $D_3 \supset C_2 \sim C_{3v} \supset C_v$

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

$D_3 : \chi^{\alpha}_{k}$	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:

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

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

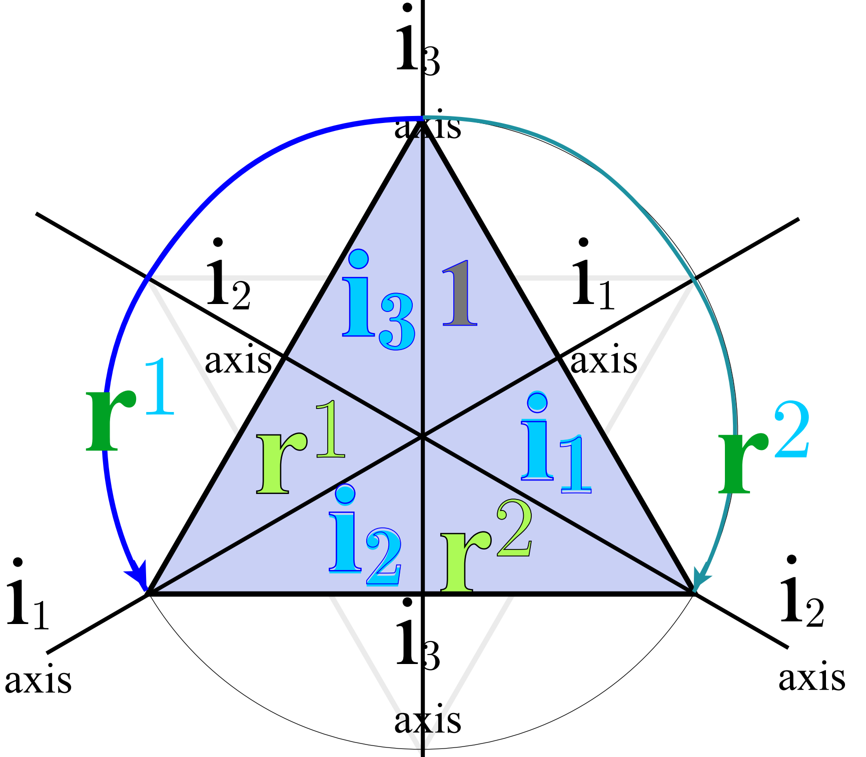
Then find nilpotent proportional to: $\mathbf{P}^{E}_{1_2 0_2} = \mathbf{P}^{E}\mathbf{p}_{1_2}\mathbf{r}\mathbf{p}_{0_2} = \mathbf{P}^{E}\,\frac{1}{2}\cdot\frac{1}{2}\left(\begin{array}{c|cc} & \mathbf{r} & +\mathbf{r}\mathbf{i}_3 \\ \hline \mathbf{1} & \mathbf{r} & +\mathbf{r}\mathbf{i}_3 \\ -\mathbf{i}_3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

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

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

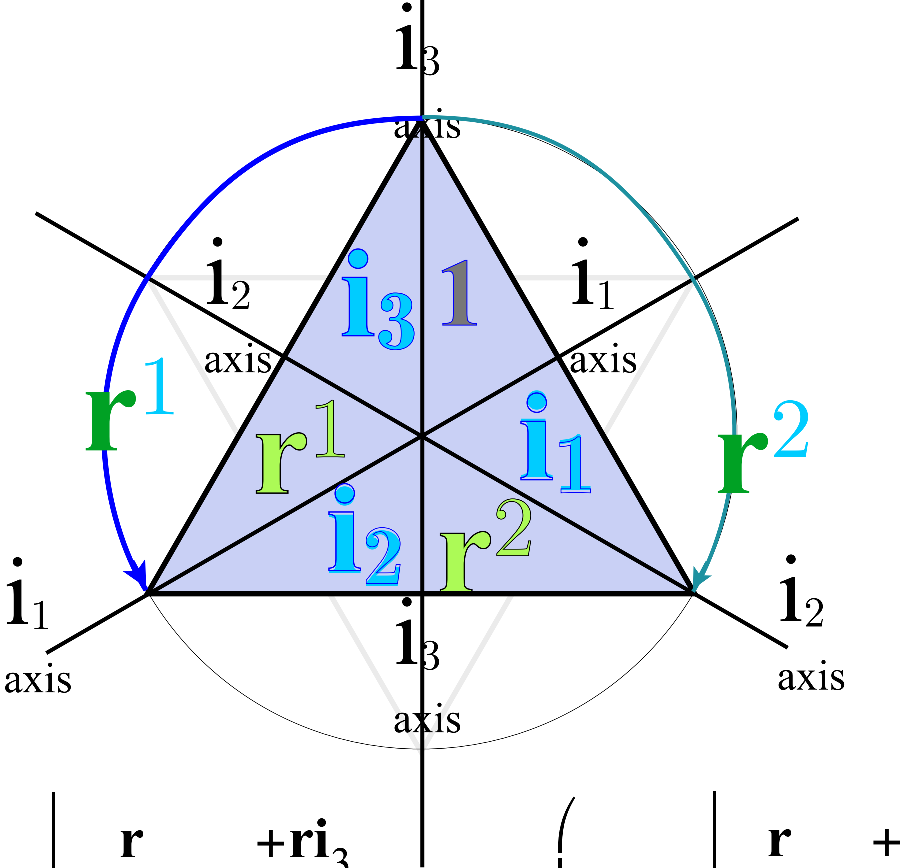
† conjugation: $(\mathbf{r}^{\dagger} = \mathbf{r}^2, \mathbf{r}^{2\dagger} = \mathbf{r}, \mathbf{i}_1^{\dagger} = \mathbf{i}_1, \mathbf{i}_2^{\dagger} = \mathbf{i}_2)$

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

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

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≠n)*

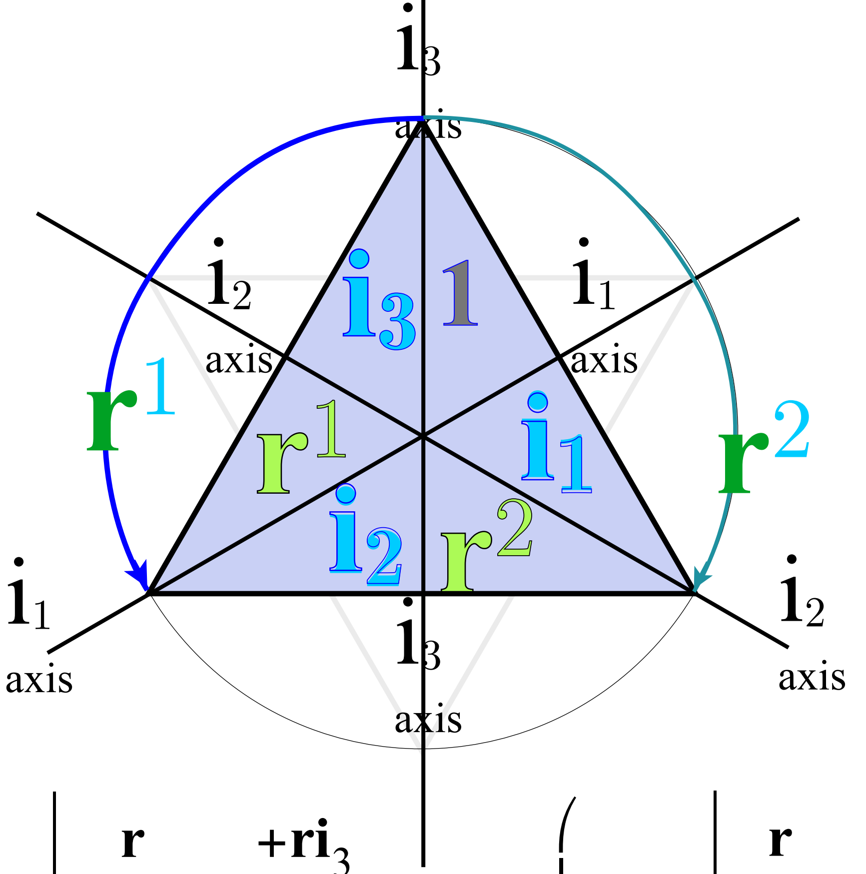
Review of $D_3 \supset C_2 \sim C_{3v} \supset C_v$

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

$D_3 : \chi^{\alpha}_{k}$	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: $\mathbf{P}^{E\dagger}_{1_2 0_2} = \mathbf{P}^{E}_{0_2 1_2} = (?)^{*}(\mathbf{r}^2 - \mathbf{r} - \mathbf{i}_1 + \mathbf{i}_2)$

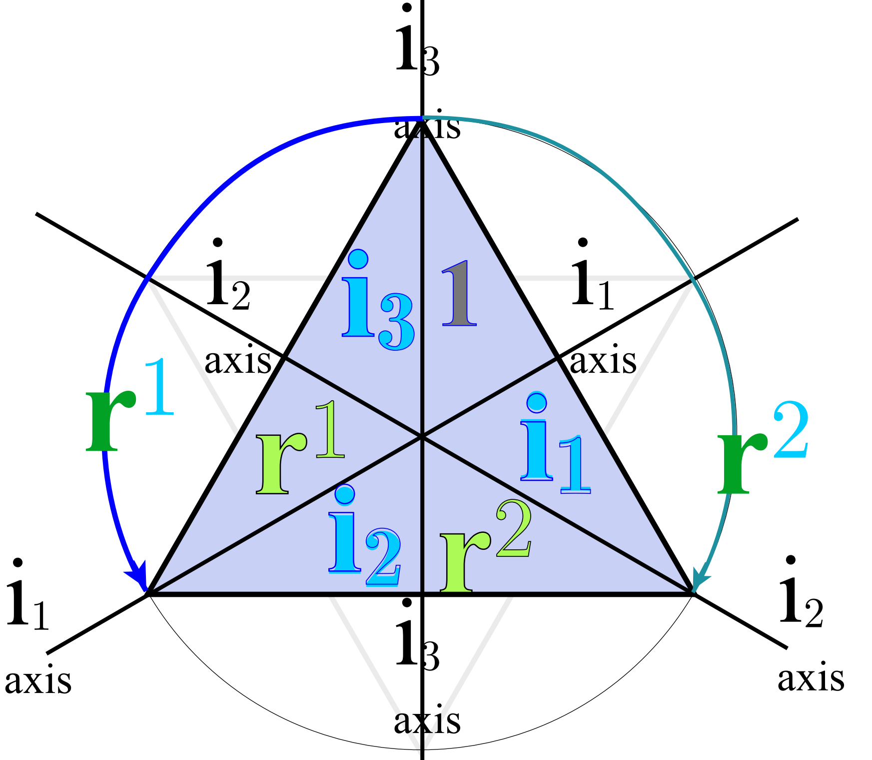
gives equation for (?)-factor: $\mathbf{P}^{E}_{0_2 1_2}\cdot\mathbf{P}^{E}_{1_2 0_2} = \mathbf{P}^{E}_{0_2 0_2} = (?)^2\cdot(\mathbf{r}^2 - \mathbf{r} - \mathbf{i}_1 + \mathbf{i}_2)(\mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 + \mathbf{i}_2)$

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

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

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

$\dagger$ 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}

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

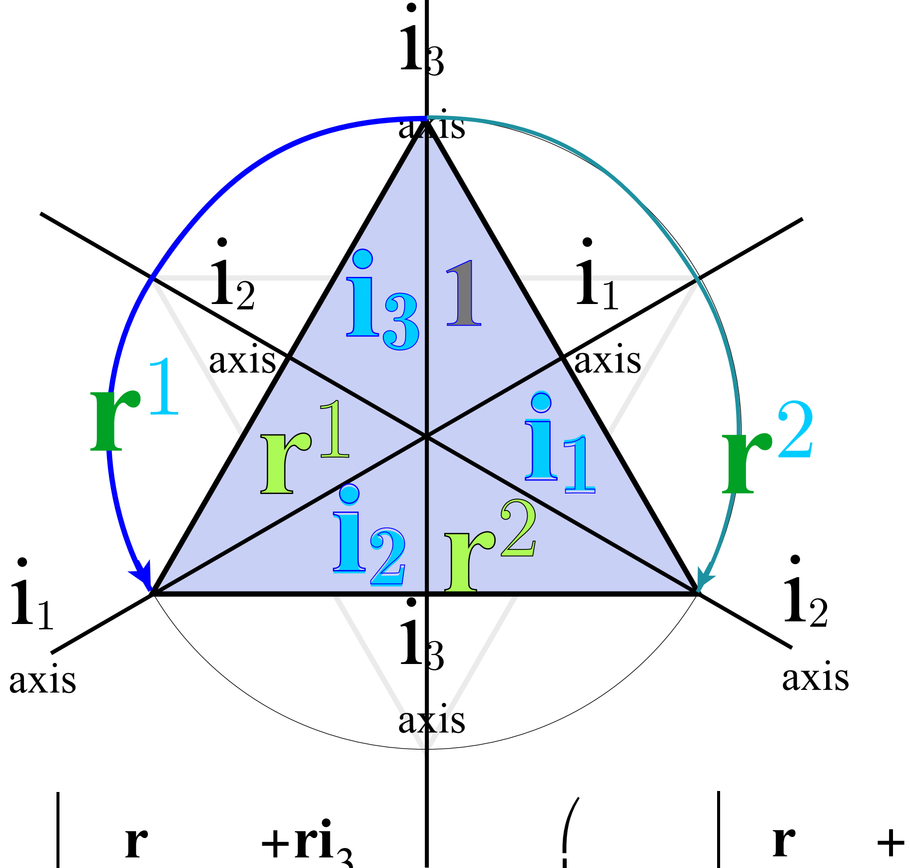
$D^{E*}_{0_2 0_2}(\mathbf{r}) = -\frac{1}{2}$

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

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

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

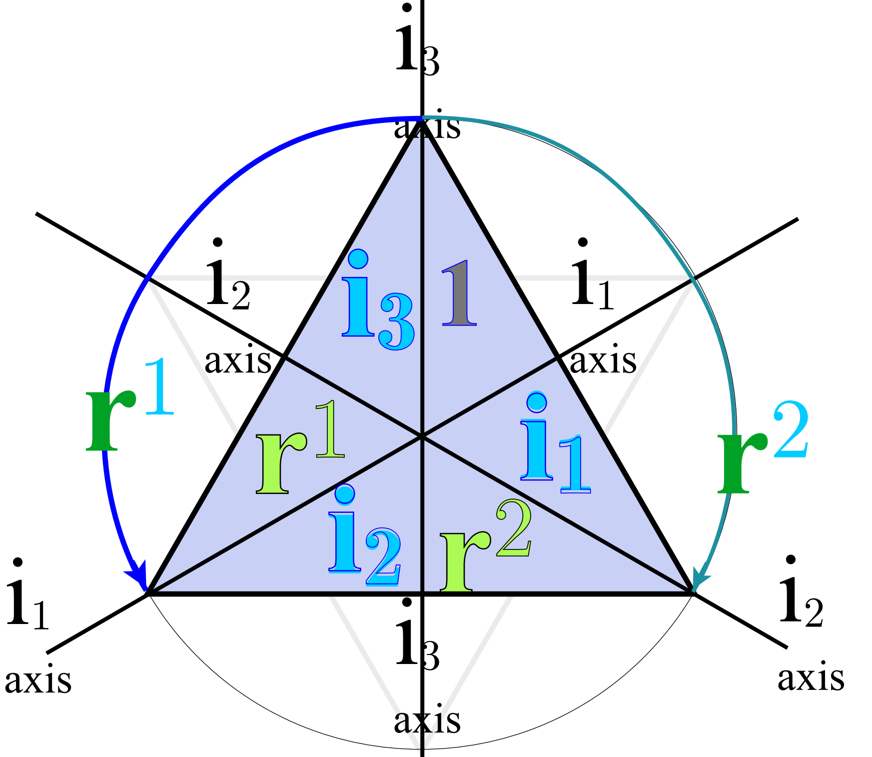
$$= \tfrac{1}{6}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 - \mathbf{i}_2 + 2\mathbf{i}_3) = (\tfrac{\ell^E}{{}^{\circ}O} = \tfrac{1}{3})(D^{E*}_{0_2 0_2}(1)\mathbf{1} + D^{E*}_{0_2 0_2}(r)\mathbf{r} + \ldots)$$

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

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

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

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

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

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

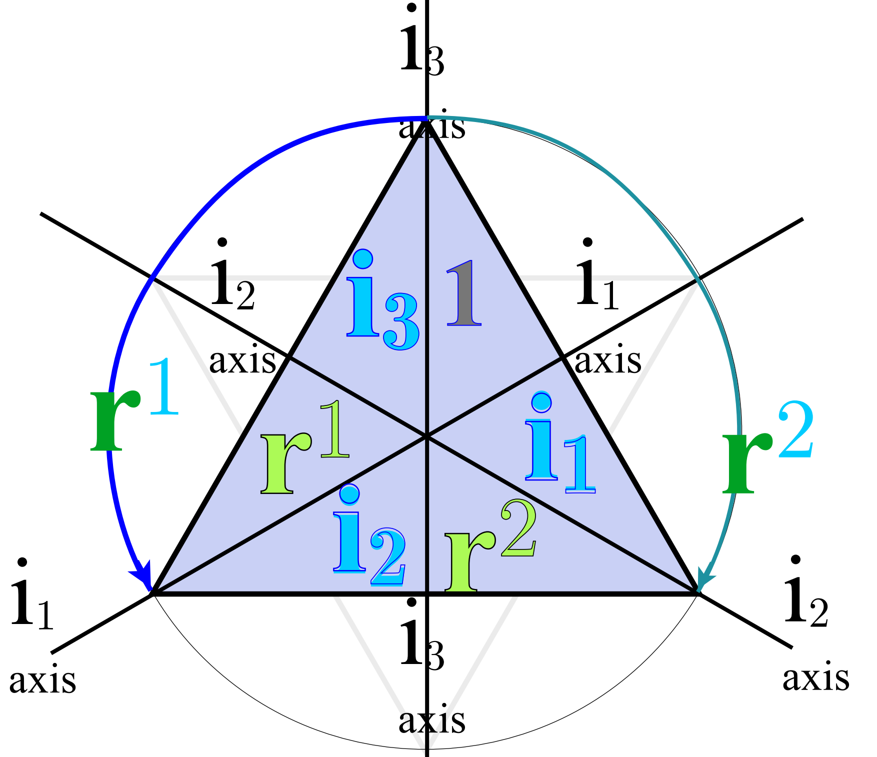
Review of $D_3 \supset C_2 \sim C_{3v} \supset C_v$

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

$D_3 : \chi^{\alpha}_{k}$	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: $\mathbf{P}^{E}_{1_2 0_2} = \mathbf{P}^{E}\mathbf{p}_{1_2}\mathbf{r}\mathbf{p}_{0_2} = \mathbf{P}^{E}\,\frac{1}{2}\cdot\frac{1}{2}\left(\begin{array}{c|cc} & \mathbf{r} & +\mathbf{r}\mathbf{i}_3 \\ \hline \mathbf{1} & \mathbf{r} & +\mathbf{r}\mathbf{i}_3 \\ -\mathbf{i}_3 & -\mathbf{i}_3\mathbf{r} & -\mathbf{i}_3\mathbf{r}\mathbf{i}_3 \end{array}\right) = \frac{1}{4}\,\mathbf{P}^{E}\left(\begin{array}{c|cc} & \mathbf{r} & +\mathbf{r}\mathbf{i}_3 \\ \hline \mathbf{1} & \mathbf{r} & +\mathbf{i}_2 \\ -\mathbf{i}_3 & -\mathbf{i}_1 & -\mathbf{r}^2 \end{array}\right)$

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

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

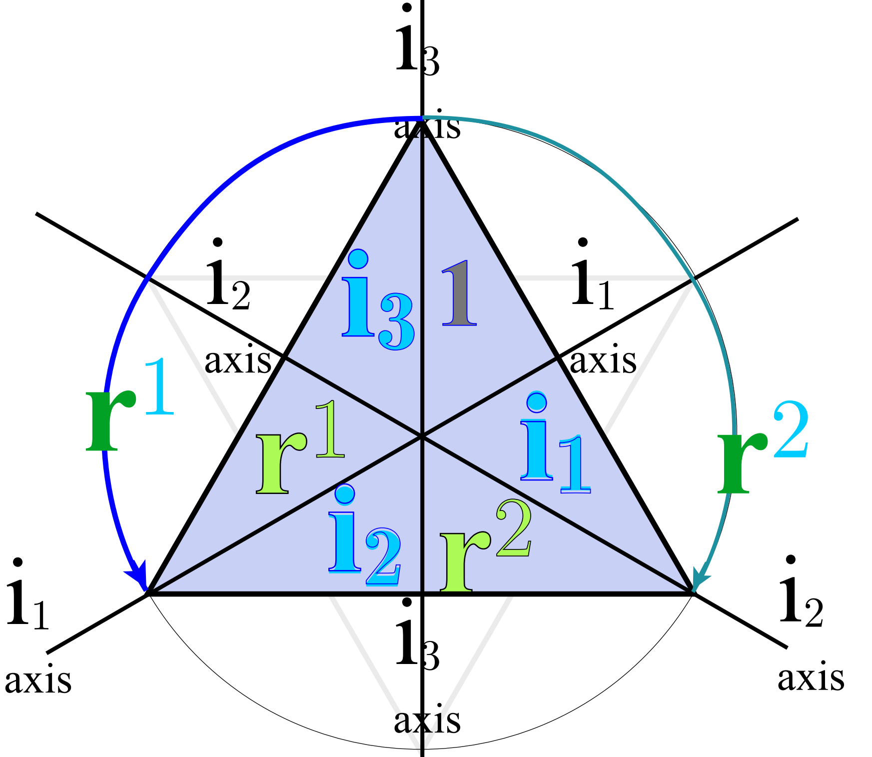
$$(?)^2\cdot 4 = \tfrac{1}{3}$$

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

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

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}

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

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

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

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

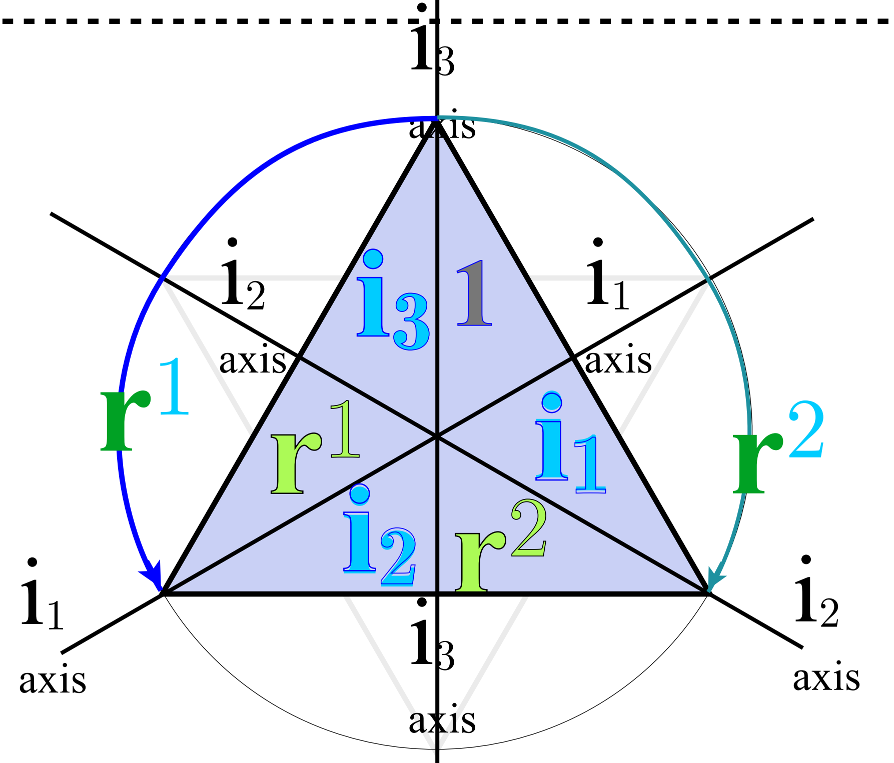
$$\mathbf{P}^{E}_{0_2 0_2} = (?)^2\cdot\left(\begin{array}{c|cccc} & +\mathbf{r} & -\mathbf{r}^2 & -\mathbf{i}_1 & +\mathbf{i}_2 \\ \hline +\mathbf{r}^2 & +\mathbf{1} & -\mathbf{r} & -\mathbf{i}_2 & +\mathbf{i}_3 \\ -\mathbf{r} & -\mathbf{r}^2 & +\mathbf{1} & +\mathbf{i}_3 & -\mathbf{i}_1 \\ -\mathbf{i}_1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

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

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

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

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

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

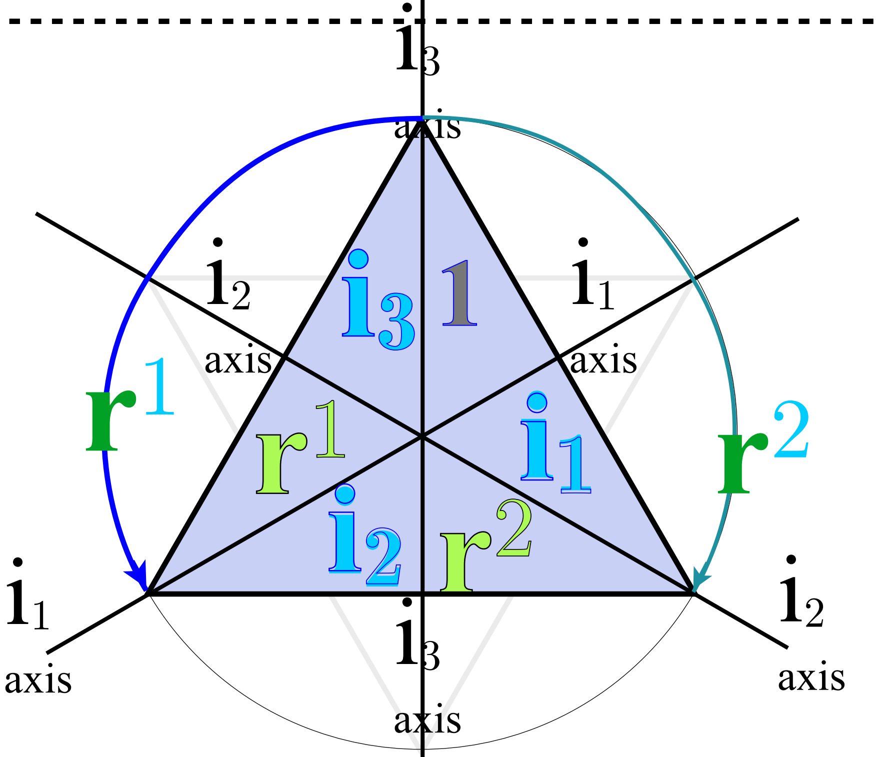
Solving gives unknown (?)-factor: (?)=±√3/6

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

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

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

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

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

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

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

This gives off-diagonal $\mathbf{P}^{E}{}_{xy}$...

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

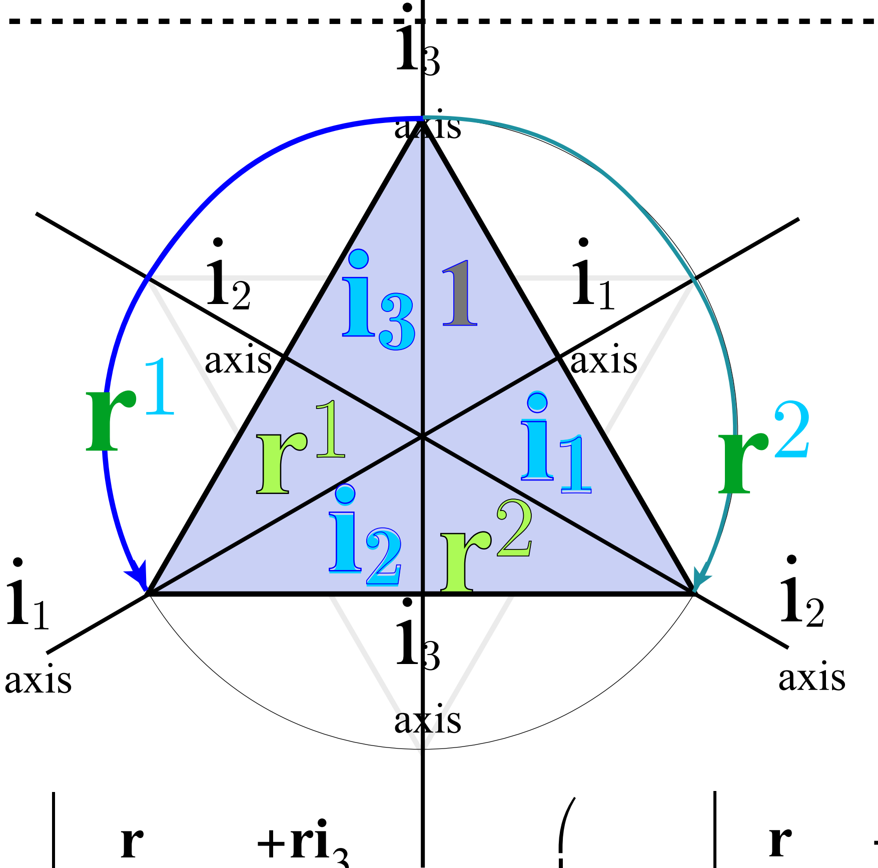
Solving gives unknown (?)-factor: (?)=±√3/6

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

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

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

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

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

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

This gives off-diagonal $\mathbf{P}^E{}_{xy}$...

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

Solving gives unknown (?)-factor: (?)=±√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...

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

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

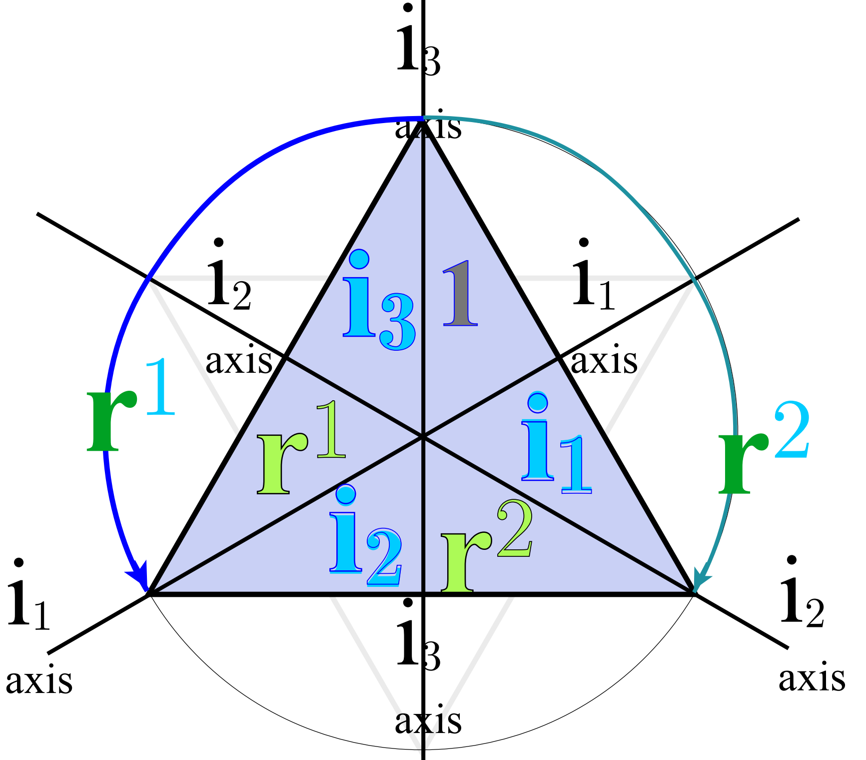
Irreducible nilpotent projectors $\mathbf{P}^{\mu}_{m,n}(m\neq n)$

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:

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

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

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...

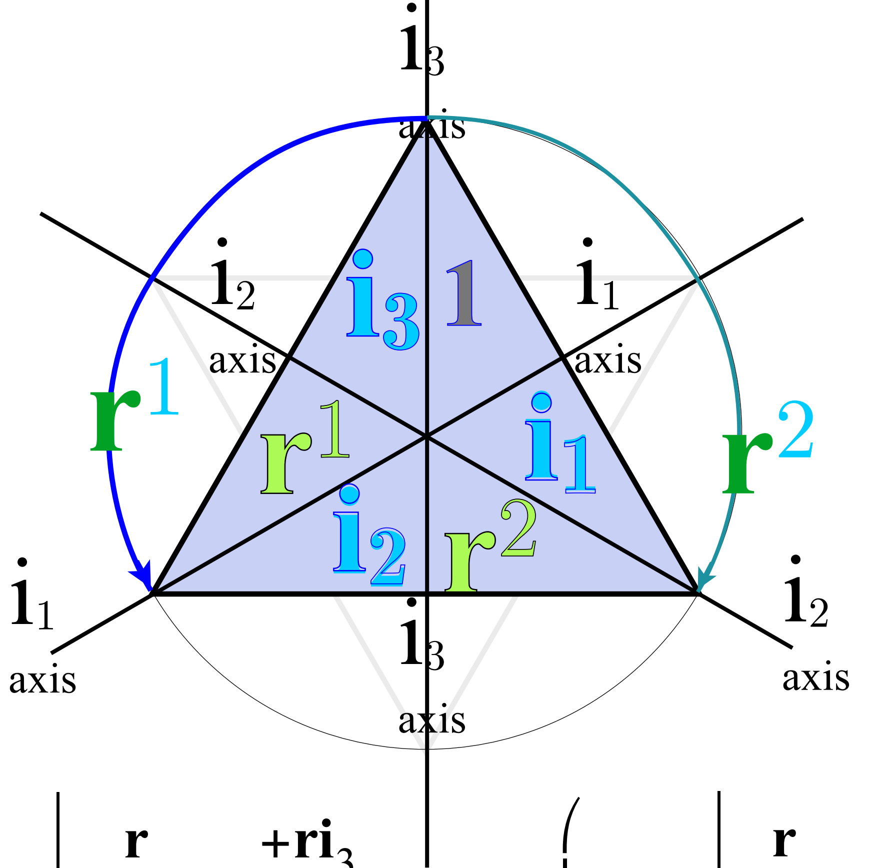
Make group space vectors:

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

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

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

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

Make group space vectors:

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

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

Do desired **g=r** transformation:

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

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

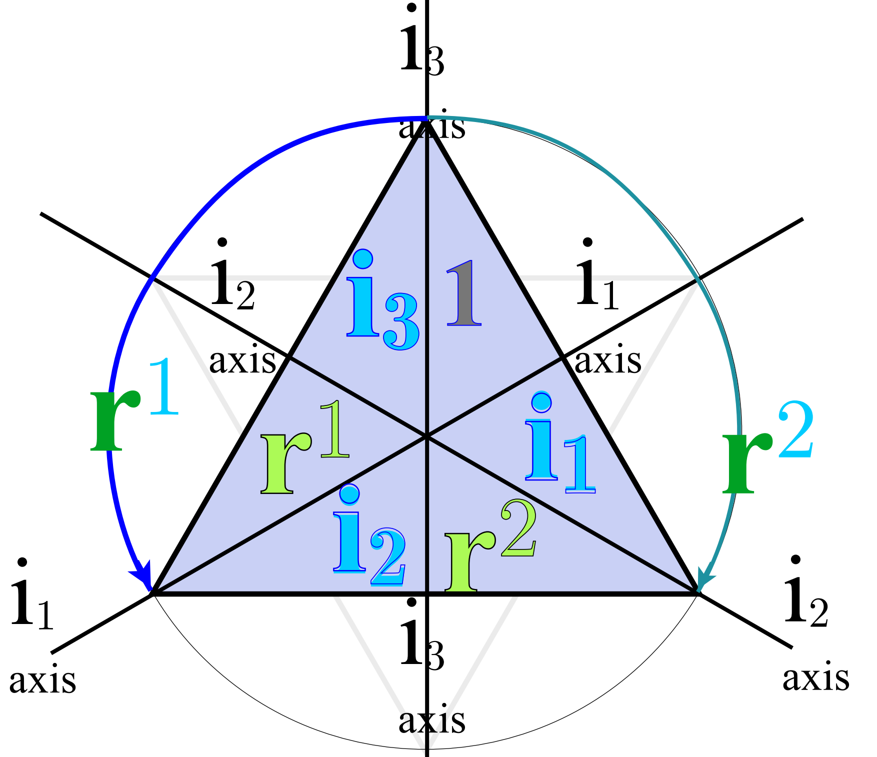
Irreducible nilpotent projectors $\mathbf{P}^{\mu}_{m,n}(m\neq n)$

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:

$$\mathbf{P}^E_{0_20_2} = \mathbf{P}^E\mathbf{p}_{0_2} = \tfrac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)\tfrac{1}{2}(\mathbf{1} + \mathbf{i}_3) = \tfrac{1}{6}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 - \mathbf{i}_2 + 2\mathbf{i}_3)$$

$$\mathbf{P}^E_{1_21_2} = \mathbf{P}^E\mathbf{p}_{1_2} = \tfrac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)\tfrac{1}{2}(\mathbf{1} - \mathbf{i}_3) = \tfrac{1}{6}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 + \mathbf{i}_1 + \mathbf{i}_2 - 2\mathbf{i}_3)$$

Then find nilpotent proportional to: $\mathbf{P}^E_{1_20_2} = \mathbf{P}^E\mathbf{p}_{1_2}\mathbf{r}\mathbf{p}_{0_2} = \mathbf{P}^E\,\frac{1}{2}\cdot\frac{1}{2}\left(\begin{array}{c|cc} & \mathbf{r} & +\mathbf{ri}_3 \\ \hline \mathbf{1} & \mathbf{r} & +\mathbf{ri}_3 \\ -\mathbf{i}_3 & -\mathbf{i}_3\mathbf{r} & -\mathbf{i}_3\mathbf{ri}_3 \end{array}\right) = \frac{1}{4}\,\mathbf{P}^E\left(\begin{array}{c|cc} & \mathbf{r} & +\mathbf{ri}_3 \\ \hline \mathbf{1} & \mathbf{r} & +\mathbf{i}_2 \\ -\mathbf{i}_3 & -\mathbf{i}_1 & -\mathbf{r}^2 \end{array}\right)$

$\pm\mathbf{P}^E_{0_21_2} = \frac{1}{3}\left(-\frac{\sqrt{3}}{2}\mathbf{r} + \frac{\sqrt{3}}{2}\mathbf{r}^2 - \frac{\sqrt{3}}{2}\mathbf{i}_1 + \frac{\sqrt{3}}{2}\mathbf{i}_2\right)$ Now, to set ± signs...

Make group space vectors:

$$\left|\mathbf{P}^E_{0_20_2}\right\rangle = \tfrac{1}{2\sqrt{3}}\left(2\left|\mathbf{1}\right\rangle - \left|\mathbf{r}\right\rangle - \left|\mathbf{r}^2\right\rangle - \left|\mathbf{i}_1\right\rangle - \left|\mathbf{i}_2\right\rangle + 2\left|\mathbf{i}_3\right\rangle\right)$$

$$\left|\mathbf{P}^E_{1_20_2}\right\rangle = \tfrac{1}{2}\left(0\left|\mathbf{1}\right\rangle + \left|\mathbf{r}\right\rangle - \left|\mathbf{r}^2\right\rangle - \left|\mathbf{i}_1\right\rangle + \left|\mathbf{i}_2\right\rangle + 0\left|\mathbf{i}_3\right\rangle\right)$$

Do desired **g=r** transformation:

$$\mathbf{r}\left|\mathbf{P}^E_{0_20_2}\right\rangle = \tfrac{1}{2\sqrt{3}}\left(2\left|\mathbf{r}\right\rangle - \left|\mathbf{r}^2\right\rangle - \left|\mathbf{1}\right\rangle - \left|\mathbf{i}_3\right\rangle - \left|\mathbf{i}_1\right\rangle + 2\left|\mathbf{i}_2\right\rangle\right)$$

$$\mathbf{r}\left|\mathbf{P}^E_{1_20_2}\right\rangle = \tfrac{1}{2}\left(0\left|\mathbf{r}\right\rangle + \left|\mathbf{r}^2\right\rangle - \left|\mathbf{1}\right\rangle - \left|\mathbf{i}_3\right\rangle + \left|\mathbf{i}_1\right\rangle + 0\left|\mathbf{i}_3\right\rangle\right)$$

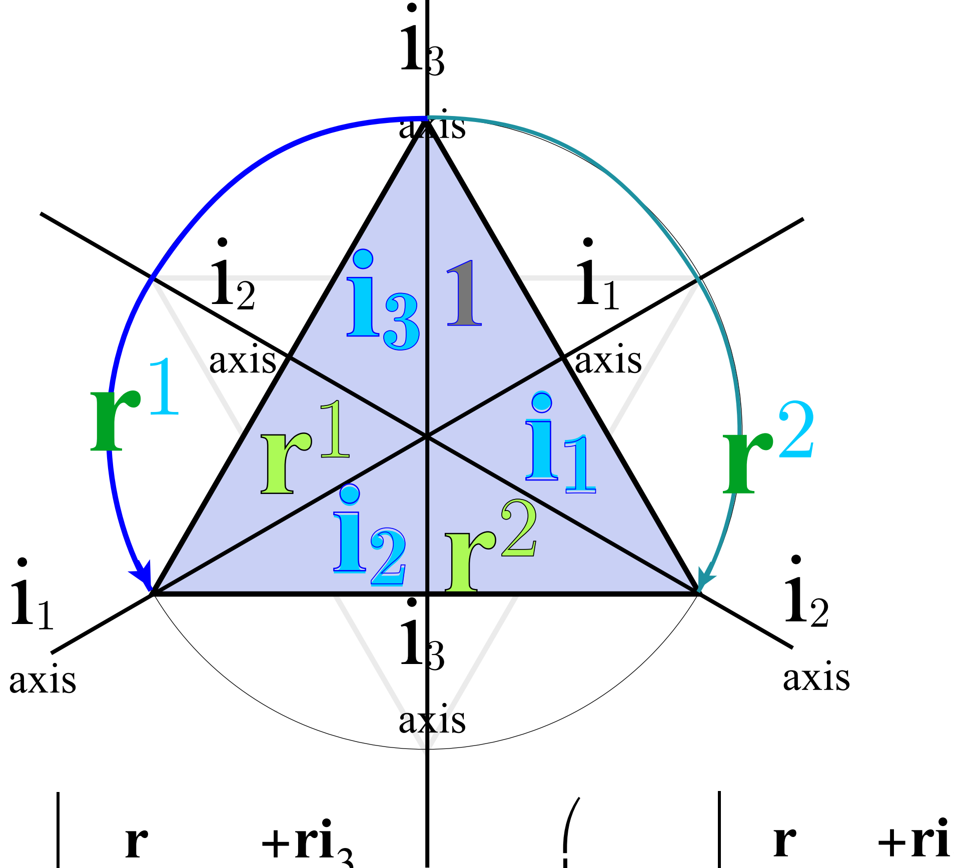
Set up to find matrix of **g=r** transformation:

$$\mathbf{r}\left|\mathbf{P}^E_{0_20_2}\right\rangle = \tfrac{1}{2\sqrt{3}}\left(-\left|\mathbf{1}\right\rangle + 2\left|\mathbf{r}\right\rangle - \left|\mathbf{r}^2\right\rangle - \left|\mathbf{i}_1\right\rangle + 2\left|\mathbf{i}_2\right\rangle - \left|\mathbf{i}_3\right\rangle\right)$$

$$\mathbf{r}\left|\mathbf{P}^E_{1_20_2}\right\rangle = \tfrac{1}{2}\left(-\left|\mathbf{1}\right\rangle + 0\left|\mathbf{r}\right\rangle + \left|\mathbf{r}^2\right\rangle + \left|\mathbf{i}_1\right\rangle + 0\left|\mathbf{i}_3\right\rangle - \left|\mathbf{i}_3\right\rangle\right)$$

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

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

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

$$\mathbf{P}^E_{0_20_2} = \mathbf{P}^E\mathbf{p}_{0_2} = \tfrac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)\tfrac{1}{2}(\mathbf{1} + \mathbf{i}_3) = \tfrac{1}{6}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 - \mathbf{i}_1 - \mathbf{i}_2 + 2\mathbf{i}_3)$$

$$\mathbf{P}^E_{1_21_2} = \mathbf{P}^E\mathbf{p}_{1_2} = \tfrac{1}{3}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)\tfrac{1}{2}(\mathbf{1} - \mathbf{i}_3) = \tfrac{1}{6}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 + \mathbf{i}_1 + \mathbf{i}_2 - 2\mathbf{i}_3)$$

Then find nilpotent proportional to: $\mathbf{P}^E_{1_20_2} = \mathbf{P}^E\mathbf{p}_{1_2}\mathbf{r}\mathbf{p}_{0_2} = \mathbf{P}^E\,\tfrac{1}{2}\cdot\tfrac{1}{2}\left(\begin{array}{c|cc} & \mathbf{r} & +\mathbf{r}\mathbf{i}_3 \\ \hline \mathbf{1} & \mathbf{r} & +\mathbf{r}\mathbf{i}_3 \\ -\mathbf{i}_3 & -\mathbf{i}_3\mathbf{r} & -\mathbf{i}_3\mathbf{r}\mathbf{i}_3 \end{array}\right) = \tfrac{1}{4}\mathbf{P}^E\left(\begin{array}{c|cc} & \mathbf{r} & +\mathbf{r}\mathbf{i}_3 \\ \hline \mathbf{1} & \mathbf{r} & +\mathbf{i}_2 \\ -\mathbf{i}_3 & -\mathbf{i}_1 & -\mathbf{r}^2 \end{array}\right)$

$\pm\mathbf{P}^E_{0_21_2} = \tfrac{1}{3}\left(-\tfrac{\sqrt{3}}{2}\mathbf{r} + \tfrac{\sqrt{3}}{2}\mathbf{r}^2 - \tfrac{\sqrt{3}}{2}\mathbf{i}_1 + \tfrac{\sqrt{3}}{2}\mathbf{i}_2\right)$ Now, to set ± signs...

Make group space vectors:

$$\left|\mathbf{P}^E_{0_20_2}\right\rangle = \tfrac{1}{2\sqrt{3}}\left(2\left|\mathbf{1}\right\rangle - \left|\mathbf{r}\right\rangle - \left|\mathbf{r}^2\right\rangle - \left|\mathbf{i}_1\right\rangle - \left|\mathbf{i}_2\right\rangle + 2\left|\mathbf{i}_3\right\rangle\right)$$

$$\left|\mathbf{P}^E_{1_20_2}\right\rangle = \tfrac{1}{2}\left(0\left|\mathbf{1}\right\rangle + \left|\mathbf{r}\right\rangle - \left|\mathbf{r}^2\right\rangle - \left|\mathbf{i}_1\right\rangle + \left|\mathbf{i}_2\right\rangle + 0\left|\mathbf{i}_3\right\rangle\right)$$

Do desired **g=r** transformation:

$$\mathbf{r}\left|\mathbf{P}^E_{0_20_2}\right\rangle = \tfrac{1}{2\sqrt{3}}\left(2\left|\mathbf{r}\right\rangle - \left|\mathbf{r}^2\right\rangle - \left|\mathbf{1}\right\rangle - \left|\mathbf{i}_3\right\rangle - \left|\mathbf{i}_1\right\rangle + 2\left|\mathbf{i}_2\right\rangle\right)$$

$$\mathbf{r}\left|\mathbf{P}^E_{1_20_2}\right\rangle = \tfrac{1}{2}\left(0\left|\mathbf{r}\right\rangle + \left|\mathbf{r}^2\right\rangle - \left|\mathbf{1}\right\rangle - \left|\mathbf{i}_3\right\rangle + \left|\mathbf{i}_1\right\rangle + 0\left|\mathbf{i}_3\right\rangle\right)$$

Set up to find matrix of **g=r** transformation:

$$\mathbf{r}\left|\mathbf{P}^E_{0_20_2}\right\rangle = \tfrac{1}{2\sqrt{3}}\left(-\left|\mathbf{1}\right\rangle + 2\left|\mathbf{r}\right\rangle - \left|\mathbf{r}^2\right\rangle - \left|\mathbf{i}_1\right\rangle + 2\left|\mathbf{i}_2\right\rangle - \left|\mathbf{i}_3\right\rangle\right)$$

$$\mathbf{r}\left|\mathbf{P}^E_{1_20_2}\right\rangle = \tfrac{1}{2}\left(-\left|\mathbf{1}\right\rangle + 0\left|\mathbf{r}\right\rangle + \left|\mathbf{r}^2\right\rangle + \left|\mathbf{i}_1\right\rangle + 0\left|\mathbf{i}_3\right\rangle - \left|\mathbf{i}_3\right\rangle\right)$$

$$\left\langle\mathbf{P}^E_{0_20_2}\middle|\mathbf{r}\middle|\mathbf{P}^E_{0_20_2}\right\rangle = \tfrac{1}{2\sqrt{3}}(2-1-1-1-1+2)\cdot\tfrac{1}{2\sqrt{3}}(-1+2-1-1+2-1) = -1/2$$

$$\left\langle\mathbf{P}^E_{1_20_2}\middle|\mathbf{r}\middle|\mathbf{P}^E_{0_20_2}\right\rangle = \tfrac{1}{2}(0+1-1-1+1+0)\cdot\tfrac{1}{2\sqrt{3}}(-1+2-1-1+2-1) = \sqrt{3}/2$$

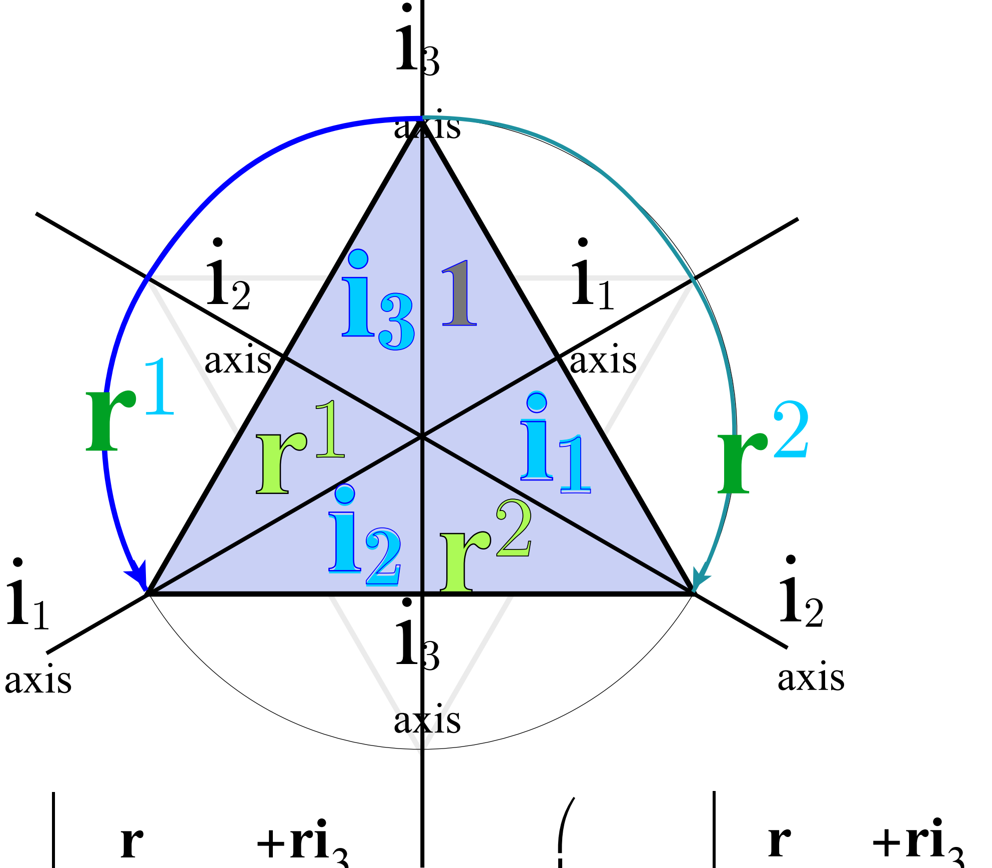
Irreducible nilpotent projectors $\mathbf{P}^{\mu}_{m,n}(m\neq n)$

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

$D_3 : \chi^{\alpha}_{k}$	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:

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

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

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

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

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

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

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

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

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

The D_{01} ± 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

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

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

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
$D^{E_1}_{x,y}(\mathbf{g}) =$	$\begin{pmatrix} 1 & \cdot \\ \cdot & 1 \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

AMOP reference links on page 2

3.12.18 class 17.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Discrete symmetry subgroups of $O(3)\supset$(Octahedral $O_h\supset O$): Part II Full $D^{(\alpha)}$-matrices defined by subgroup-chains $O\supset D_4\supset C_4$, D_2, or C_3 applied to eigensolutions of O_h-tensors $\mathbf{T}^{[4]}+\mathbf{T}^{[6]}$

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

Review Coset factored splitting of projectors for $O\supset D_4\supset C_4$ *into split classes and level structure*

Hamiltonian level cluster models with subgroup-defined tunneling parameters

Diagonal idempotent $\mathbf{P}^{\mu}_{m,m}$ *parameter sets for* $O\supset C_4$ *and* $O\supset C_3$ *case of* SF_6 *level clusters*

Off-diagonal nilpotent $\mathbf{P}^{\mu}_{m,n}$ $(m\neq n)$ *parameter sets needed for* $O\supset C_2$ *clusters*

Deriving nilpotent projectors $\mathbf{P}^{\mu}_{m,n}$ *and ireps* $D^{\mu}_{m,n}$ *by fundamental* $\mathbf{g}\rightleftarrows\mathbf{P}^{\mu}_{m,n}$ *relations:*

(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 nilpotent projectors for simple $D_3\supset C_2\sim C_{3v}\supset C_v$ *chains* (Lect13p95)

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

Structure and applications of coset tabulated $D^{\mu}_{m,n}$ *irreps for various* O_h *subgroup chains*

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

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 *cluster spectra of* O_h*-symmetric tensors* $\mathbf{T}^{[4]}+\mathbf{T}^{[6]}$

Monster clusters: When local C_2 *symmetry dominates*

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

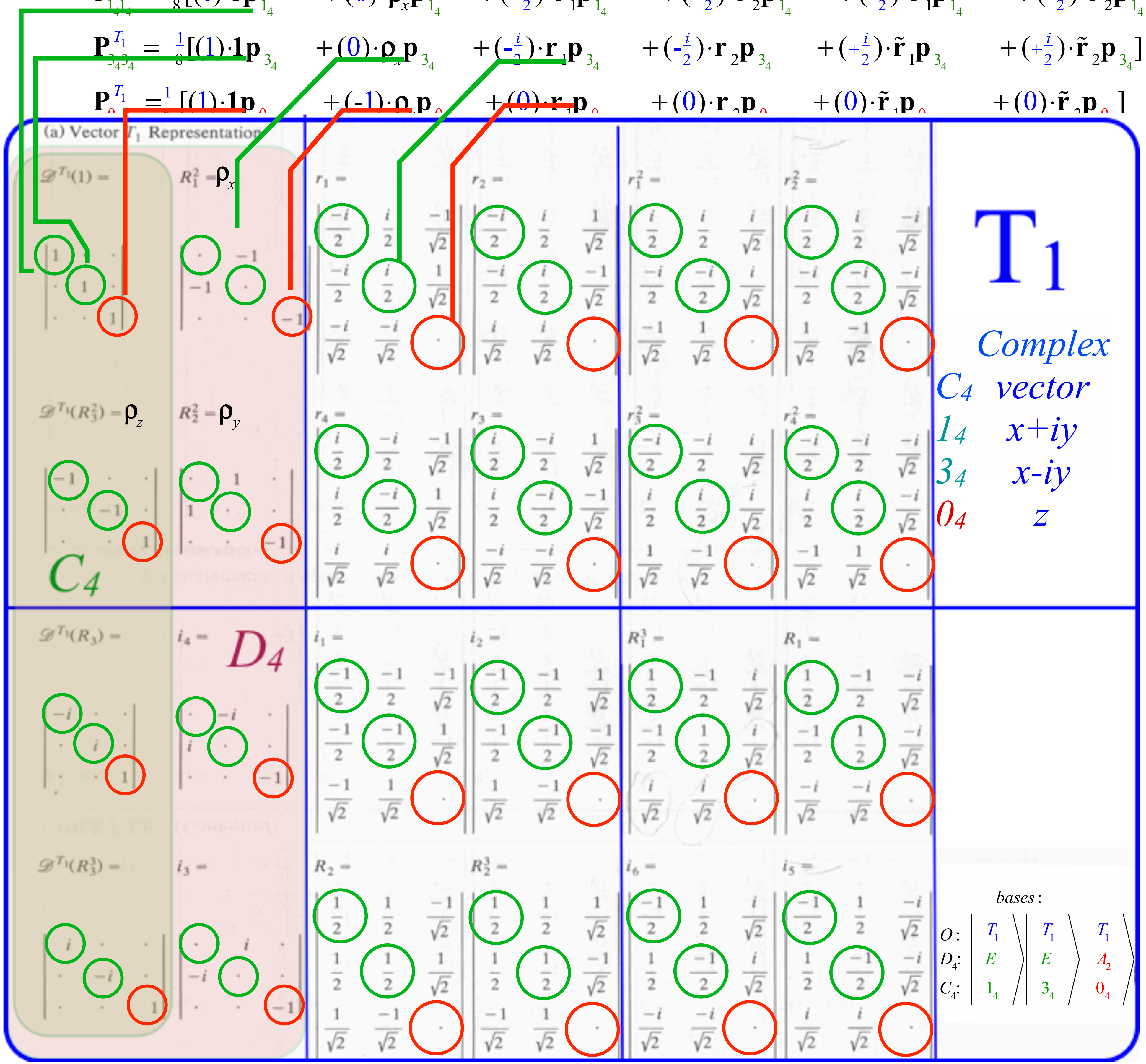
Irreducible nilpotent projectors $\mathbf{P}^{\mu}{}_{m,n}$

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

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

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

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



(a) Vector T_1 Representation

$\mathscr{D}^{T_1}(1) = \begin{vmatrix} 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \end{vmatrix}$ $\quad R_1^2 = \boldsymbol{\rho}_x \begin{vmatrix} \cdot & -1 & \cdot \\ -1 & \cdot & \cdot \\ \cdot & \cdot & -1 \end{vmatrix}$ $\quad r_1 = \begin{vmatrix} \frac{-i}{2} & \frac{i}{2} & \frac{-1}{\sqrt2} \\ \frac{-i}{2} & \frac{i}{2} & \frac{1}{\sqrt2} \\ \frac{-i}{\sqrt2} & \frac{-i}{\sqrt2} & \cdot \end{vmatrix}$ $\quad r_2 = \begin{vmatrix} \frac{-i}{2} & \frac{i}{2} & \frac{1}{\sqrt2} \\ \frac{-i}{2} & \frac{i}{2} & \frac{-1}{\sqrt2} \\ \frac{i}{\sqrt2} & \frac{i}{\sqrt2} & \cdot \end{vmatrix}$ $\quad r_1^2 = \begin{vmatrix} \frac{i}{2} & \frac{i}{2} & \frac{i}{\sqrt2} \\ \frac{-i}{2} & \frac{-i}{2} & \frac{i}{\sqrt2} \\ \frac{-1}{\sqrt2} & \frac{1}{\sqrt2} & \cdot \end{vmatrix}$ $\quad r_2^2 = \begin{vmatrix} \frac{i}{2} & \frac{i}{2} & \frac{-i}{\sqrt2} \\ \frac{-i}{2} & \frac{-i}{2} & \frac{-i}{\sqrt2} \\ \frac{1}{\sqrt2} & \frac{-1}{\sqrt2} & \cdot \end{vmatrix}$

$\mathscr{D}^{T_1}(R_3^2) = \boldsymbol{\rho}_z \begin{vmatrix} -1 & \cdot & \cdot \\ \cdot & -1 & \cdot \\ \cdot & \cdot & 1 \end{vmatrix}$ $\quad R_2^2 = \boldsymbol{\rho}_y \begin{vmatrix} \cdot & 1 & \cdot \\ 1 & \cdot & \cdot \\ \cdot & \cdot & -1 \end{vmatrix}$ $\quad r_4 = \begin{vmatrix} \frac{i}{2} & \frac{-i}{2} & \frac{-1}{\sqrt2} \\ \frac{i}{2} & \frac{-i}{2} & \frac{1}{\sqrt2} \\ \frac{i}{\sqrt2} & \frac{i}{\sqrt2} & \cdot \end{vmatrix}$ $\quad r_3 = \begin{vmatrix} \frac{i}{2} & \frac{-i}{2} & \frac{1}{\sqrt2} \\ \frac{i}{2} & \frac{-i}{2} & \frac{-1}{\sqrt2} \\ \frac{-i}{\sqrt2} & \frac{-i}{\sqrt2} & \cdot \end{vmatrix}$ $\quad r_3^2 = \begin{vmatrix} \frac{-i}{2} & \frac{-i}{2} & \frac{i}{\sqrt2} \\ \frac{i}{2} & \frac{i}{2} & \frac{i}{\sqrt2} \\ \frac{1}{\sqrt2} & \frac{-1}{\sqrt2} & \cdot \end{vmatrix}$ $\quad r_4^2 = \begin{vmatrix} \frac{-i}{2} & \frac{-i}{2} & \frac{-i}{\sqrt2} \\ \frac{i}{2} & \frac{i}{2} & \frac{-i}{\sqrt2} \\ \frac{-1}{\sqrt2} & \frac{1}{\sqrt2} & \cdot \end{vmatrix}$

C_4

$\mathscr{D}^{T_1}(R_3) = \begin{vmatrix} -i & \cdot & \cdot \\ \cdot & i & \cdot \\ \cdot & \cdot & 1 \end{vmatrix}$ $\quad i_4 = \begin{vmatrix} \cdot & -i & \cdot \\ i & \cdot & \cdot \\ \cdot & \cdot & -1 \end{vmatrix}$ $\quad i_1 = \begin{vmatrix} \frac{-1}{2} & \frac{-1}{2} & \frac{-1}{\sqrt2} \\ \frac{-1}{2} & \frac{-1}{2} & \frac{1}{\sqrt2} \\ \frac{-1}{\sqrt2} & \frac{1}{\sqrt2} & \cdot \end{vmatrix}$ $\quad i_2 = \begin{vmatrix} \frac{-1}{2} & \frac{-1}{2} & \frac{1}{\sqrt2} \\ \frac{-1}{2} & \frac{-1}{2} & \frac{-1}{\sqrt2} \\ \frac{1}{\sqrt2} & \frac{-1}{\sqrt2} & \cdot \end{vmatrix}$ $\quad R_1^3 = \begin{vmatrix} \frac{1}{2} & \frac{-1}{2} & \frac{i}{\sqrt2} \\ \frac{-1}{2} & \frac{1}{2} & \frac{i}{\sqrt2} \\ \frac{i}{\sqrt2} & \frac{i}{\sqrt2} & \cdot \end{vmatrix}$ $\quad R_1 = \begin{vmatrix} \frac{1}{2} & \frac{-1}{2} & \frac{-i}{\sqrt2} \\ \frac{-1}{2} & \frac{1}{2} & \frac{-i}{\sqrt2} \\ \frac{-i}{\sqrt2} & \frac{-i}{\sqrt2} & \cdot \end{vmatrix}$

D_4

$\mathscr{D}^{T_1}(R_3^3) = \begin{vmatrix} i & \cdot & \cdot \\ \cdot & -i & \cdot \\ \cdot & \cdot & 1 \end{vmatrix}$ $\quad i_3 = \begin{vmatrix} \cdot & i & \cdot \\ -i & \cdot & \cdot \\ \cdot & \cdot & -1 \end{vmatrix}$ $\quad R_2 = \begin{vmatrix} \frac{1}{2} & \frac{1}{2} & \frac{-1}{\sqrt2} \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{\sqrt2} \\ \frac{1}{\sqrt2} & \frac{-1}{\sqrt2} & \cdot \end{vmatrix}$ $\quad R_2^3 = \begin{vmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{\sqrt2} \\ \frac{1}{2} & \frac{1}{2} & \frac{-1}{\sqrt2} \\ \frac{-1}{\sqrt2} & \frac{1}{\sqrt2} & \cdot \end{vmatrix}$ $\quad i_6 = \begin{vmatrix} \frac{-1}{2} & \frac{1}{2} & \frac{i}{\sqrt2} \\ \frac{1}{2} & \frac{-1}{2} & \frac{i}{\sqrt2} \\ \frac{-i}{\sqrt2} & \frac{-i}{\sqrt2} & \cdot \end{vmatrix}$ $\quad i_5 = \begin{vmatrix} \frac{-1}{2} & \frac{1}{2} & \frac{-i}{\sqrt2} \\ \frac{1}{2} & \frac{-1}{2} & \frac{-i}{\sqrt2} \\ \frac{i}{\sqrt2} & \frac{i}{\sqrt2} & \cdot \end{vmatrix}$

T1

	Complex
C_4	vector
1_4	$x+iy$
3_4	$x-iy$
0_4	z

bases:

$$\begin{matrix} O: \\ D_4: \\ C_4: \end{matrix} \left| \begin{matrix} T_1 \\ E \\ 1_4 \end{matrix} \right\rangle \left| \begin{matrix} T_1 \\ E \\ 3_4 \end{matrix} \right\rangle \left| \begin{matrix} T_1 \\ A_2 \\ 0_4 \end{matrix} \right\rangle$$

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

$O \supset C_4$
left cosets

$\{\mathbf{1}, \boldsymbol{\rho}_z, \mathbf{R}_z, \tilde{\mathbf{R}}_z\}$

$\{\boldsymbol{\rho}_x, \boldsymbol{\rho}_y, \mathbf{i}_4, \mathbf{i}_3\}$

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

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

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

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

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

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

O⊃C₄ left cosets

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

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

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

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

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

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

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

$O \supset C_4$

left cosets

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

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

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

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

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

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

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

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* $D^{T_1 *}_{jk}(\mathbf{g})$

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

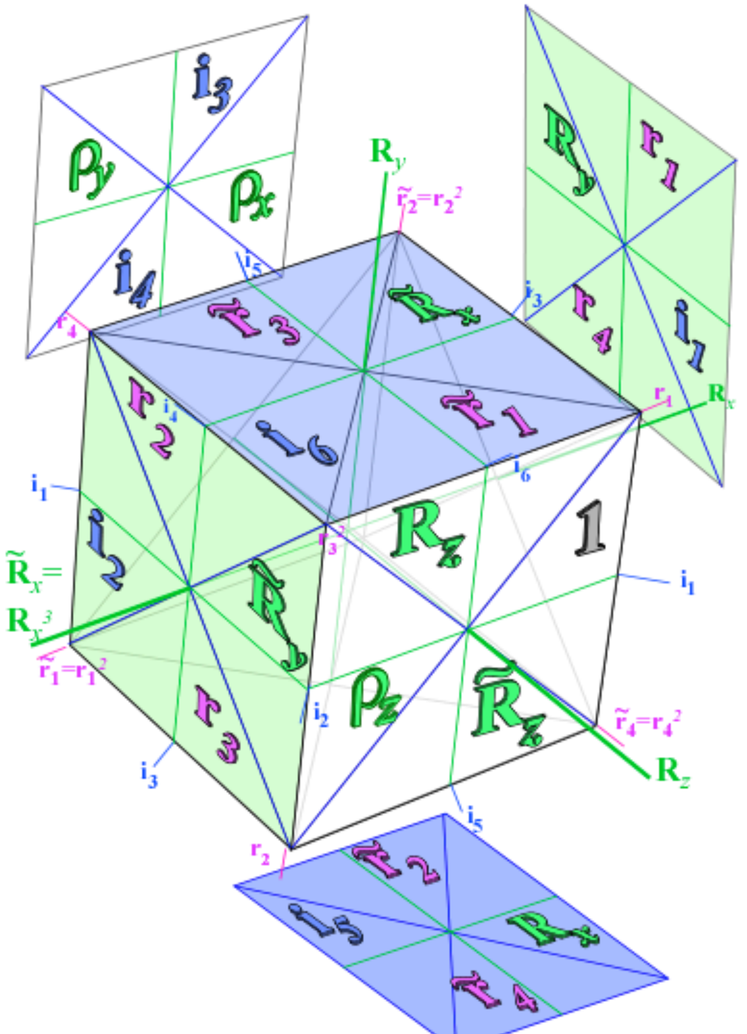
$$\mathbf{P}^{T_1}_{3_43_4} = \tfrac{1}{8}[(1)\cdot\mathbf{1p}_{3_4} + (0)\cdot\rho_x\mathbf{p}_{3_4} + (-\tfrac{i}{2})\cdot\mathbf{r}_1\mathbf{p}_{3_4} + (-\tfrac{i}{2})\cdot\mathbf{r}_2\mathbf{p}_{3_4} + (+\tfrac{i}{2})\cdot\tilde{\mathbf{r}}_1\mathbf{p}_{3_4} + (+\tfrac{i}{2})\cdot\tilde{\mathbf{r}}_2\mathbf{p}_{3_4}]$$

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

Calculating: $\mathbf{P}^{T_1}_{1_41_4}\mathbf{r}_1\mathbf{P}^{T_1}_{0_40_4} = D^{T_1}_{1_40_4}(\mathbf{r}_1)\mathbf{P}^{T_1}_{1_40_4} = \mathbf{P}^{T_1}\mathbf{p}_{1_4}\mathbf{r}_1\mathbf{p}_{0_4}$

Then find nilpotent proportional to: $\mathbf{p}_{1_4}\mathbf{r}_1\mathbf{p}_{0_4} = \frac{1}{16}$

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



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

Consistent with standard: $\mathbf{P}^{\mu}_{m_4m_4} = \sum_{g}^{\circ O}\frac{\ell^{\mu}}{\circ G}D^{\mu *}_{m_4m_4}(g)\mathbf{g}$

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

$O\supset C_4$

left cosets

$\{\mathbf{1},\boldsymbol{\rho}_z,\mathbf{R}_z,\tilde{\mathbf{R}}_z\}$

$\{\boldsymbol{\rho}_x,\boldsymbol{\rho}_y,\mathbf{i}_4,\mathbf{i}_3\}$

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

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

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

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

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

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

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

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

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: $\mathbf{p}_{1_4}\mathbf{r}_1\mathbf{p}_{0_4} = \dfrac{1}{16}$

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

$$=[(\mathbf{r}_1+\mathbf{r}_4+\mathbf{i}_1+\mathbf{R}_y)-(\mathbf{r}_2+\mathbf{r}_3+\mathbf{i}_2+\tilde{\mathbf{R}}_y)-i(\tilde{\mathbf{r}}_1+\tilde{\mathbf{r}}_3+\tilde{\mathbf{R}}_x+\mathbf{i}_6)+i(\tilde{\mathbf{r}}_2+\tilde{\mathbf{r}}_4+\mathbf{R}_x+\mathbf{i}_5)]/16$$

$$=[\mathbf{r}_1\mathbf{p}_{0_4}-\mathbf{r}_2\mathbf{p}_{0_4}-i\tilde{\mathbf{r}}_1\mathbf{p}_{0_4}+i\tilde{\mathbf{r}}_2\mathbf{p}_{0_4}]/4$$

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

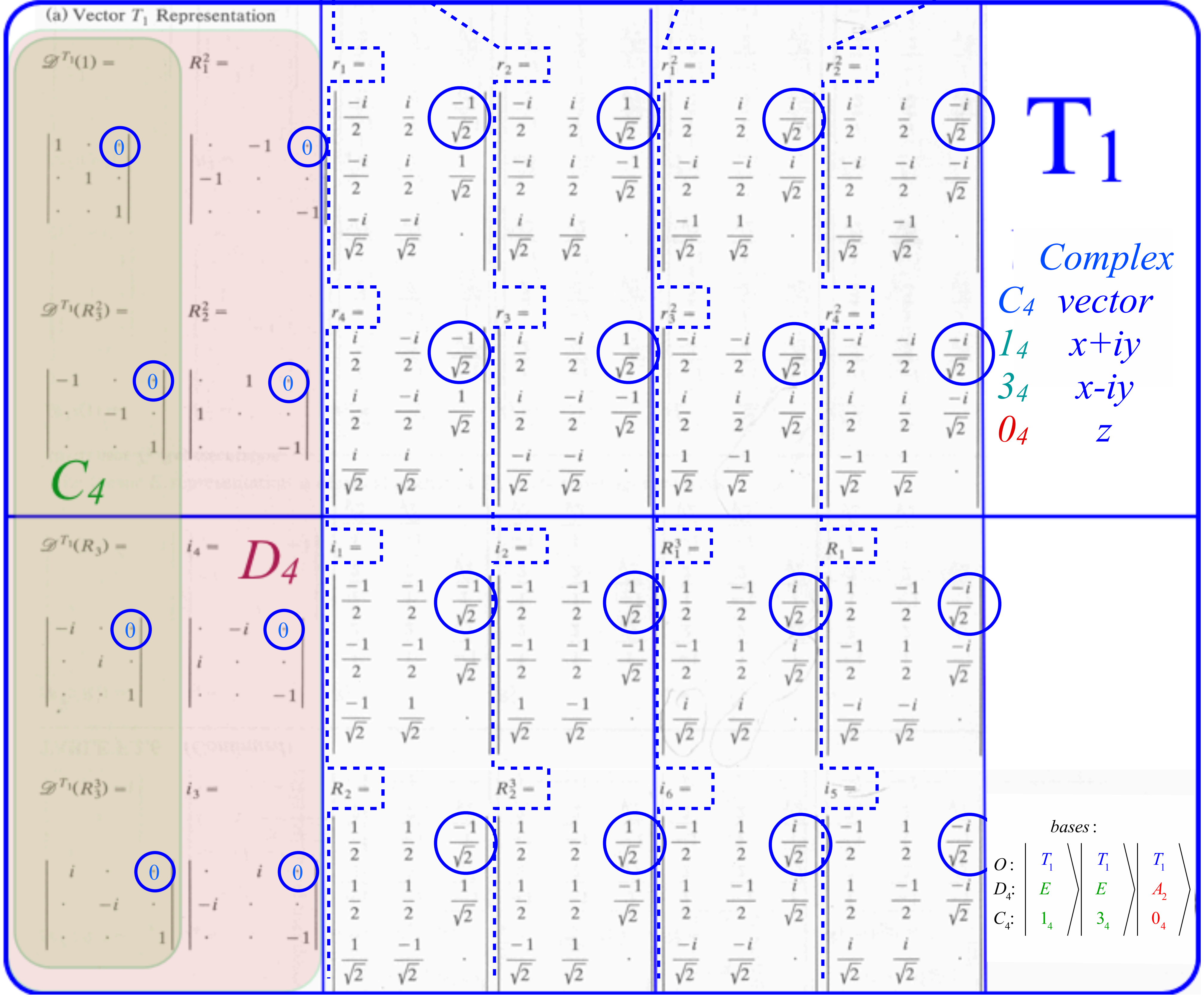
Consistent with standard: $\mathbf{P}^{\mu}_{m_4 m_4}=\sum_{g}^{\circ O}\frac{\ell^{\mu}}{\circ G}D^{\mu *}_{m_4 m_4}(g)\mathbf{g}$

Relating off-diagonal $1_4 0_4$ components $D^{T_1}_{1_4 0_4}(\mathbf{g})$ to coefficients of $\frac{-1}{\sqrt{2}}\mathbf{p}_{1_4}\mathbf{r}_1\mathbf{p}_{0_4}$:

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

$$\frac{-1}{\sqrt{2}}\mathbf{p}_{1_4}\mathbf{r}_1\mathbf{p}_{0_4} = \frac{1}{\sqrt{2}}\left[-\mathbf{r}_1\mathbf{p}_{0_4} + \mathbf{r}_2\mathbf{p}_{0_4} + i\tilde{\mathbf{r}}_1\mathbf{p}_{0_4} - i\tilde{\mathbf{r}}_2\mathbf{p}_{0_4}\right] =$$

$$\frac{1}{\sqrt{2}}\left[-(\mathbf{r}_1 + \mathbf{r}_4 + \mathbf{i}_1 + \mathbf{R}_y) + (\mathbf{r}_2 + \mathbf{r}_3 + \mathbf{i}_2 + \tilde{\mathbf{R}}_y) + i(\tilde{\mathbf{r}}_1 + \tilde{\mathbf{r}}_3 + \tilde{\mathbf{R}}_x + \mathbf{i}_6) - i(\tilde{\mathbf{r}}_2 + \tilde{\mathbf{r}}_4 + \mathbf{R}_x + \mathbf{i}_5)\right]$$



(a) Vector T_1 Representation

$\mathscr{D}^{T_1}(1) = \begin{vmatrix} 1 & \cdot & 0 \\ \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \end{vmatrix}$ $R_1^2 = \begin{vmatrix} \cdot & -1 & 0 \\ -1 & \cdot & \cdot \\ \cdot & \cdot & -1 \end{vmatrix}$ $r_1 = \begin{vmatrix} \frac{-i}{2} & \frac{i}{2} & \frac{-1}{\sqrt2} \\ \frac{-i}{2} & \frac{i}{2} & \frac{1}{\sqrt2} \\ \frac{-i}{\sqrt2} & \frac{-i}{\sqrt2} & \cdot \end{vmatrix}$ $r_2 = \begin{vmatrix} \frac{-i}{2} & \frac{i}{2} & \frac{1}{\sqrt2} \\ \frac{-i}{2} & \frac{i}{2} & \frac{-1}{\sqrt2} \\ \frac{i}{\sqrt2} & \frac{i}{\sqrt2} & \cdot \end{vmatrix}$ $r_1^2 = \begin{vmatrix} \frac{i}{2} & \frac{i}{2} & \frac{i}{\sqrt2} \\ \frac{-i}{2} & \frac{-i}{2} & \frac{i}{\sqrt2} \\ \frac{-1}{\sqrt2} & \frac{1}{\sqrt2} & \cdot \end{vmatrix}$ $r_2^2 = \begin{vmatrix} \frac{i}{2} & \frac{i}{2} & \frac{-i}{\sqrt2} \\ \frac{-i}{2} & \frac{-i}{2} & \frac{-i}{\sqrt2} \\ \frac{1}{\sqrt2} & \frac{-1}{\sqrt2} & \cdot \end{vmatrix}$

$\mathscr{D}^{T_1}(R_3^2) = \begin{vmatrix} -1 & \cdot & 0 \\ \cdot & -1 & \cdot \\ \cdot & \cdot & 1 \end{vmatrix}$ $R_2^2 = \begin{vmatrix} \cdot & 1 & 0 \\ 1 & \cdot & \cdot \\ \cdot & \cdot & -1 \end{vmatrix}$ $r_4 = \begin{vmatrix} \frac{i}{2} & \frac{-i}{2} & \frac{-1}{\sqrt2} \\ \frac{i}{2} & \frac{-i}{2} & \frac{1}{\sqrt2} \\ \frac{i}{\sqrt2} & \frac{i}{\sqrt2} & \cdot \end{vmatrix}$ $r_3 = \begin{vmatrix} \frac{i}{2} & \frac{-i}{2} & \frac{1}{\sqrt2} \\ \frac{i}{2} & \frac{-i}{2} & \frac{-1}{\sqrt2} \\ \frac{-i}{\sqrt2} & \frac{-i}{\sqrt2} & \cdot \end{vmatrix}$ $r_3^2 = \begin{vmatrix} \frac{-i}{2} & \frac{-i}{2} & \frac{i}{\sqrt2} \\ \frac{i}{2} & \frac{i}{2} & \frac{i}{\sqrt2} \\ \frac{1}{\sqrt2} & \frac{-1}{\sqrt2} & \cdot \end{vmatrix}$ $r_4^2 = \begin{vmatrix} \frac{-i}{2} & \frac{-i}{2} & \frac{-i}{\sqrt2} \\ \frac{i}{2} & \frac{i}{2} & \frac{-i}{\sqrt2} \\ \frac{-1}{\sqrt2} & \frac{1}{\sqrt2} & \cdot \end{vmatrix}$

$\mathscr{D}^{T_1}(R_3) = \begin{vmatrix} -i & \cdot & 0 \\ \cdot & i & \cdot \\ \cdot & \cdot & 1 \end{vmatrix}$ $i_4 = \begin{vmatrix} \cdot & -i & 0 \\ i & \cdot & \cdot \\ \cdot & \cdot & -1 \end{vmatrix}$ $i_1 = \begin{vmatrix} \frac{-1}{2} & \frac{-1}{2} & \frac{-1}{\sqrt2} \\ \frac{-1}{2} & \frac{-1}{2} & \frac{1}{\sqrt2} \\ \frac{-1}{\sqrt2} & \frac{1}{\sqrt2} & \cdot \end{vmatrix}$ $i_2 = \begin{vmatrix} \frac{-1}{2} & \frac{-1}{2} & \frac{1}{\sqrt2} \\ \frac{-1}{2} & \frac{-1}{2} & \frac{-1}{\sqrt2} \\ \frac{1}{\sqrt2} & \frac{-1}{\sqrt2} & \cdot \end{vmatrix}$ $R_1^3 = \begin{vmatrix} \frac{1}{2} & \frac{-1}{2} & \frac{i}{\sqrt2} \\ \frac{-1}{2} & \frac{1}{2} & \frac{i}{\sqrt2} \\ \frac{i}{\sqrt2} & \frac{i}{\sqrt2} & \cdot \end{vmatrix}$ $R_1 = \begin{vmatrix} \frac{1}{2} & \frac{-1}{2} & \frac{-i}{\sqrt2} \\ \frac{-1}{2} & \frac{1}{2} & \frac{-i}{\sqrt2} \\ \frac{-i}{\sqrt2} & \frac{-i}{\sqrt2} & \cdot \end{vmatrix}$

$\mathscr{D}^{T_1}(R_3^3) = \begin{vmatrix} i & \cdot & 0 \\ \cdot & -i & \cdot \\ \cdot & \cdot & 1 \end{vmatrix}$ $i_3 = \begin{vmatrix} \cdot & i & 0 \\ -i & \cdot & \cdot \\ \cdot & \cdot & -1 \end{vmatrix}$ $R_2 = \begin{vmatrix} \frac{1}{2} & \frac{1}{2} & \frac{-1}{\sqrt2} \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{\sqrt2} \\ \frac{1}{\sqrt2} & \frac{-1}{\sqrt2} & \cdot \end{vmatrix}$ $R_2^3 = \begin{vmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{\sqrt2} \\ \frac{1}{2} & \frac{1}{2} & \frac{-1}{\sqrt2} \\ \frac{-1}{\sqrt2} & \frac{1}{\sqrt2} & \cdot \end{vmatrix}$ $i_6 = \begin{vmatrix} \frac{-1}{2} & \frac{1}{2} & \frac{i}{\sqrt2} \\ \frac{1}{2} & \frac{-1}{2} & \frac{i}{\sqrt2} \\ \frac{-i}{\sqrt2} & \frac{-i}{\sqrt2} & \cdot \end{vmatrix}$ $i_5 = \begin{vmatrix} \frac{-1}{2} & \frac{1}{2} & \frac{-i}{\sqrt2} \\ \frac{1}{2} & \frac{-1}{2} & \frac{-i}{\sqrt2} \\ \frac{i}{\sqrt2} & \frac{i}{\sqrt2} & \cdot \end{vmatrix}$

C_4	Complex vector
1_4	$x+iy$
3_4	$x-iy$
0_4	z

bases :

$$\begin{array}{l} O: \\ D_4: \\ C_4: \end{array} \left| \begin{array}{c} T_1 \\ E \\ 1_4 \end{array} \right\rangle \left| \begin{array}{c} T_1 \\ E \\ 3_4 \end{array} \right\rangle \left| \begin{array}{c} T_1 \\ A_2 \\ 0_4 \end{array} \right\rangle$$

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

$O\supset C_4$

left cosets

$\{\mathbf{1},\boldsymbol{\rho}_z,\mathbf{R}_z,\tilde{\mathbf{R}}_z\}$

$\{\boldsymbol{\rho}_x,\boldsymbol{\rho}_y,\mathbf{i}_4,\mathbf{i}_3\}$

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

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

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

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

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

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

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

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

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: $\mathbf{p}_{1_4}\mathbf{r}_1\mathbf{p}_{0_4} = \frac{1}{16}$

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

$$=[(\mathbf{r}_1+\mathbf{r}_4+\mathbf{i}_1+\mathbf{R}_y)-(\mathbf{r}_2+\mathbf{r}_3+\mathbf{i}_2+\tilde{\mathbf{R}}_y)+i(\tilde{\mathbf{r}}_1+\tilde{\mathbf{r}}_3+\tilde{\mathbf{R}}_x+\mathbf{i}_6)-i(\tilde{\mathbf{r}}_2+\tilde{\mathbf{r}}_4+\mathbf{R}_x+\mathbf{i}_5)]/16$$

$$=[\mathbf{r}_1\mathbf{p}_{0_4}-\mathbf{r}_2\mathbf{p}_{0_4}+i\tilde{\mathbf{r}}_1\mathbf{p}_{0_4}-i\tilde{\mathbf{r}}_2\mathbf{p}_{0_4}]/4 = (\mathbf{r}_1-\mathbf{r}_2+i\tilde{\mathbf{r}}_1-i\tilde{\mathbf{r}}_2)\mathbf{p}_{0_4}/4$$

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

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:*

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

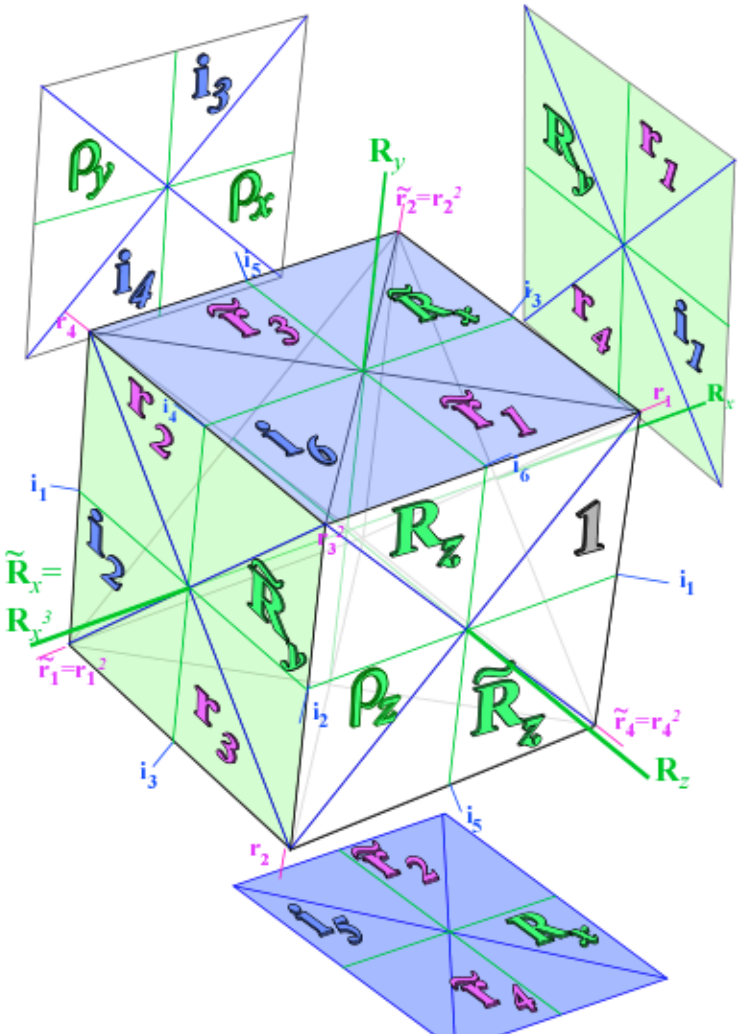
$$\mathbf{P}^{T_1}_{3_4 3_4} = \tfrac{1}{8}[(1)\cdot\mathbf{1}\mathbf{p}_{3_4} \quad + (0)\cdot\rho_x\mathbf{p}_{3_4} \quad + (-\tfrac{i}{2})\cdot\mathbf{r}_1\mathbf{p}_{3_4} \quad + (-\tfrac{i}{2})\cdot\mathbf{r}_2\mathbf{p}_{3_4} \quad + (+\tfrac{i}{2})\cdot\tilde{\mathbf{r}}_1\mathbf{p}_{3_4} \quad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

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

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

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

Then find nilpotent proportional to: $\mathbf{p}_{0_4}\tilde{\mathbf{r}}_1\mathbf{p}_{1_4} = \frac{1}{16}\rho_z$



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

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

$\{\mathbf{1},\boldsymbol{\rho}_z,\mathbf{R}_z,\tilde{\mathbf{R}}_z\}$

$\{\boldsymbol{\rho}_x,\boldsymbol{\rho}_y,\mathbf{i}_4,\mathbf{i}_3\}$

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

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

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

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

Coset-factored T$_1$*-sum:*

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

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

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

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

Then find nilpotent proportional to: $\mathbf{p}_{0_4}\tilde{\mathbf{r}}_1\mathbf{p}_{1_4} = \frac{1}{16}$

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

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

$$= \mathbf{p}_{0_4}\tilde{\mathbf{r}}_1 - \mathbf{p}_{0_4}\tilde{\mathbf{r}}_3 - i\mathbf{p}_{0_4}\tilde{\mathbf{R}}_x + i\mathbf{p}_{0_4}\mathbf{i}_6$$

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

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⊃C₄ left cosets

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

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

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

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

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

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

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

Then find nilpotent proportional to: $\mathbf{p}_{1_4}\mathbf{r}_1\mathbf{p}_{3_4} = \frac{1}{16}$

$$\begin{array}{c|cccc} & \mathbf{r}_1 & -\mathbf{r}_4 & -i\mathbf{i}_1 & +i\mathbf{R}_y \\ \hline \mathbf{1} & \mathbf{r}_1 & -\mathbf{r}_4 & -i\mathbf{i}_1 & +i\mathbf{R}_y \\ -\rho_z & -\mathbf{r}_3 & +\mathbf{r}_2 & +i\tilde{\mathbf{R}}_y & -i\mathbf{i}_2 \\ +i\mathbf{R}_z & +i\mathbf{i}_6 & -i\tilde{\mathbf{R}}_x & +\tilde{\mathbf{r}}_1 & -\tilde{\mathbf{r}}_3 \\ -i\tilde{\mathbf{R}}_z & -i\mathbf{R}_x & +i\mathbf{i}_5 & -\tilde{\mathbf{r}}_4 & +\tilde{\mathbf{r}}_2 \end{array}$$

$$=[(\mathbf{r}_1 - \mathbf{r}_4 - i\mathbf{i}_1 + i\mathbf{R}_y) + (\mathbf{r}_2 - \mathbf{r}_3 - i\mathbf{i}_2 + i\tilde{\mathbf{R}}_y) + (\tilde{\mathbf{r}}_1 - \tilde{\mathbf{r}}_3 - i\tilde{\mathbf{R}}_x + i\mathbf{i}_6) + (\tilde{\mathbf{r}}_2 - \tilde{\mathbf{r}}_4 - i\mathbf{R}_x + i\mathbf{i}_5)]/16$$

$$=[\mathbf{r}_1\mathbf{p}_{3_4} + \mathbf{r}_2\mathbf{p}_{3_4} + \tilde{\mathbf{r}}_1\mathbf{p}_{3_4} + \tilde{\mathbf{r}}_2\mathbf{p}_{3_4}]/4$$

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

AMOP reference links on page 2

3.12.18 class 17.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Discrete symmetry subgroups of O(3)⊃(Octahedral O_h⊃O): Part II Full $D^{(\alpha)}$-matrices defined by subgroup-chains $O\supset D_4\supset C_4$, D_2, or C_3 applied to eigensolutions of O_h-tensors $\mathbf{T}^{[4]}+\mathbf{T}^{[6]}$

Review Idempotent projector splits $\mathbf{P}^{\mu}_{m,m}$ *of* $O\supset C_4$ $\mathbf{P}^{E}_{0404}$ $\mathbf{P}^{E}_{2424}$ $\mathbf{P}^{T_1}_{0404}$ $\mathbf{P}^{T_1}_{1414}$ $\mathbf{P}^{T_2}_{2424}$ $\mathbf{P}^{T_2}_{1414}$

Review Coset factored splitting of projectors for $O\supset D_4\supset C_4$ *into split classes and level structure*

Hamiltonian level cluster models with subgroup-defined tunneling parameters

Diagonal idempotent $\mathbf{P}^{\mu}_{m,m}$ *parameter sets for* $O\supset C_4$ *and* $O\supset C_3$ *case of* SF_6 *level clusters*

Off-diagonal nilpotent $\mathbf{P}^{\mu}_{m,n}$ $(m\neq n)$ *parameter sets needed for* $O\supset C_2$ *clusters*

Deriving nilpotent projectors $\mathbf{P}^{\mu}_{m,n}$ *and ireps* $D^{\mu}_{m,n}$ *by fundamental* $\mathbf{g}\rightleftarrows\mathbf{P}^{\mu}_{m,n}$ *relations:*

(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 nilpotent projectors for simple $D_3\supset C_2\sim C_{3v}\supset C_v$ *chains* (Lect13p95)

Calculating and Factoring $\mathbf{P}^{T_1}_{1404}$ *and* $\mathbf{P}^{T_1}_{1434}$

Structure and applications of coset tabulated $D^{\mu}_{m,n}$ *irreps for various* O_h *subgroup chains*

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

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}_{0424}

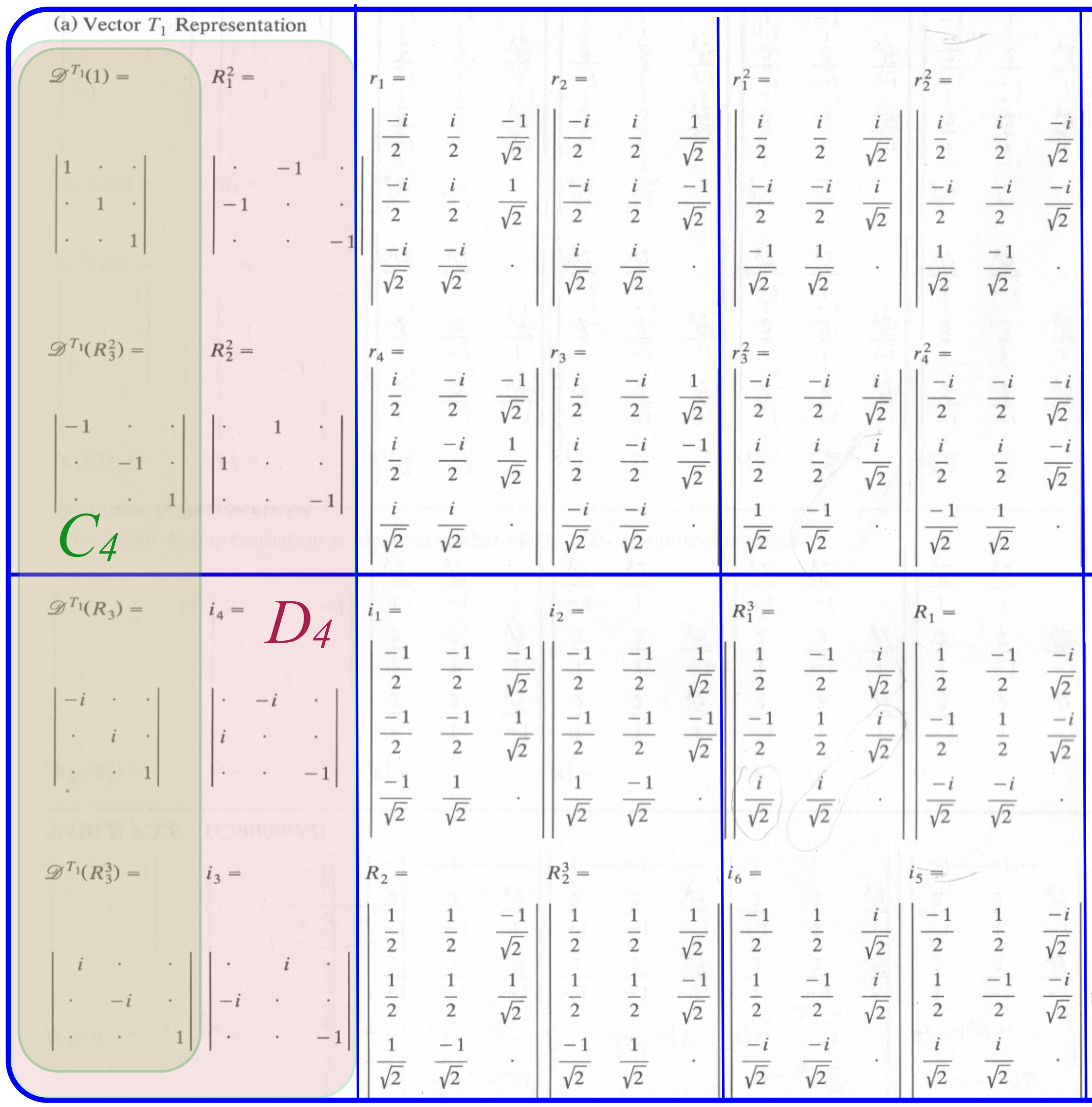
Comparing local C_4, C_3, *and* C_2 *cluster spectra of* O_h*-symmetric tensors* $\mathbf{T}^{[4]}+\mathbf{T}^{[6]}$

Monster clusters: When local C_2 *symmetry dominates*

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

Are these "accidents" or not?

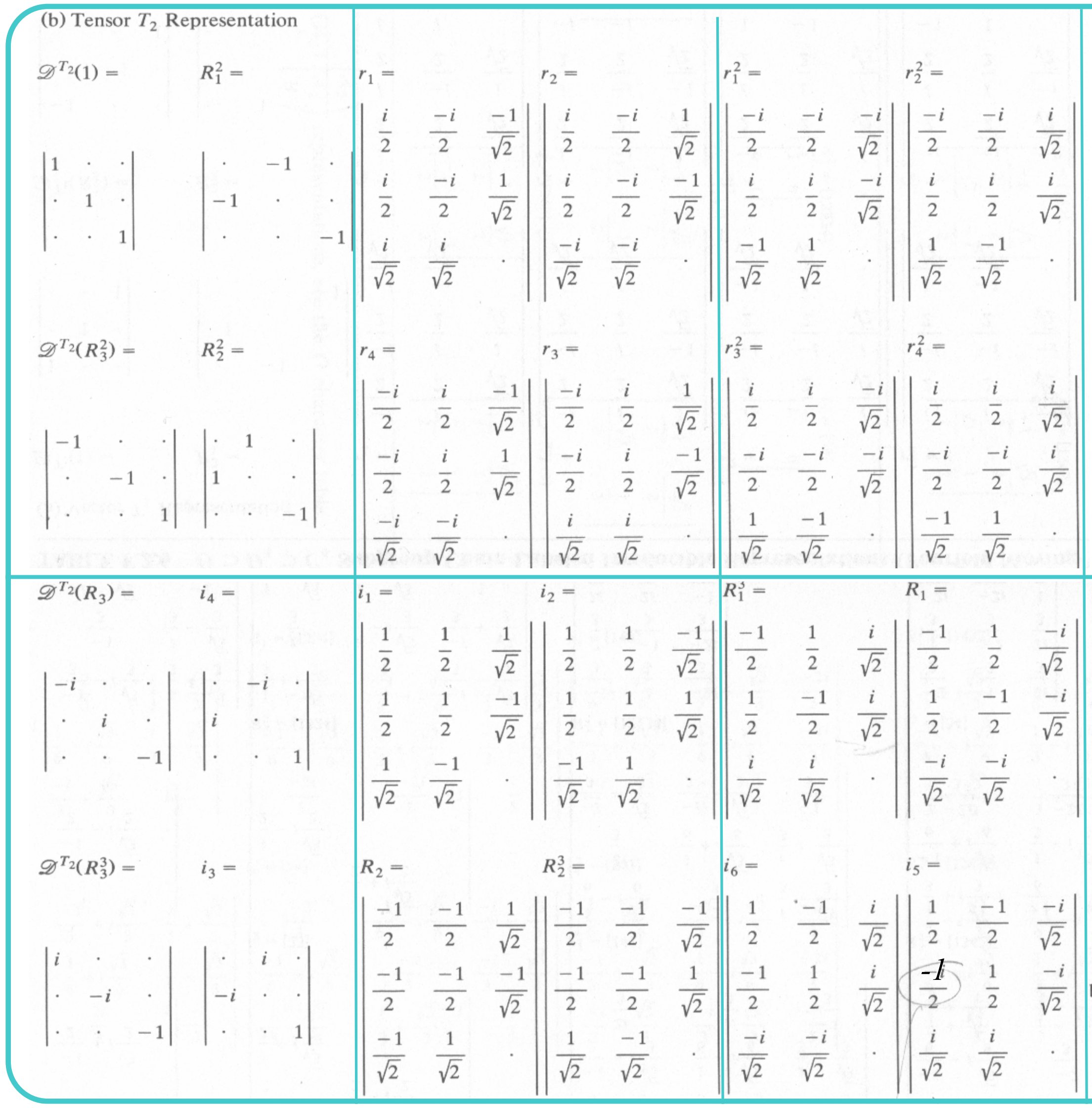
Ireps for O⊃D_4⊃C_4 *subgroup chain*



T$_1$

Vector
x+iy
x-iy
z

basis $O: \left|T_1\right\rangle \left|T_1\right\rangle \left|T_1\right\rangle$, $D_4: E, E, A_2$, $C_4: 1_4, 3_4, 0_4$



T$_2$

Tensor
(x+iy)z
(x-iy)z
xy

basis $O: \left|T_2\right\rangle \left|T_2\right\rangle \left|T_2\right\rangle$, $D_4: E, E, B_2$, $C_4: 1_4, 3_4, 2_4$

$1=[1][2][3][4]$ $\begin{pmatrix}1&0\\0&1\end{pmatrix}$ $R_1^2=[13][24]$ $\begin{pmatrix}1&0\\0&1\end{pmatrix}$

$r_1=[132]$ $\begin{pmatrix}-\frac{1}{2}&-\frac{\sqrt{3}}{2}\\+\frac{\sqrt{3}}{2}&-\frac{1}{2}\end{pmatrix}$ $r_2=[124]$ $\begin{pmatrix}-\frac{1}{2}&-\frac{\sqrt{3}}{2}\\+\frac{\sqrt{3}}{2}&-\frac{1}{2}\end{pmatrix}$

$r_1^2=[123]$ $\begin{pmatrix}-\frac{1}{2}&+\frac{\sqrt{3}}{2}\\-\frac{\sqrt{3}}{2}&-\frac{1}{2}\end{pmatrix}$ $r_2^2=[142]$ $\begin{pmatrix}-\frac{1}{2}&+\frac{\sqrt{3}}{2}\\-\frac{\sqrt{3}}{2}&-\frac{1}{2}\end{pmatrix}$

$R_3^2=[12][34]$ $\begin{pmatrix}1&0\\0&1\end{pmatrix}$ $R_2^2=[14][23]$ $\begin{pmatrix}1&0\\0&1\end{pmatrix}$

$r_4=[234]$ $\begin{pmatrix}-\frac{1}{2}&-\frac{\sqrt{3}}{2}\\+\frac{\sqrt{3}}{2}&-\frac{1}{2}\end{pmatrix}$ $r_3=[124]$ $\begin{pmatrix}-\frac{1}{2}&-\frac{\sqrt{3}}{2}\\+\frac{\sqrt{3}}{2}&-\frac{1}{2}\end{pmatrix}$

$r_3^2=[134]$ $\begin{pmatrix}-\frac{1}{2}&+\frac{\sqrt{3}}{2}\\-\frac{\sqrt{3}}{2}&-\frac{1}{2}\end{pmatrix}$ $r_4^2=[243]$ $\begin{pmatrix}-\frac{1}{2}&+\frac{\sqrt{3}}{2}\\-\frac{\sqrt{3}}{2}&-\frac{1}{2}\end{pmatrix}$

$R_3=[1423]$ $\begin{pmatrix}1&0\\0&-1\end{pmatrix}$ $i_4=[12]$ $\begin{pmatrix}1&0\\0&-1\end{pmatrix}$

$i_1=[14]$ $\begin{pmatrix}-\frac{1}{2}&+\frac{\sqrt{3}}{2}\\+\frac{\sqrt{3}}{2}&+\frac{1}{2}\end{pmatrix}$ $i_2=[23]$ $\begin{pmatrix}-\frac{1}{2}&+\frac{\sqrt{3}}{2}\\+\frac{\sqrt{3}}{2}&+\frac{1}{2}\end{pmatrix}$

$R_1^3=[1432]$ $\begin{pmatrix}-\frac{1}{2}&-\frac{\sqrt{3}}{2}\\-\frac{\sqrt{3}}{2}&+\frac{1}{2}\end{pmatrix}$ $R_1=[1234]$ $\begin{pmatrix}-\frac{1}{2}&-\frac{\sqrt{3}}{2}\\-\frac{\sqrt{3}}{2}&+\frac{1}{2}\end{pmatrix}$

$R_3^3=[1324]$ $\begin{pmatrix}1&0\\0&-1\end{pmatrix}$ $i_3=[34]$ $\begin{pmatrix}1&0\\0&-1\end{pmatrix}$

$R_2=[1243]$ $\begin{pmatrix}-\frac{1}{2}&+\frac{\sqrt{3}}{2}\\+\frac{\sqrt{3}}{2}&+\frac{1}{2}\end{pmatrix}$ $R_2^3=[1342]$ $\begin{pmatrix}-\frac{1}{2}&+\frac{\sqrt{3}}{2}\\+\frac{\sqrt{3}}{2}&+\frac{1}{2}\end{pmatrix}$

$i_6=[24]$ $\begin{pmatrix}-\frac{1}{2}&-\frac{\sqrt{3}}{2}\\-\frac{\sqrt{3}}{2}&+\frac{1}{2}\end{pmatrix}$ $i_5=[13]$ $\begin{pmatrix}-\frac{1}{2}&-\frac{\sqrt{3}}{2}\\-\frac{\sqrt{3}}{2}&+\frac{1}{2}\end{pmatrix}$

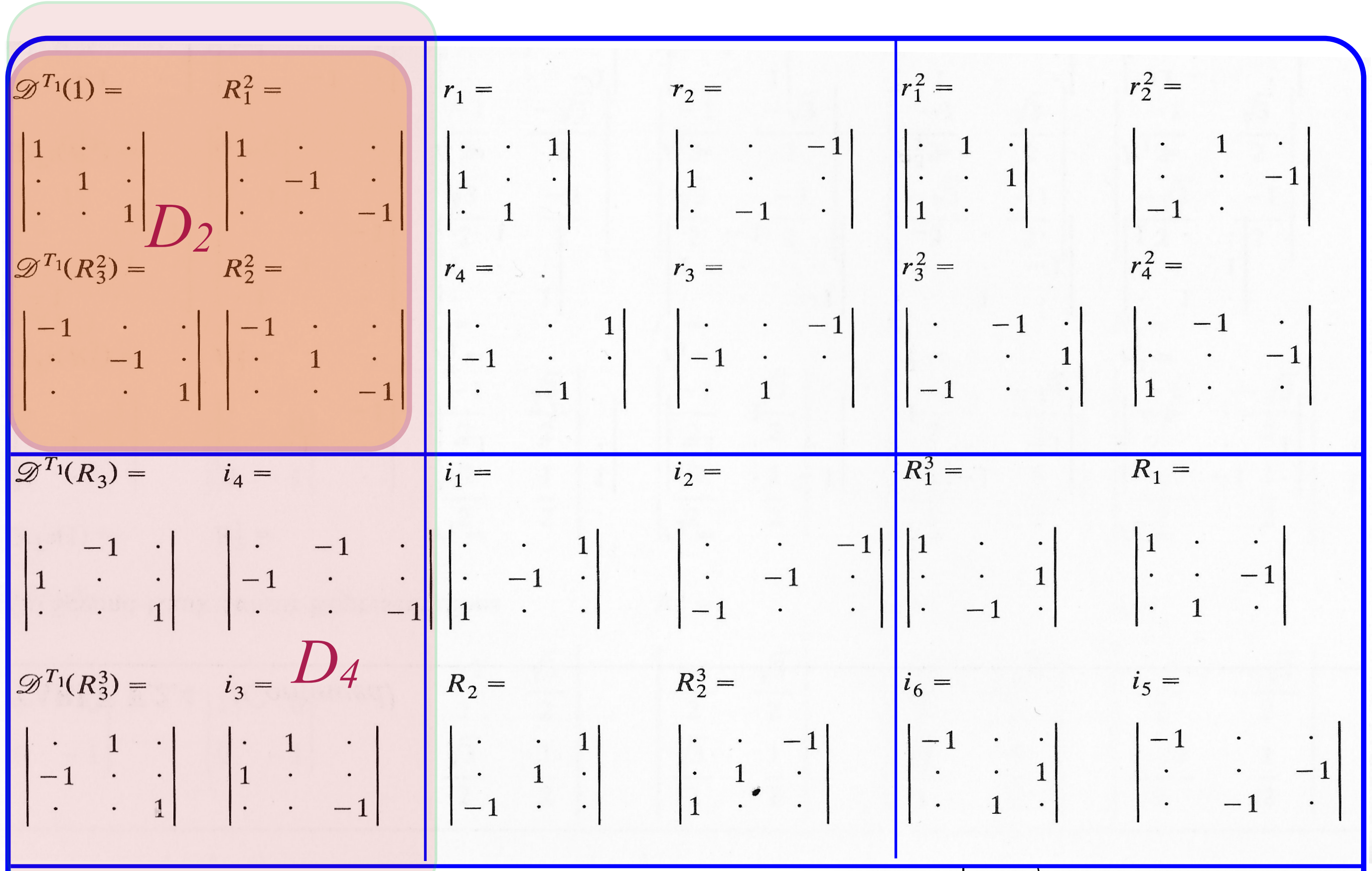
E

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

basis: $O: \left|E\right\rangle \left|E\right\rangle$, $D_4: A_1, B_1$, $C_4: 0_4, 2_4$

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

Ireps for O$\supset D_4 \supset D_2$ subgroup chain



$$\mathscr{D}^{T_1}(1) = \begin{vmatrix} 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \end{vmatrix} \quad R_1^2 = \begin{vmatrix} 1 & \cdot & \cdot \\ \cdot & -1 & \cdot \\ \cdot & \cdot & -1 \end{vmatrix} \quad r_1 = \begin{vmatrix} \cdot & \cdot & 1 \\ 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \end{vmatrix} \quad r_2 = \begin{vmatrix} \cdot & \cdot & -1 \\ 1 & \cdot & \cdot \\ \cdot & -1 & \cdot \end{vmatrix} \quad r_1^2 = \begin{vmatrix} \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \\ 1 & \cdot & \cdot \end{vmatrix} \quad r_2^2 = \begin{vmatrix} \cdot & 1 & \cdot \\ \cdot & \cdot & -1 \\ -1 & \cdot & \cdot \end{vmatrix}$$

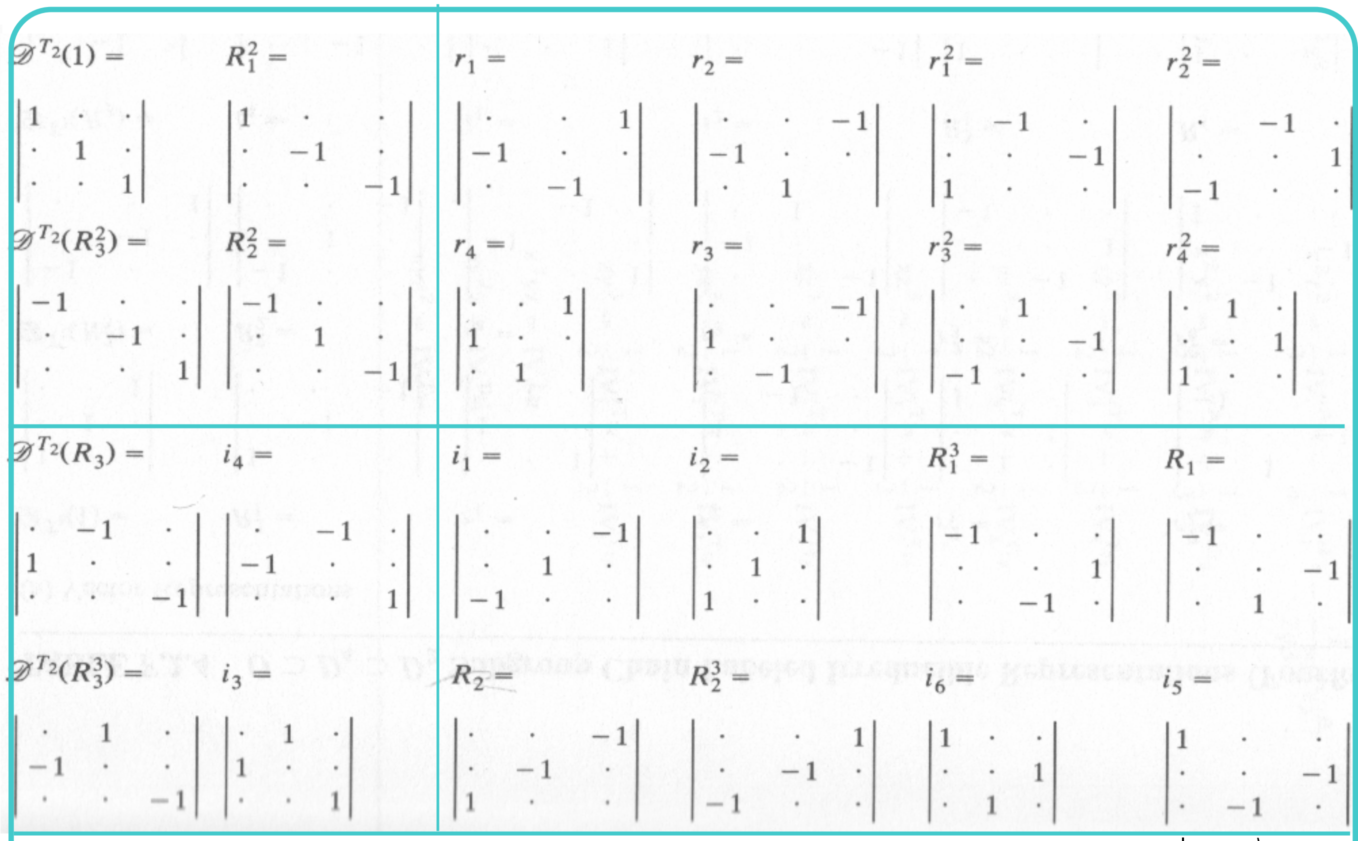
$$\mathscr{D}^{T_1}(R_3^2) = \begin{vmatrix} -1 & \cdot & \cdot \\ \cdot & -1 & \cdot \\ \cdot & \cdot & 1 \end{vmatrix} \quad R_2^2 = \begin{vmatrix} -1 & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & -1 \end{vmatrix} \quad r_4 = \begin{vmatrix} \cdot & \cdot & 1 \\ -1 & \cdot & \cdot \\ \cdot & -1 & \cdot \end{vmatrix} \quad r_3 = \begin{vmatrix} \cdot & \cdot & -1 \\ -1 & \cdot & \cdot \\ \cdot & 1 & \cdot \end{vmatrix} \quad r_3^2 = \begin{vmatrix} \cdot & -1 & \cdot \\ \cdot & \cdot & 1 \\ -1 & \cdot & \cdot \end{vmatrix} \quad r_4^2 = \begin{vmatrix} \cdot & -1 & \cdot \\ \cdot & \cdot & -1 \\ 1 & \cdot & \cdot \end{vmatrix}$$

$$\mathscr{D}^{T_1}(R_3) = \begin{vmatrix} \cdot & -1 & \cdot \\ 1 & \cdot & \cdot \\ \cdot & \cdot & 1 \end{vmatrix} \quad i_4 = \begin{vmatrix} \cdot & -1 & \cdot \\ -1 & \cdot & \cdot \\ \cdot & \cdot & -1 \end{vmatrix} \quad i_1 = \begin{vmatrix} \cdot & \cdot & 1 \\ \cdot & -1 & \cdot \\ 1 & \cdot & \cdot \end{vmatrix} \quad i_2 = \begin{vmatrix} \cdot & \cdot & -1 \\ \cdot & -1 & \cdot \\ -1 & \cdot & \cdot \end{vmatrix} \quad R_1^3 = \begin{vmatrix} 1 & \cdot & \cdot \\ \cdot & \cdot & 1 \\ \cdot & -1 & \cdot \end{vmatrix} \quad R_1 = \begin{vmatrix} 1 & \cdot & \cdot \\ \cdot & \cdot & -1 \\ \cdot & 1 & \cdot \end{vmatrix}$$

$$\mathscr{D}^{T_1}(R_3^3) = \begin{vmatrix} \cdot & 1 & \cdot \\ -1 & \cdot & \cdot \\ \cdot & \cdot & 1 \end{vmatrix} \quad i_3 = \begin{vmatrix} \cdot & 1 & \cdot \\ 1 & \cdot & \cdot \\ \cdot & \cdot & -1 \end{vmatrix} \quad R_2 = \begin{vmatrix} \cdot & \cdot & 1 \\ \cdot & 1 & \cdot \\ -1 & \cdot & \cdot \end{vmatrix} \quad R_2^3 = \begin{vmatrix} \cdot & \cdot & -1 \\ \cdot & 1 & \cdot \\ 1 & \cdot & \cdot \end{vmatrix} \quad i_6 = \begin{vmatrix} -1 & \cdot & \cdot \\ \cdot & \cdot & 1 \\ \cdot & 1 & \cdot \end{vmatrix} \quad i_5 = \begin{vmatrix} -1 & \cdot & \cdot \\ \cdot & \cdot & -1 \\ \cdot & -1 & \cdot \end{vmatrix}$$

T_1 *Vector* *x,y,z*

basis: $\begin{matrix} O \\ D_4 \\ D_2 \end{matrix} \left| \begin{matrix} T_1 \\ E \\ B_1 \end{matrix} \right\rangle \left| \begin{matrix} T_1 \\ E \\ B_2 \end{matrix} \right\rangle \left| \begin{matrix} T_1 \\ A_2 \\ A_2 \end{matrix} \right\rangle$



$$\mathscr{D}^{T_2}(1) = \begin{vmatrix} 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \end{vmatrix} \quad R_1^2 = \begin{vmatrix} 1 & \cdot & \cdot \\ \cdot & -1 & \cdot \\ \cdot & \cdot & -1 \end{vmatrix} \quad r_1 = \begin{vmatrix} \cdot & \cdot & 1 \\ -1 & \cdot & \cdot \\ \cdot & -1 & \cdot \end{vmatrix} \quad r_2 = \begin{vmatrix} \cdot & \cdot & -1 \\ -1 & \cdot & \cdot \\ \cdot & 1 & \cdot \end{vmatrix} \quad r_1^2 = \begin{vmatrix} \cdot & -1 & \cdot \\ \cdot & \cdot & -1 \\ 1 & \cdot & \cdot \end{vmatrix} \quad r_2^2 = \begin{vmatrix} \cdot & -1 & \cdot \\ \cdot & \cdot & 1 \\ -1 & \cdot & \cdot \end{vmatrix}$$

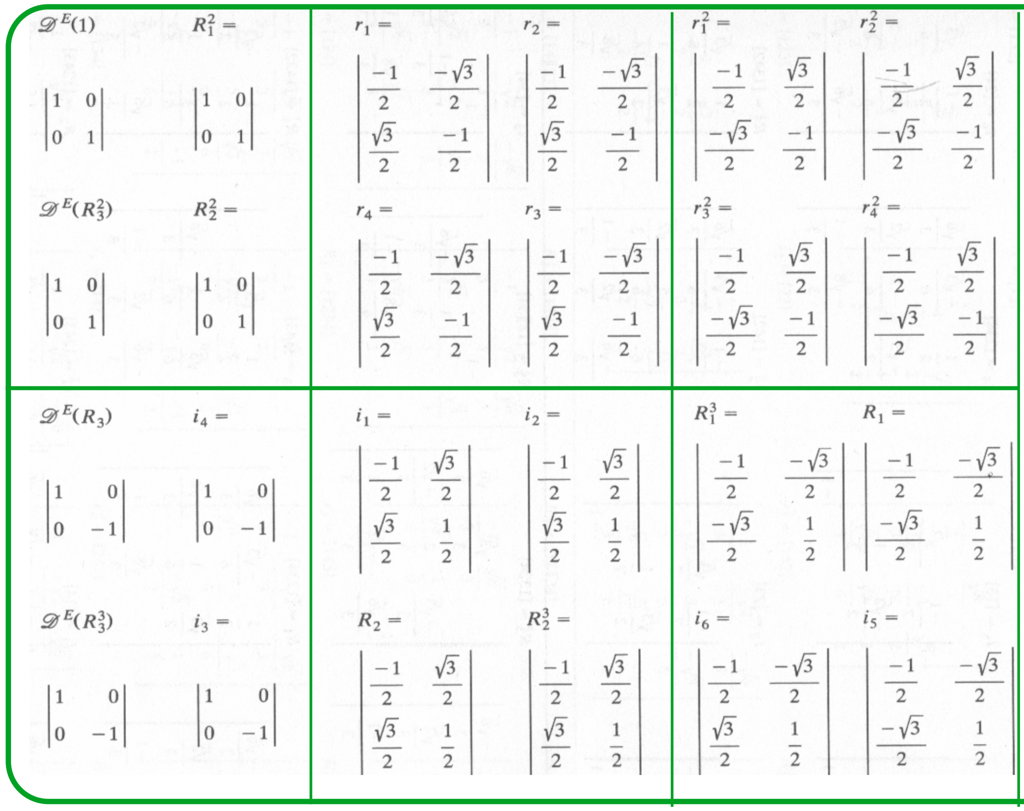
$$\mathscr{D}^{T_2}(R_3^2) = \begin{vmatrix} -1 & \cdot & \cdot \\ \cdot & -1 & \cdot \\ \cdot & \cdot & 1 \end{vmatrix} \quad R_2^2 = \begin{vmatrix} -1 & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & -1 \end{vmatrix} \quad r_4 = \begin{vmatrix} \cdot & \cdot & 1 \\ 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \end{vmatrix} \quad r_3 = \begin{vmatrix} \cdot & \cdot & -1 \\ 1 & \cdot & \cdot \\ \cdot & -1 & \cdot \end{vmatrix} \quad r_3^2 = \begin{vmatrix} \cdot & 1 & \cdot \\ \cdot & \cdot & -1 \\ -1 & \cdot & \cdot \end{vmatrix} \quad r_4^2 = \begin{vmatrix} \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \\ 1 & \cdot & \cdot \end{vmatrix}$$

$$\mathscr{D}^{T_2}(R_3) = \begin{vmatrix} \cdot & -1 & \cdot \\ 1 & \cdot & \cdot \\ \cdot & \cdot & -1 \end{vmatrix} \quad i_4 = \begin{vmatrix} \cdot & -1 & \cdot \\ -1 & \cdot & \cdot \\ \cdot & \cdot & 1 \end{vmatrix} \quad i_1 = \begin{vmatrix} \cdot & \cdot & -1 \\ \cdot & 1 & \cdot \\ -1 & \cdot & \cdot \end{vmatrix} \quad i_2 = \begin{vmatrix} \cdot & \cdot & 1 \\ \cdot & 1 & \cdot \\ 1 & \cdot & \cdot \end{vmatrix} \quad R_1^3 = \begin{vmatrix} -1 & \cdot & \cdot \\ \cdot & \cdot & 1 \\ \cdot & -1 & \cdot \end{vmatrix} \quad R_1 = \begin{vmatrix} -1 & \cdot & \cdot \\ \cdot & \cdot & -1 \\ \cdot & 1 & \cdot \end{vmatrix}$$

$$\mathscr{D}^{T_2}(R_3^3) = \begin{vmatrix} \cdot & 1 & \cdot \\ -1 & \cdot & \cdot \\ \cdot & \cdot & -1 \end{vmatrix} \quad i_3 = \begin{vmatrix} \cdot & 1 & \cdot \\ 1 & \cdot & \cdot \\ \cdot & \cdot & 1 \end{vmatrix} \quad R_2 = \begin{vmatrix} \cdot & \cdot & -1 \\ \cdot & -1 & \cdot \\ 1 & \cdot & \cdot \end{vmatrix} \quad R_2^3 = \begin{vmatrix} \cdot & \cdot & 1 \\ \cdot & -1 & \cdot \\ -1 & \cdot & \cdot \end{vmatrix} \quad i_6 = \begin{vmatrix} 1 & \cdot & \cdot \\ \cdot & \cdot & 1 \\ \cdot & 1 & \cdot \end{vmatrix} \quad i_5 = \begin{vmatrix} 1 & \cdot & \cdot \\ \cdot & \cdot & -1 \\ \cdot & -1 & \cdot \end{vmatrix}$$

T_2 *Tensor* *yz,xz,xy*

basis: $\begin{matrix} O \\ D_4 \\ D_2 \end{matrix} \left| \begin{matrix} T_2 \\ E \\ B_1 \end{matrix} \right\rangle \left| \begin{matrix} T_2 \\ E \\ B_2 \end{matrix} \right\rangle \left| \begin{matrix} T_2 \\ B_2 \\ A_2 \end{matrix} \right\rangle$



$$\mathscr{D}^{E}(1) \begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix} \quad R_1^2 = \begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix} \quad r_1 = \begin{vmatrix} \frac{-1}{2} & \frac{-\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{-1}{2} \end{vmatrix} \quad r_2 = \begin{vmatrix} \frac{-1}{2} & \frac{-\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{-1}{2} \end{vmatrix} \quad r_1^2 = \begin{vmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ \frac{-\sqrt{3}}{2} & \frac{-1}{2} \end{vmatrix} \quad r_2^2 = \begin{vmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ \frac{-\sqrt{3}}{2} & \frac{-1}{2} \end{vmatrix}$$

$$\mathscr{D}^{E}(R_3^2) \begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix} \quad R_2^2 = \begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix} \quad r_4 = \begin{vmatrix} \frac{-1}{2} & \frac{-\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{-1}{2} \end{vmatrix} \quad r_3 = \begin{vmatrix} \frac{-1}{2} & \frac{-\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{-1}{2} \end{vmatrix} \quad r_3^2 = \begin{vmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ \frac{-\sqrt{3}}{2} & \frac{-1}{2} \end{vmatrix} \quad r_4^2 = \begin{vmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ \frac{-\sqrt{3}}{2} & \frac{-1}{2} \end{vmatrix}$$

$$\mathscr{D}^{E}(R_3) \begin{vmatrix} 1 & 0 \\ 0 & -1 \end{vmatrix} \quad i_4 = \begin{vmatrix} 1 & 0 \\ 0 & -1 \end{vmatrix} \quad i_1 = \begin{vmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{vmatrix} \quad i_2 = \begin{vmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{vmatrix} \quad R_1^3 = \begin{vmatrix} \frac{-1}{2} & \frac{-\sqrt{3}}{2} \\ \frac{-\sqrt{3}}{2} & \frac{1}{2} \end{vmatrix} \quad R_1 = \begin{vmatrix} \frac{-1}{2} & \frac{-\sqrt{3}}{2} \\ \frac{-\sqrt{3}}{2} & \frac{1}{2} \end{vmatrix}$$

$$\mathscr{D}^{E}(R_3^3) \begin{vmatrix} 1 & 0 \\ 0 & -1 \end{vmatrix} \quad i_3 = \begin{vmatrix} 1 & 0 \\ 0 & -1 \end{vmatrix} \quad R_2 = \begin{vmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{vmatrix} \quad R_2^3 = \begin{vmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{vmatrix} \quad i_6 = \begin{vmatrix} \frac{-1}{2} & \frac{-\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{vmatrix} \quad i_5 = \begin{vmatrix} \frac{-1}{2} & \frac{-\sqrt{3}}{2} \\ \frac{-\sqrt{3}}{2} & \frac{1}{2} \end{vmatrix}$$

E

Tensor

$x^2+y^2-2z^2$

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

basis: $\begin{matrix} O \\ D_4 \\ D_2 \end{matrix} \left| \begin{matrix} E \\ A_1 \\ A_1 \end{matrix} \right\rangle \left| \begin{matrix} E \\ B_1 \\ A_1 \end{matrix} \right\rangle$

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

Ireps for O⊃D_3⊃C_2 subgroup chain (Also permutation group Young Tableau chain S_4⊃S_3⊃S_2⊃S_1)

C_2

$\mathscr{D}^{T_1}(1) =$ $\begin{vmatrix}1&\cdot&\cdot\\\cdot&1&\cdot\\\cdot&\cdot&1\end{vmatrix}$

$i_4 = [12]$ $\begin{vmatrix}1&\cdot&\cdot\\\cdot&-1&\cdot\\\cdot&\cdot&-1\end{vmatrix}$

D_3

$r_1 = [132]$ $\begin{vmatrix}\frac{-1}{2}&\frac{-\sqrt{3}}{2}&\cdot\\\frac{\sqrt{3}}{2}&\frac{-1}{2}&\cdot\\\cdot&\cdot&1\end{vmatrix}$

$i_5 = [13]$ $\begin{vmatrix}\frac{-1}{2}&\frac{-\sqrt{3}}{2}&\cdot\\\frac{-\sqrt{3}}{2}&\frac{1}{2}&\cdot\\\cdot&\cdot&-1\end{vmatrix}$

$r_1^2 = [123]$ $\begin{vmatrix}\frac{-1}{2}&\frac{\sqrt{3}}{2}&\cdot\\\frac{-\sqrt{3}}{2}&\frac{-1}{2}&\cdot\\\cdot&\cdot&1\end{vmatrix}$

$i_2 = [23]$ $\begin{vmatrix}\frac{-1}{2}&\frac{\sqrt{3}}{2}&\cdot\\\frac{\sqrt{3}}{2}&\frac{1}{2}&\cdot\\\cdot&\cdot&-1\end{vmatrix}$

$R_1^2 = [13][24]$ $\begin{vmatrix}\cdot&\frac{\sqrt{3}}{3}&\frac{\sqrt{6}}{3}\\\frac{\sqrt{3}}{3}&\frac{-2}{3}&\frac{\sqrt{2}}{3}\\\frac{\sqrt{6}}{3}&\frac{\sqrt{2}}{3}&\frac{-1}{3}\end{vmatrix}$

$R_3 = [1423]$ $\begin{vmatrix}\cdot&\frac{-\sqrt{3}}{3}&\frac{-\sqrt{6}}{3}\\\frac{\sqrt{3}}{3}&\frac{2}{3}&\frac{-\sqrt{2}}{3}\\\frac{\sqrt{6}}{3}&\frac{-\sqrt{2}}{3}&\frac{1}{3}\end{vmatrix}$

$r_4 = [234]$ $\begin{vmatrix}\frac{1}{2}&\frac{-\sqrt{3}}{6}&\frac{\sqrt{6}}{3}\\\frac{-\sqrt{3}}{2}&\frac{-1}{6}&\frac{\sqrt{2}}{3}\\\cdot&\frac{-\sqrt{8}}{3}&\frac{-1}{3}\end{vmatrix}$

$i_6 = [24]$ $\begin{vmatrix}\frac{-1}{2}&\frac{\sqrt{3}}{6}&\frac{-\sqrt{6}}{3}\\\frac{\sqrt{3}}{6}&\frac{-5}{6}&\frac{-\sqrt{2}}{3}\\\frac{-\sqrt{6}}{3}&\frac{-\sqrt{2}}{3}&\frac{1}{3}\end{vmatrix}$

$r_2^2 = [142]$ $\begin{vmatrix}\frac{-1}{2}&\frac{-\sqrt{3}}{6}&\frac{\sqrt{6}}{3}\\\frac{\sqrt{3}}{6}&\frac{5}{6}&\frac{\sqrt{2}}{3}\\\frac{-\sqrt{6}}{3}&\frac{\sqrt{2}}{3}&\frac{-1}{3}\end{vmatrix}$

$R_2^3 = [1342]$ $\begin{vmatrix}\frac{1}{2}&\frac{\sqrt{3}}{6}&\frac{-\sqrt{6}}{3}\\\frac{-\sqrt{3}}{2}&\frac{1}{6}&\frac{-\sqrt{2}}{3}\\\cdot&\frac{\sqrt{8}}{3}&\frac{1}{3}\end{vmatrix}$

$R_2^2 = [14][23]$ $\begin{vmatrix}\cdot&\frac{-\sqrt{3}}{3}&\frac{-\sqrt{6}}{3}\\\frac{-\sqrt{3}}{3}&\frac{-2}{3}&\frac{\sqrt{2}}{3}\\\frac{-\sqrt{6}}{3}&\frac{\sqrt{2}}{3}&\frac{-1}{3}\end{vmatrix}$

$R_3^3 = [1324]$ $\begin{vmatrix}\cdot&\frac{\sqrt{3}}{3}&\frac{\sqrt{6}}{3}\\\frac{-\sqrt{3}}{3}&\frac{2}{3}&\frac{-\sqrt{2}}{3}\\\frac{-\sqrt{6}}{3}&\frac{-\sqrt{2}}{3}&\frac{1}{3}\end{vmatrix}$

$r_2 = [124]$ $\begin{vmatrix}\frac{-1}{2}&\frac{\sqrt{3}}{6}&\frac{-\sqrt{6}}{3}\\\frac{-\sqrt{3}}{6}&\frac{5}{6}&\frac{\sqrt{2}}{3}\\\frac{\sqrt{6}}{3}&\frac{\sqrt{2}}{3}&\frac{-1}{3}\end{vmatrix}$

$R_1 = [1234]$ $\begin{vmatrix}\frac{1}{2}&\frac{-\sqrt{3}}{6}&\frac{\sqrt{6}}{3}\\\frac{\sqrt{3}}{2}&\frac{1}{6}&\frac{-\sqrt{2}}{3}\\\cdot&\frac{\sqrt{8}}{3}&\frac{1}{3}\end{vmatrix}$

$r_3^2 = [134]$ $\begin{vmatrix}\frac{1}{2}&\frac{\sqrt{3}}{6}&\frac{-\sqrt{6}}{3}\\\frac{\sqrt{3}}{2}&\frac{-1}{6}&\frac{\sqrt{2}}{3}\\\cdot&\frac{-\sqrt{8}}{3}&\frac{-1}{3}\end{vmatrix}$

$i_1 = [14]$ $\begin{vmatrix}\frac{-1}{2}&\frac{-\sqrt{3}}{6}&\frac{\sqrt{6}}{3}\\\frac{-\sqrt{3}}{6}&\frac{-5}{6}&\frac{-\sqrt{2}}{3}\\\frac{\sqrt{6}}{3}&\frac{-\sqrt{2}}{3}&\frac{1}{3}\end{vmatrix}$

$R_3^2 = [12][34]$ $\begin{vmatrix}-1&\cdot&\cdot\\\cdot&\frac{1}{3}&\frac{-\sqrt{8}}{3}\\\cdot&\frac{-\sqrt{8}}{3}&\frac{-1}{3}\end{vmatrix}$

$i_3 = [34]$ $\begin{vmatrix}-1&\cdot&\cdot\\\cdot&\frac{-1}{3}&\frac{\sqrt{8}}{3}\\\cdot&\frac{\sqrt{8}}{3}&\frac{1}{3}\end{vmatrix}$

$r_3 = [143]$ $\begin{vmatrix}\frac{1}{2}&\frac{\sqrt{3}}{2}&\cdot\\\frac{\sqrt{3}}{6}&\frac{-1}{6}&\frac{-\sqrt{8}}{3}\\\frac{-\sqrt{6}}{3}&\frac{\sqrt{2}}{3}&\frac{-1}{3}\end{vmatrix}$

$R_1^3 = [1432]$ $\begin{vmatrix}\frac{1}{2}&\frac{\sqrt{3}}{2}&\cdot\\\frac{-\sqrt{3}}{6}&\frac{1}{6}&\frac{\sqrt{8}}{3}\\\frac{\sqrt{6}}{3}&\frac{-\sqrt{2}}{3}&\frac{1}{3}\end{vmatrix}$

$r_4^2 = [243]$ $\begin{vmatrix}\frac{1}{2}&\frac{-\sqrt{3}}{2}&\cdot\\\frac{-\sqrt{3}}{6}&\frac{-1}{6}&\frac{-\sqrt{8}}{3}\\\frac{\sqrt{6}}{3}&\frac{\sqrt{2}}{3}&\frac{-1}{3}\end{vmatrix}$

$R_2 = [1243]$ $\begin{vmatrix}\frac{1}{2}&\frac{-\sqrt{3}}{2}&\cdot\\\frac{\sqrt{3}}{6}&\frac{1}{6}&\frac{\sqrt{8}}{3}\\\frac{-\sqrt{6}}{3}&\frac{-\sqrt{2}}{3}&\frac{1}{3}\end{vmatrix}$

T_1 *Vector* *u,v,w* $\begin{array}{|c|c|}\hline 1&2\\\hline 3\\\cline{1-1} 4\\\cline{1-1}\end{array}$ $\begin{array}{|c|c|}\hline 1&3\\\hline 2\\\cline{1-1} 4\\\cline{1-1}\end{array}$ $\begin{array}{|c|c|}\hline 1&4\\\hline 2\\\cline{1-1} 3\\\cline{1-1}\end{array}$

basis: $\begin{matrix}O\\D_3\\C_2\end{matrix}\left|\begin{matrix}T_1\\E\\0_2\end{matrix}\right\rangle\left|\begin{matrix}T_1\\E\\1_2\end{matrix}\right\rangle\left|\begin{matrix}T_1\\A_2\\1_2\end{matrix}\right\rangle$

$\mathscr{D}^{T_2}(1) =$ $\begin{vmatrix}1&\cdot&\cdot\\\cdot&1&\cdot\\\cdot&\cdot&1\end{vmatrix}$

$i_4 = [12]$ $\begin{vmatrix}1&\cdot&\cdot\\\cdot&1&\cdot\\\cdot&\cdot&-1\end{vmatrix}$

$r_1 = [132]$ $\begin{vmatrix}1&\cdot&\cdot\\\cdot&\frac{-1}{2}&\frac{-\sqrt{3}}{2}\\\cdot&\frac{\sqrt{3}}{2}&\frac{-1}{2}\end{vmatrix}$

$i_5 = [13]$ $\begin{vmatrix}1&\cdot&\cdot\\\cdot&\frac{-1}{2}&\frac{-\sqrt{3}}{2}\\\cdot&\frac{-\sqrt{3}}{2}&\frac{1}{2}\end{vmatrix}$

$r_1^2 = [123]$ $\begin{vmatrix}1&\cdot&\cdot\\\cdot&\frac{-1}{2}&\frac{\sqrt{3}}{2}\\\cdot&\frac{-\sqrt{3}}{2}&\frac{-1}{2}\end{vmatrix}$

$i_2 = [23]$ $\begin{vmatrix}1&\cdot&\cdot\\\cdot&\frac{-1}{2}&\frac{\sqrt{3}}{2}\\\cdot&\frac{\sqrt{3}}{2}&\frac{1}{2}\end{vmatrix}$

$R_1^2 = [13][24]$ $\begin{vmatrix}\frac{-1}{3}&\frac{-\sqrt{2}}{3}&\frac{\sqrt{6}}{3}\\\frac{-\sqrt{2}}{3}&\frac{-2}{3}&\frac{-\sqrt{3}}{3}\\\frac{\sqrt{6}}{3}&\frac{-\sqrt{3}}{3}&\cdot\end{vmatrix}$

$R_3 = [1423]$ $\begin{vmatrix}\frac{-1}{3}&\frac{-\sqrt{2}}{3}&\frac{-\sqrt{6}}{3}\\\frac{-\sqrt{2}}{3}&\frac{-2}{3}&\frac{\sqrt{3}}{3}\\\frac{\sqrt{6}}{3}&\frac{-\sqrt{3}}{3}&\cdot\end{vmatrix}$

$r_4 = [234]$ $\begin{vmatrix}\frac{-1}{3}&\frac{\sqrt{8}}{3}&\cdot\\\frac{-\sqrt{2}}{3}&\frac{-1}{6}&\frac{\sqrt{3}}{2}\\\frac{\sqrt{6}}{3}&\frac{\sqrt{3}}{6}&\frac{1}{2}\end{vmatrix}$

$i_6 = [24]$ $\begin{vmatrix}\frac{-1}{3}&\frac{-\sqrt{2}}{3}&\frac{\sqrt{6}}{3}\\\frac{-\sqrt{2}}{3}&\frac{5}{6}&\frac{\sqrt{3}}{6}\\\frac{\sqrt{6}}{3}&\frac{\sqrt{3}}{6}&\frac{1}{2}\end{vmatrix}$

$r_2^2 = [142]$ $\begin{vmatrix}\frac{-1}{3}&\frac{-\sqrt{2}}{3}&\frac{-\sqrt{6}}{3}\\\frac{-\sqrt{2}}{3}&\frac{5}{6}&\frac{-\sqrt{3}}{6}\\\frac{\sqrt{6}}{3}&\frac{\sqrt{3}}{6}&\frac{-1}{2}\end{vmatrix}$

$R_2^3 = [1342]$ $\begin{vmatrix}\frac{-1}{3}&\frac{\sqrt{8}}{3}&\cdot\\\frac{-\sqrt{2}}{3}&\frac{-1}{6}&\frac{-\sqrt{3}}{2}\\\frac{\sqrt{6}}{3}&\frac{\sqrt{3}}{6}&\frac{-1}{2}\end{vmatrix}$

$R_2^2 = [14][23]$ $\begin{vmatrix}\frac{-1}{3}&\frac{-\sqrt{2}}{3}&\frac{-\sqrt{6}}{3}\\\frac{-\sqrt{2}}{3}&\frac{-2}{3}&\frac{\sqrt{3}}{3}\\\frac{-\sqrt{6}}{3}&\frac{\sqrt{3}}{3}&\cdot\end{vmatrix}$

$R_3^3 = [1324]$ $\begin{vmatrix}\frac{-1}{3}&\frac{-\sqrt{2}}{3}&\frac{\sqrt{6}}{3}\\\frac{-\sqrt{2}}{3}&\frac{-2}{3}&\frac{\sqrt{3}}{3}\\\frac{-\sqrt{6}}{3}&\frac{\sqrt{3}}{3}&\cdot\end{vmatrix}$

$r_2 = [124]$ $\begin{vmatrix}\frac{-1}{3}&\frac{-\sqrt{2}}{3}&\frac{\sqrt{6}}{3}\\\frac{-\sqrt{2}}{3}&\frac{5}{6}&\frac{\sqrt{3}}{6}\\\frac{-\sqrt{6}}{3}&\frac{-\sqrt{3}}{6}&\frac{-1}{2}\end{vmatrix}$

$R_1 = [1234]$ $\begin{vmatrix}\frac{-1}{3}&\frac{\sqrt{8}}{3}&\cdot\\\frac{-\sqrt{2}}{3}&\frac{-1}{6}&\frac{\sqrt{3}}{2}\\\frac{-\sqrt{6}}{3}&\frac{-\sqrt{3}}{6}&\frac{-1}{2}\end{vmatrix}$

$r_3^2 = [134]$ $\begin{vmatrix}\frac{-1}{3}&\frac{\sqrt{8}}{3}&\cdot\\\frac{-\sqrt{2}}{3}&\frac{-1}{6}&\frac{-\sqrt{3}}{2}\\\frac{-\sqrt{6}}{3}&\frac{-\sqrt{3}}{6}&\frac{1}{2}\end{vmatrix}$

$i_1 = [14]$ $\begin{vmatrix}\frac{-1}{3}&\frac{-\sqrt{2}}{3}&\frac{-\sqrt{6}}{3}\\\frac{-\sqrt{2}}{3}&\frac{5}{6}&\frac{-\sqrt{3}}{6}\\\frac{-\sqrt{6}}{3}&\frac{-\sqrt{3}}{6}&\frac{1}{2}\end{vmatrix}$

$R_3^2 = [12][34]$ $\begin{vmatrix}\frac{-1}{3}&\frac{\sqrt{8}}{3}&\cdot\\\frac{\sqrt{8}}{3}&\frac{1}{3}&\cdot\\\cdot&\cdot&-1\end{vmatrix}$

$i_3 = [34]$ $\begin{vmatrix}\frac{-1}{3}&\frac{\sqrt{8}}{3}&\cdot\\\frac{\sqrt{8}}{3}&\frac{1}{3}&\cdot\\\cdot&\cdot&1\end{vmatrix}$

$r_3 = [143]$ $\begin{vmatrix}\frac{-1}{3}&\frac{-\sqrt{2}}{3}&\frac{-\sqrt{6}}{3}\\\frac{\sqrt{8}}{3}&\frac{-1}{6}&\frac{-\sqrt{3}}{6}\\\cdot&\frac{-\sqrt{3}}{2}&\frac{1}{2}\end{vmatrix}$

$R_1^3 = [1432]$ $\begin{vmatrix}\frac{-1}{3}&\frac{-\sqrt{2}}{3}&\frac{-\sqrt{6}}{3}\\\frac{\sqrt{8}}{3}&\frac{-1}{6}&\frac{-\sqrt{3}}{6}\\\cdot&\frac{\sqrt{3}}{2}&\frac{-1}{2}\end{vmatrix}$

$r_4^2 = [243]$ $\begin{vmatrix}\frac{-1}{3}&\frac{-\sqrt{2}}{3}&\frac{\sqrt{6}}{3}\\\frac{\sqrt{8}}{3}&\frac{-1}{6}&\frac{\sqrt{3}}{6}\\\cdot&\frac{\sqrt{3}}{2}&\frac{1}{2}\end{vmatrix}$

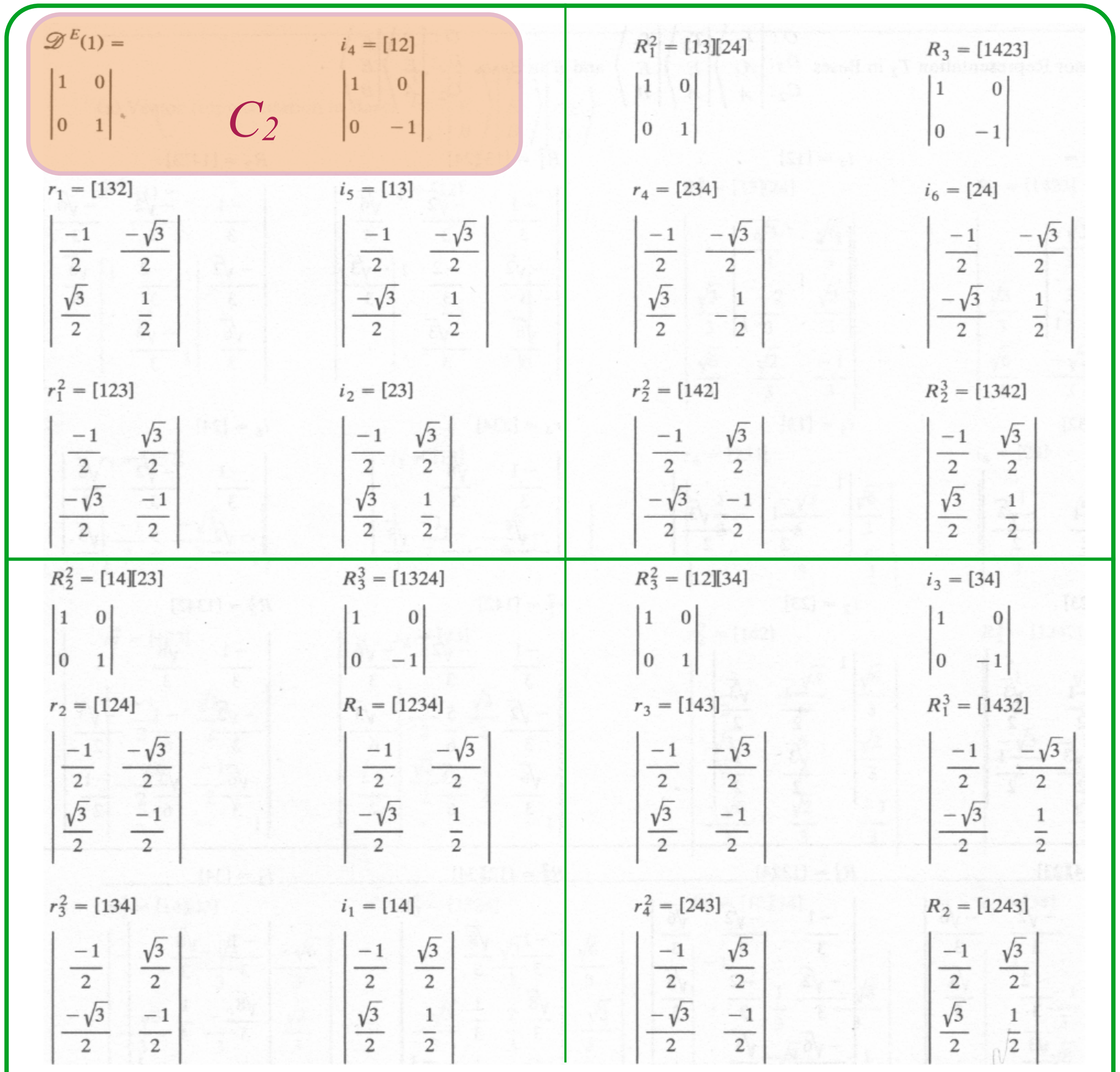
$R_2 = [1243]$ $\begin{vmatrix}\frac{-1}{3}&\frac{-\sqrt{2}}{3}&\frac{\sqrt{6}}{3}\\\frac{\sqrt{8}}{3}&\frac{-1}{6}&\frac{\sqrt{3}}{6}\\\cdot&\frac{-\sqrt{3}}{2}&\frac{-1}{2}\end{vmatrix}$

T_2 *Tensor* *vw,uw,uv* $\begin{array}{|c|c|c|}\hline 1&3&4\\\hline 2\\\cline{1-1}\end{array}$ $\begin{array}{|c|c|c|}\hline 1&2&4\\\hline 3\\\cline{1-1}\end{array}$ $\begin{array}{|c|c|c|}\hline 1&2&3\\\hline 4\\\cline{1-1}\end{array}$

basis: $\begin{matrix}O\\D_3\\C_2\end{matrix}\left|\begin{matrix}T_2\\B_2\\0_2\end{matrix}\right\rangle\left|\begin{matrix}T_2\\E\\0_2\end{matrix}\right\rangle\left|\begin{matrix}T_2\\E\\1_2\end{matrix}\right\rangle$

Ireps for O⊃D_3⊃C_2 subgroup chain (contd)

(Also permutation group Young Tableau chain $S_4 \supset S_3 \supset S_2 \supset S_1$)



$\mathscr{D}^E(1) = \begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix}$ $\quad i_4 = [12]$ $\begin{vmatrix} 1 & 0 \\ 0 & -1 \end{vmatrix}$ $\quad R_1^2 = [13][24]$ $\begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix}$ $\quad R_3 = [1423]$ $\begin{vmatrix} 1 & 0 \\ 0 & -1 \end{vmatrix}$

C_2

$r_1 = [132]$ $\begin{vmatrix} \frac{-1}{2} & \frac{-\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{vmatrix}$ $\quad i_5 = [13]$ $\begin{vmatrix} \frac{-1}{2} & \frac{-\sqrt{3}}{2} \\ \frac{-\sqrt{3}}{2} & \frac{1}{2} \end{vmatrix}$ $\quad r_4 = [234]$ $\begin{vmatrix} \frac{-1}{2} & \frac{-\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{vmatrix}$ $\quad i_6 = [24]$ $\begin{vmatrix} \frac{-1}{2} & \frac{-\sqrt{3}}{2} \\ \frac{-\sqrt{3}}{2} & \frac{1}{2} \end{vmatrix}$

$r_1^2 = [123]$ $\begin{vmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ \frac{-\sqrt{3}}{2} & \frac{-1}{2} \end{vmatrix}$ $\quad i_2 = [23]$ $\begin{vmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{vmatrix}$ $\quad r_2^2 = [142]$ $\begin{vmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ \frac{-\sqrt{3}}{2} & \frac{-1}{2} \end{vmatrix}$ $\quad R_2^3 = [1342]$ $\begin{vmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{vmatrix}$

$R_2^2 = [14][23]$ $\begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix}$ $\quad R_3^3 = [1324]$ $\begin{vmatrix} 1 & 0 \\ 0 & -1 \end{vmatrix}$ $\quad R_3^2 = [12][34]$ $\begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix}$ $\quad i_3 = [34]$ $\begin{vmatrix} 1 & 0 \\ 0 & -1 \end{vmatrix}$

$r_2 = [124]$ $\begin{vmatrix} \frac{-1}{2} & \frac{-\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{-1}{2} \end{vmatrix}$ $\quad R_1 = [1234]$ $\begin{vmatrix} \frac{-1}{2} & \frac{-\sqrt{3}}{2} \\ \frac{-\sqrt{3}}{2} & \frac{1}{2} \end{vmatrix}$ $\quad r_3 = [143]$ $\begin{vmatrix} \frac{-1}{2} & \frac{-\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{-1}{2} \end{vmatrix}$ $\quad R_1^3 = [1432]$ $\begin{vmatrix} \frac{-1}{2} & \frac{-\sqrt{3}}{2} \\ \frac{-\sqrt{3}}{2} & \frac{1}{2} \end{vmatrix}$

$r_3^2 = [134]$ $\begin{vmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ \frac{-\sqrt{3}}{2} & \frac{-1}{2} \end{vmatrix}$ $\quad i_1 = [14]$ $\begin{vmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{vmatrix}$ $\quad r_4^2 = [243]$ $\begin{vmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ \frac{-\sqrt{3}}{2} & \frac{-1}{2} \end{vmatrix}$ $\quad R_2 = [1243]$ $\begin{vmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{vmatrix}$

E *Tensor*

$u^2+v^2-2w^2$

$(u^2-v^2)\sqrt{3}$

$$\begin{array}{|c|c|}\hline 1 & 2 \\ \hline 3 & 4 \\ \hline\end{array} \quad \begin{array}{|c|c|}\hline 1 & 3 \\ \hline 2 & 4 \\ \hline\end{array}$$

$$\text{basis: } \begin{matrix} O \\ D_3 \\ C_2 \end{matrix} \left| \begin{matrix} E \\ E \\ 0_2 \end{matrix} \right\rangle \left| \begin{matrix} E \\ E \\ 1_2 \end{matrix} \right\rangle$$

O: $\chi_{\mathbf{g}}^{\mu}$	**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

AMOP reference links on page 2

3.12.18 class 17.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Discrete symmetry subgroups of O(3)⊃(Octahedral O_h⊃O): Part II Full $D^{(\alpha)}$-matrices defined by subgroup-chains $O\supset D_4\supset C_4$, D_2, or C_3 applied to eigensolutions of O_h-tensors $\mathbf{T}^{[4]}+\mathbf{T}^{[6]}$

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

Review Coset factored splitting of projectors for $O\supset D_4\supset C_4$ *into split classes and level structure*

Hamiltonian level cluster models with subgroup-defined tunneling parameters

- *Diagonal idempotent* $\mathbf{P}^{\mu}_{m,m}$ *parameter sets* $\boxed{\textit{for } O\supset C_4}$ *and* $\boxed{O\supset C_3}$ *case of* SF_6 *level clusters*
- *Off-diagonal nilpotent* $\mathbf{P}^{\mu}_{m,n}$ $(m\neq n)$ *parameter sets needed for* $\boxed{O\supset C_2}$ *clusters*

Deriving nilpotent projectors $\mathbf{P}^{\mu}_{m,n}$ *and ireps* $D^{\mu}_{m,n}$ *by fundamental* $\mathbf{g}\rightleftarrows\mathbf{P}^{\mu}_{m,n}$ *relations:*

(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 nilpotent projectors for simple* $D_3\supset C_2\sim C_{3v}\supset C_v$ *chains* (Lect13p95)
- *Calculating and Factoring* $\mathbf{P}^{T_1}_{1_4 0_4}$ *and* $\mathbf{P}^{T_1}_{1_4 3_4}$

Structure and applications of coset tabulated $D^{\mu}_{m,n}$ *irreps for various* O_h *subgroup chains*

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

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* $D^{E}_{0_4 2_4}$

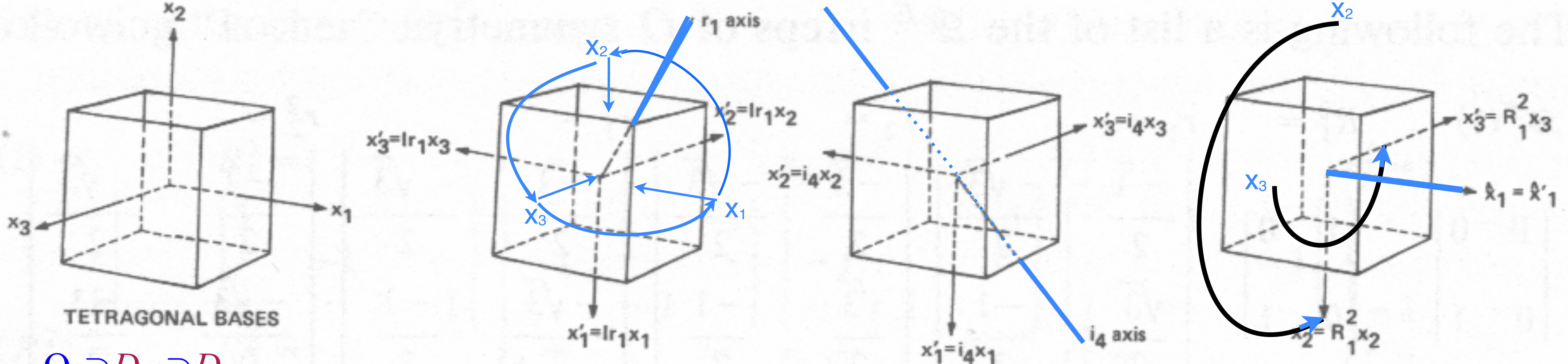
Comparing local C_4, C_3, *and* C_2 *cluster spectra of* O_h*-symmetric tensors* $\mathbf{T}^{[4]}+\mathbf{T}^{[6]}$

- *Monster clusters: When local* C_2 *symmetry dominates*

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

Are these "accidents" or not?

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*

$$D^{T_{1u}}(Ir_1) = \begin{pmatrix} 0 & 0 & -1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix}$$

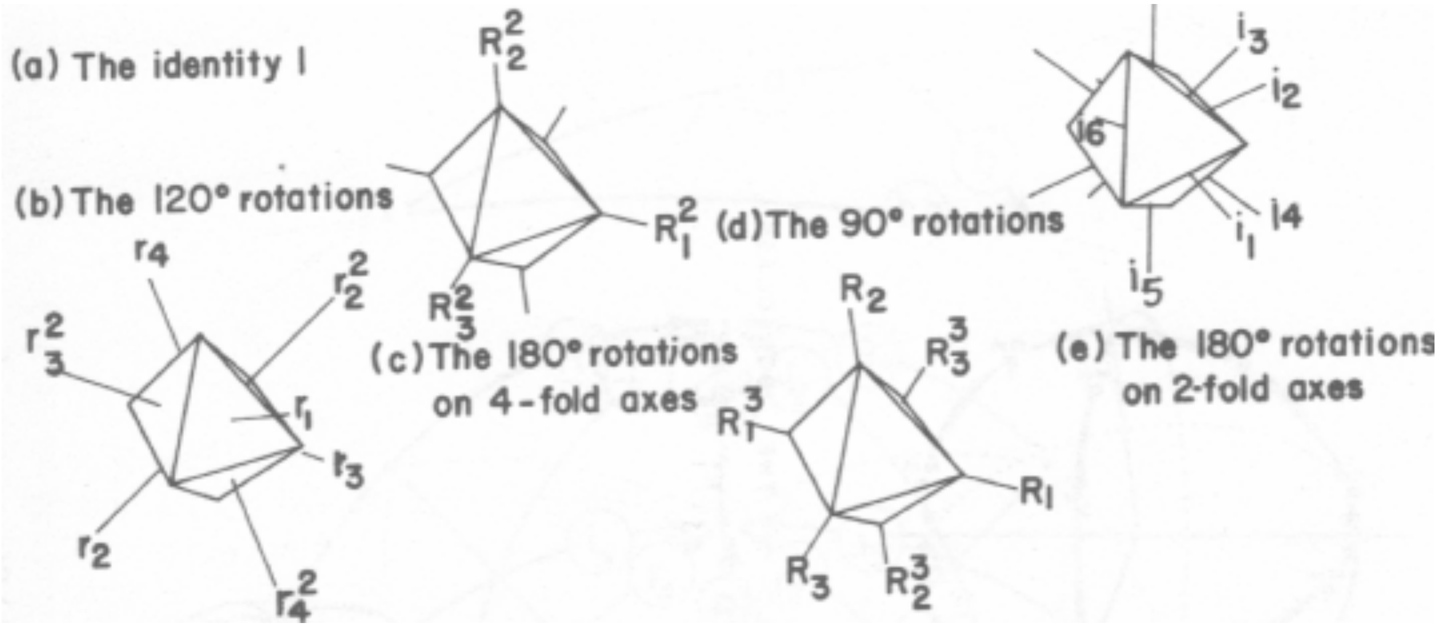
3-by-3 block

$$D^{T_{1u}}(i_4) = \begin{pmatrix} \begin{vmatrix} 0 & -1 \\ -1 & 0 \end{vmatrix} & \begin{matrix} 0 \\ 0 \end{matrix} \\ \begin{matrix} 0 & 0 \end{matrix} & -1 \end{pmatrix}$$

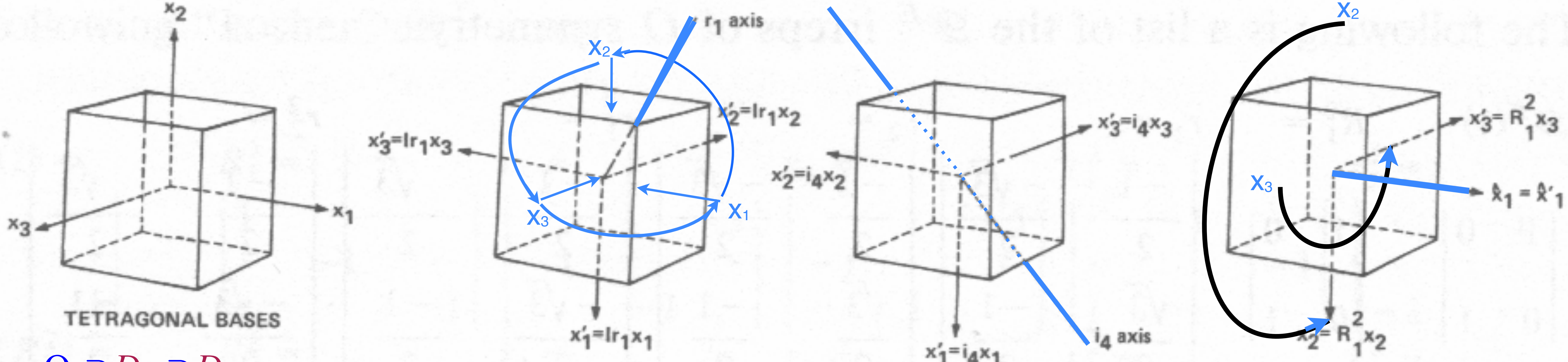
2-by-2 and 1-by-1 blocks

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

diagonal



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



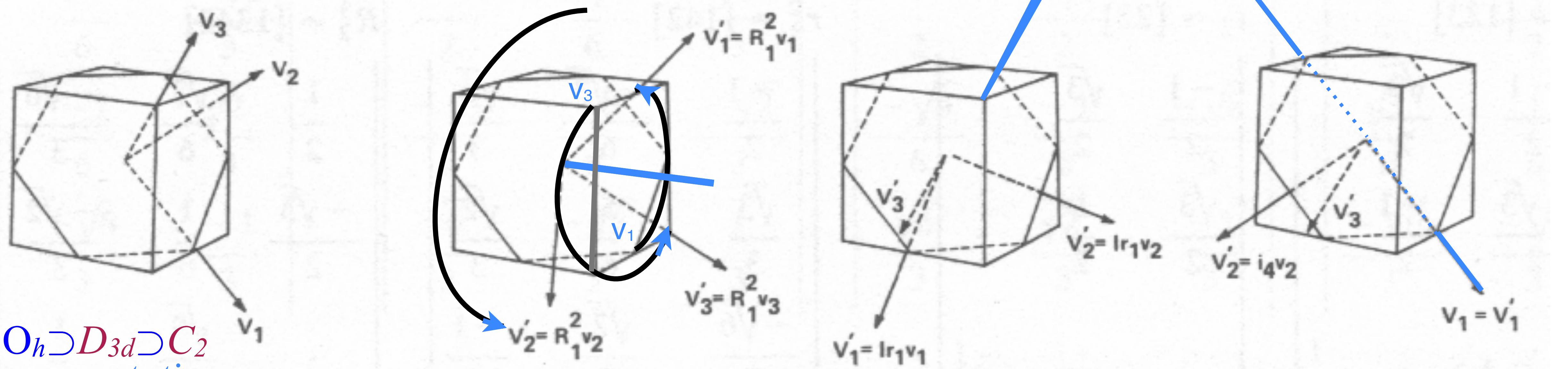
$O_h \supset D_{4h} \supset D_{2h}$
x-*representation*

$$D^{T_{1u}}(Ir_1) = \begin{pmatrix} 0 & 0 & -1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix} \qquad D^{T_{1u}}(i_4) = \begin{pmatrix} \begin{vmatrix} 0 & -1 \\ -1 & 0 \end{vmatrix} & \begin{matrix} 0 \\ 0 \end{matrix} \\ \begin{matrix} 0 & 0 \end{matrix} & -1 \end{pmatrix} \qquad D^{T_{1u}}(R_1^2) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

3-by-3 block *2-by-2 and 1-by-1 blocks* *diagonal*

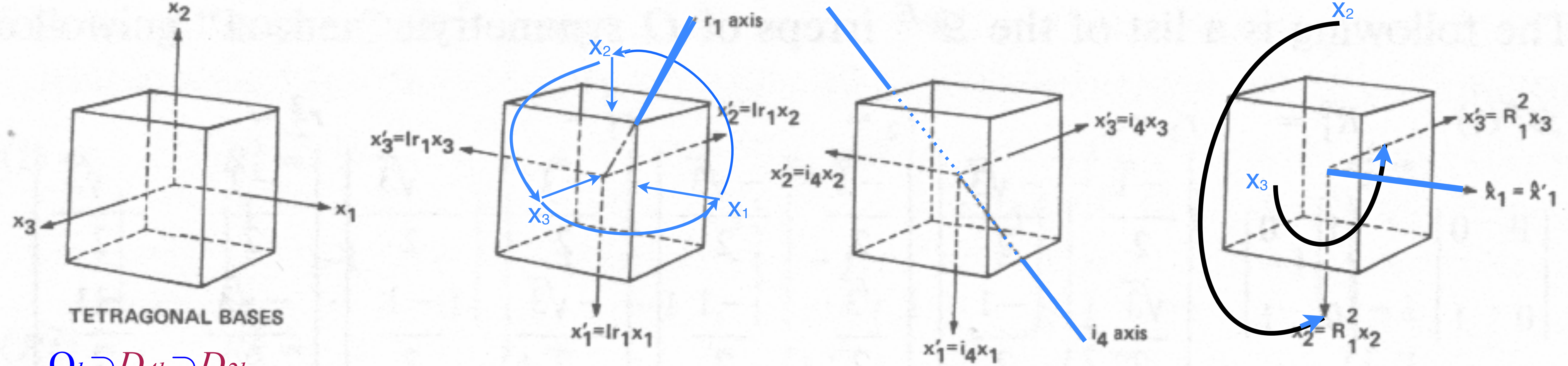
TRIGONAL BASES

$$D^{T_{1u}}(R_1^2) = \begin{pmatrix} 0 & \sqrt{3}/3 & \sqrt{6}/3 \\ \sqrt{3}/3 & -2/3 & \sqrt{2}/3 \\ \sqrt{6}/3 & \sqrt{2}/3 & -1/3 \end{pmatrix} \qquad D^{T_{1u}}(Ir_1) = \begin{pmatrix} \begin{pmatrix} 1/2 & \sqrt{3}/2 \\ -\sqrt{3}/2 & 1/2 \end{pmatrix} & \begin{matrix} 0 \\ 0 \end{matrix} \\ \begin{matrix} 0 & 0 \end{matrix} & -1 \end{pmatrix} \qquad D^{T_{1u}}(i_4) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$



$O_h \supset D_{3d} \supset C_2$
v-*representation*

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

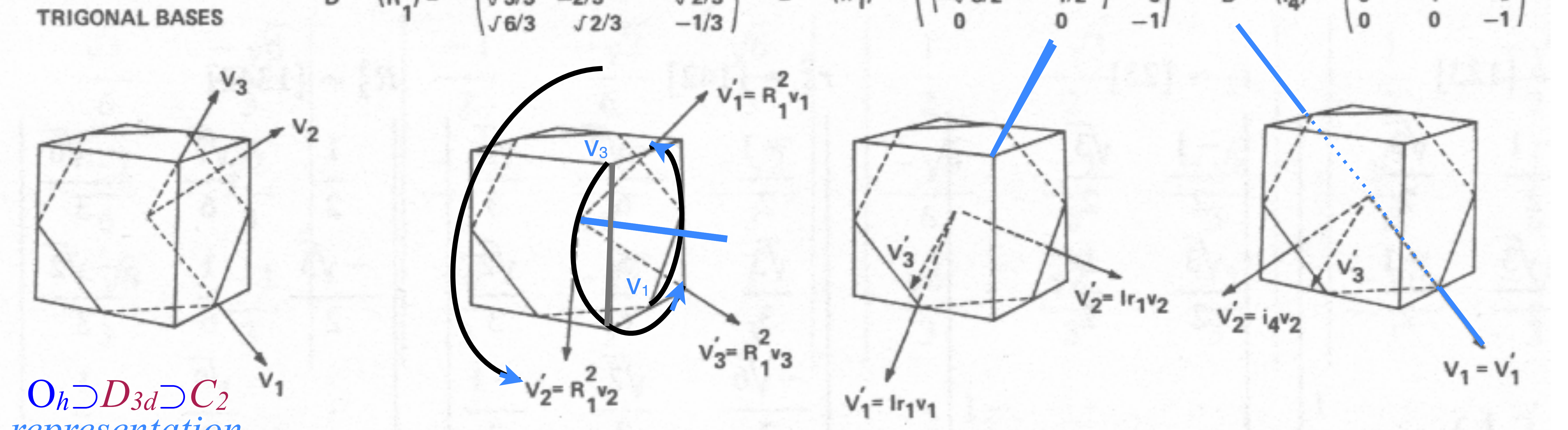
$$D^{T_{1u}}(R_1^2) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

diagonal

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

$$D^{T_{1u}}(Ir_1) = \begin{pmatrix} \begin{bmatrix} 1/2 & \sqrt{3}/2 \\ -\sqrt{3}/2 & 1/2 \end{bmatrix} & \begin{matrix} 0 \\ 0 \end{matrix} \\ \begin{matrix} 0 & 0 \end{matrix} & -1 \end{pmatrix}$$

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



$O_h \supset D_{3d} \supset C_2$

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*

AMOP reference links on page 2

3.12.18 class 17.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Discrete symmetry subgroups of O(3)⊃(Octahedral O_h⊃O): Part II Full $D^{(\alpha)}$-matrices defined by subgroup-chains $O \supset D_4 \supset C_4$, D_2, or C_3 applied to eigensolutions of O_h-tensors $\mathbf{T}^{[4]}+\mathbf{T}^{[6]}$

Review Idempotent projector splits $\mathbf{P}^{\mu}_{m,m}$ *of* $O \supset C_4$ $\mathbf{P}^{E}_{0404}$ $\mathbf{P}^{E}_{2424}$ $\mathbf{P}^{T_1}_{0404}$ $\mathbf{P}^{T_1}_{1414}$ $\mathbf{P}^{T_2}_{2424}$ $\mathbf{P}^{T_2}_{1414}$

Review Coset factored splitting of projectors for $O \supset D_4 \supset C_4$ *into split classes and level structure*

Hamiltonian level cluster models with subgroup-defined tunneling parameters

Diagonal idempotent $\mathbf{P}^{\mu}_{m,m}$ *parameter sets for* $O \supset C_4$ *and* $O \supset C_3$ *case of* SF_6 *level clusters*

Off-diagonal nilpotent $\mathbf{P}^{\mu}_{m,n}$ $(m \neq n)$ *parameter sets needed for* $O \supset C_2$ *clusters*

Deriving nilpotent projectors $\mathbf{P}^{\mu}_{m,n}$ *and ireps* $D^{\mu}_{m,n}$ *by fundamental* $\mathbf{g} \rightleftarrows \mathbf{P}^{\mu}_{m,n}$ *relations:*

(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 nilpotent projectors for simple $D_3 \supset C_2 \sim C_{3v} \supset C_v$ *chains* *(Lect13p95)*

Calculating and Factoring $\mathbf{P}^{T_1}_{1404}$ *and* $\mathbf{P}^{T_1}_{1434}$

Structure and applications of coset tabulated $D^{\mu}_{m,n}$ *irreps for various* O_h *subgroup chains*

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

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}_{0424}

Comparing local C_4, C_3, *and* C_2 *cluster spectra of* O_h*-symmetric tensors* $\mathbf{T}^{[4]}+\mathbf{T}^{[6]}$

Monster clusters: When local C_2 *symmetry dominates*

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

Are these "accidents" or not?

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

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

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

$$\text{basis: } \begin{array}{c|c|c} O & E & E \\ D_4 & A_1 & B_1 \\ C_4 & 0_4 & 2_4 \end{array}\rangle\,\rangle$$

$1 = [1][2][3][4]$ $\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

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

$r_1 = [132]$ $\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ +\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$

$r_2 = [124]$ $\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ +\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$

$r_1^2 = [123]$ $\begin{pmatrix} -\frac{1}{2} & +\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$

$r_2^2 = [142]$ $\begin{pmatrix} -\frac{1}{2} & +\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$

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

$R_2^2 = [14][23]$ $\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

$r_4 = [234]$ $\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ +\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$

$r_3 = [124]$ $\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ +\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$

$r_3^2 = [134]$ $\begin{pmatrix} -\frac{1}{2} & +\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$

$r_4^2 = [243]$ $\begin{pmatrix} -\frac{1}{2} & +\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$

$R_3 = [1423]$ $\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

$i_4 = [12]$ $\begin{pmatrix} 1 & \boxed{0} \\ 0 & -1 \end{pmatrix}$

$i_1 = [14]$ $\begin{pmatrix} -\frac{1}{2} & \boxed{+\frac{\sqrt{3}}{2}} \\ +\frac{\sqrt{3}}{2} & +\frac{1}{2} \end{pmatrix}$

$i_2 = [23]$ $\begin{pmatrix} -\frac{1}{2} & \boxed{+\frac{\sqrt{3}}{2}} \\ +\frac{\sqrt{3}}{2} & +\frac{1}{2} \end{pmatrix}$

$R_1^3 = [1432]$ $\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & +\frac{1}{2} \end{pmatrix}$

$R_1 = [1234]$ $\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & +\frac{1}{2} \end{pmatrix}$

$R_3^3 = [1324]$ $\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

$i_3 = [34]$ $\begin{pmatrix} 1 & \boxed{0} \\ 0 & -1 \end{pmatrix}$

$R_2 = [1243]$ $\begin{pmatrix} -\frac{1}{2} & +\frac{\sqrt{3}}{2} \\ +\frac{\sqrt{3}}{2} & +\frac{1}{2} \end{pmatrix}$

$R_2^3 = [1342]$ $\begin{pmatrix} -\frac{1}{2} & +\frac{\sqrt{3}}{2} \\ +\frac{\sqrt{3}}{2} & +\frac{1}{2} \end{pmatrix}$

$i_6 = [24]$ $\begin{pmatrix} -\frac{1}{2} & \boxed{-\frac{\sqrt{3}}{2}} \\ -\frac{\sqrt{3}}{2} & +\frac{1}{2} \end{pmatrix}$

$i_5 = [13]$ $\begin{pmatrix} -\frac{1}{2} & \boxed{-\frac{\sqrt{3}}{2}} \\ -\frac{\sqrt{3}}{2} & +\frac{1}{2} \end{pmatrix}$

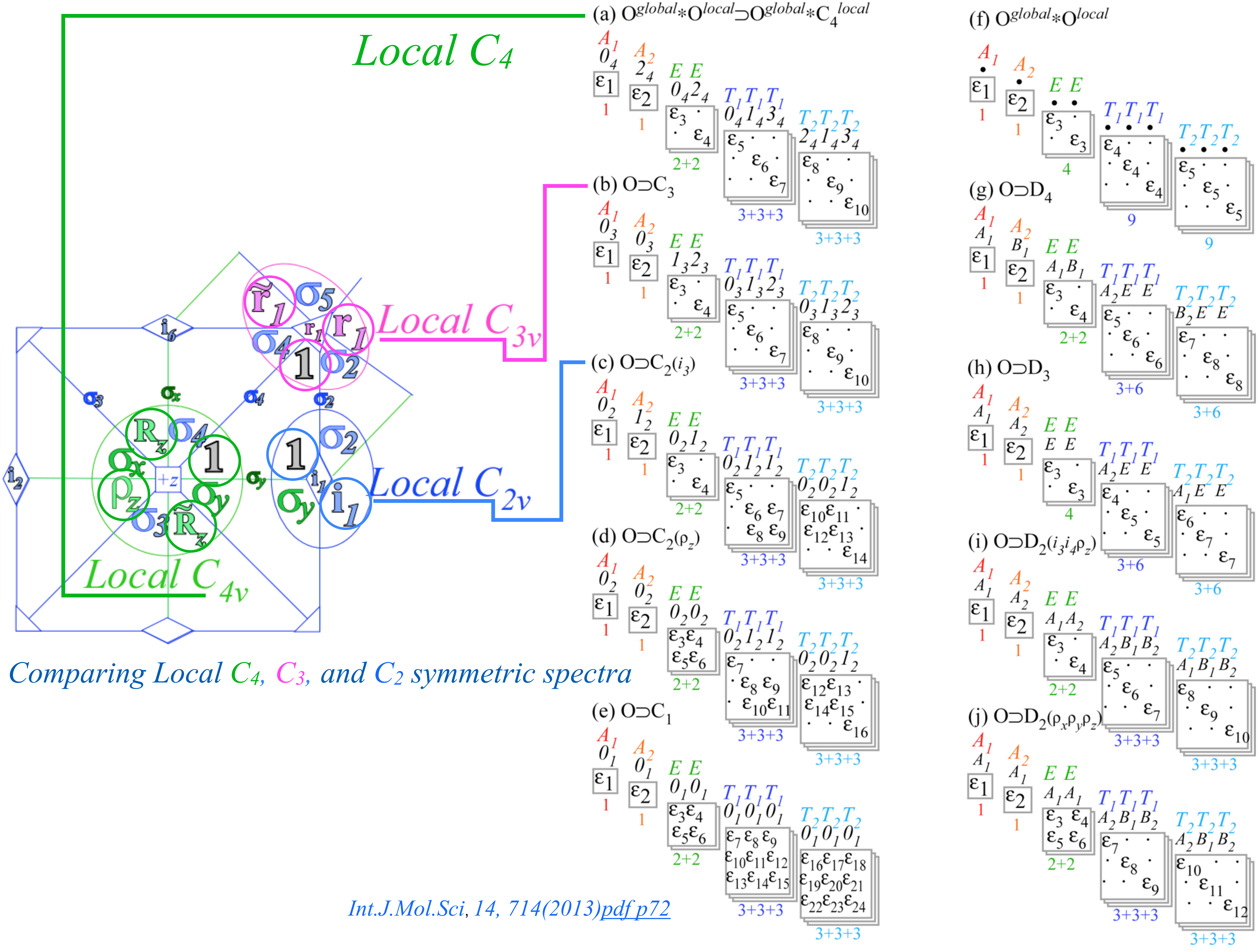
$D^{E*}(i_k \mathbf{i}_k)$	0_4	2_4
0_4	$-\frac{1}{2}(i_1+i_2+i_5+i_6)+i_3+i_4$	$\frac{\sqrt{3}}{2}(i_1+i_2-i_5-i_6)$
2_4	*h.c.*	$\frac{1}{2}(i_1+i_2+i_3+i_4+i_5+i_6)-i_3-i_4$

$D^{T_1*}(i_k \mathbf{i}_k)$	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.

Int.J.Mol.Sci, 14, 714(2013)pdf p68



Comparing Local C_4, C_3, and C_2 symmetric spectra

Int.J.Mol.Sci, 14, 714(2013)pdf p72

AMOP
reference links
on page 2

3.12.18 class 17.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Discrete symmetry subgroups of O(3)⊃(Octahedral O_h⊃O): Part II Full $D^{(\alpha)}$-matrices defined by subgroup-chains $O \supset D_4 \supset C_4$, D_2, or C_3 applied to eigensolutions of O_h-tensors $\mathbf{T}^{[4]}+\mathbf{T}^{[6]}$

Review Idempotent projector splits $\mathbf{P}^{\mu}_{m,m}$ *of* $O \supset C_4$ $\mathbf{P}^{E}_{0404}$ $\mathbf{P}^{E}_{2424}$ $\mathbf{P}^{T_1}_{0404}$ $\mathbf{P}^{T_1}_{1414}$ $\mathbf{P}^{T_2}_{2424}$ $\mathbf{P}^{T_2}_{1414}$

Review Coset factored splitting of projectors for $O \supset D_4 \supset C_4$ *into split classes and level structure*

Hamiltonian level cluster models with subgroup-defined tunneling parameters

Diagonal idempotent $\mathbf{P}^{\mu}_{m,m}$ *parameter sets for* $O \supset C_4$ *and* $O \supset C_3$ *case of* SF_6 *level clusters*

Off-diagonal nilpotent $\mathbf{P}^{\mu}_{m,n}$ $(m \neq n)$ *parameter sets needed for* $O \supset C_2$ *clusters*

Deriving nilpotent projectors $\mathbf{P}^{\mu}_{m,n}$ *and ireps* $D^{\mu}_{m,n}$ *by fundamental* $\mathbf{g} \rightleftarrows \mathbf{P}^{\mu}_{m,n}$ *relations:*

(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 nilpotent projectors for simple $D_3 \supset C_2 \sim C_{3v} \supset C_v$ *chains* (Lect13p95)

Calculating and Factoring $\mathbf{P}^{T_1}_{1404}$ *and* $\mathbf{P}^{T_1}_{1434}$

Structure and applications of coset tabulated $D^{\mu}_{m,n}$ *irreps for various* O_h *subgroup chains*

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

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}_{0424}

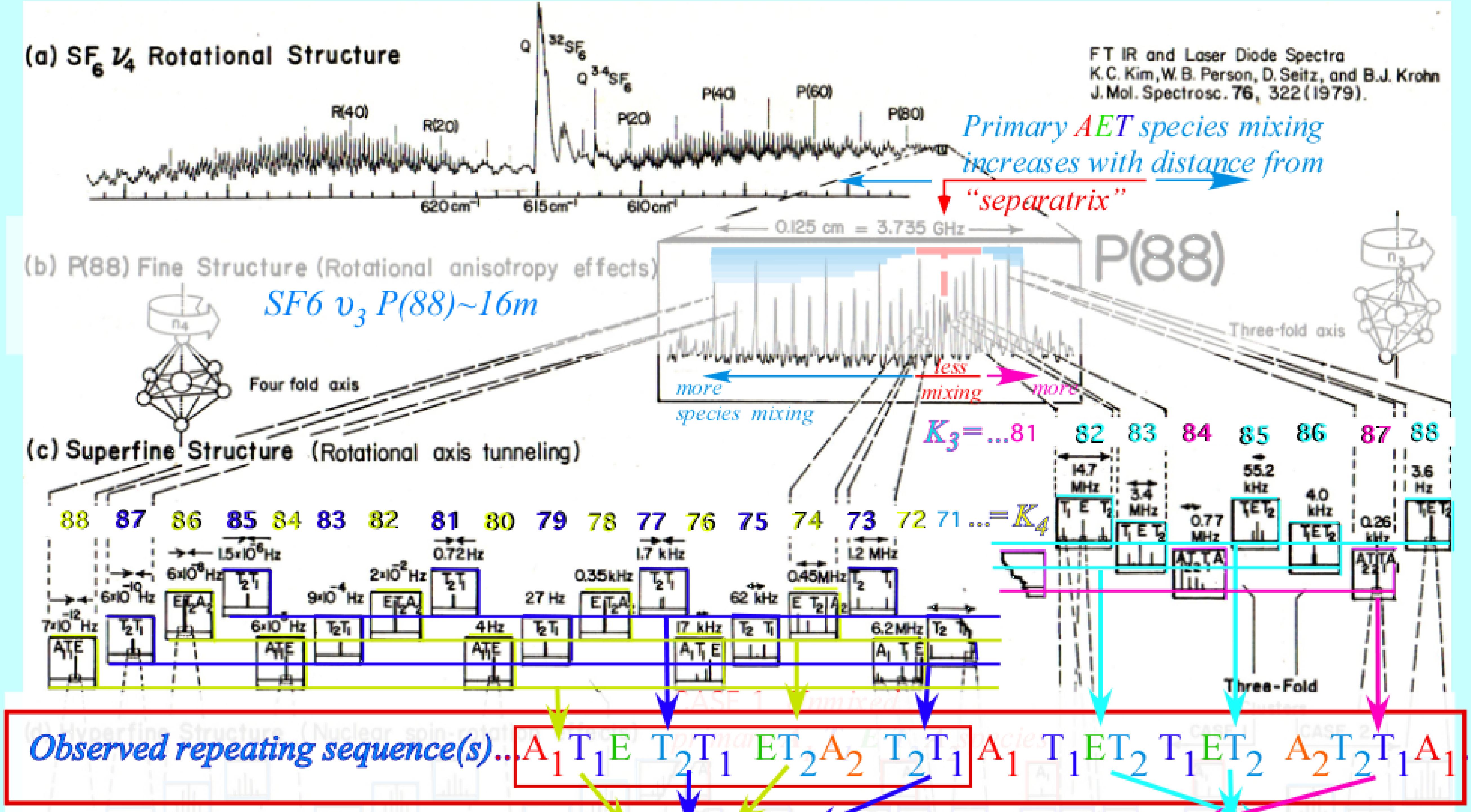
Comparing local C_4, C_3, *and* C_2 *cluster spectra of* O_h*-symmetric tensors* $\mathbf{T}^{[4]}+\mathbf{T}^{[6]}$

Monster clusters: When local C_2 *symmetry dominates*

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

Are these "accidents" or not?

Comparing Local C_4, C_3, and C_2 symmetric spectra



Primary AET species mixing increases with distance from "separatrix"

SF6 υ_3 P(88)~16m

Observed repeating sequence(s)...$A_1T_1E\ \ T_2T_1\ \ ET_2A_2\ \ T_2T_1\ \ A_1\ \ T_1ET_2\ \ T_1ET_2\ \ A_2T_2T_1A_1$...

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

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

...and physical consequences?

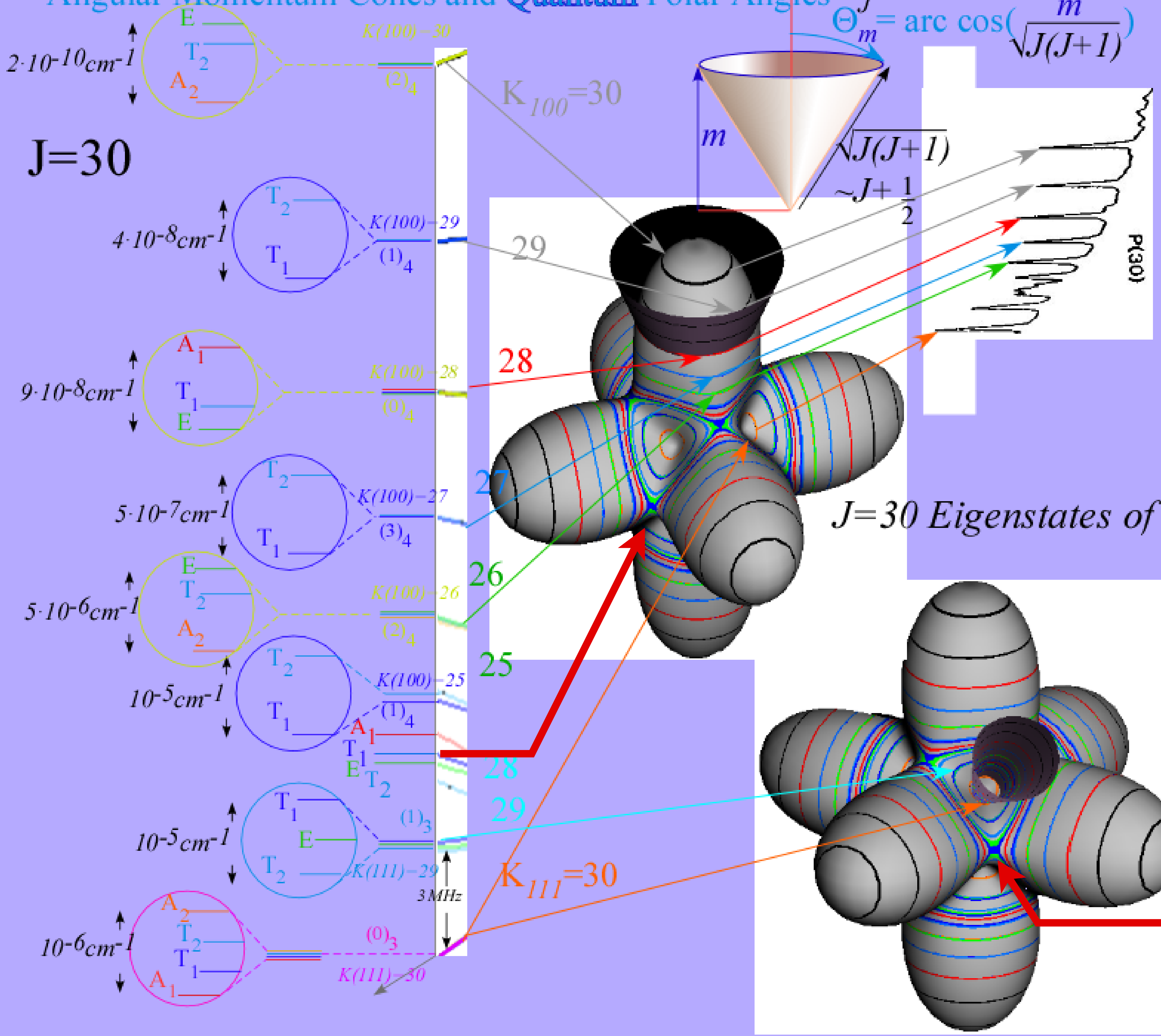
NO C_2 symmetry clusters between C_4 and C_3 bands

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

$$\Theta^J_m = \arccos\left(\frac{m}{\sqrt{J(J+1)}}\right)$$



Cubane C_8H_8 ν_{11} P(30)

A.S. Pines, A.G. Maki,
A. G. Robiette, B. J. Krohn,
J.K.G. Watson, & T. Urbanek,
J.Am.Chem.Soc. 106, 891 (1984)

J=30 Eigenstates of $\mathbf{H}=B\mathbf{J}^2+T^{[4]}$

NO C_2 symmetry clusters between C_4 and C_3 bands because C_2 axes are on SADDLE POINTS

(12 of them)

AMOP reference links on page 2

3.12.18 class 17.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Discrete symmetry subgroups of O(3)⊃(Octahedral O_h⊃O): Part II Full $D^{(\alpha)}$-matrices defined by subgroup-chains $O\supset D_4\supset C_4$, D_2, or C_3 applied to eigensolutions of O_h-tensors $\mathbf{T}^{[4]}+\mathbf{T}^{[6]}$

Review Idempotent projector splits $\mathbf{P}^{\mu}_{m,m}$ *of* $O\supset C_4$ $\mathbf{P}^{E}_{0404}$ $\mathbf{P}^{E}_{2424}$ $\mathbf{P}^{T_1}_{0404}$ $\mathbf{P}^{T_1}_{1414}$ $\mathbf{P}^{T_2}_{2424}$ $\mathbf{P}^{T_2}_{1414}$

Review Coset factored splitting of projectors for $O\supset D_4\supset C_4$ *into split classes and level structure*

Hamiltonian level cluster models with subgroup-defined tunneling parameters

Diagonal idempotent $\mathbf{P}^{\mu}_{m,m}$ *parameter sets for* $O\supset C_4$ *and* $O\supset C_3$ *case of* SF_6 *level clusters*

Off-diagonal nilpotent $\mathbf{P}^{\mu}_{m,n}$ $(m\neq n)$ *parameter sets needed for* $O\supset C_2$ *clusters*

Deriving nilpotent projectors $\mathbf{P}^{\mu}_{m,n}$ *and ireps* $D^{\mu}_{m,n}$ *by fundamental* $\mathbf{g}\rightleftarrows\mathbf{P}^{\mu}_{m,n}$ *relations:*

(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 nilpotent projectors for simple $D_3\supset C_2\sim C_{3v}\supset C_v$ *chains* (Lect13p95)

Calculating and Factoring $\mathbf{P}^{T_1}_{1404}$ *and* $\mathbf{P}^{T_1}_{1434}$

Structure and applications of coset tabulated $D^{\mu}_{m,n}$ *irreps for various* O_h *subgroup chains*

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

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}_{0424}

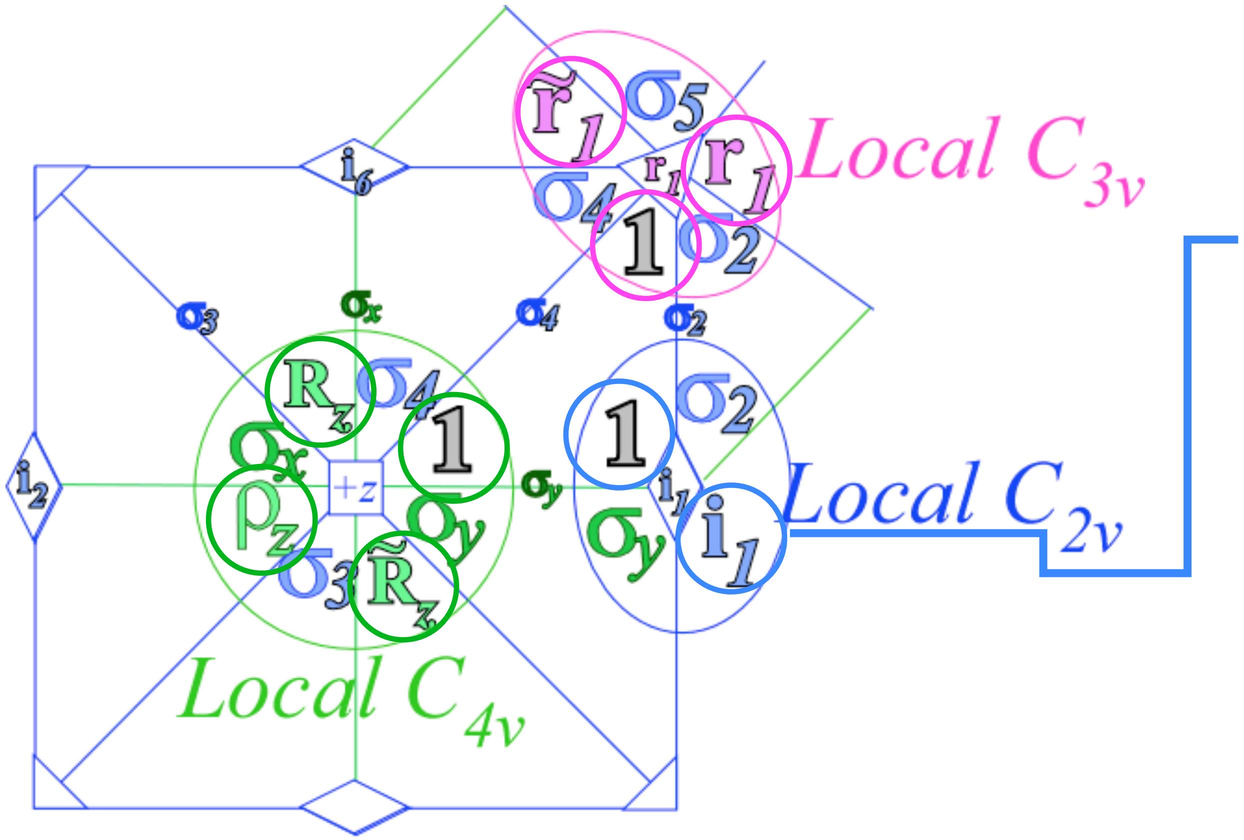
Comparing local C_4, C_3, *and* C_2 *cluster spectra of* O_h*-symmetric tensors* $\mathbf{T}^{[4]}+\mathbf{T}^{[6]}$

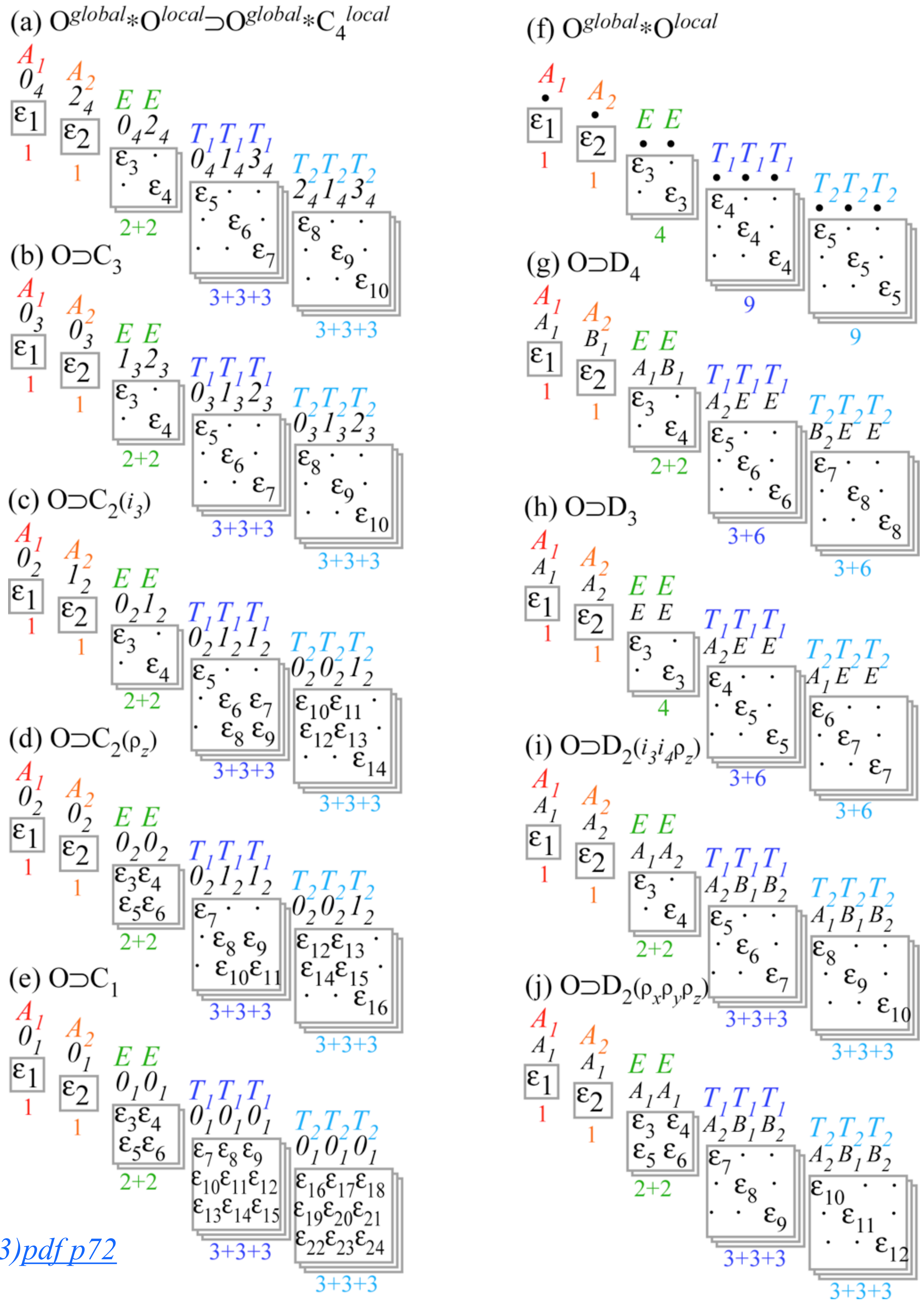
➡ *Monster clusters: When local* C_2 *symmetry dominates*

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

Are these "accidents" or not?

When Local C_2 symmetry dominates
Due to 4th and 6th rank $T^{[4]}+T^{[6]}$ *combo*





Int.J.Mol.Sci, *14, 714(2013)*[*pdf p72*]

When Local C_2 symmetry dominates
Due to 4^{th} and 6^{th} rank $T^{[4]}+T^{[6]}$ *combo*

$$T^{[6]} = (1/\sqrt{8})\left[T_0^6 - (\sqrt{7}/\sqrt{2})(T_4^6 + T_{-4}^6)\right]$$

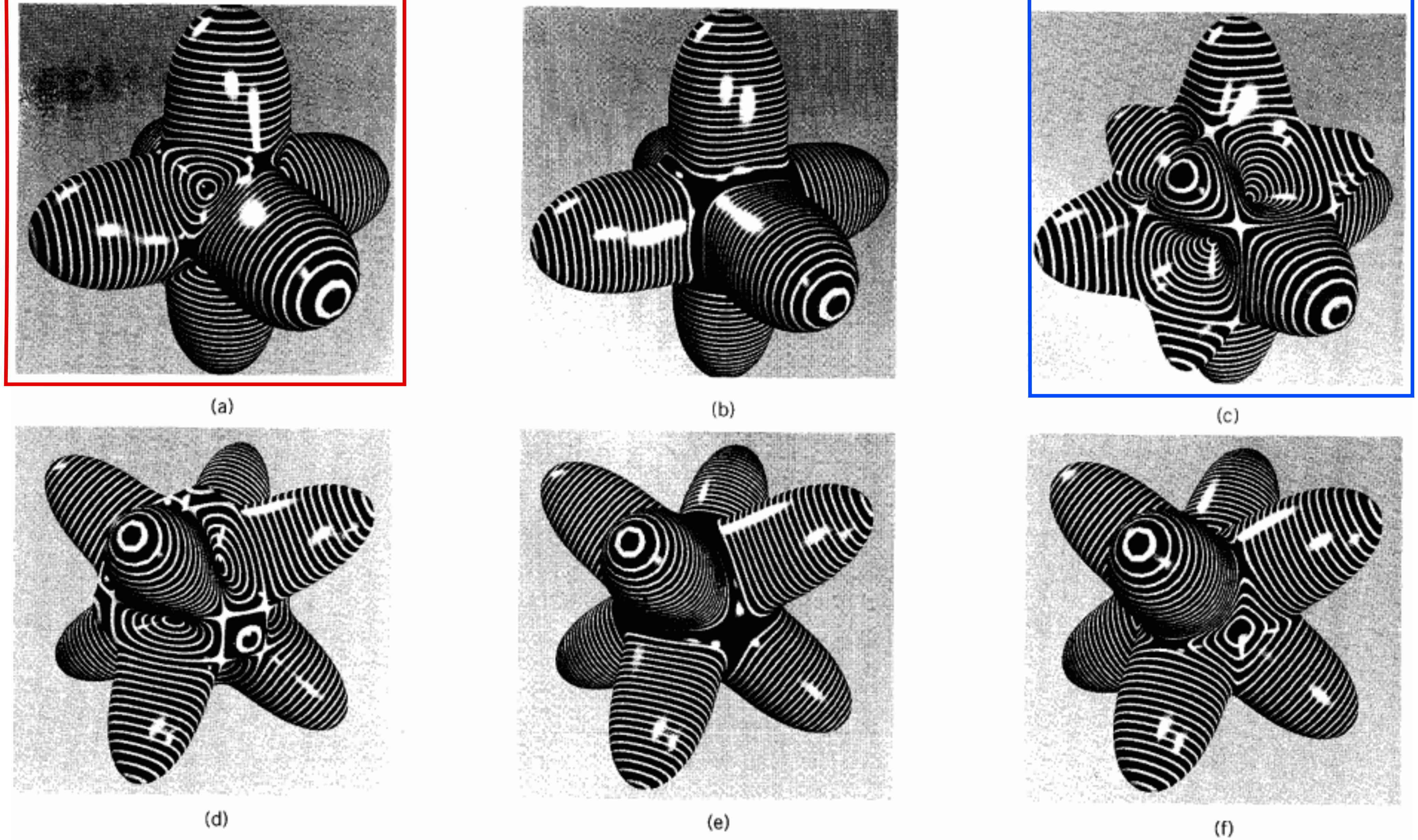
$$E^{[6]}(\beta,\gamma) = (1/8)^{1/2}(13/4\pi)^{1/2}(231\cos^6\beta - 315\cos^4\beta + 105\cos^2\beta - 5$$
$$-21\sin^4\beta(11\cos^2\beta - 1)\cos 4\gamma)/16.$$

$$H = B\mathbf{J}^2 + 10t_{044}\left(J_x^4 + J_y^4 + J_z^4 - \tfrac{3}{5}\mathbf{J}\right)^4$$

$$H = BT_0^0 + 4t_{044}\left[T_0^4 + \sqrt{\frac{5}{14}}\,(T_4^4 + T_{-4}^4)\right]$$

$$E = B\langle J^2\rangle + t_{044}\langle J^4\rangle(35\cos^4\beta - 30\cos^2\beta + 3 + 5\sin^4\beta\cos 4\gamma)/2$$

$$T^{4,6}(\nu) = T^{[4]}\cos\nu + T^{[6]}\sin\nu$$



(a) (b) (c)

(d) (e) (f)

Figure 7.4.11 *RE* surfaces corresponding to selected ν values in Fig. 7.4.10. (a) $\nu = 0.0$, (b) $\nu = 0.4\ (\pi/6)$, (c) $\nu = 2.0\ (\pi/6)$, (d) $\nu = 4.0\ (\pi/6)$, (e) $\nu = 4.6\ (\pi/6)$, (f) $\nu = 5.0\ (\pi/6)$.

PSDS Ch.7p.76.

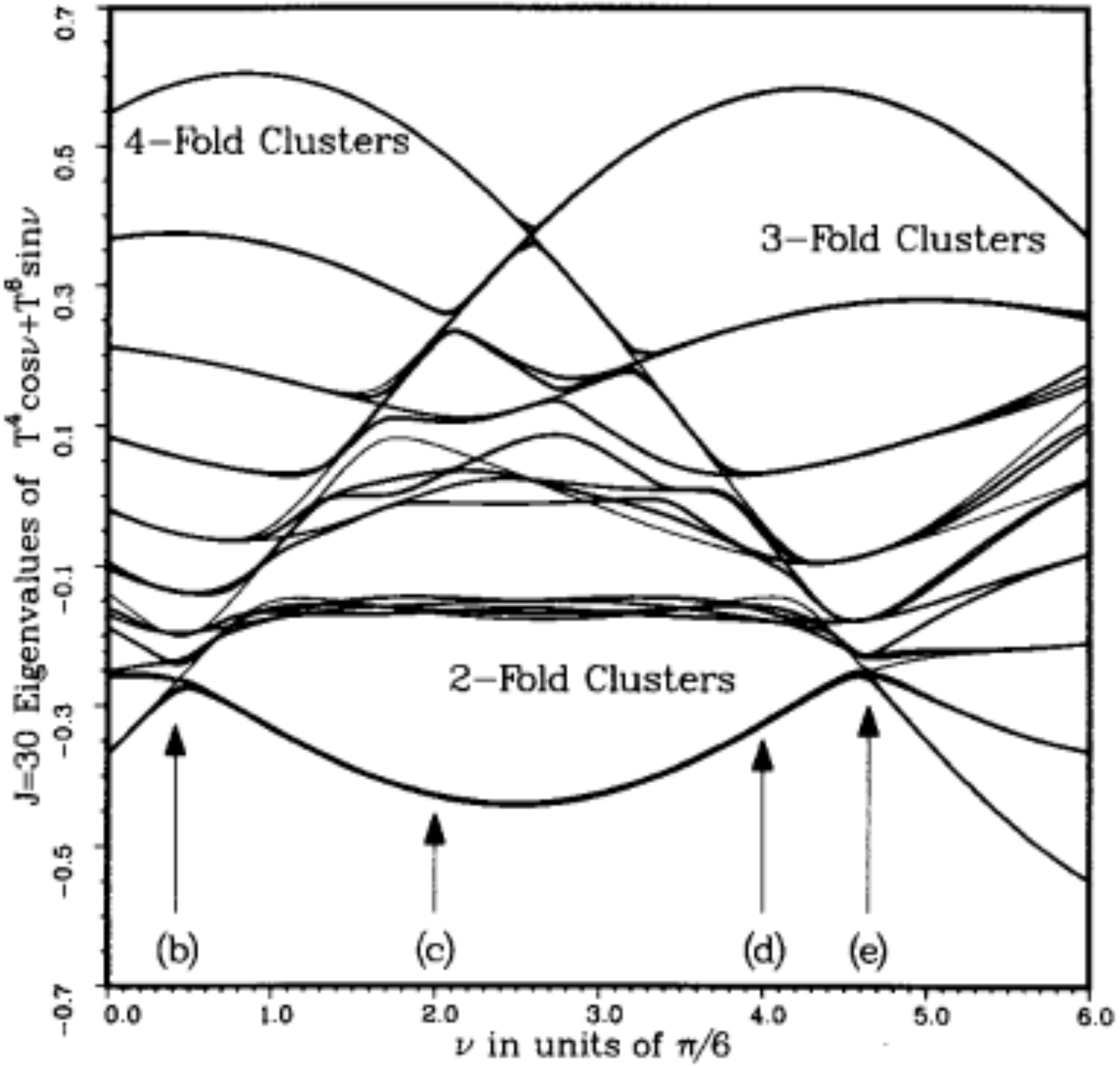
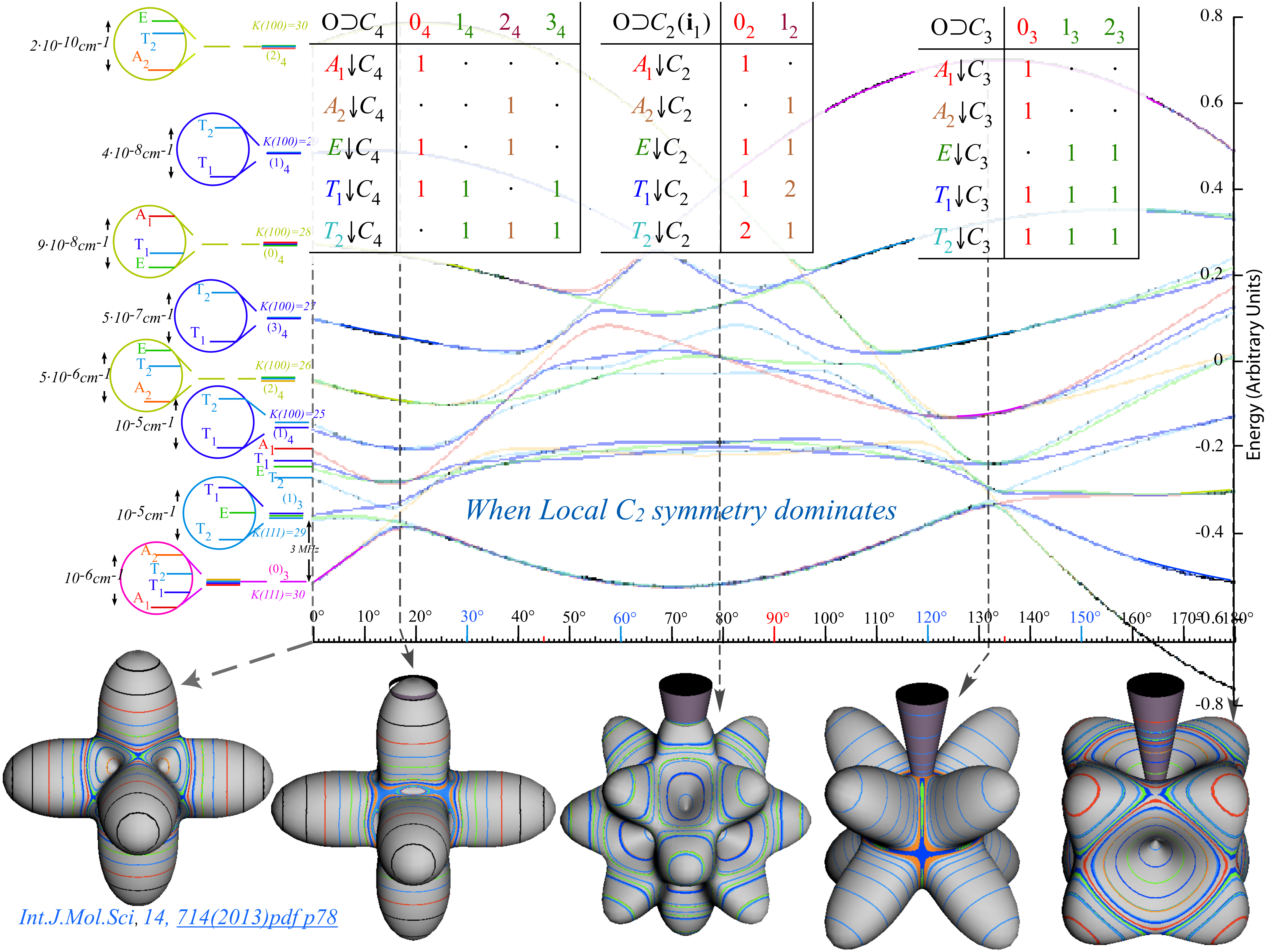


Figure 7.4.10 $J = 30$ eigenvalues of varying mixtures of fourth- and sixth-rank tensors. ($\nu = 0$) corresponds to levels in Figure 7.4.6.

PSDS Ch.7p.74.



$O \supset C_4$	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

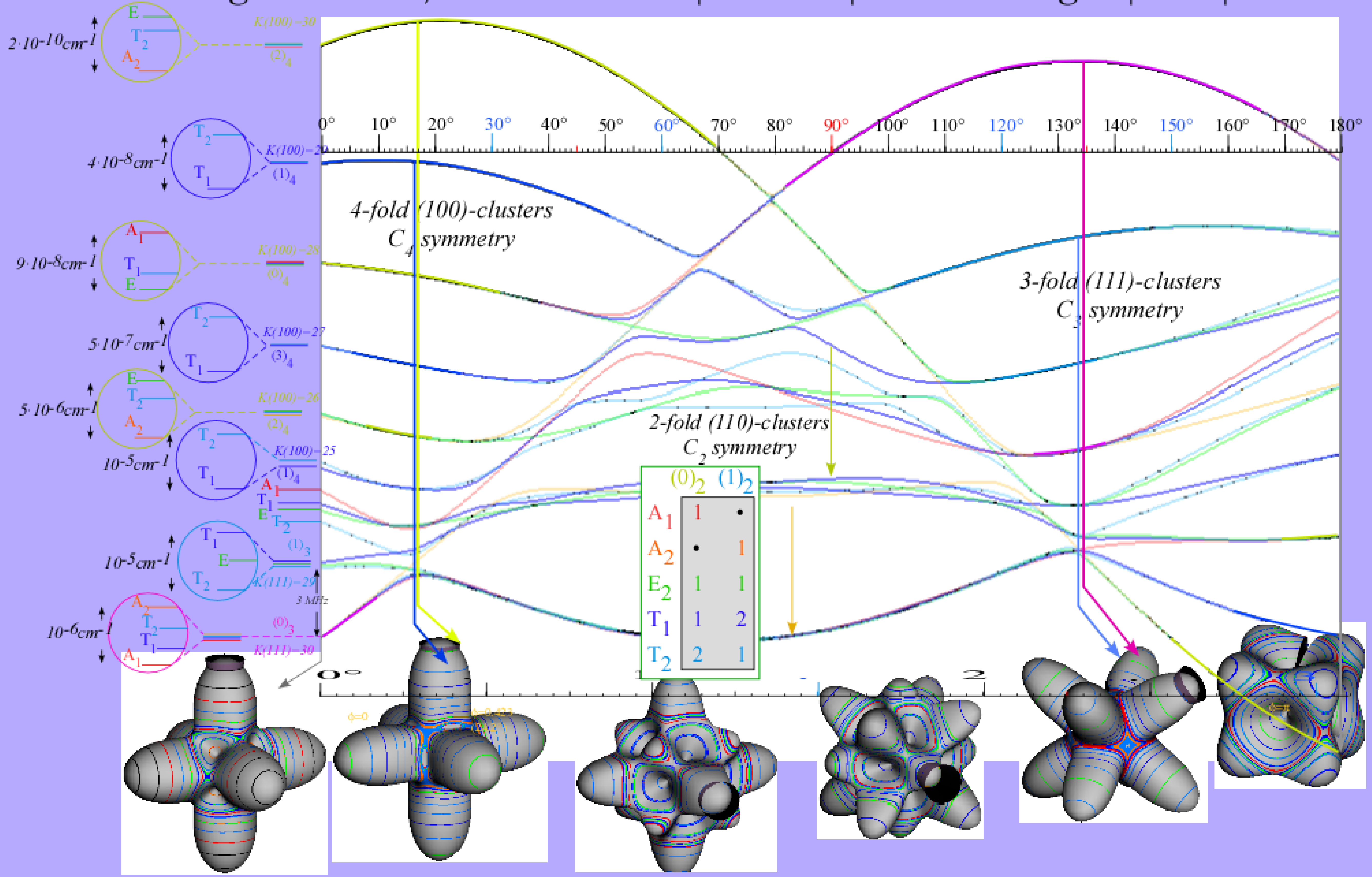
$O \supset C_3$	0_3	1_3	2_3
$A_1 \downarrow C_3$	1	·	·
$A_2 \downarrow C_3$	1	·	·
$E \downarrow C_3$	·	1	1
$T_1 \downarrow C_3$	1	1	1
$T_2 \downarrow C_3$	1	1	1

When Local C_2 symmetry dominates

Int.J.Mol.Sci, 14, 714(2013)pdf p78

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)pdf p78*

AMOP reference links on page 2

3.12.18 class 17.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Discrete symmetry subgroups of O(3)⊃(Octahedral $O_h \supset O$): Part II Full $D^{(\alpha)}$-matrices defined by subgroup-chains $O\supset D_4 \supset C_4$, D_2, or C_3 applied to eigensolutions of O_h-tensors $\mathbf{T}^{[4]}+\mathbf{T}^{[6]}$

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

Review Coset factored splitting of projectors for $O\supset D_4 \supset C_4$ *into split classes and level structure*

Hamiltonian level cluster models with subgroup-defined tunneling parameters

Diagonal idempotent $\mathbf{P}^{\mu}_{m,m}$ *parameter sets for* $O\supset C_4$ *and* $O\supset C_3$ *case of* SF_6 *level clusters*

Off-diagonal nilpotent $\mathbf{P}^{\mu}_{m,n}$ $(m\neq n)$ *parameter sets needed for* $O\supset C_2$ *clusters*

Deriving nilpotent projectors $\mathbf{P}^{\mu}_{m,n}$ *and ireps* $D^{\mu}_{m,n}$ *by fundamental* $\mathbf{g}\rightleftarrows\mathbf{P}^{\mu}_{m,n}$ *relations:*

(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 nilpotent projectors for simple $D_3\supset C_2 \sim C_{3v}\supset C_v$ *chains* *(Lect13p95)*

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

Structure and applications of coset tabulated $D^{\mu}_{m,n}$ *irreps for various* O_h *subgroup chains*

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

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 *cluster spectra of* O_h*-symmetric tensors* $\mathbf{T}^{[4]}+\mathbf{T}^{[6]}$

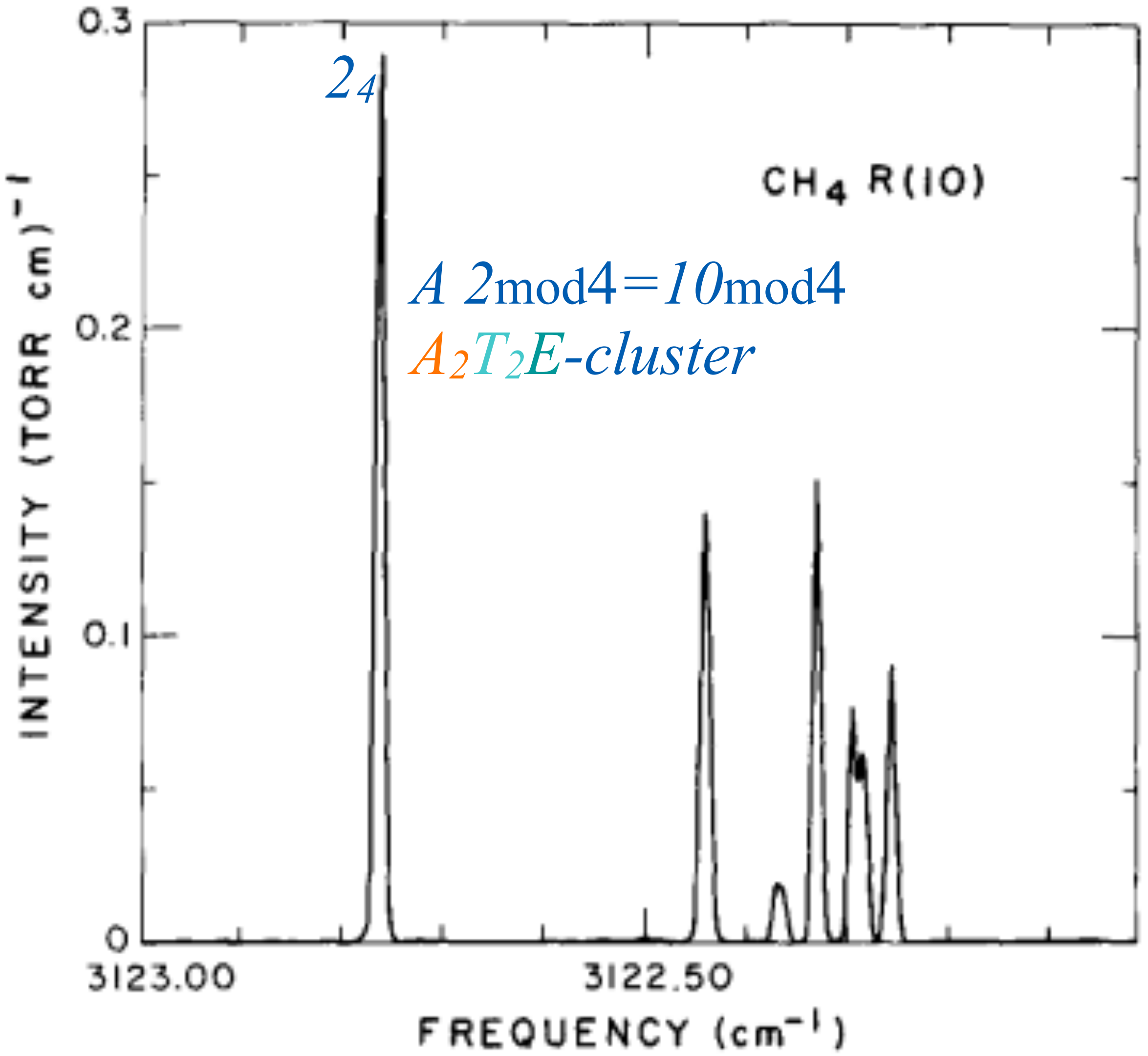
Monster clusters: When local C_2 *symmetry dominates*

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

Are these "accidents" or not?

Examples of triple-level crossing points in low-J low-inertia molecule (CH_4 J=10)

Are these "accidents" or not?



2_4

*A 2*mod4=*10*mod4

A_2T_2E-cluster

FIG. 7. *R* (10) Laser spectra of CH_4 (courtesy of Allen S. Pine, MIT Lincoln Laboratory). Symmetry species can be identified by fitting the spectrum with Fig. 6 ($\nu \cong 0.5/6\pi$). This is further verified by the heights of the lines which approximately correspond to the well-known statistical weights: 5 for A_1, 3 for T_1 or T_2, and 2 for *E*.

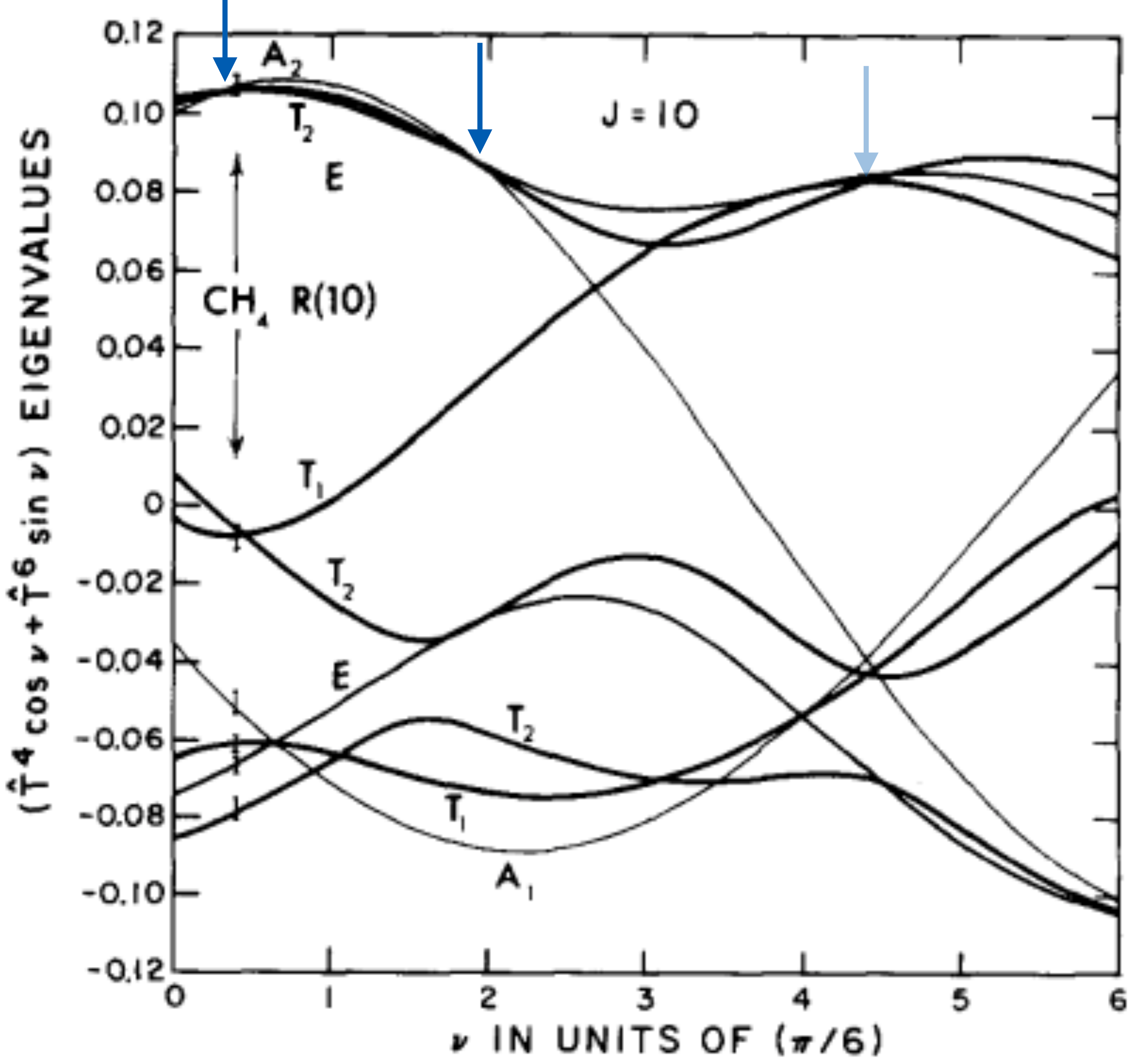


FIG. 6. ($J = 10$) Eigenvalue spectrum of $T(\nu)$.

W. G. Harter and C. W. Patterson 1457

J. Math. Phys. **20**,7,1457 *(1979). pdf p7.*

When Local C_2 symmetry dominates
Due to 4^{th} and 6^{th} rank $T^{[4]}+T^{[6]}$ combo

$O\supset C_2(\mathbf{i}_1)$	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

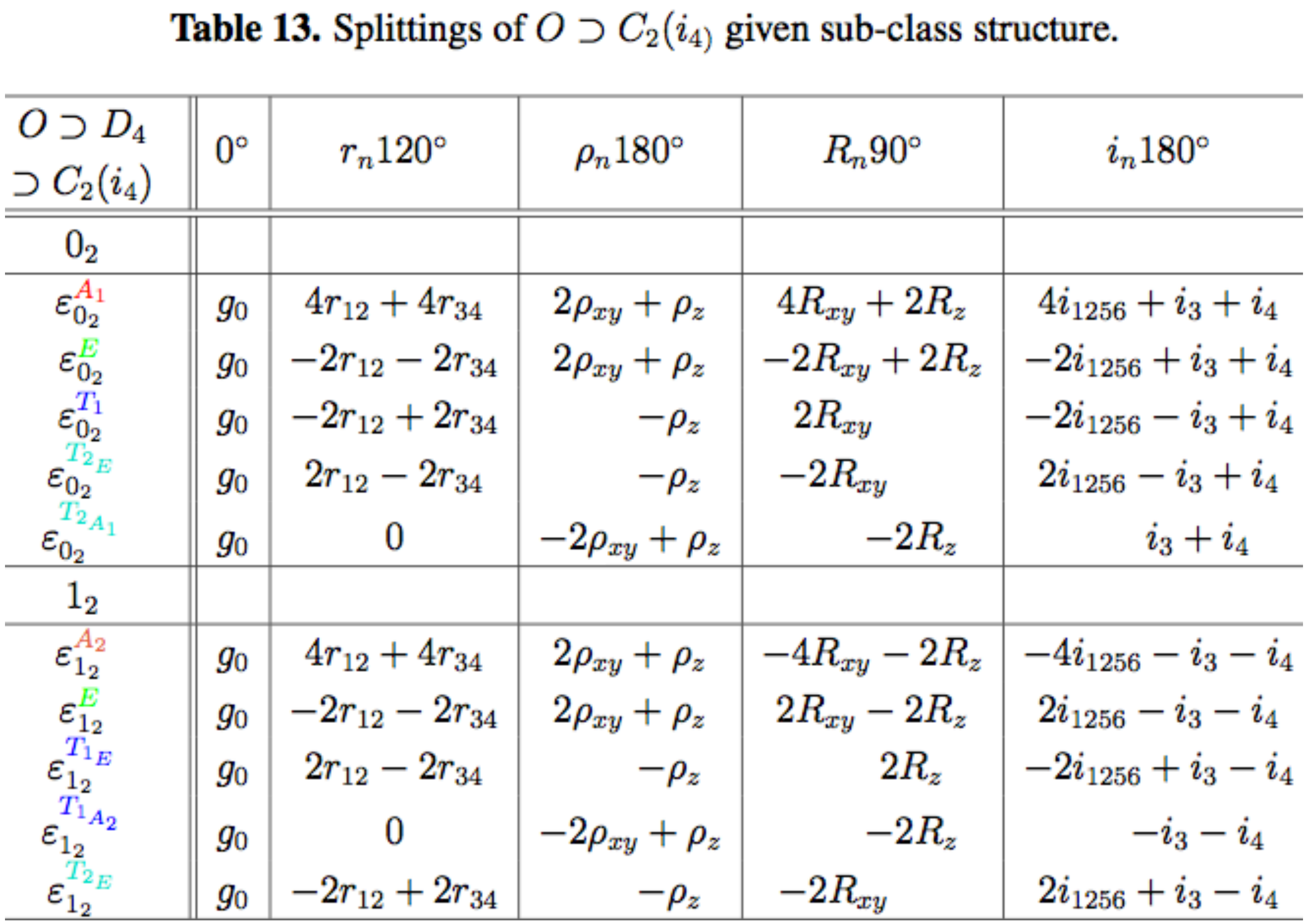


Table 13. Splittings of $O\supset C_2(i_4)$ given sub-class structure.

$O\supset D_4$ $\supset C_2(i_4)$	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	$-2r_{12}+2r_{34}$	$-\rho_z$	$-2R_{xy}$	$2i_{1256}+i_3-i_4$

Int.J.Mol.Sci, *14, 714(2013)pdf p76*

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

Int.J.Mol.Sci, *14, 714(2013)pdf p77*

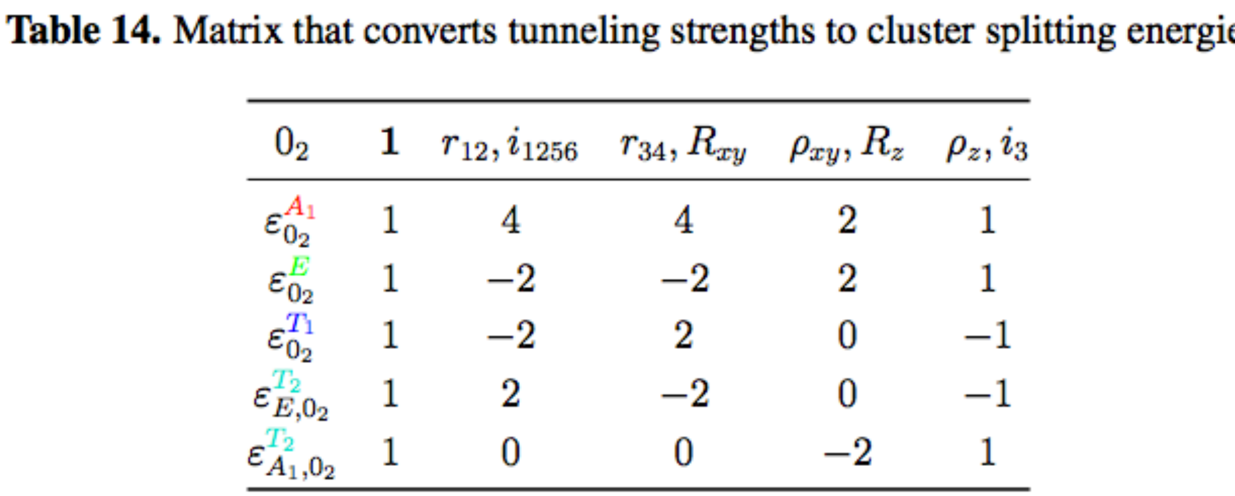


Table 14. Matrix that converts tunneling strengths to cluster splitting energie

0_2	**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

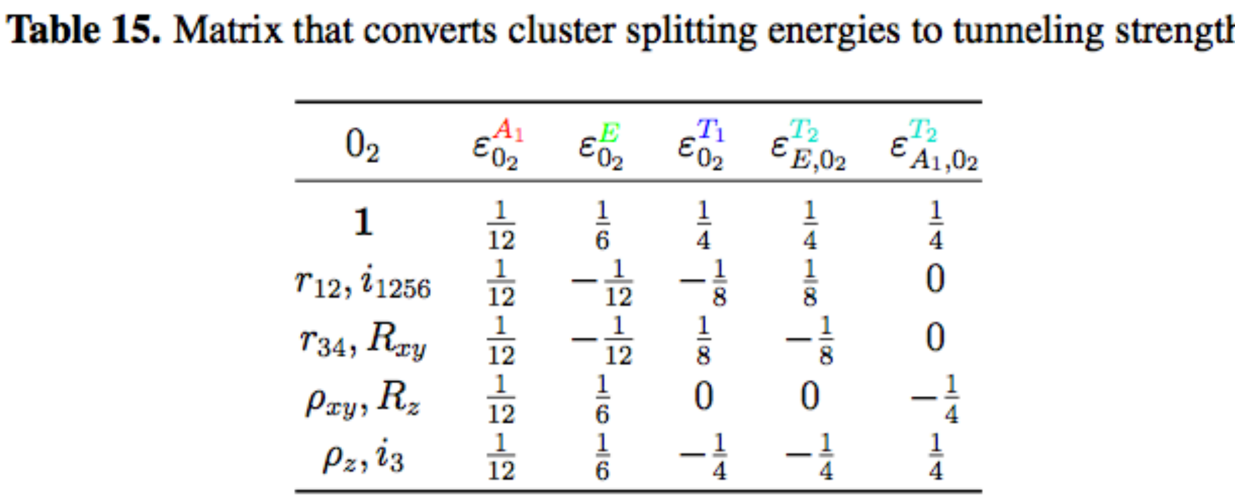


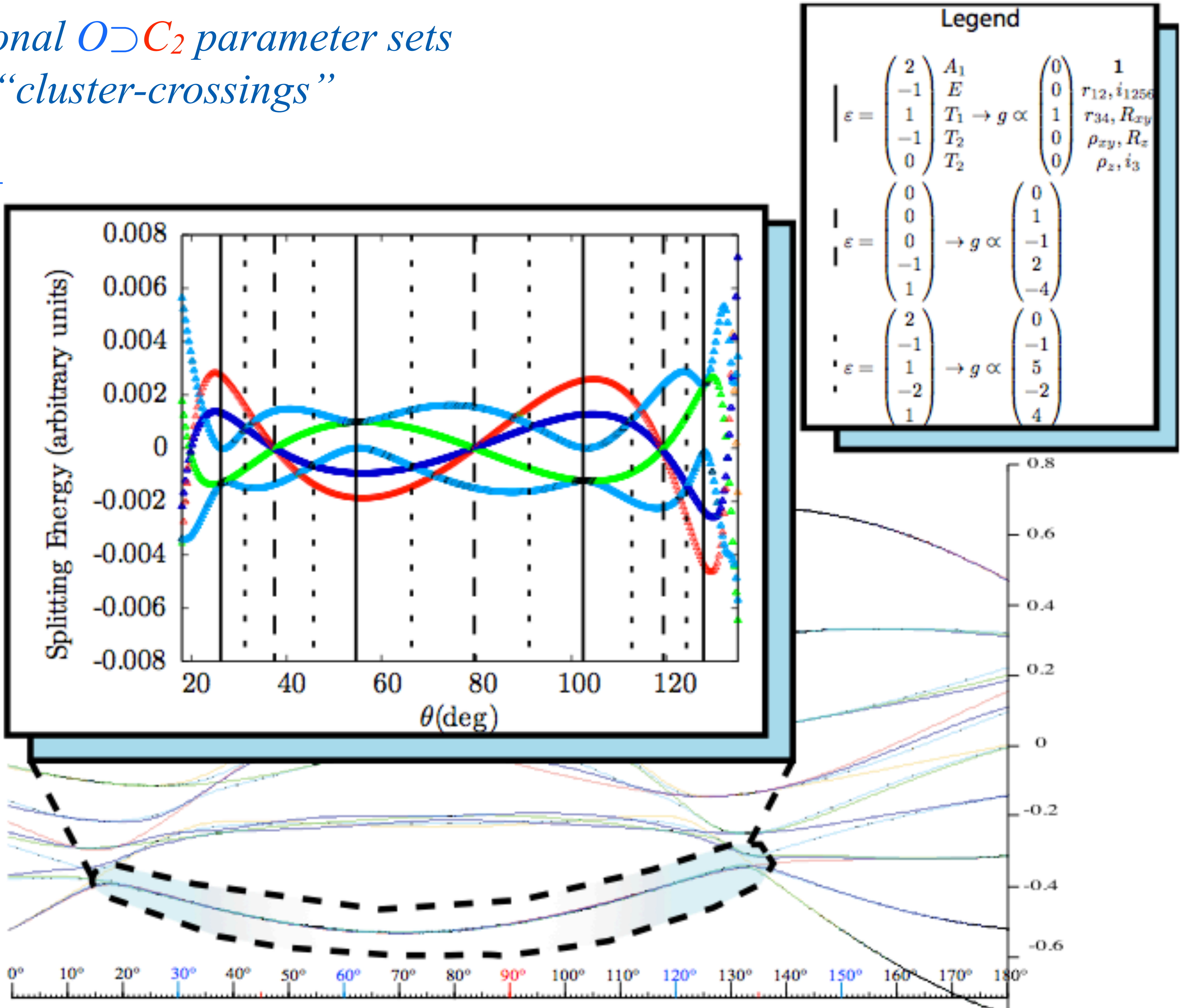
Table 15. Matrix that converts cluster splitting energies to tunneling strengt

0_2	$\varepsilon_{0_2}^{A_1}$	$\varepsilon_{0_2}^{E}$	$\varepsilon_{0_2}^{T_1}$	$\varepsilon_{E,0_2}^{T_2}$	$\varepsilon_{A_1,0_2}^{T_2}$
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	$\frac{1}{12}$	$\frac{1}{6}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$\frac{1}{4}$

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)*



AMOP
reference links
on page 2

3.12.18 class 17.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Discrete symmetry subgroups of O(3)⊃(Octahedral O_h⊃O): Part II Full $D^{(\alpha)}$-matrices defined by subgroup-chains $O\supset D_4\supset C_4$, D_2, or C_3 applied to eigensolutions of O_h-tensors $\mathbf{T}^{[4]}+\mathbf{T}^{[6]}$

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

Review Coset factored splitting of projectors for $O\supset D_4\supset C_4$ *into split classes and level structure*

Hamiltonian level cluster models with subgroup-defined tunneling parameters

Diagonal idempotent $\mathbf{P}^{\mu}_{m,m}$ *parameter sets for* $O\supset C_4$ *and* $O\supset C_3$ *case of* SF_6 *level clusters*

Off-diagonal nilpotent $\mathbf{P}^{\mu}_{m,n}$ $(m\neq n)$ *parameter sets needed for* $O\supset C_2$ *clusters*

Deriving nilpotent projectors $\mathbf{P}^{\mu}_{m,n}$ *and ireps* $D^{\mu}_{m,n}$ *by fundamental* $\mathbf{g}\rightleftarrows\mathbf{P}^{\mu}_{m,n}$ *relations:*

(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 nilpotent projectors for simple $D_3\supset C_2\sim C_{3v}\supset C_v$ *chains* *(Lect13p95)*

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

Structure and applications of coset tabulated $D^{\mu}_{m,n}$ *irreps for various* O_h *subgroup chains*

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

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 $D^{E}_{0_4 2_4}$

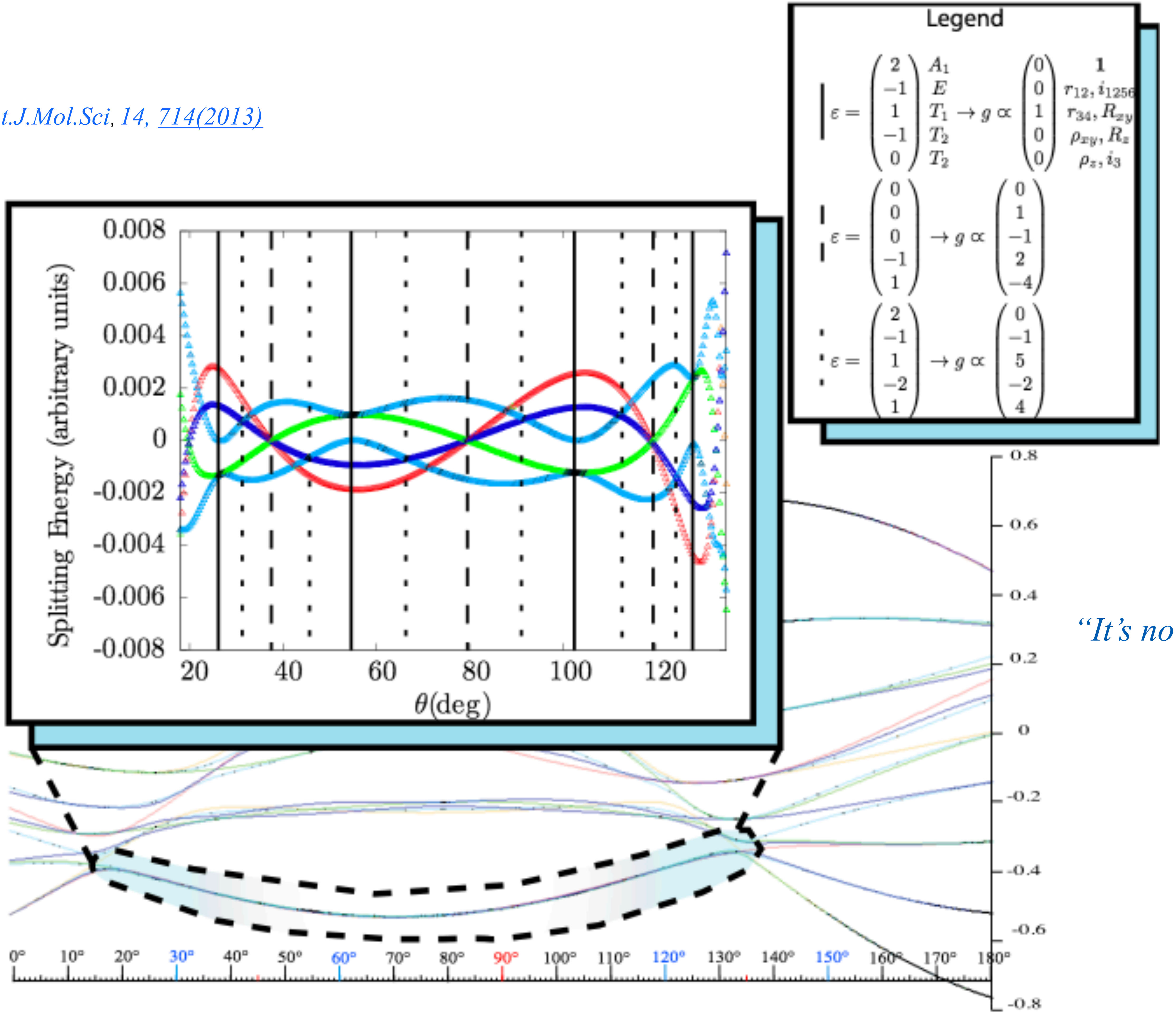
Comparing local C_4, C_3, *and* C_2 *cluster spectra of* O_h*-symmetric tensors* $\mathbf{T}^{[4]}+\mathbf{T}^{[6]}$

Monster clusters: When local C_2 *symmetry dominates*

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

Are these "accidents" or not? NOT!

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



"It's no "accident!"

End of Lecture 17. Following are O_h-related tables some given previously

$O\supset C_4$	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
$A_{1u}\downarrow C_{4v}$	·	·	1	·	·
$A_{2u}\downarrow C_{4v}$	·	·	·	1	·
$E_u\downarrow C_{4v}$	·	·	1	1	·
$T_{1u}\downarrow C_{4v}$	1	·	·	·	1
$T_{2u}\downarrow C_{4v}$	·	1	·	·	1

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

$O_h\supset C^i_{2v}$	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
$A_{1u}\downarrow C^i_{2v}$	·	·	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
$A_{1u}\downarrow C^z_{2v}$	·	·	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

	1	ρ_z	R_z	$\tilde{R}_z$
1	1	ρ_z	R_z	$\tilde{R}_z$
ρ_z	ρ_z	1	$\tilde{R}_z$	R_z
R_z	$\tilde{R}_z$	R_z	1	ρ_z
$\tilde{R}_z$	R_z	$\tilde{R}_z$	ρ_z	1

	ρ_x	ρ_y	i_4	i_3
ρ_x	1	ρ_z	R_z	$\tilde{R}_z$
ρ_y	ρ_z	1	$\tilde{R}_z$	R_z
i_4	$\tilde{R}_z$	R_z	1	ρ_z
i_3	R_z	$\tilde{R}_z$	ρ_z	1

	r_1	r_4	i_1	R_y
r_1	1	ρ_z	R_z	$\tilde{R}_z$
r_4	ρ_z	1	$\tilde{R}_z$	R_z
i_1	$\tilde{R}_z$	R_z	1	ρ_z
R_y	R_z	$\tilde{R}_z$	ρ_z	1

	r_2	r_3	i_2	$\tilde{R}_y$
r_2	1	ρ_z	R_z	$\tilde{R}_z$
r_3	ρ_z	1	$\tilde{R}_z$	R_z
i_2	$\tilde{R}_z$	R_z	1	ρ_z
$\tilde{R}_y$	R_z	$\tilde{R}_z$	ρ_z	1

	$\tilde{r}_1$	$\tilde{r}_3$	$\tilde{R}_x$	i_6
$\tilde{r}_1$	1	ρ_z	R_z	$\tilde{R}_z$
$\tilde{r}_3$	ρ_z	1	$\tilde{R}_z$	R_z
$\tilde{R}_x$	$\tilde{R}_z$	R_z	1	ρ_z
i_6	R_z	$\tilde{R}_z$	ρ_z	1

	$\tilde{r}_2$	$\tilde{r}_4$	R_x	i_5
$\tilde{r}_2$	1	ρ_z	R_z	$\tilde{R}_z$
$\tilde{r}_4$	ρ_z	1	$\tilde{R}_z$	R_z
R_x	$\tilde{R}_z$	R_z	1	ρ_z
i_5	R_z	$\tilde{R}_z$	ρ_z	1

	1	ρ_z	R_z	$\tilde{R}_z$
1	1	ρ_z	R_z	$\tilde{R}_z$
ρ_z	ρ_z	1	$\tilde{R}_z$	R_z
R_z	$\tilde{R}_z$	R_z	1	ρ_z
$\tilde{R}_z$	R_z	$\tilde{R}_z$	ρ_z	1

	ρ_x	ρ_y	i_4	i_3
ρ_x	1	ρ_z	R_z	$\tilde{R}_z$
ρ_y	ρ_z	1	$\tilde{R}_z$	R_z
i_4	$\tilde{R}_z$	R_z	1	ρ_z
i_3	R_z	$\tilde{R}_z$	ρ_z	1

	r_1	r_4	i_1	R_y
r_1	1	ρ_z	R_z	$\tilde{R}_z$
r_4	ρ_z	1	$\tilde{R}_z$	R_z
i_1	$\tilde{R}_z$	R_z	1	ρ_z
R_y	R_z	$\tilde{R}_z$	ρ_z	1

	r_2	r_3	i_2	$\tilde{R}_y$
r_2	1	ρ_z	R_z	$\tilde{R}_z$
r_3	ρ_z	1	$\tilde{R}_z$	R_z
i_2	$\tilde{R}_z$	R_z	1	ρ_z
$\tilde{R}_y$	R_z	$\tilde{R}_z$	ρ_z	1

	$\tilde{r}_1$	$\tilde{r}_3$	$\tilde{R}_x$	i_6
$\tilde{r}_1$	1	ρ_z	R_z	$\tilde{R}_z$
$\tilde{r}_3$	ρ_z	1	$\tilde{R}_z$	R_z
$\tilde{R}_x$	$\tilde{R}_z$	R_z	1	ρ_z
i_6	R_z	$\tilde{R}_z$	ρ_z	1

	$\tilde{r}_2$	$\tilde{r}_4$	R_x	i_5
$\tilde{r}_2$	1	ρ_z	R_z	$\tilde{R}_z$
$\tilde{r}_4$	ρ_z	1	$\tilde{R}_z$	R_z
R_x	$\tilde{R}_z$	R_z	1	ρ_z
i_5	R_z	$\tilde{R}_z$	ρ_z	1

$[1,\rho_z,R_z,\tilde{R}_z]$ $[\rho_x,\rho_y,i_4,i_3]$ $[r_1,r_4,i_1,R_y]$ $[r_2,r_3,i_2,\tilde{R}_y]$ $[\tilde{r}_1,\tilde{r}_3,\tilde{R}_x,i_6]$ $[\tilde{r}_2,\tilde{r}_4,R_x,i_5]$ Cosets of C_4

$1\,(1,\rho_z,R_z,\tilde{R}_z)$, $\rho_x(1,\rho_z,R_z,\tilde{R}_z)$, $r_1(1,\rho_z,R_z,\tilde{R}_z)$, $r_2(1,\rho_z,R_z,\tilde{R}_z)$, $\tilde{r}_1(1,\rho_z,R_z,\tilde{R}_z)$, $\tilde{r}_2(1,\rho_z,R_z,\tilde{R}_z)$

$\rho_z(\rho_z,1,\tilde{R}_z,R_z)$, $\rho_y(\rho_z,1,\tilde{R}_z,R_z)$, $r_4(\rho_z,1,\tilde{R}_z,R_z)$, $r_3(\rho_z,1,\tilde{R}_z,R_z)$, $\tilde{r}_3(\rho_z,1,\tilde{R}_z,R_z)$, $\tilde{r}_4(\rho_z,1,\tilde{R}_z,R_z)$

$R_z(\tilde{R}_z,R_z,1,\rho_z)$, $i_4(\tilde{R}_z,R_z,1,\rho_z)$, $i_1(\tilde{R}_z,R_z,1,\rho_z)$, $i_2(\tilde{R}_z,R_z,1,\rho_z)$, $\tilde{R}_x(\tilde{R}_z,R_z,1,\rho_z)$, $R_x(\tilde{R}_z,R_z,1,\rho_z)$

$\tilde{R}_z(R_z,\tilde{R}_z,\rho_z,1)$, $i_3(R_z,\tilde{R}_z,\rho_z,1)$, $R_y(R_z,\tilde{R}_z,\rho_z,1)$, $\tilde{R}_y(R_z,\tilde{R}_z,\rho_z,1)$, $i_6(R_z,\tilde{R}_z,\rho_z,1)$, $i_5(R_z,\tilde{R}_z,\rho_z,1)$