AMOP reference links on following page

3.07.18 class 16.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Discrete symmetry subgroups of $O(3)\supset$(Octahedral $O_h\supset O$): Deriving $D^{(\alpha)}$-matrices defined by subgroup-chains $O\supset D_4\supset C_4$, $O\supset D_4\supset D_2$, and $O\supset D_3\supset C_3$ applications to IR spectra of SF_6

Review *Octahedral* $O_h\supset O$ *group operator structure*

Review *Octahedral* $O_h\supset O\supset D_4\supset C_4$ *subgroup chain correlations*

Comparison of $O\supset D_4\supset C_4$ *and* $O\supset D_4\supset D_2$ *correlations and level/projector splitting*

- $O\supset D_4\supset C_4$ *subgroup chain splitting*
- $O\supset D_4\supset D_2$ *subgroup chain splitting (nOrmal* D_2 *vs. unOrmal* D_2*)*
- $O_h\supset O\supset D_4\supset C_{4v}$ *and* $O_h\supset O\supset D_4\supset C_{4v}\supset C_{2v}$ *subgroup splitting*

Splitting O *class projectors* $\mathbf{P}^{\mu}$ *into irreducible projectors* $\mathbf{P}^{\mu}_{m_4m_4}$ *for* $O\supset C_4$

- *Left-cosets and coefficient arrays*

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- *Calculating* $\mathbf{P}^{E}_{0_40_4}$, $\mathbf{P}^{E}_{2_42_4}$, $\mathbf{P}^{T_1}_{0_40_4}$, $\mathbf{P}^{T_1}_{1_41_4}$, $\mathbf{P}^{T_2}_{2_42_4}$, $\mathbf{P}^{T_2}_{1_41_4}$, *Collected* $\mathbf{P}_{mm}$ *results Table*

$O\supset C_4$ *induced representation* $0_4(C_4)\uparrow O \sim A_1\oplus T_1\oplus E$ *and spectral analysis examples*

- *Elementary induced representation* $0_4(C_4)\uparrow O$
- *Projection reduction of induced representation* $0_4(C_4)\uparrow O$
- *Introduction to ortho-complete eigenvalue-parameter relations*
  - *Examples for* SF_6 *spectroscopy*

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 - ajp-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

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Discrete symmetry subgroups of O(3)⊃(Octahedral O_h⊃O): Deriving $D^{(\alpha)}$-matrices defined by subgroup-chains $O\supset D_4\supset C_4$, $O\supset D_4\supset D_2$, and $O\supset D_3\supset C_3$ applications to IR spectra of SF_6

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Example: $G=O$ *Cubic-Octahedral Group O*

$\ell^{A_1}=1$

$\ell^{A_2}=1$

$\ell^{E}=2$

$\ell^{T_1}=3$

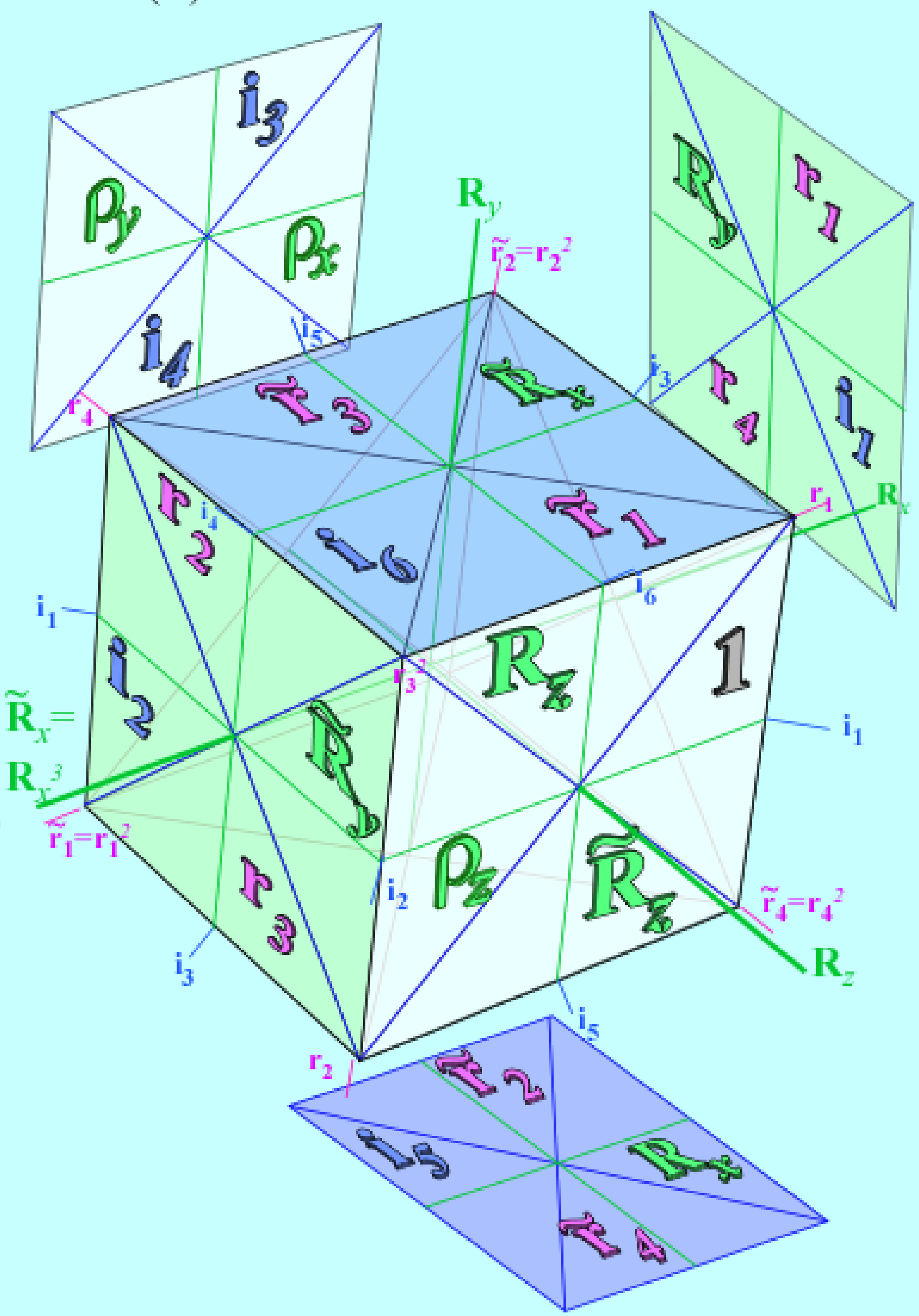
$\ell^{T_2}=3$

Centrum: $\kappa(O)=\Sigma_{(\alpha)}(\ell^{\alpha})^0=1^0+1^0+2^0+3^0+3^0=5$

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

Order: $^{o}(O)=\Sigma_{(\alpha)}(\ell^{\alpha})^0=1^2+1^2+2^2+3^2+3^2=24$

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



$O\supset C_4$

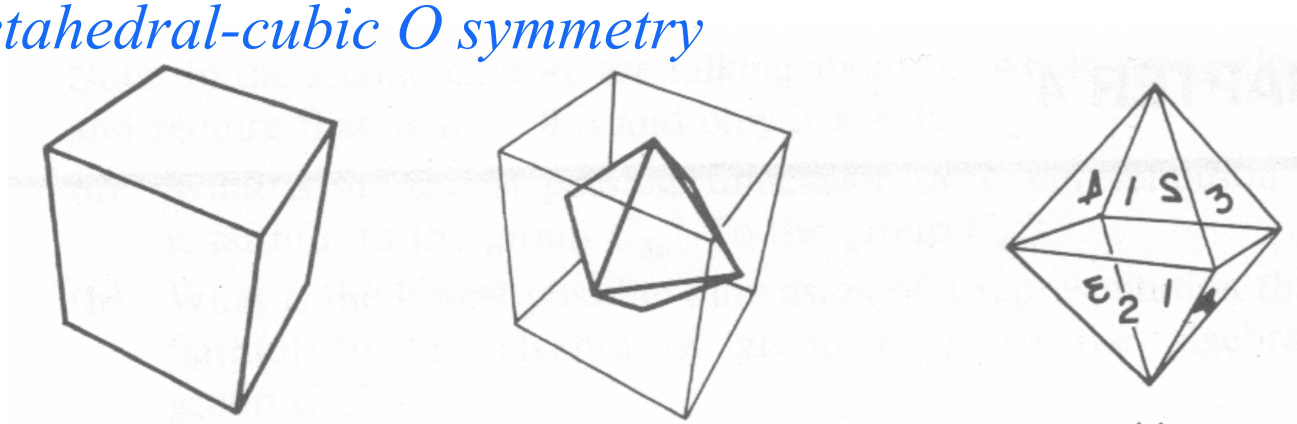
	$(0)_4$	$(1)_4$	$(2)_4$	$(3)_4=(-1)_4$
A_1	1	•	•	•
A_2	•	•	1	•
E	1	•	1	•
T_1	1	1	•	1
T_2	•	1	1	1

$O\supset C_3$

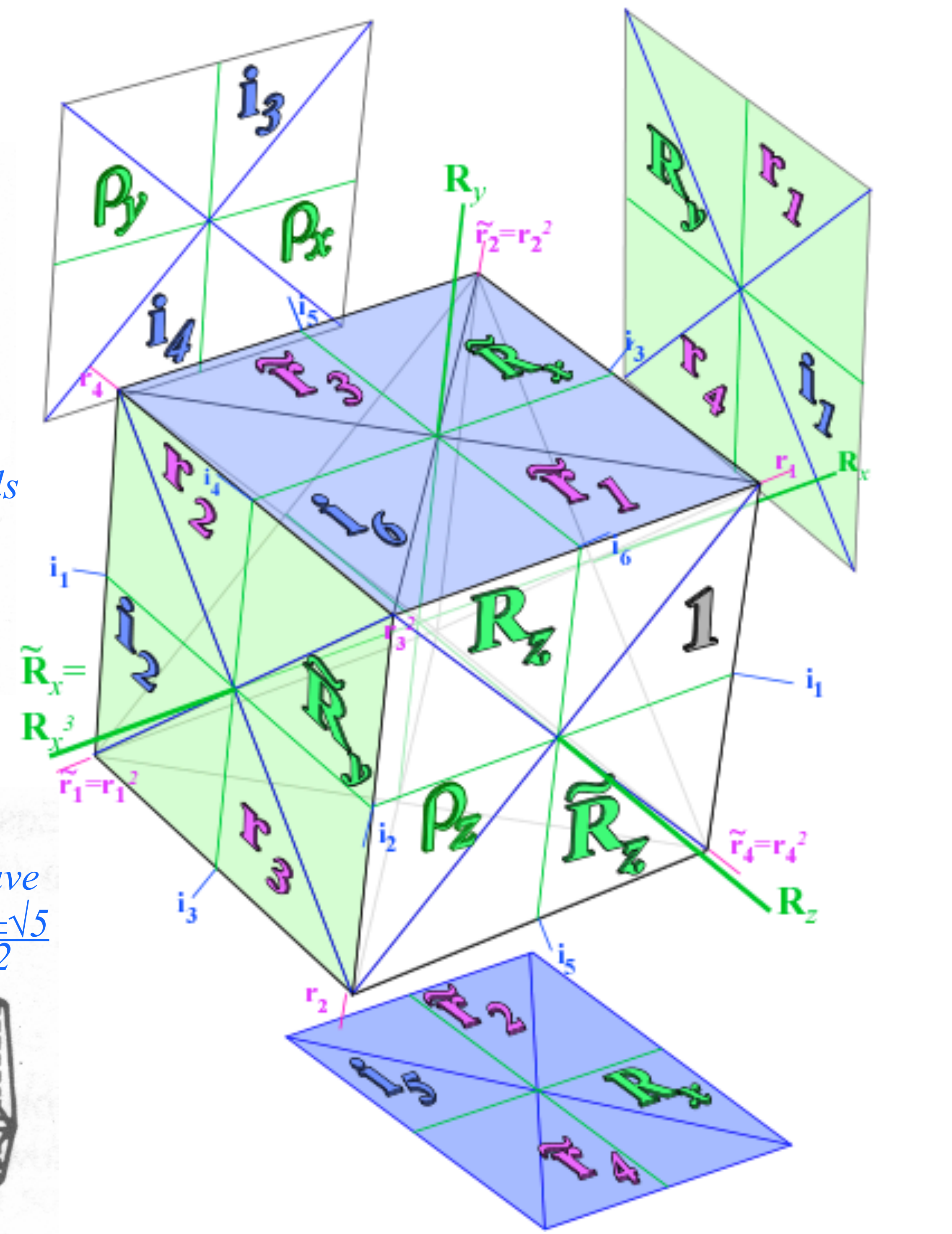
	$(0)_3$	$(1)_3$	$(2)_3=(-1)_3$
A_1	1	•	•
A_2	1	•	•
E	•	1	1
T_1	1	1	1
T_2	1	1	1

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

Octahedral-cubic O symmetry



Order °O=6 hexahedron squares · 4 pts =24
=8 octahedron triangles · 3 pts =24
=12 lines · 2 pts =24 positions

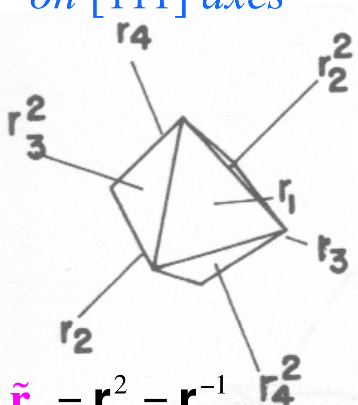


Octahedral group O operations

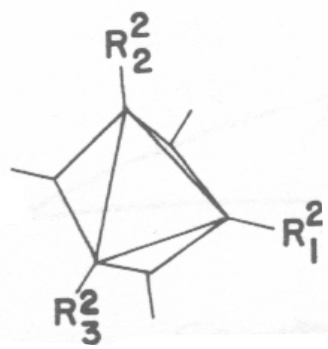
Class of 1: **1**

$\mathbf{r}_k = \mathbf{r}_k$

Class of 8:
±120° rotations
on [111] axes



$\tilde{\mathbf{r}}_k = \mathbf{r}_k^2 = \mathbf{r}_k^{-1}$

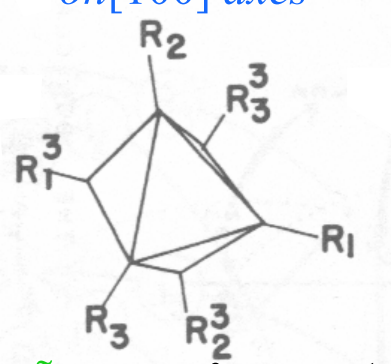


Class of 3:
180° rotations
on [100] axes

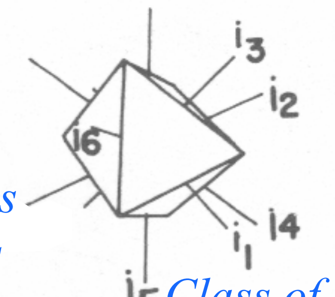
$\rho_{x,y,z} = \mathbf{R}^2_{1,2,3}$

$\mathbf{R}_{x,y,z} = \mathbf{R}_{1,2,3}$

Class of 6:
±90° rotations
on[100] axes



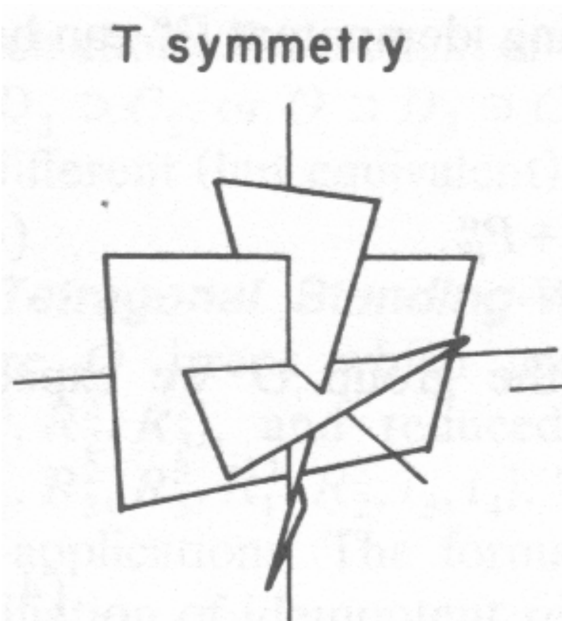
$\tilde{\mathbf{R}}_{x,y,z} = \mathbf{R}^3_{1,2,3} = \mathbf{R}^{-1}_{1,2,3}$

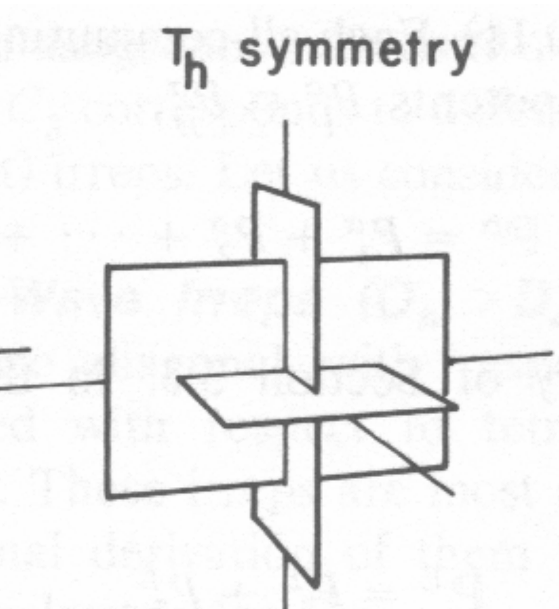


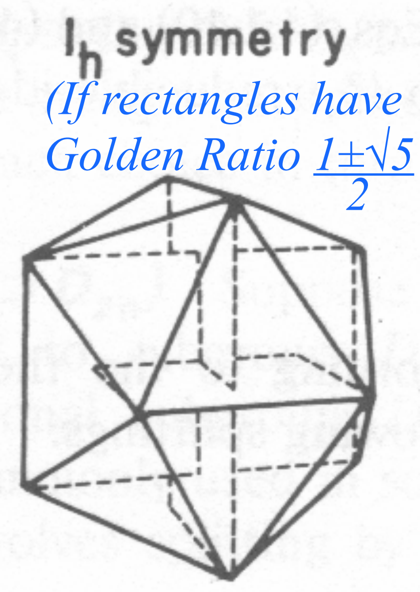
Class of 6:
180° rotations
on [110] diagonals

$\mathbf{i}_k = \mathbf{i}_k$

Tetrahedral symmetry becomes Icosahedral







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

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

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

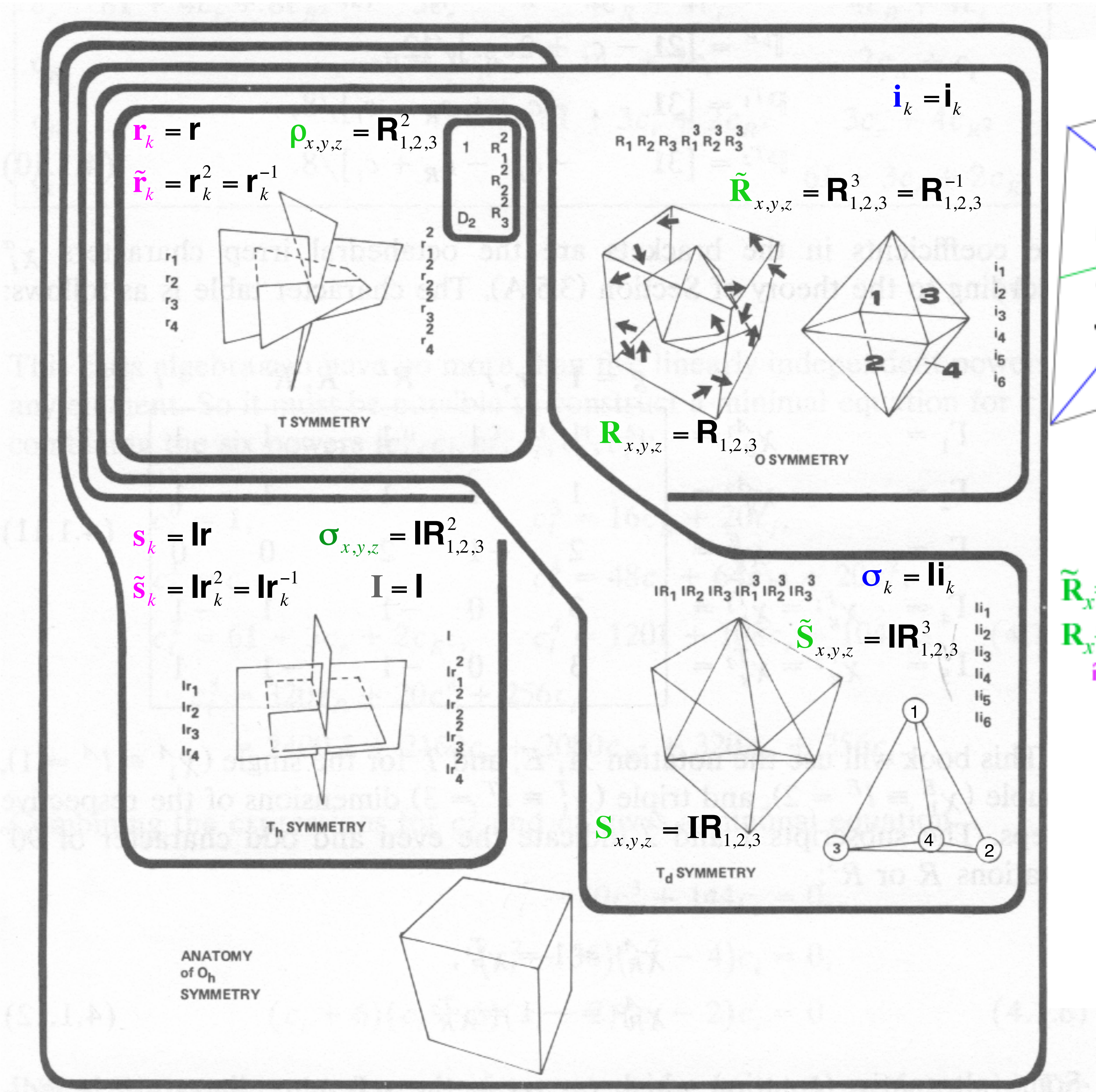
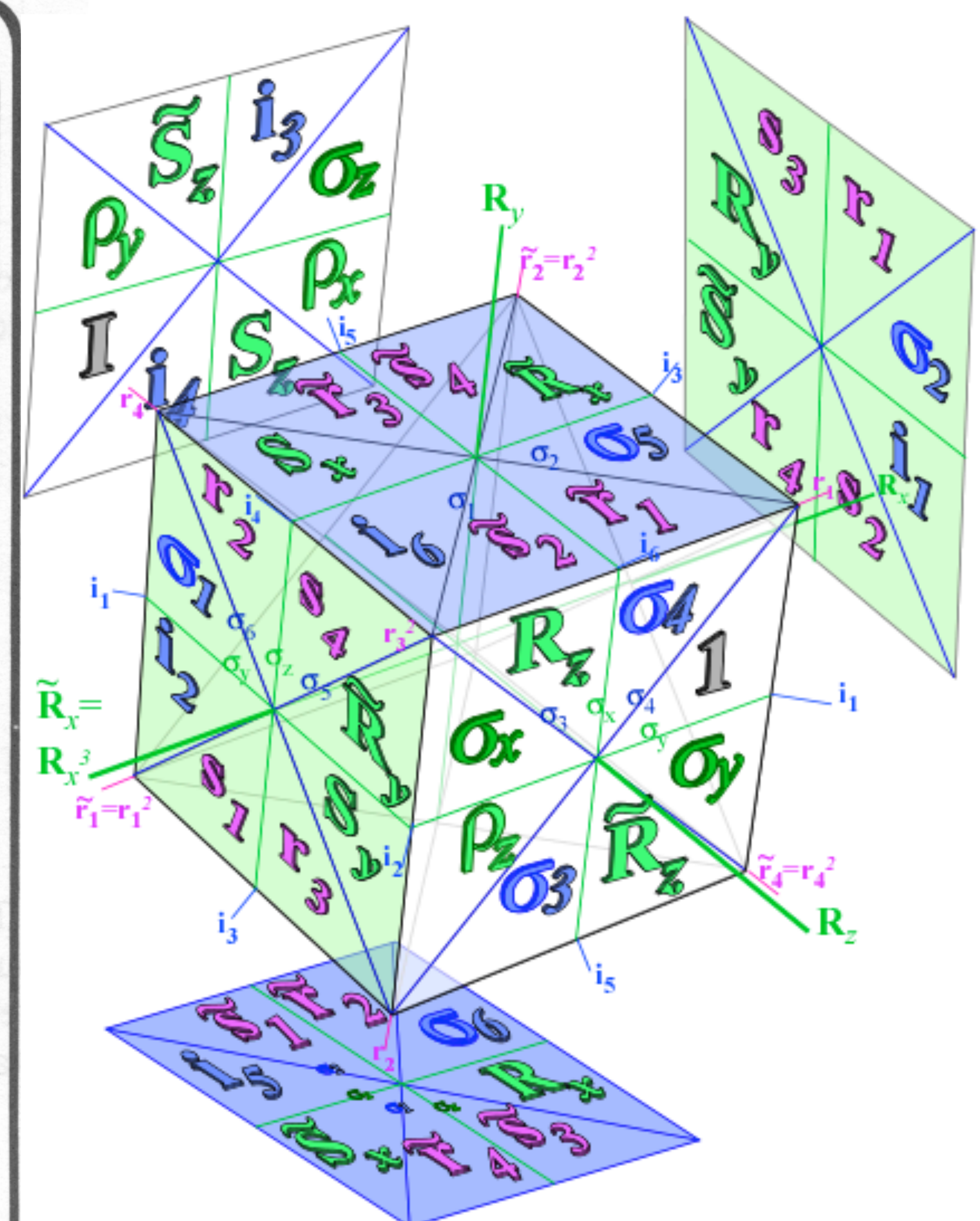


Figure 4.1.5 The full octahedral group (O_h) and four non-Abelian subgroups T, T_h, T_d, and O. The Abelian D_2 subgroup of T is indicated also.

Fig. 4.1.5 from Principles of Symmetry, Dynamics and Spectroscopy



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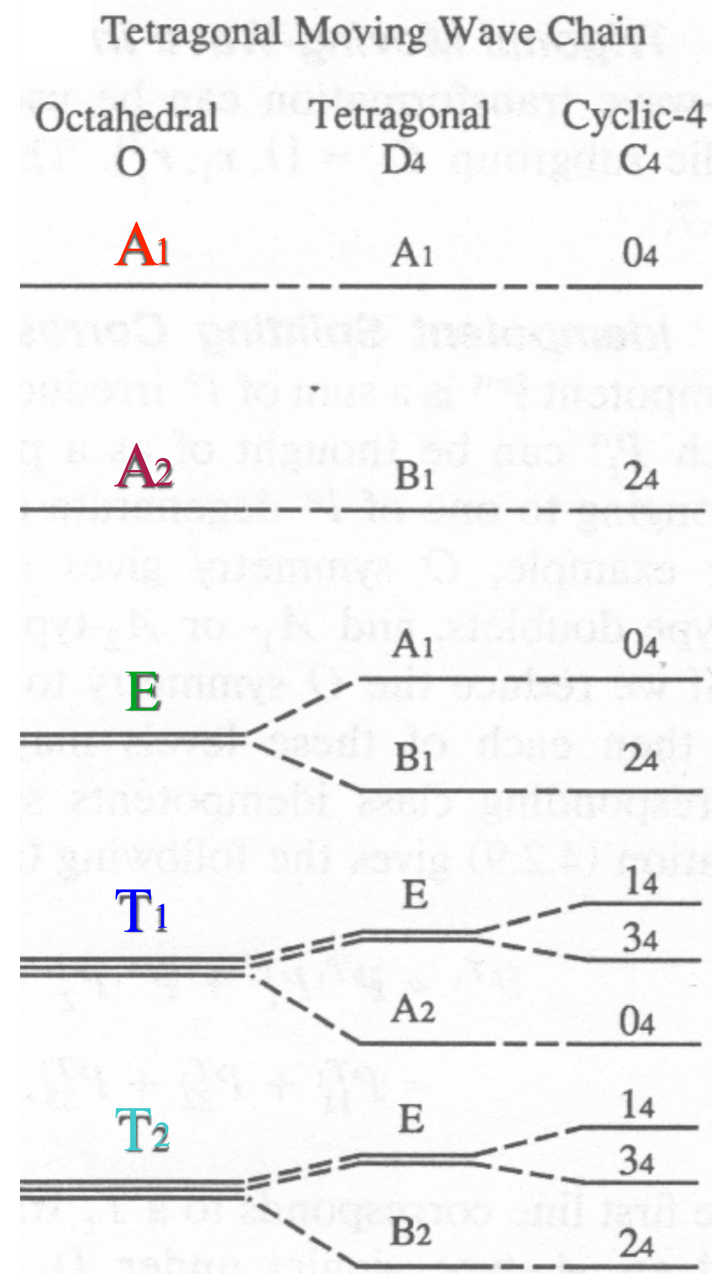
$O \supset D_4 \supset C_4$ level splitting

D_4	$\mathbf{1}$	ρ_z	$\mathbf{R}_z$	$\rho_{x,y}$	$\mathbf{i}_{3,4}$
A_1	1	1	1	1	1
B_1	1	1	-1	1	-1
A_2	1	1	1	-1	-1
B_2	1	1	-1	-1	1
E	2	-2	0	0	0



$C_4 \; \{ \mathbf{1}, \mathbf{R}_z^1, \mathbf{R}_z^2, \mathbf{R}_z^3 \}$

$\{ \mathbf{1}, \mathbf{R}_3^2, \mathbf{R}_3^2, \mathbf{R}_3^3 \}$

0_4	1	1	1	1
1_4	1	i	-1	$-i$
2_4	1	-1	1	-1
3_4	1	$-i$	-1	i

$-1_4 =$

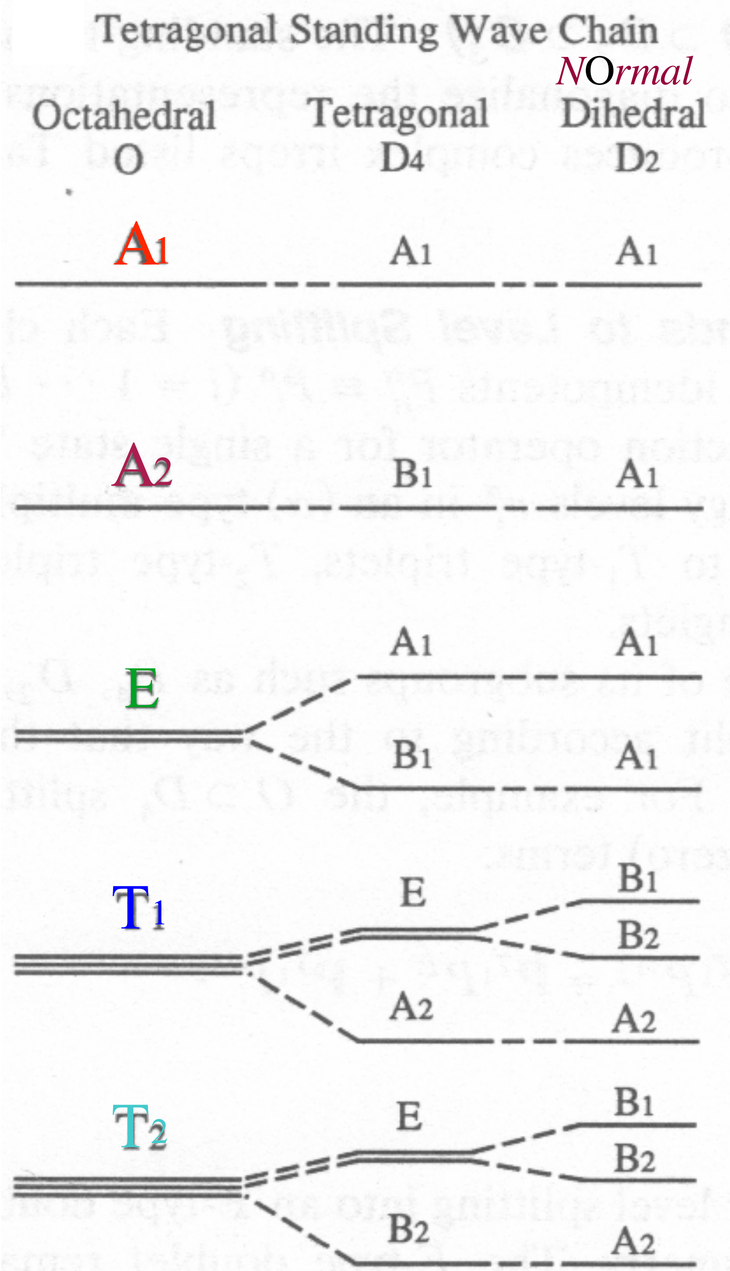
$D_4 \downarrow C_4$	0_4	1_4	2_4	3_4
A_1	1	·	·	·
B_1	·	·	1	·
A_2	1	·	·	·
B_2	·	·	1	·
E	·	1	·	1

	$\mathbf{r}, \tilde{\mathbf{r}}_i$	ρ_{xyz}	$\mathbf{R}, \tilde{\mathbf{R}}_{xyz}$		
O	$\mathbf{1}$	$\mathbf{r}$	$\mathbf{R}^2$	$\mathbf{R}^3$	$\mathbf{i}_k$
A_1	1	1	1	1	1
A_2	1	1	1	-1	-1
E	2	-1	2	0	0
T_1	3	0	-1	1	-1
T_2	3	0	-1	-1	1

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

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

O⊃D_4⊃D_2 *level splitting*

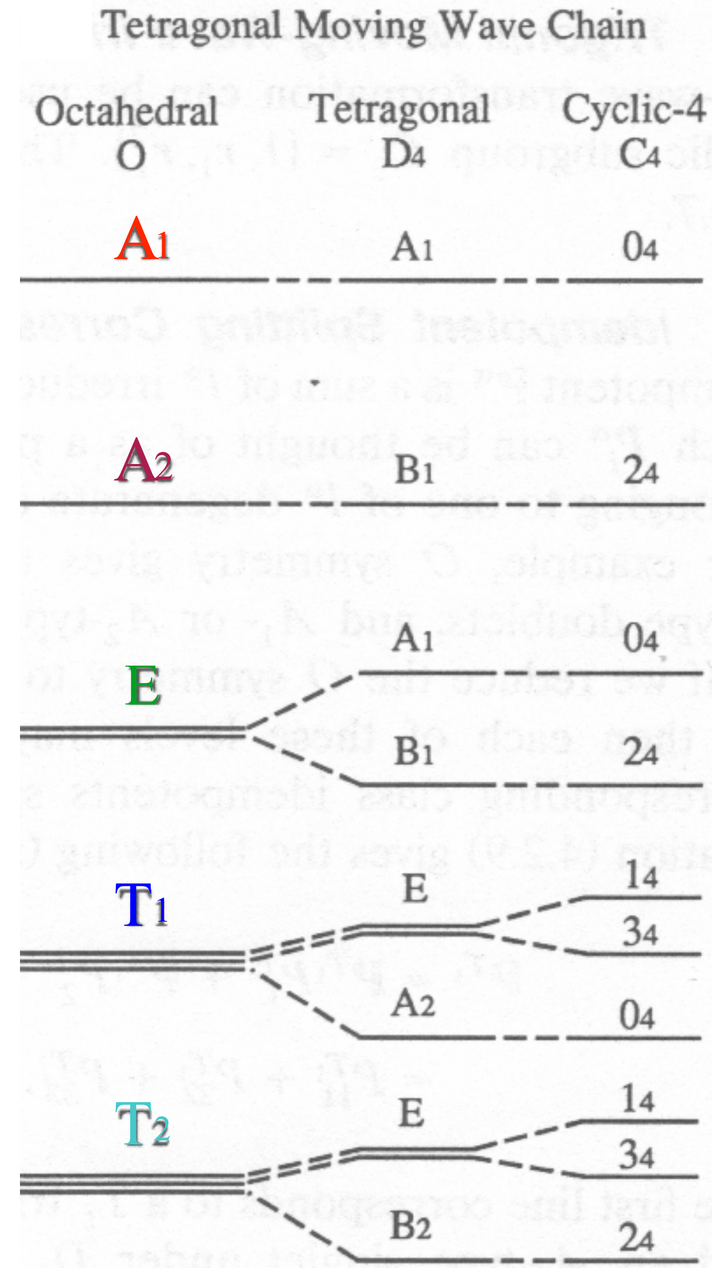


D_4	1	ρ_z	$\mathbf{R}_z$	$\rho_{x,y}$	$\mathbf{i}_{3,4}$
A_1	1	1	1	1	1
B_1	1	1	-1	1	-1
A_2	1	1	1	-1	-1
B_2	1	1	-1	-1	1
E	2	-2	0	0	0

NOrmal $D_2 = \{1, \mathbf{R}_3^2, \mathbf{R}_1^2, \mathbf{R}_2^2\}$

$D_4 \downarrow D_2$	A_1	B_1	A_2	B_2
A_1	1	·	·	·
B_1	1	·	·	·
A_2	·	·	1	·
B_2	·	·	1	·
E	·	1	·	1

O⊃D_4⊃C_4 *level splitting*



D_2^{Nm}	$\{1,$	$\mathbf{R}_z^2,$	$\mathbf{R}_x^2,$	$\mathbf{R}_y^2\}$
A_1	1	1	1	1
B_1	1	-1	1	-1
A_2	1	1	-1	-1
B_2	1	-1	-1	1

$-1_4 =$

$D_4 \downarrow C_4$	0_4	1_4	2_4	3_4
A_1	1	·	·	·
B_1	·	·	1	·
A_2	1	·	·	·
B_2	·	·	1	·
E	·	1	·	1

		$\mathbf{r}, \tilde{\mathbf{r}}_i$	ρ_{xyz}	$\mathbf{R}, \tilde{\mathbf{R}}_{xyz}$	
O	1	r	$\mathbf{R}^2$	$\mathbf{R}^3$	$\mathbf{i}_k$
A_1	1	1	1	1	1
A_2	1	1	1	-1	-1
E	2	-1	2	0	0
T_1	3	0	-1	1	-1
T_2	3	0	-1	-1	1

NOrmal $D_2 = \{1, \mathbf{R}_3^2, \mathbf{R}_1^2, \mathbf{R}_2^2\}$

$O \downarrow D_2$	A_1	B_1	A_2	B_2
A_1	1	·	·	·
A_2	1	·	·	·
E	2	·	·	·
T_1	·	1	1	1
T_2	·	1	1	1

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

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

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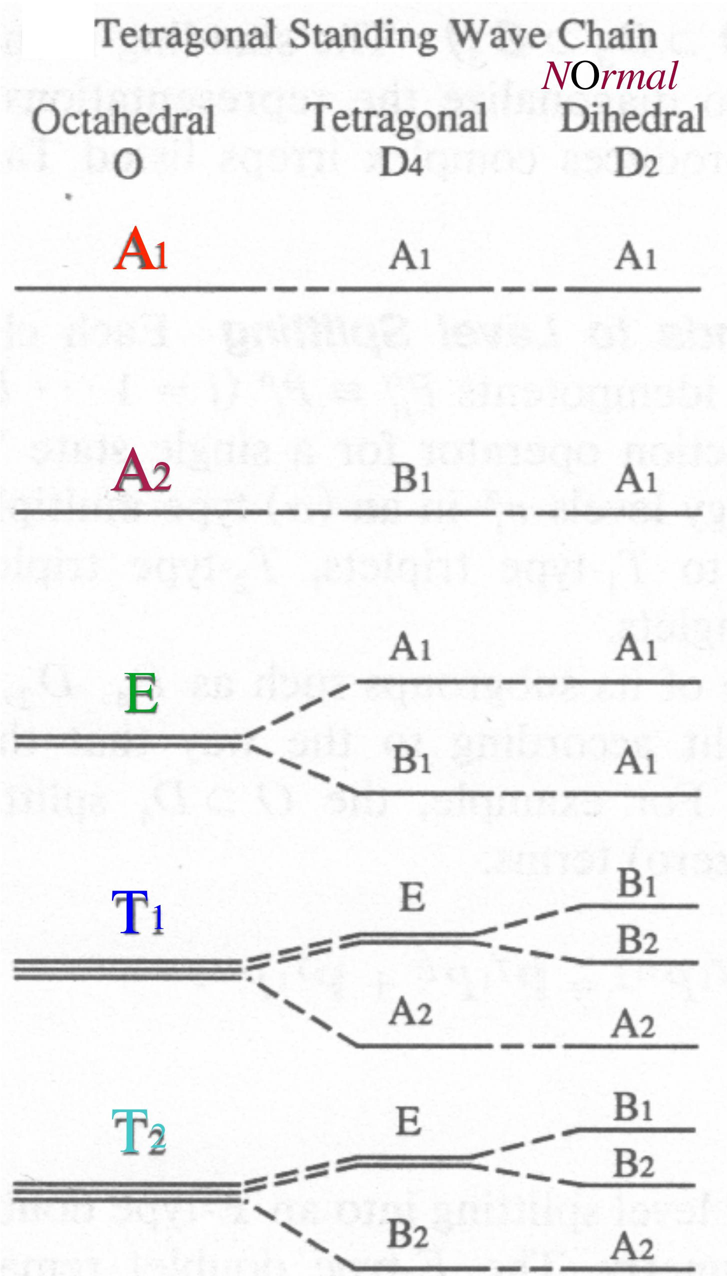
$O_h \supset O \supset D_4 \supset D_2$ subgroup splitting



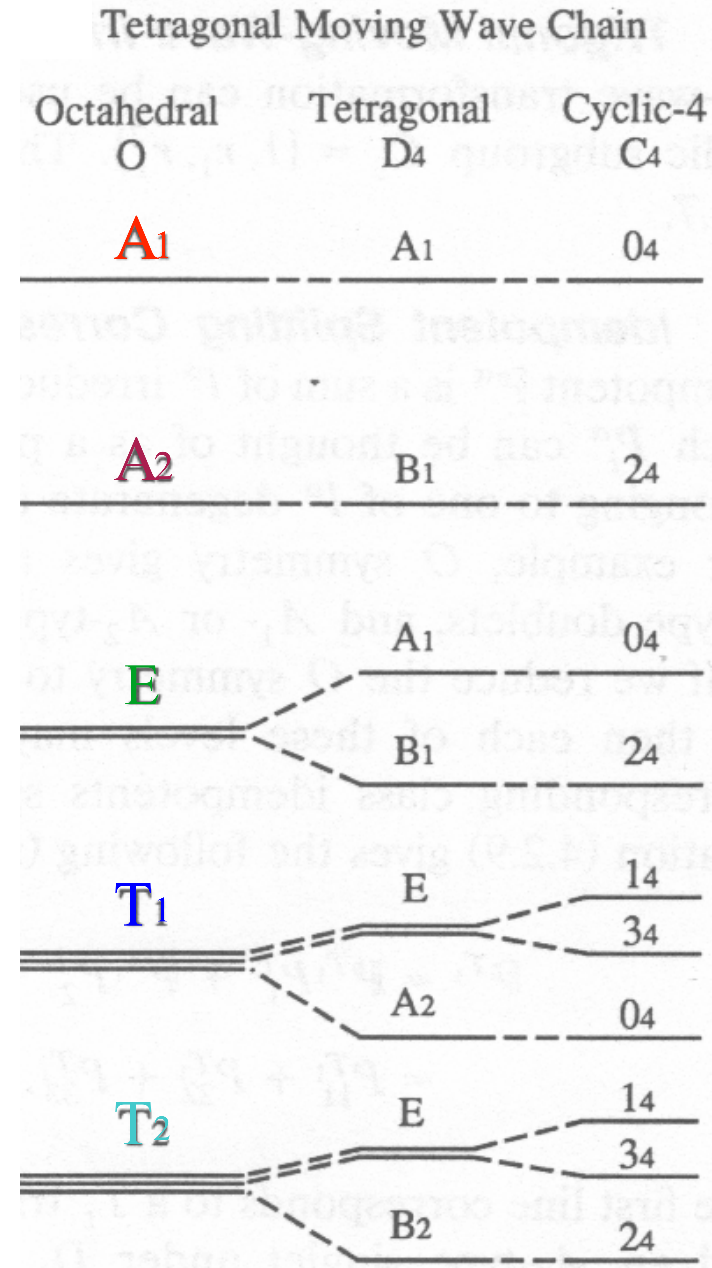
D_4	$\mathbf{1}$	ρ_z	$\mathbf{R}_z$	$\rho_{x,y}$	$\mathbf{i}_{3,4}$
A_1	1	1	1	1	1
B_1	1	1	-1	1	-1
A_2	1	1	1	-1	-1
B_2	1	1	-1	-1	1
E	2	-2	0	0	0

NOrmal $D_2 = \{1, \mathbf{R}_3^2, \mathbf{R}_1^2, \mathbf{R}_2^2\}$

$D_4 \downarrow D_2$	A_1	B_1	A_2	B_2
A_1	1	·	·	·
B_1	1	·	·	·
A_2	·	·	1	·
B_2	·	·	1	·
E	·	1	·	1

UnOrmal $D_2 = \{1, \mathbf{R}_3^2, \mathbf{i}_3, \mathbf{i}_4\}$

$D_4 \downarrow D_2$	A_1	B_1	A_2	B_2
A_1	1	·	·	·
B_1	·	·	1	·
A_2	·	·	1	·
B_2	1	·	·	·
E	·	1	·	1



$D_2^{Nm}\{\ \mathbf{1},\ \mathbf{R}_z^2,\ \mathbf{R}_x^2,\ \mathbf{R}_y^2\}$
$D_2^{Un}\{\ \mathbf{1},\ \mathbf{R}_z^2,\ \mathbf{i}_3,\ \mathbf{i}_4\}$

A_1	1	1	1	1
B_1	1	-1	1	-1
A_2	1	1	-1	-1
B_2	1	-1	-1	1

$-1_4 =$

$D_4 \downarrow C_4$	0_4	1_4	2_4	3_4
A_1	1	·	·	·
B_1	·	·	1	·
A_2	1	·	·	·
B_2	·	·	1	·
E	·	1	·	1

	$\mathbf{r}, \tilde{\mathbf{r}}_i$	ρ_{xyz}	$\mathbf{R}, \tilde{\mathbf{R}}_{xyz}$		
O	$\mathbf{1}$	$\mathbf{r}$	$\mathbf{R}^2$	$\mathbf{R}^3$	$\mathbf{i}_k$
A_1	1	1	1	1	1
A_2	1	1	1	-1	-1
E	2	-1	2	0	0
T_1	3	0	-1	1	-1
T_2	3	0	-1	-1	1

two kinds of D_2 subgroup

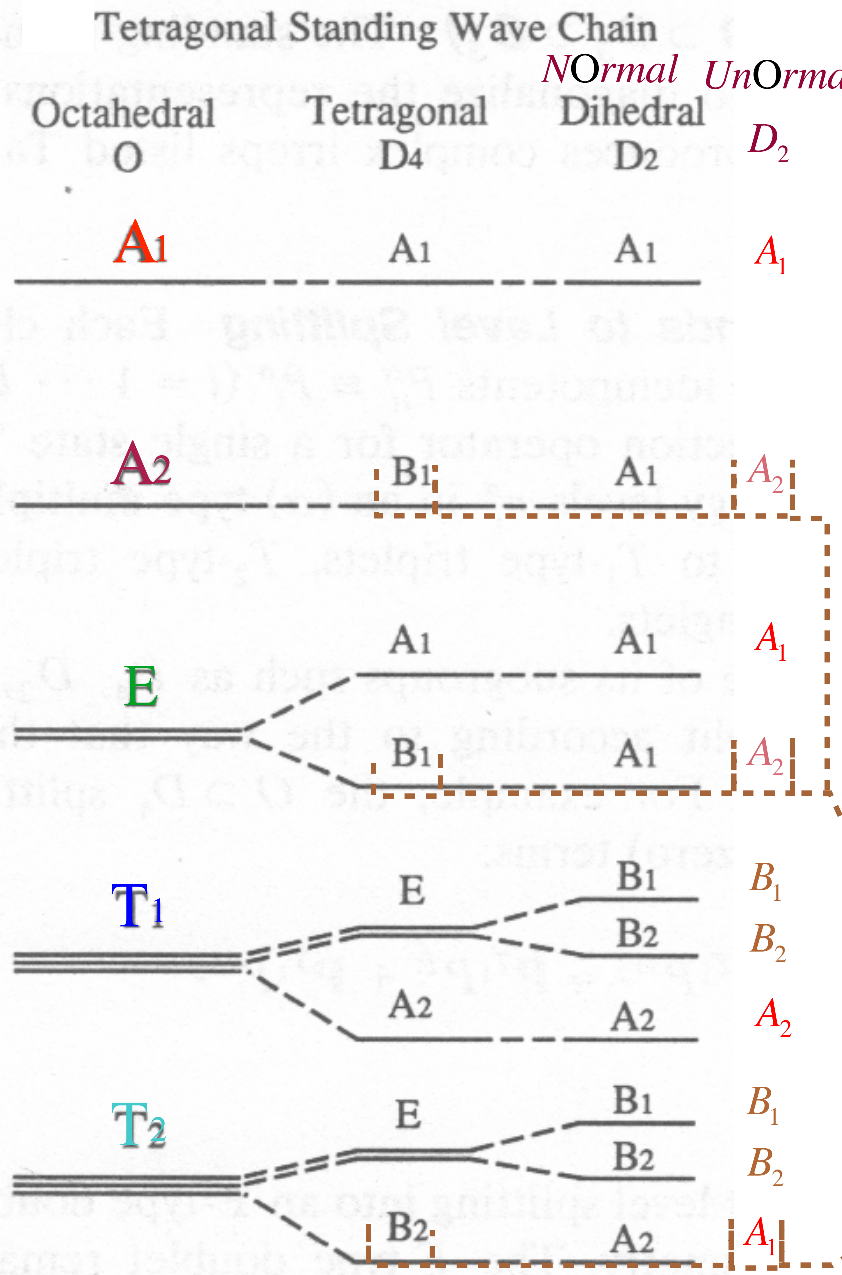
NOrmal $D_2 = \{1, \mathbf{R}_3^2, \mathbf{R}_1^2, \mathbf{R}_2^2\}$

$O \downarrow D_2$	A_1	B_1	A_2	B_2
A_1	1	·	·	·
A_2	1	·	·	·
E	2	·	·	·
T_1	·	1	1	1
T_2	·	1	1	1

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

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

$O_h \supset O \supset D_4 \supset D_2$ subgroup splitting



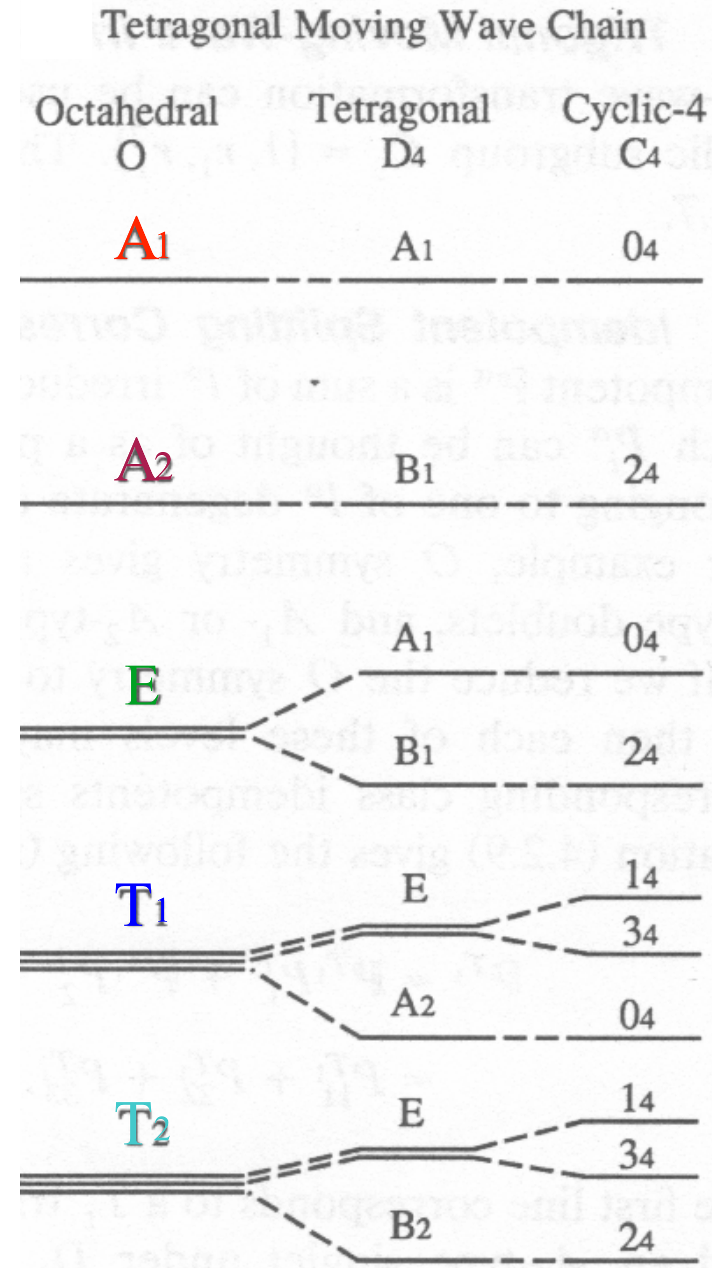
D_4	$\mathbf{1}$	ρ_z	$\mathbf{R}_z$	$\rho_{x,y}$	$\mathbf{i}_{3,4}$
A_1	1	1	1	1	1
B_1	1	1	-1	1	-1
A_2	1	1	1	-1	-1
B_2	1	1	-1	-1	1
E	2	-2	0	0	0

*NO*rmal $D_2 = \{1, \mathbf{R}_3^2, \mathbf{R}_1^2, \mathbf{R}_2^2\}$

$D_4 \downarrow D_2$	A_1	B_1	A_2	B_2
A_1	1	·	·	·
B_1	1	·	·	·
A_2	·	·	1	·
B_2	·	·	1	·
E	·	1	·	1

*UnO*rmal $D_2 = \{1, \mathbf{R}_3^2, \mathbf{i}_3, \mathbf{i}_4\}$

$D_4 \downarrow D_2$	A_1	B_1	A_2	B_2
A_1	1	·	·	·
B_1	·	·	1	·
A_2	·	·	1	·
B_2	1	·	·	·
E	·	1	·	1



D_2^{Nm}	$\mathbf{1}$	$\mathbf{R}_z^2$	$\mathbf{R}_x^2$	$\mathbf{R}_y^2$
D_2^{Un}	$\mathbf{1}$	$\mathbf{R}_z^2$	$\mathbf{i}_3$	$\mathbf{i}_4$
A_1	1	1	1	1
B_1	1	-1	1	-1
A_2	1	1	-1	-1
B_2	1	-1	-1	1

$-1_4 =$

$D_4 \downarrow C_4$	0_4	1_4	2_4	3_4
A_1	1	·	·	·
B_1	·	·	1	·
A_2	1	·	·	·
B_2	·	·	1	·
E	·	1	·	1

	$\mathbf{r}, \tilde{\mathbf{r}}_i$		ρ_{xyz}	$\mathbf{R}, \tilde{\mathbf{R}}_{xyz}$	
O	$\mathbf{1}$	$\mathbf{r}$	$\mathbf{R}^2$	$\mathbf{R}^3$	$\mathbf{i}_k$
A_1	1	1	1	1	1
A_2	1	1	1	-1	-1
E	2	-1	2	0	0
T_1	3	0	-1	1	-1
T_2	3	0	-1	-1	1

two kinds of D_2 subgroup splitting

*NO*rmal $D_2 = \{1, \mathbf{R}_3^2, \mathbf{R}_1^2, \mathbf{R}_2^2\}$ *UnO*rmal $D_2 = \{1, \mathbf{R}_3^2, \mathbf{i}_3, \mathbf{i}_4\}$

$O \downarrow D_2$	A_1	B_1	A_2	B_2
A_1	1	·	·	·
A_2	1	·	·	·
E	2	*degeneracy ambiguity*		·
T_1	·	1	1	1
T_2	·	1	1	1

$O \downarrow D_2$	A_1	B_1	A_2	B_2
A_1	1	·	·	·
A_2	·	·	1	·
E	1	·	1	·
T_1	·	1	1	1
T_2	1	1	·	1

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

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

AMOP reference links on page 2

3.07.18 class 16.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Discrete symmetry subgroups of O(3)⊃(Octahedral O_h⊃O): Deriving $D^{(\alpha)}$-matrices defined by subgroup-chains $O\supset D_4\supset C_4$, $O\supset D_4\supset D_2$, and $O\supset D_3\supset C_3$ applications to IR spectra of SF_6

Review Octahedral $O_h\supset O$ *group operator structure*

Review Octahedral $O_h\supset O\supset D_4\supset C_4$ *subgroup chain correlations*

Comparison of $O\supset D_4\supset C_4$ *and* $O\supset D_4\supset D_2$ *correlations and level/projector splitting*

- $O\supset D_4\supset C_4$ *subgroup chain splitting*
- $O\supset D_4\supset D_2$ *subgroup chain splitting (nOrmal* D_2 *vs. unOrmal* D_2*)*
- $O_h\supset O\supset D_4\supset C_{4v}$ *and* $O_h\supset O\supset D_4\supset C_{4v}\supset C_{2v}$ *subgroup splitting*

Splitting O class projectors $\mathbf{P}^{\mu}$ *into irreducible projectors* $\mathbf{P}^{\mu}_{m_4m_4}$ *for* $O\supset C_4$

- *Left-cosets and coefficient arrays*

Development of irreducible projectors $\mathbf{P}^{\mu}_{m_4m_4}$ *and representations* $D^{\mu}_{m_4m_4}$

- *Calculating* $\mathbf{P}^{E}_{0_40_4}$, $\mathbf{P}^{E}_{2_42_4}$, $\mathbf{P}^{T_1}_{0_40_4}$, $\mathbf{P}^{T_1}_{1_41_4}$, $\mathbf{P}^{T_2}_{2_42_4}$, $\mathbf{P}^{T_2}_{1_41_4}$,

$O\supset C_4$ *induced representation* $0_4(C_4)\uparrow O\sim A_1\oplus T_1\oplus E$ *and spectral analysis examples*

- *Elementary induced representation* $0_4(C_4)\uparrow O$
- *Projection reduction of induced representation* $0_4(C_4)\uparrow O$
- *Introduction to ortho-complete eigenvalue-parameter relations*
  - *Examples in* SF_6 *spectroscopy*

$O_h \supset D_{4h} \supset C_{4v} \supset C_4$ *subgroup splitting*

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

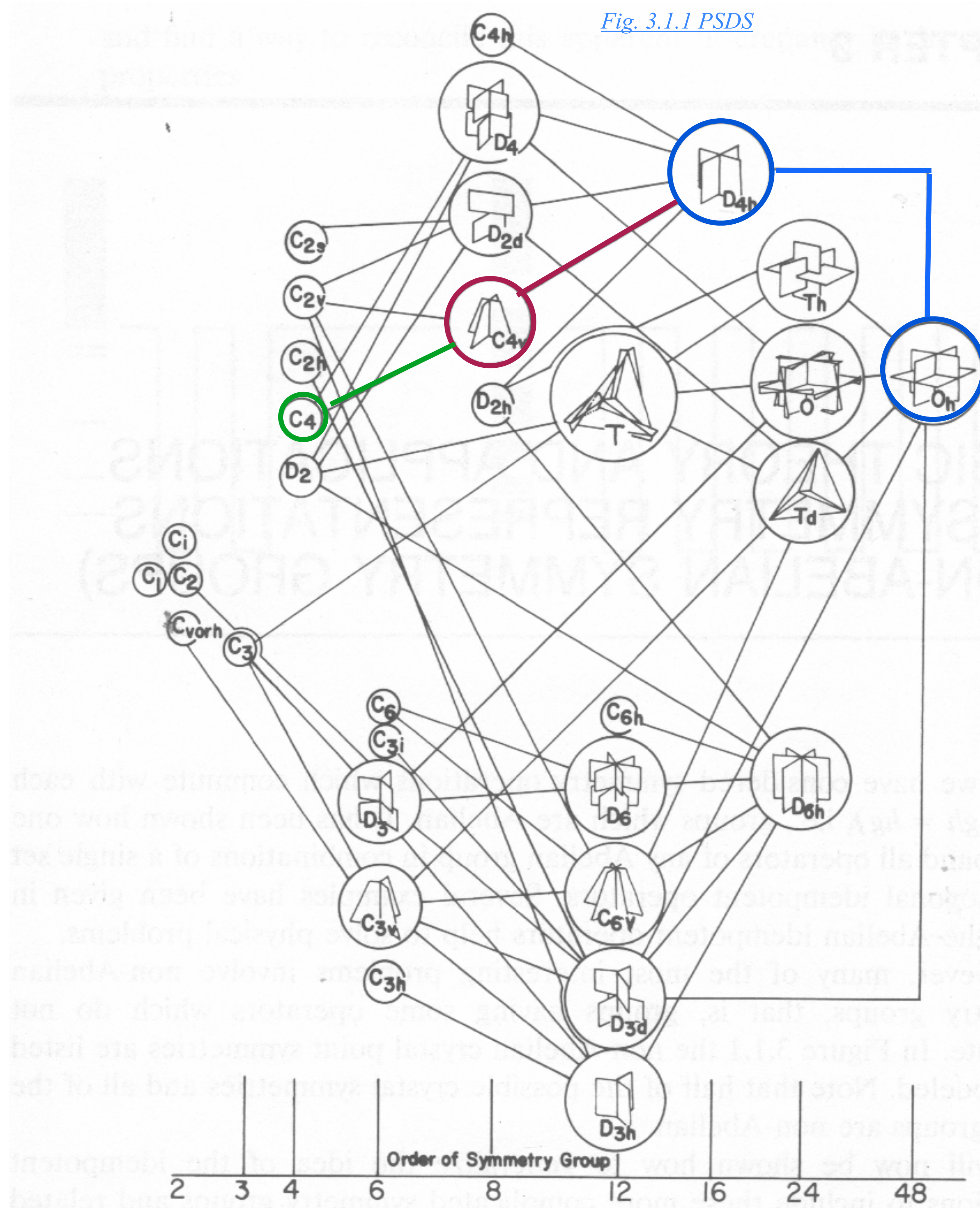


Fig. 3.1.1 PSDS

$O_h \supset D_{4h} \supset C_{4v} \supset C_{2v}$ subgroup splitting

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

has degeneracy ambiguity

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

has no degeneracy ambiguity

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

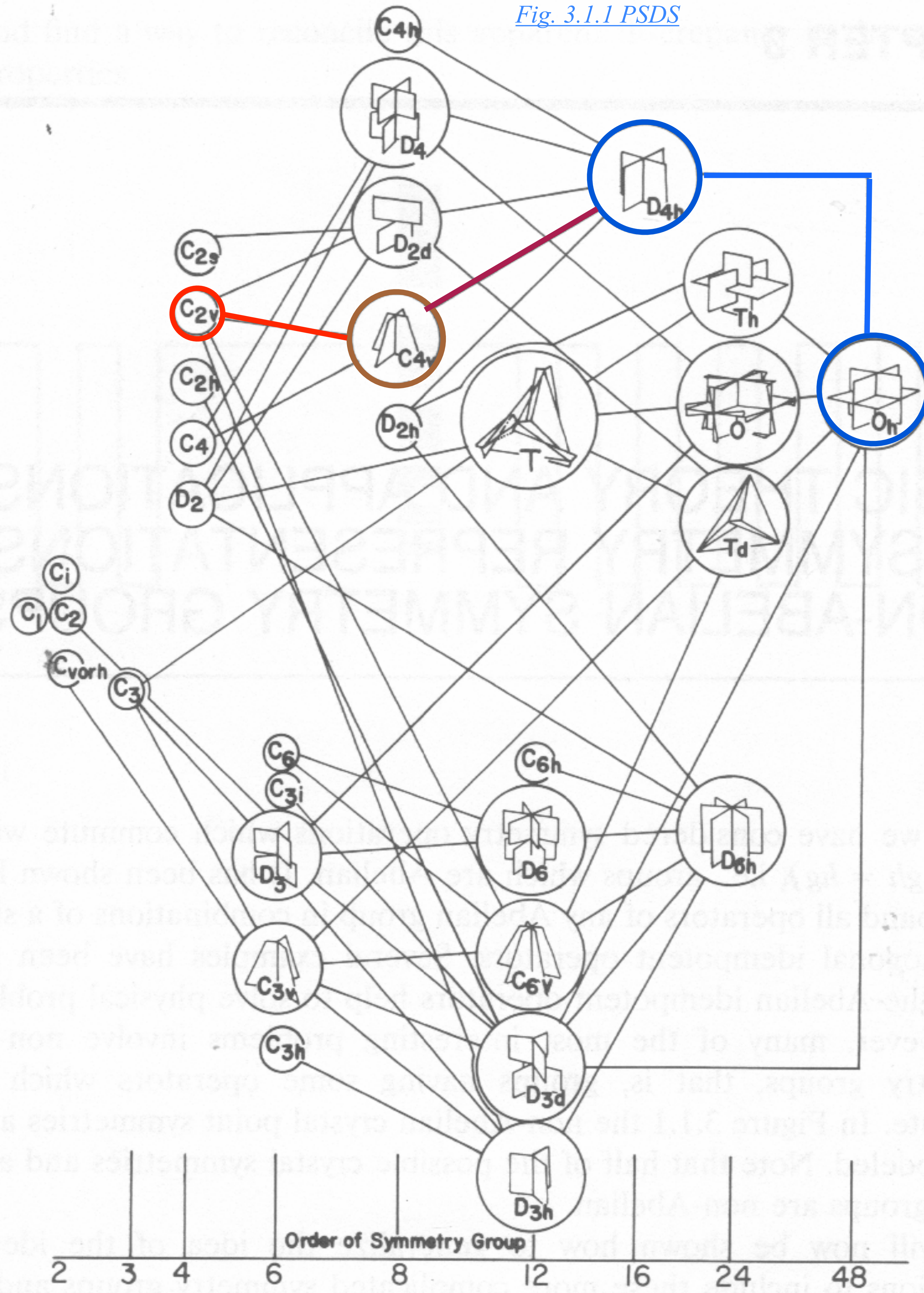


Fig. 3.1.1 PSDS

AMOP reference links on page 2

3.07.18 class 16.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Discrete symmetry subgroups of O(3)⊃(Octahedral O_h⊃O): Deriving $D^{(\alpha)}$-matrices defined by subgroup-chains $O\supset D_4\supset C_4$, $O\supset D_4\supset D_2$, and $O\supset D_3\supset C_3$ applications to IR spectra of SF_6

Review Octahedral $O_h\supset O$ group operator structure

Review Octahedral $O_h\supset O\supset D_4\supset C_4$ subgroup chain correlations

Comparison of $O\supset D_4\supset C_4$ and $O\supset D_4\supset D_2$ correlations and level/projector splitting

- *$O\supset D_4\supset C_4$ subgroup chain splitting*
- *$O\supset D_4\supset D_2$ subgroup chain splitting (nOrmal D_2 vs. unOrmal D_2)*
- *$O_h\supset O\supset D_4\supset C_{4v}$ and $O_h\supset O\supset D_4\supset C_{4v}\supset C_{2v}$ subgroup splitting*

➡ *Splitting O class projectors $\mathbf{P}^{\mu}$ into irreducible projectors $\mathbf{P}^{\mu}_{m_4m_4}$ for $O\supset C_4$*

- *Left-cosets and coefficient arrays*

Development of irreducible projectors $\mathbf{P}^{\mu}_{m_4m_4}$ and representations $D^{\mu}_{m_4m_4}$

- *Calculating $\mathbf{P}^{E}_{0_40_4}$, $\mathbf{P}^{E}_{2_42_4}$, $\mathbf{P}^{T_1}_{0_40_4}$, $\mathbf{P}^{T_1}_{1_41_4}$, $\mathbf{P}^{T_2}_{2_42_4}$, $\mathbf{P}^{T_2}_{1_41_4}$, Collected $\mathbf{P}_{mm}$ results Table*

$O\supset C_4$ induced representation $0_4(C_4)\uparrow O \sim A_1\oplus T_1\oplus E$ and spectral analysis examples

- *Elementary induced representation $0_4(C_4)\uparrow O$*
- *Projection reduction of induced representation $0_4(C_4)\uparrow O$*
- *Introduction to ortho-complete eigenvalue-parameter relations*
  - *Examples in SF_6 spectroscopy*

Splitting **O** *class projectors* $\mathbf{P}^{\mu}$ *into irreducible projectors* $\mathbf{P}^{\mu}_{m_4 m_4}$ *for* $O\supset C_4$

$O\supset C_4$ *Correlation table shows which* $\mathbf{P}^{\mu}$ *splittings are allowed:*

$O\supset C_4$	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

$\mathbf{P}^{A_1}=\mathbf{P}^{A_1}_{0_4 0_4}$ and $\mathbf{P}^{A_2}=\mathbf{P}^{A_2}_{2_4 2_4}$ *cannot* split

O characters

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

C_4 characters

$C_4:d^{m_4}_{\mathbf{R}^p}$	$\mathbf{g}=\mathbf{1}$	$\mathbf{R}^1_z$	$\rho_z=\mathbf{R}^2_z$	$\tilde{\mathbf{R}}_z=\mathbf{R}^3_z$
$m_4=0_4$	1	1	1	1
1_4	1	$-i$	-1	i
2_4	1	-1	1	-1
3_4	1	$-i$	-1	$-i$

O operators (Two notations: Older Princ.of Symm.Dynamics and Spectra. *and Newer* Int.J.Mol.Sci*)*

PSDS:	$\mathbf{1}$	$\mathbf{r}_1$	$\mathbf{r}_2$	$\mathbf{r}_3$	$\mathbf{r}_4$	$\mathbf{r}^2_1$	$\mathbf{r}^2_2$	$\mathbf{r}^2_3$	$\mathbf{r}^2_4$	$\mathbf{R}^2_1$	$\mathbf{R}^2_2$	$\mathbf{R}^2_3$	$\mathbf{R}_1$	$\mathbf{R}_2$	$\mathbf{R}_3$	$\mathbf{R}^3_1$	$\mathbf{R}^3_2$	$\mathbf{R}^3_3$	$\mathbf{i}_1$	$\mathbf{i}_2$	$\mathbf{i}_3$	$\mathbf{i}_4$	$\mathbf{i}_5$	$\mathbf{i}_6$
IJMS:	$\mathbf{1}$	$\mathbf{r}_1$	$\mathbf{r}_2$	$\mathbf{r}_3$	$\mathbf{r}_4$	$\tilde{\mathbf{r}}_1$	$\tilde{\mathbf{r}}_2$	$\tilde{\mathbf{r}}_3$	$\tilde{\mathbf{r}}_4$	ρ_x	ρ_y	ρ_z	$\mathbf{R}_x$	$\mathbf{R}_y$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_x$	$\tilde{\mathbf{R}}_y$	$\tilde{\mathbf{R}}_z$	$\mathbf{i}_1$	$\mathbf{i}_2$	$\mathbf{i}_3$	$\mathbf{i}_4$	$\mathbf{i}_5$	$\mathbf{i}_6$

Splitting O class projectors $\mathbf{P}^{\mu}$ into irreducible projectors $\mathbf{P}^{\mu}_{m_4 m_4}$ for $O \supset C_4$

$O \supset C_4$ Correlation table shows which $\mathbf{P}^{\mu}$ splittings are allowed:

$O \supset C_4$	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

$\mathbf{P}^{A_1} = \mathbf{P}^{A_1}_{0_4 0_4}$ and $\mathbf{P}^{A_2} = \mathbf{P}^{A_2}_{2_4 2_4}$ *cannot* split

$1 \cdot \mathbf{P}^{\mu} =$	$(\mathbf{p}_{0_4}$	$+\mathbf{p}_{1_4}$	$+\mathbf{p}_{2_4}$	$+\mathbf{p}_{3_4}) \cdot \mathbf{P}^{\mu}$
$1 \cdot \mathbf{P}^{A_1} =$	$\mathbf{P}^{A_1}_{0_4 0_4}$	+0	+0	+0
$1 \cdot \mathbf{P}^{A_2} =$	0	+0	$+\mathbf{P}^{A_2}_{2_4 2_4}$	+0
$1 \cdot \mathbf{P}^{E} =$	$\mathbf{P}^{E}_{0_4 0_4}$	+0	$+\mathbf{P}^{E}_{2_4 2_4}$	+0
$1 \cdot \mathbf{P}^{T_1} =$	$\mathbf{P}^{T_1}_{0_4 0_4}$	$+\mathbf{P}^{T_1}_{1_4 1_4}$	+0	$+\mathbf{P}^{T_1}_{3_4 3_4}$
$1 \cdot \mathbf{P}^{T_2} =$	0	$+\mathbf{P}^{T_2}_{1_4 1_4}$	$+\mathbf{P}^{T_2}_{2_4 2_4}$	$+\mathbf{P}^{T_2}_{3_4 3_4}$

O characters

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

C_4 characters

$C_4 : d^{m_4}_{\mathbf{R}^p}$	$\mathbf{g}=1$	$\mathbf{R}^1_z$	$\rho_z = \mathbf{R}^2_z$	$\tilde{\mathbf{R}}_z = \mathbf{R}^3_z$
$m_4 = 0_4$	1	1	1	1
1_4	1	$-i$	-1	i
2_4	1	-1	1	-1
3_4	1	$-i$	-1	$-i$

O operators (Two notations: Older Princ.of Symm.Dynamics and Spectra. *and Newer* Int.J.Mol.Sci*)*

PSDS:	$\mathbf{1}$	$\mathbf{r}_1$	$\mathbf{r}_2$	$\mathbf{r}_3$	$\mathbf{r}_4$	$\mathbf{r}^2_1$	$\mathbf{r}^2_2$	$\mathbf{r}^2_3$	$\mathbf{r}^2_4$	$\mathbf{R}^2_1$	$\mathbf{R}^2_2$	$\mathbf{R}^2_3$	$\mathbf{R}_1$	$\mathbf{R}_2$	$\mathbf{R}_3$	$\mathbf{R}^3_1$	$\mathbf{R}^3_2$	$\mathbf{R}^3_3$	$\mathbf{i}_1$	$\mathbf{i}_2$	$\mathbf{i}_3$	$\mathbf{i}_4$	$\mathbf{i}_5$	$\mathbf{i}_6$
IJMS:	$\mathbf{1}$	$\mathbf{r}_1$	$\mathbf{r}_2$	$\mathbf{r}_3$	$\mathbf{r}_4$	$\tilde{\mathbf{r}}_1$	$\tilde{\mathbf{r}}_2$	$\tilde{\mathbf{r}}_3$	$\tilde{\mathbf{r}}_4$	ρ_x	ρ_y	ρ_z	$\mathbf{R}_x$	$\mathbf{R}_y$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_x$	$\tilde{\mathbf{R}}_y$	$\tilde{\mathbf{R}}_z$	$\mathbf{i}_1$	$\mathbf{i}_2$	$\mathbf{i}_3$	$\mathbf{i}_4$	$\mathbf{i}_5$	$\mathbf{i}_6$

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$O \supset C_4$ Correlation table shows which $\mathbf{P}^{\mu}$ splittings are allowed:

$O \supset C_4$	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

$\mathbf{P}^{A_1} = \mathbf{P}^{A_1}_{0_4 0_4}$ and $\mathbf{P}^{A_2} = \mathbf{P}^{A_2}_{2_4 2_4}$ *cannot* split

$\mathbf{1}\cdot\mathbf{P}^{\mu} =$	$(\mathbf{p}_{0_4}$	$+\mathbf{p}_{1_4}$	$+\mathbf{p}_{2_4}$	$+\mathbf{p}_{3_4})\cdot\mathbf{P}^{\mu}$
$\mathbf{1}\cdot\mathbf{P}^{A_1} =$	$\mathbf{P}^{A_1}_{0_4 0_4}$	$+0$	$+0$	$+0$
$\mathbf{1}\cdot\mathbf{P}^{A_2} =$	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	$+\mathbf{P}^{T_2}_{1_4 1_4}$	$+\mathbf{P}^{T_2}_{2_4 2_4}$	$+\mathbf{P}^{T_2}_{3_4 3_4}$

O characters

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

C_4 characters

$C_4: d^{m_4}_{\mathbf{R}^p}$	$\mathbf{g}=\mathbf{1}$	$\mathbf{R}^1_z$	$\rho_z = \mathbf{R}^2_z$	$\tilde{\mathbf{R}}_z = \mathbf{R}^3_z$
$m_4 = 0_4$	1	1	1	1
1_4	1	$-i$	-1	i
2_4	1	-1	1	-1
3_4	1	$-i$	-1	$-i$

$O \supset C_4$ splitting done by C_4 projectors applied to O class projectors

$$\mathbf{P}^{E} = \frac{2}{8}\mathbf{1} - \frac{1}{8}\mathbf{c}_r + \frac{2}{8}\mathbf{c}_\rho + \frac{0}{8}\mathbf{c}_R - \frac{0}{8}\mathbf{c}_i$$

$$\mathbf{P}^{T_1} = \frac{3}{8}\mathbf{1} + \frac{0}{8}\mathbf{c}_r - \frac{1}{8}\mathbf{c}_\rho + \frac{1}{8}\mathbf{c}_R - \frac{1}{8}\mathbf{c}_i$$

$$\mathbf{P}^{T_2} = \frac{3}{8}\mathbf{1} + \frac{0}{8}\mathbf{c}_r - \frac{1}{8}\mathbf{c}_\rho - \frac{1}{8}\mathbf{c}_R + \frac{1}{8}\mathbf{c}_i$$

O operators (Two notations: Older Princ.of Symm.Dynamics and Spectra. *and Newer* Int.J.Mol.Sci*)*

PSDS:	$\mathbf{1}$	$\mathbf{r}_1$	$\mathbf{r}_2$	$\mathbf{r}_3$	$\mathbf{r}_4$	$\mathbf{r}^2_1$	$\mathbf{r}^2_2$	$\mathbf{r}^2_3$	$\mathbf{r}^2_4$	$\mathbf{R}^2_1$	$\mathbf{R}^2_2$	$\mathbf{R}^2_3$	$\mathbf{R}_1$	$\mathbf{R}_2$	$\mathbf{R}_3$	$\mathbf{R}^3_1$	$\mathbf{R}^3_2$	$\mathbf{R}^3_3$	$\mathbf{i}_1$	$\mathbf{i}_2$	$\mathbf{i}_3$	$\mathbf{i}_4$	$\mathbf{i}_5$	$\mathbf{i}_6$
IJMS:	$\mathbf{1}$	$\mathbf{r}_1$	$\mathbf{r}_2$	$\mathbf{r}_3$	$\mathbf{r}_4$	$\tilde{\mathbf{r}}_1$	$\tilde{\mathbf{r}}_2$	$\tilde{\mathbf{r}}_3$	$\tilde{\mathbf{r}}_4$	ρ_x	ρ_y	ρ_z	$\mathbf{R}_x$	$\mathbf{R}_y$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_x$	$\tilde{\mathbf{R}}_y$	$\tilde{\mathbf{R}}_z$	$\mathbf{i}_1$	$\mathbf{i}_2$	$\mathbf{i}_3$	$\mathbf{i}_4$	$\mathbf{i}_5$	$\mathbf{i}_6$

Splitting O class projectors $\mathbf{P}^\mu$ into irreducible projectors $\mathbf{P}^\mu_{m_4 m_4}$ for $O\supset C_4$

$O\supset C_4$ Correlation table shows which $\mathbf{P}^\mu$ splittings are allowed:

$O\supset C_4$	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

$\mathbf{P}^{A_1}=\mathbf{P}^{A_1}_{0_4 0_4}$ and $\mathbf{P}^{A_2}=\mathbf{P}^{A_2}_{2_4 2_4}$ *cannot* split

$\mathbf{1}\cdot\mathbf{P}^\mu =$	$(\mathbf{p}_{0_4}$	$+\mathbf{p}_{1_4}$	$+\mathbf{p}_{2_4}$	$+\mathbf{p}_{3_4})\cdot\mathbf{P}^\mu$
$\mathbf{1}\cdot\mathbf{P}^{A_1} =$	$\mathbf{P}^{A_1}_{0_4 0_4}$	$+0$	$+0$	$+0$
$\mathbf{1}\cdot\mathbf{P}^{A_2} =$	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	$+\mathbf{P}^{T_2}_{1_4 1_4}$	$+\mathbf{P}^{T_2}_{2_4 2_4}$	$+\mathbf{P}^{T_2}_{3_4 3_4}$

O characters

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

C_4 characters

$C_4: d^{m_4}_{\mathbf{R}^p}$	$\mathbf{g}=\mathbf{1}$	$\mathbf{R}_z^1$	$\rho_z=\mathbf{R}_z^2$	$\tilde{\mathbf{R}}_z=\mathbf{R}_z^3$
$m_4=0_4$	1	1	1	1
1_4	1	$-i$	-1	i
2_4	1	-1	1	-1
3_4	1	$-i$	-1	$-i$

$O\supset C_4$ splitting done by C_4 projectors applied to O class projectors

$$\mathbf{p}_{m_4}=\frac{1}{4}\sum_{p=0}^{3}\underbrace{e^{\frac{2\pi i m_4\cdot p}{4}}}_{C_4\ \text{characters}}\mathbf{R}_z^p=\begin{cases}\mathbf{p}_{0_4}=(\mathbf{1}+\mathbf{R}_z+\rho_z+\tilde{\mathbf{R}}_z)/4\\ \mathbf{p}_{1_4}=(\mathbf{1}+i\mathbf{R}_z-\rho_z-i\tilde{\mathbf{R}}_z)/4\\ \mathbf{p}_{2_4}=(\mathbf{1}-\mathbf{R}_z+\rho_z-\tilde{\mathbf{R}}_z)/4\\ \mathbf{p}_{3_4}=(\mathbf{1}-i\mathbf{R}_z-\rho_z+i\tilde{\mathbf{R}}_z)/4\end{cases}$$

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

$$\mathbf{P}^E=\frac{2}{8}\mathbf{1}-\frac{1}{8}\mathbf{c}_r+\frac{2}{8}\mathbf{c}_\rho+\frac{0}{8}\mathbf{c}_R-\frac{0}{8}\mathbf{c}_i$$

$$\mathbf{P}^{T_1}=\frac{3}{8}\mathbf{1}+\frac{0}{8}\mathbf{c}_r-\frac{1}{8}\mathbf{c}_\rho+\frac{1}{8}\mathbf{c}_R-\frac{1}{8}\mathbf{c}_i$$

$$\mathbf{P}^{T_2}=\frac{3}{8}\mathbf{1}+\frac{0}{8}\mathbf{c}_r-\frac{1}{8}\mathbf{c}_\rho-\frac{1}{8}\mathbf{c}_R+\frac{1}{8}\mathbf{c}_i$$

O operators (Two notations: Older Princ.of Symm.Dynamics and Spectra. *and Newer* Int.J.Mol.Sci*)*

PSDS:	$\mathbf{1}$	$\mathbf{r}_1$	$\mathbf{r}_2$	$\mathbf{r}_3$	$\mathbf{r}_4$	$\mathbf{r}_1^2$	$\mathbf{r}_2^2$	$\mathbf{r}_3^2$	$\mathbf{r}_4^2$	$\mathbf{R}_1^2$	$\mathbf{R}_2^2$	$\mathbf{R}_3^2$	$\mathbf{R}_1$	$\mathbf{R}_2$	$\mathbf{R}_3$	$\mathbf{R}_1^3$	$\mathbf{R}_2^3$	$\mathbf{R}_3^3$	$\mathbf{i}_1$	$\mathbf{i}_2$	$\mathbf{i}_3$	$\mathbf{i}_4$	$\mathbf{i}_5$	$\mathbf{i}_6$
IJMS:	$\mathbf{1}$	$\mathbf{r}_1$	$\mathbf{r}_2$	$\mathbf{r}_3$	$\mathbf{r}_4$	$\tilde{\mathbf{r}}_1$	$\tilde{\mathbf{r}}_2$	$\tilde{\mathbf{r}}_3$	$\tilde{\mathbf{r}}_4$	ρ_x	ρ_y	ρ_z	$\mathbf{R}_x$	$\mathbf{R}_y$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_x$	$\tilde{\mathbf{R}}_y$	$\tilde{\mathbf{R}}_z$	$\mathbf{i}_1$	$\mathbf{i}_2$	$\mathbf{i}_3$	$\mathbf{i}_4$	$\mathbf{i}_5$	$\mathbf{i}_6$

Splitting O class projectors $\mathbf{P}^{\mu}$ into irreducible projectors $\mathbf{P}^{\mu}_{m_4 m_4}$ for $O \supset C_4$

$O \supset C_4$ Correlation table shows which $\mathbf{P}^{\mu}$ splittings are allowed:

$O \supset C_4$	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

$\mathbf{P}^{A_1} = \mathbf{P}^{A_1}_{0_4 0_4}$ and $\mathbf{P}^{A_2} = \mathbf{P}^{A_2}_{2_4 2_4}$ *cannot* split

$1 \cdot \mathbf{P}^{\mu} =$	$(\mathbf{p}_{0_4}$	$+\mathbf{p}_{1_4}$	$+\mathbf{p}_{2_4}$	$+\mathbf{p}_{3_4}) \cdot \mathbf{P}^{\mu}$
$1 \cdot \mathbf{P}^{A_1} =$	$\mathbf{P}^{A_1}_{0_4 0_4}$	+0	+0	+0
$1 \cdot \mathbf{P}^{A_2} =$	0	+0	$+\mathbf{P}^{A_2}_{2_4 2_4}$	+0
$1 \cdot \mathbf{P}^{E} =$	$\mathbf{P}^{E}_{0_4 0_4}$	+0	$+\mathbf{P}^{E}_{2_4 2_4}$	+0
$1 \cdot \mathbf{P}^{T_1} =$	$\mathbf{P}^{T_1}_{0_4 0_4}$	$+\mathbf{P}^{T_1}_{1_4 1_4}$	+0	$+\mathbf{P}^{T_1}_{3_4 3_4}$
$1 \cdot \mathbf{P}^{T_2} =$	0	$+\mathbf{P}^{T_2}_{1_4 1_4}$	$+\mathbf{P}^{T_2}_{2_4 2_4}$	$+\mathbf{P}^{T_2}_{3_4 3_4}$

O characters

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

C_4 characters

$C_4: d^{m_4}_{\mathbf{R}^p}$	$\mathbf{g}=1$	$\mathbf{R}^1_z$	$\rho_z = \mathbf{R}^2_z$	$\tilde{\mathbf{R}}_z = \mathbf{R}^3_z$
$m_4 = 0_4$	1	1	1	1
1_4	1	$-i$	-1	i
2_4	1	-1	1	-1
3_4	1	$-i$	-1	$-i$

$O \supset C_4$ splitting done by C_4 projectors applied to O class projectors

$$\mathbf{p}_{m_4} = \frac{1}{4}\sum_{p=0}^{3} \underbrace{e^{\frac{2\pi i m_4 \cdot p}{4}}}_{C_4 \text{ characters}} \mathbf{R}^p_z = \begin{cases} \mathbf{p}_{0_4} = (1+\mathbf{R}_z+\rho_z+\tilde{\mathbf{R}}_z)/4 \\ \mathbf{p}_{1_4} = (1+i\mathbf{R}_z-\rho_z-i\tilde{\mathbf{R}}_z)/4 \\ \mathbf{p}_{2_4} = (1-\mathbf{R}_z+\rho_z-\tilde{\mathbf{R}}_z)/4 \\ \mathbf{p}_{3_4} = (1-i\mathbf{R}_z-\rho_z+i\tilde{\mathbf{R}}_z)/4 \end{cases}$$

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

$$\mathbf{P}^{E} = \frac{2}{8}\mathbf{1} - \frac{1}{8}\mathbf{c}_r + \frac{2}{8}\mathbf{c}_\rho + \frac{0}{8}\mathbf{c}_R - \frac{0}{8}\mathbf{c}_i$$

$$\mathbf{P}^{T_1} = \frac{3}{8}\mathbf{1} + \frac{0}{8}\mathbf{c}_r - \frac{1}{8}\mathbf{c}_\rho + \frac{1}{8}\mathbf{c}_R - \frac{1}{8}\mathbf{c}_i$$

$$\mathbf{P}^{T_2} = \frac{3}{8}\mathbf{1} + \frac{0}{8}\mathbf{c}_r - \frac{1}{8}\mathbf{c}_\rho - \frac{1}{8}\mathbf{c}_R + \frac{1}{8}\mathbf{c}_i$$

Following development of irreducible projectors:

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

O operators (Two notations: Older Princ.of Symm.Dynamics and Spectra. and Newer Int.J.Mol.Sci)

PSDS:	$\mathbf{1}$	$\mathbf{r}_1$	$\mathbf{r}_2$	$\mathbf{r}_3$	$\mathbf{r}_4$	$\mathbf{r}^2_1$	$\mathbf{r}^2_2$	$\mathbf{r}^2_3$	$\mathbf{r}^2_4$	$\mathbf{R}^2_1$	$\mathbf{R}^2_2$	$\mathbf{R}^2_3$	$\mathbf{R}_1$	$\mathbf{R}_2$	$\mathbf{R}_3$	$\mathbf{R}^3_1$	$\mathbf{R}^3_2$	$\mathbf{R}^3_3$	$\mathbf{i}_1$	$\mathbf{i}_2$	$\mathbf{i}_3$	$\mathbf{i}_4$	$\mathbf{i}_5$	$\mathbf{i}_6$
IJMS:	$\mathbf{1}$	$\mathbf{r}_1$	$\mathbf{r}_2$	$\mathbf{r}_3$	$\mathbf{r}_4$	$\tilde{\mathbf{r}}_1$	$\tilde{\mathbf{r}}_2$	$\tilde{\mathbf{r}}_3$	$\tilde{\mathbf{r}}_4$	ρ_x	ρ_y	ρ_z	$\mathbf{R}_x$	$\mathbf{R}_y$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_x$	$\tilde{\mathbf{R}}_y$	$\tilde{\mathbf{R}}_z$	$\mathbf{i}_1$	$\mathbf{i}_2$	$\mathbf{i}_3$	$\mathbf{i}_4$	$\mathbf{i}_5$	$\mathbf{i}_6$

Splitting O *class projectors* $\mathbf{P}^{\mu}$ *into irreducible projectors* $\mathbf{P}^{\mu}_{m_4 m_4}$ *for* O⊃C_4

O⊃C_4 *Correlation table shows which* $\mathbf{P}^{\mu}$ *splittings are allowed:*

O⊃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

$\mathbf{P}^{A_1}=\mathbf{P}^{A_1}_{0_4 0_4}$ and $\mathbf{P}^{A_2}=\mathbf{P}^{A_2}_{2_4 2_4}$ *cannot* split

$\mathbf{1}\cdot\mathbf{P}^{\mu}=$	$(\mathbf{p}_{0_4}$	$+\mathbf{p}_{1_4}$	$+\mathbf{p}_{2_4}$	$+\mathbf{p}_{3_4})\cdot\mathbf{P}^{\mu}$
$\mathbf{1}\cdot\mathbf{P}^{A_1}=$	$\mathbf{P}^{A_1}_{0_4 0_4}$	+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	$+\mathbf{P}^{T_2}_{1_4 1_4}$	$+\mathbf{P}^{T_2}_{2_4 2_4}$	$+\mathbf{P}^{T_2}_{3_4 3_4}$

O characters

$O:\chi^{\mu}_{\mathbf{g}}$	$\mathbf{g}$=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

C_4 characters

$C_4:d^{m_4}_{\mathbf{R}^p}$	$\mathbf{g}$=1	$\mathbf{R}^1_z$	$\rho_z=\mathbf{R}^2_z$	$\tilde{\mathbf{R}}_z=\mathbf{R}^3_z$
$m_4=0_4$	1	1	1	1
1_4	1	$-i$	-1	i
2_4	1	-1	1	-1
3_4	1	$-i$	-1	$-i$

O⊃C_4 *splitting done by* C_4 *projectors applied to O class projectors*

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

C_4 characters

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

$$\mathbf{P}^{E}=\frac{2}{8}\mathbf{1}-\frac{1}{8}\mathbf{c}_r+\frac{2}{8}\mathbf{c}_\rho+\frac{0}{8}\mathbf{c}_R-\frac{0}{8}\mathbf{c}_i$$

$$\mathbf{P}^{T_1}=\frac{3}{8}\mathbf{1}+\frac{0}{8}\mathbf{c}_r-\frac{1}{8}\mathbf{c}_\rho+\frac{1}{8}\mathbf{c}_R-\frac{1}{8}\mathbf{c}_i$$

$$\mathbf{P}^{T_2}=\frac{3}{8}\mathbf{1}+\frac{0}{8}\mathbf{c}_r-\frac{1}{8}\mathbf{c}_\rho-\frac{1}{8}\mathbf{c}_R+\frac{1}{8}\mathbf{c}_i$$

Following development of irreducible projectors:

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

...with examples:

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

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

etc.

O operators (Two notations: Older Princ.of Symm.Dynamics and Spectra. *and Newer* Int.J.Mol.Sci*)*

PSDS:	1	$\mathbf{r}_1$	$\mathbf{r}_2$	$\mathbf{r}_3$	$\mathbf{r}_4$	$\mathbf{r}^2_1$	$\mathbf{r}^2_2$	$\mathbf{r}^2_3$	$\mathbf{r}^2_4$	$\mathbf{R}^2_1$	$\mathbf{R}^2_2$	$\mathbf{R}^2_3$	$\mathbf{R}_1$	$\mathbf{R}_2$	$\mathbf{R}_3$	$\mathbf{R}^3_1$	$\mathbf{R}^3_2$	$\mathbf{R}^3_3$	$\mathbf{i}_1$	$\mathbf{i}_2$	$\mathbf{i}_3$	$\mathbf{i}_4$	$\mathbf{i}_5$	$\mathbf{i}_6$
IJMS:	1	$\mathbf{r}_1$	$\mathbf{r}_2$	$\mathbf{r}_3$	$\mathbf{r}_4$	$\tilde{\mathbf{r}}_1$	$\tilde{\mathbf{r}}_2$	$\tilde{\mathbf{r}}_3$	$\tilde{\mathbf{r}}_4$	ρ_x	ρ_y	ρ_z	$\mathbf{R}_x$	$\mathbf{R}_y$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_x$	$\tilde{\mathbf{R}}_y$	$\tilde{\mathbf{R}}_z$	$\mathbf{i}_1$	$\mathbf{i}_2$	$\mathbf{i}_3$	$\mathbf{i}_4$	$\mathbf{i}_5$	$\mathbf{i}_6$

AMOP reference links on page 2

3.07.18 class 16.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Discrete symmetry subgroups of O(3)⊃(Octahedral O_h⊃O): Deriving $D^{(\alpha)}$-matrices defined by subgroup-chains $O\supset D_4\supset C_4$, $O\supset D_4\supset D_2$, and $O\supset D_3\supset C_3$ applications to IR spectra of SF_6

Review Octahedral $O_h\supset O$ *group operator structure*

Review Octahedral $O_h\supset O\supset D_4\supset C_4$ *subgroup chain correlations*

Comparison of $O\supset D_4\supset C_4$ *and* $O\supset D_4\supset D_2$ *correlations and level/projector splitting*

- $O\supset D_4\supset C_4$ *subgroup chain splitting*
- $O\supset D_4\supset D_2$ *subgroup chain splitting (nOrmal* D_2 *vs. unOrmal* D_2*)*
- $O_h\supset O\supset D_4\supset C_{4v}$ *and* $O_h\supset O\supset D_4\supset C_{4v}\supset C_{2v}$ *subgroup splitting*

Splitting O *class projectors* $\mathbf{P}^\mu$ *into irreducible projectors* $\mathbf{P}^\mu_{m_4m_4}$ *for* $O\supset C_4$

- *Left-cosets and coefficient arrays*

Development of irreducible projectors $\mathbf{P}^\mu_{m_4m_4}$ *and representations* $D^\mu_{m_4m_4}$

- *Calculating* $\mathbf{P}^E_{0_40_4}$, $\mathbf{P}^E_{2_42_4}$, $\mathbf{P}^{T_1}_{0_40_4}$, $\mathbf{P}^{T_1}_{1_41_4}$, $\mathbf{P}^{T_2}_{2_42_4}$, $\mathbf{P}^{T_2}_{1_41_4}$, *Collected* $\mathbf{P}_{mm}$ *results Table*

$O\supset C_4$ *induced representation* $0_4(C_4)\uparrow O \sim A_1\oplus T_1\oplus E$ *and spectral analysis examples*

- *Elementary induced representation* $0_4(C_4)\uparrow O$
- *Projection reduction of induced representation* $0_4(C_4)\uparrow O$
- *Introduction to ortho-complete eigenvalue-parameter relations*
  - *Examples in* SF_6 *spectroscopy*

Splitting O *class projectors* $\mathbf{P}^{\mu}$ *into irreducible projectors* $\mathbf{P}^{\mu}_{m_4 m_4}$ *for* O⊃C_4

O⊃C_4 *Correlation table shows which* $\mathbf{P}^{\mu}$ *splittings are allowed:*

O⊃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

$\mathbf{P}^{A_1} = \mathbf{P}^{A_1}_{0_4 0_4}$ and $\mathbf{P}^{A_2} = \mathbf{P}^{A_2}_{2_4 2_4}$ *cannot* split

$1\cdot\mathbf{P}^{\mu} =$	$(\mathbf{p}_{0_4}$	$+\mathbf{p}_{1_4}$	$+\mathbf{p}_{2_4}$	$+\mathbf{p}_{3_4})\cdot\mathbf{P}^{\mu}$
$1\cdot\mathbf{P}^{A_1} =$	$\mathbf{P}^{A_1}_{0_4 0_4}$	+0	+0	+0
$1\cdot\mathbf{P}^{A_2} =$	0	+0	$+\mathbf{P}^{A_2}_{2_4 2_4}$	+0
$1\cdot\mathbf{P}^{E} =$	$\mathbf{P}^{E}_{0_4 0_4}$	+0	$+\mathbf{P}^{E}_{2_4 2_4}$	+0
$1\cdot\mathbf{P}^{T_1} =$	$\mathbf{P}^{T_1}_{0_4 0_4}$	$+\mathbf{P}^{T_1}_{1_4 1_4}$	+0	$+\mathbf{P}^{T_1}_{3_4 3_4}$
$1\cdot\mathbf{P}^{T_2} =$	0	$+\mathbf{P}^{T_2}_{1_4 1_4}$	$+\mathbf{P}^{T_2}_{2_4 2_4}$	$+\mathbf{P}^{T_2}_{3_4 3_4}$

O characters

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

C_4 characters

$C_4: d^{m_4}_{\mathbf{R}^p}$	$\mathbf{g}=1$	$\mathbf{R}^1_z$	$\rho_z=\mathbf{R}^2_z$	$\tilde{\mathbf{R}}_z=\mathbf{R}^3_z$
$m_4=0_4$	1	1	1	1
1_4	1	$-i$	-1	i
2_4	1	-1	1	-1
3_4	1	$-i$	-1	$-i$

O⊃C_4 *splitting done by* C_4 *projectors applied to O class projectors*

$$\mathbf{p}_{m_4} = \frac{1}{4}\sum_{p=0}^{3} \underbrace{e^{\frac{2\pi i m_4\cdot p}{4}}}_{C_4 \text{ characters}} \mathbf{R}^p_z = \begin{cases} \mathbf{p}_{0_4} = (1+\mathbf{R}_z+\rho_z+\tilde{\mathbf{R}}_z)/4 \\ \mathbf{p}_{1_4} = (1+i\mathbf{R}_z-\rho_z-i\tilde{\mathbf{R}}_z)/4 \\ \mathbf{p}_{2_4} = (1-\mathbf{R}_z+\rho_z-\tilde{\mathbf{R}}_z)/4 \\ \mathbf{p}_{3_4} = (1-i\mathbf{R}_z-\rho_z+i\tilde{\mathbf{R}}_z)/4 \end{cases}$$

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

$$\mathbf{P}^{E} = \frac{2}{8}\mathbf{1} - \frac{1}{8}\mathbf{c}_r + \frac{2}{8}\mathbf{c}_\rho + \frac{0}{8}\mathbf{c}_R - \frac{0}{8}\mathbf{c}_i$$

$$\mathbf{P}^{T_1} = \frac{3}{8}\mathbf{1} + \frac{0}{8}\mathbf{c}_r - \frac{1}{8}\mathbf{c}_\rho + \frac{1}{8}\mathbf{c}_R - \frac{1}{8}\mathbf{c}_i$$

$$\mathbf{P}^{T_2} = \frac{3}{8}\mathbf{1} + \frac{0}{8}\mathbf{c}_r - \frac{1}{8}\mathbf{c}_\rho - \frac{1}{8}\mathbf{c}_R + \frac{1}{8}\mathbf{c}_i$$

Following development of irreducible projectors:

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

...with examples:

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

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

etc.

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

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

O operators (Two notations: Older Princ.of Symm.Dynamics and Spectra. *and Newer* Int.J.Mol.Sci*)*

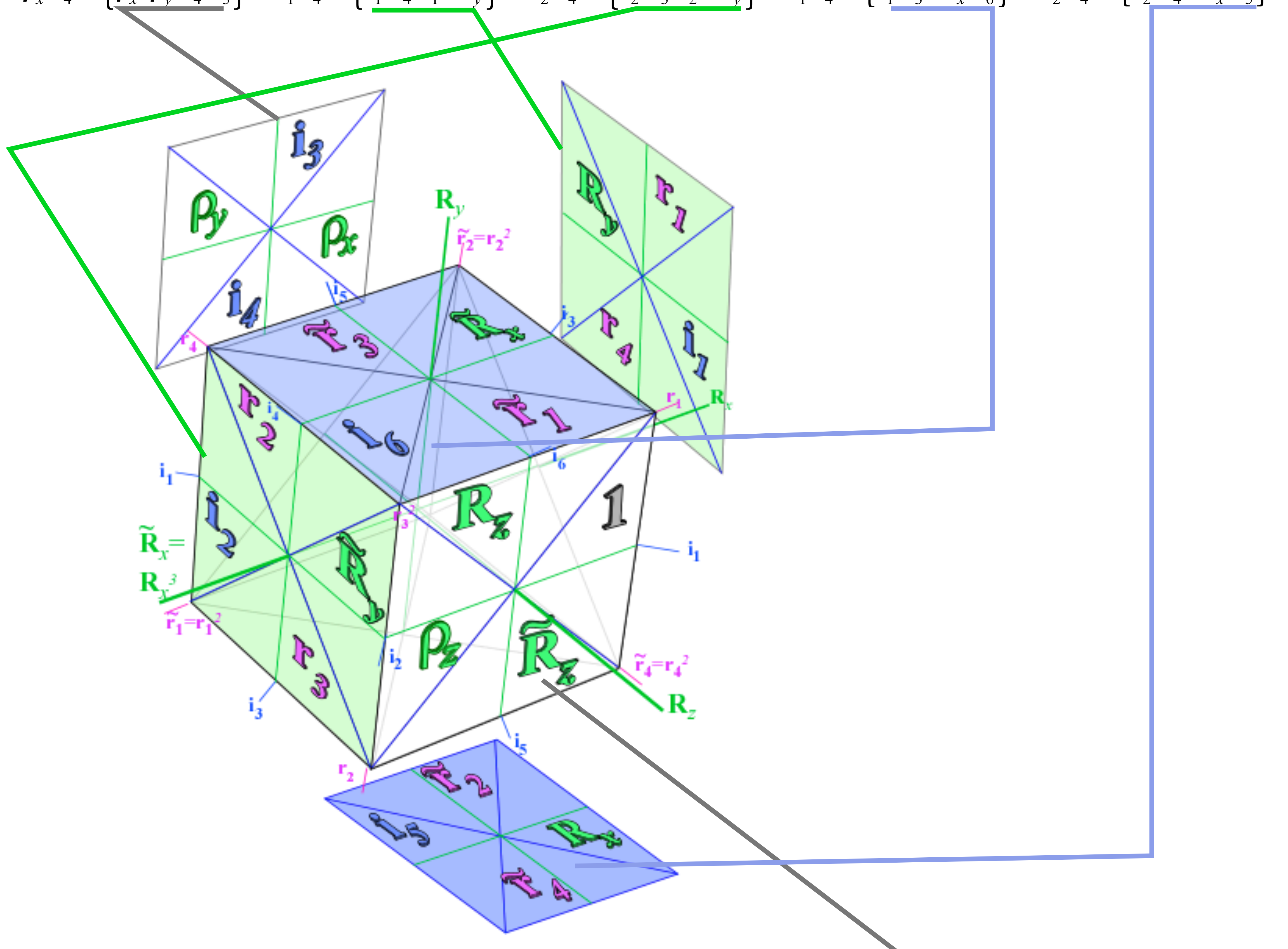
PSDS:	1	$\mathbf{r}_1$	$\mathbf{r}_2$	$\mathbf{r}_3$	$\mathbf{r}_4$	$\mathbf{r}^2_1$	$\mathbf{r}^2_2$	$\mathbf{r}^2_3$	$\mathbf{r}^2_4$	$\mathbf{R}^2_1$	$\mathbf{R}^2_2$	$\mathbf{R}^2_3$	$\mathbf{R}_1$	$\mathbf{R}_2$	$\mathbf{R}_3$	$\mathbf{R}^3_1$	$\mathbf{R}^3_2$	$\mathbf{R}^3_3$	$\mathbf{i}_1$	$\mathbf{i}_2$	$\mathbf{i}_3$	$\mathbf{i}_4$	$\mathbf{i}_5$	$\mathbf{i}_6$
IJMS:	1	$\mathbf{r}_1$	$\mathbf{r}_2$	$\mathbf{r}_3$	$\mathbf{r}_4$	$\tilde{\mathbf{r}}_1$	$\tilde{\mathbf{r}}_2$	$\tilde{\mathbf{r}}_3$	$\tilde{\mathbf{r}}_4$	ρ_x	ρ_y	ρ_z	$\mathbf{R}_x$	$\mathbf{R}_y$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_x$	$\tilde{\mathbf{R}}_y$	$\tilde{\mathbf{R}}_z$	$\mathbf{i}_1$	$\mathbf{i}_2$	$\mathbf{i}_3$	$\mathbf{i}_4$	$\mathbf{i}_5$	$\mathbf{i}_6$

Following development of irreducible projectors:

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

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

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

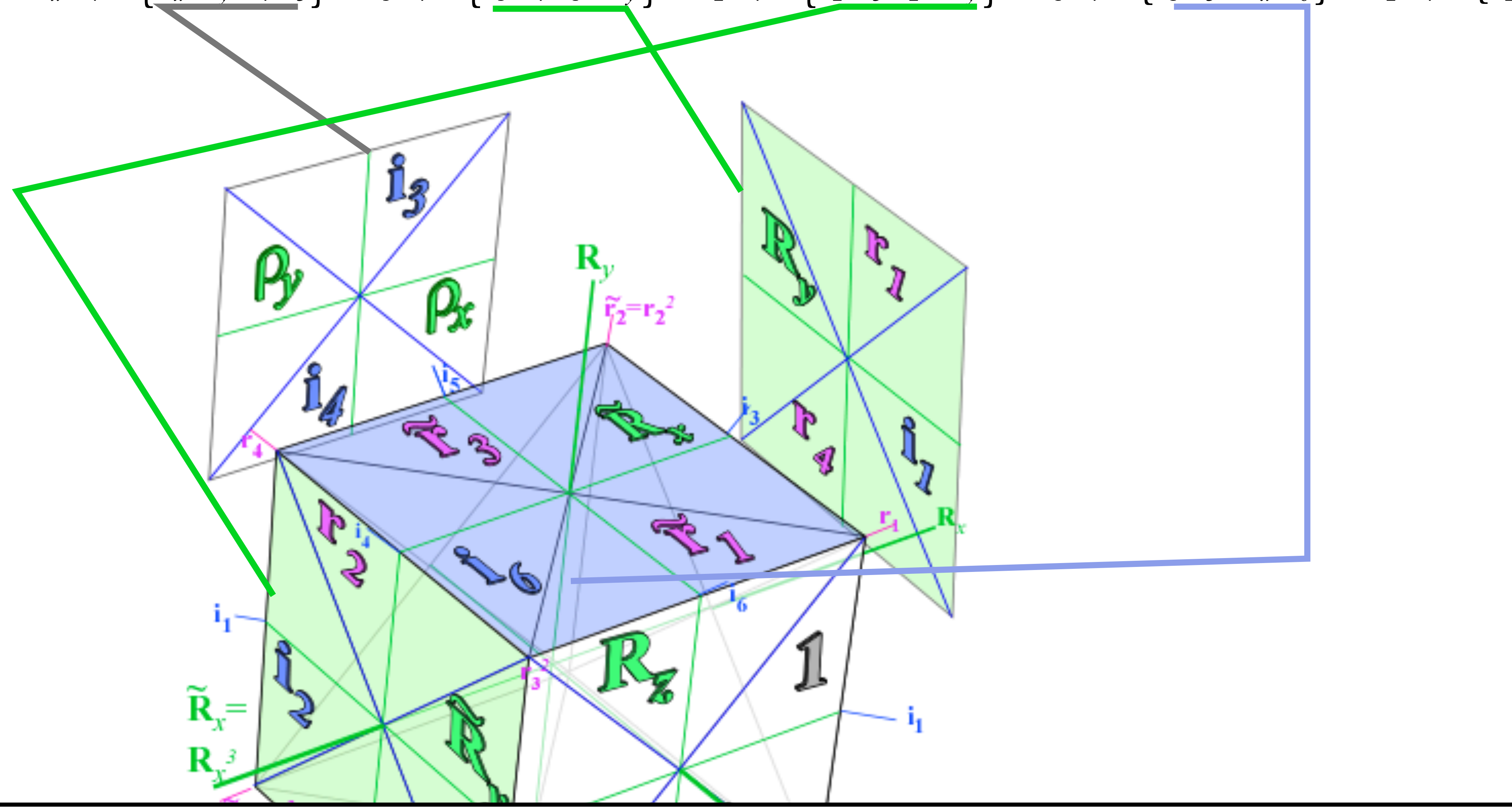


Following development of irreducible projectors:

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

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

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



$[1,\rho_z,R_z,\tilde{R}_z]$	$[\rho_x,\rho_y,i_4,i_3]$	$[r_1,r_4,i_1,R_y]$	$[r_2,r_3,i_2,\tilde{R}_y]$	$[\tilde{r}_1,\tilde{r}_3,\tilde{R}_x,i_6]$	$[\tilde{r}_2,\tilde{r}_4,R_x,i_5]$	Cosets of C_4
$1\ (1,\rho_z,R_z,\tilde{R}_z)$,	$\rho_x(1,\rho_z,R_z,\tilde{R}_z)$,	$r_1(1,\rho_z,R_z,\tilde{R}_z)$,	$r_2(1,\rho_z,R_z,\tilde{R}_z)$,	$\tilde{r}_1(1,\rho_z,R_z,\tilde{R}_z)$,	$\tilde{r}_2(1,\rho_z,R_z,\tilde{R}_z)$	made from
$\rho_z(\rho_z,1,\tilde{R}_z,R_z)$,	$\rho_y(\rho_z,1,\tilde{R}_z,R_z)$,	$r_4(\rho_z,1,\tilde{R}_z,R_z)$,	$r_3(\rho_z,1,\tilde{R}_z,R_z)$,	$\tilde{r}_3(\rho_z,1,\tilde{R}_z,R_z)$,	$\tilde{r}_4(\rho_z,1,\tilde{R}_z,R_z)$	C_4 operators
$R_z(\tilde{R}_z,R_z,1,\rho_z)$,	$i_4(\tilde{R}_z,R_z,1,\rho_z)$,	$i_1(\tilde{R}_z,R_z,1,\rho_z)$,	$i_2(\tilde{R}_z,R_z,1,\rho_z)$,	$\tilde{R}_x(\tilde{R}_z,R_z,1,\rho_z)$,	$R_x(\tilde{R}_z,R_z,1,\rho_z)$	reordered by
$\tilde{R}_z(R_z,\tilde{R}_z,\rho_z,1)$,	$i_3(R_z,\tilde{R}_z,\rho_z,1)$,	$R_y(R_z,\tilde{R}_z,\rho_z,1)$,	$\tilde{R}_y(R_z,\tilde{R}_z,\rho_z,1)$,	$i_6(R_z,\tilde{R}_z,\rho_z,1)$,	$i_5(R_z,\tilde{R}_z,\rho_z,1)$	their own action!

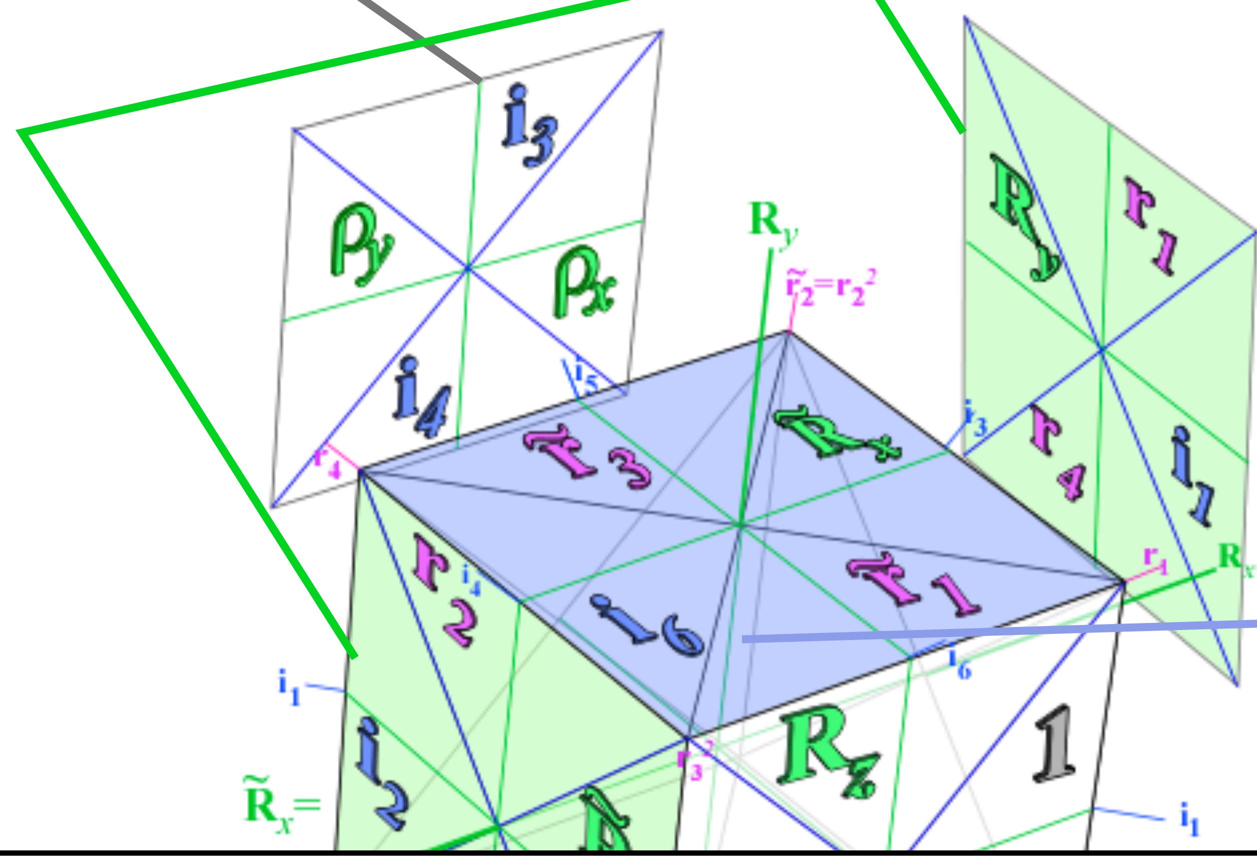
C_4 reodering itself

Following development of irreducible projectors:

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

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

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



Coset array that helps sum character products for O projector splitting

	$\mathbf{1}$	ρ_z	R_z	$\tilde{R}_z$
$\mathbf{1}$	$\mathbf{1}$	ρ_z	R_z	$\tilde{R}_z$
ρ_z	ρ_z	$\mathbf{1}$	$\tilde{R}_z$	R_z
R_z	$\tilde{R}_z$	R_z	$\mathbf{1}$	ρ_z
$\tilde{R}_z$	R_z	$\tilde{R}_z$	ρ_z	$\mathbf{1}$

	ρ_x	ρ_y	i_4	i_3
ρ_x	$\mathbf{1}$	ρ_z	R_z	$\tilde{R}_z$
ρ_y	ρ_z	$\mathbf{1}$	$\tilde{R}_z$	R_z
i_4	$\tilde{R}_z$	R_z	$\mathbf{1}$	ρ_z
i_3	R_z	$\tilde{R}_z$	ρ_z	$\mathbf{1}$

	r_1	r_4	i_1	R_y
r_1	$\mathbf{1}$	ρ_z	R_z	$\tilde{R}_z$
r_4	ρ_z	$\mathbf{1}$	$\tilde{R}_z$	R_z
i_1	$\tilde{R}_z$	R_z	$\mathbf{1}$	ρ_z
R_y	R_z	$\tilde{R}_z$	ρ_z	$\mathbf{1}$

	r_2	r_3	i_2	$\tilde{R}_y$
r_2	$\mathbf{1}$	ρ_z	R_z	$\tilde{R}_z$
r_3	ρ_z	$\mathbf{1}$	$\tilde{R}_z$	R_z
i_2	$\tilde{R}_z$	R_z	$\mathbf{1}$	ρ_z
$\tilde{R}_y$	R_z	$\tilde{R}_z$	ρ_z	$\mathbf{1}$

	$\tilde{r}_1$	$\tilde{r}_3$	$\tilde{R}_x$	i_6
$\tilde{r}_1$	$\mathbf{1}$	ρ_z	R_z	$\tilde{R}_z$
$\tilde{r}_3$	ρ_z	$\mathbf{1}$	$\tilde{R}_z$	R_z
$\tilde{R}_x$	$\tilde{R}_z$	R_z	$\mathbf{1}$	ρ_z
i_6	R_z	$\tilde{R}_z$	ρ_z	$\mathbf{1}$

	$\tilde{r}_2$	$\tilde{r}_4$	R_x	i_5
$\tilde{r}_2$	$\mathbf{1}$	ρ_z	R_z	$\tilde{R}_z$
$\tilde{r}_4$	ρ_z	$\mathbf{1}$	$\tilde{R}_z$	R_z
R_x	$\tilde{R}_z$	R_z	$\mathbf{1}$	ρ_z
i_5	R_z	$\tilde{R}_z$	ρ_z	$\mathbf{1}$

AMOP reference links on page 2

3.07.18 class 16.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Discrete symmetry subgroups of O(3)⊃(Octahedral O_h⊃O): Deriving $D^{(\alpha)}$-matrices defined by subgroup-chains $O\supset D_4\supset C_4$, $O\supset D_4\supset D_2$, and $O\supset D_3\supset C_3$ applications to IR spectra of SF_6

Review Octahedral $O_h\supset O$ group operator structure

Review Octahedral $O_h\supset O\supset D_4\supset C_4$ subgroup chain correlations

Comparison of $O\supset D_4\supset C_4$ and $O\supset D_4\supset D_2$ correlations and level/projector splitting

- *$O\supset D_4\supset C_4$ subgroup chain splitting*
- *$O\supset D_4\supset D_2$ subgroup chain splitting (nOrmal D_2 vs. unOrmal D_2)*
- *$O_h\supset O\supset D_4\supset C_{4v}$ and $O_h\supset O\supset D_4\supset C_{4v}\supset C_{2v}$ subgroup splitting*

Splitting O class projectors $\mathbf{P}^{\mu}$ into irreducible projectors $\mathbf{P}^{\mu}_{m_4m_4}$ for $O\supset C_4$

- *Left-cosets and coefficient arrays*

Development of irreducible projectors $\mathbf{P}^{\mu}_{m_4m_4}$ and representations $D^{\mu}_{m_4m_4}$

- *Calculating $\mathbf{P}^{E}_{0_40_4}$, $\mathbf{P}^{E}_{2_42_4}$, $\mathbf{P}^{T_1}_{0_40_4}$, $\mathbf{P}^{T_1}_{1_41_4}$, $\mathbf{P}^{T_2}_{2_42_4}$, $\mathbf{P}^{T_2}_{1_41_4}$, Collected $\mathbf{P}_{mm}$ results Table*

$O\supset C_4$ induced representation $0_4(C_4)\uparrow O\sim A_1\oplus T_1\oplus E$ and spectral analysis examples

- *Elementary induced representation $0_4(C_4)\uparrow O$*
- *Projection reduction of induced representation $0_4(C_4)\uparrow O$*
- *Introduction to ortho-complete eigenvalue-parameter relations*
  - *Examples in SF_6 spectroscopy*

General development of O⊃C_4 *irreducible projectors* $\mathbf{P}^{\mu}_{m_4 m_4} = \sum_g^{{}^\circ O} \frac{\ell^\mu}{{}^\circ O} D^{\mu *}_{m_4 m_4}(g)\,\mathbf{g}$

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

Deriving diagonal irreducible O-representation components $D^{\mu *}_{m_4 m_4}(g)$

$$= \sum_g^{{}^\circ O} \frac{\ell^\mu}{{}^\circ O}(\chi_g^{\mu *})\cdot \mathbf{g}\left(\mathbf{p}^{m_4}\right)$$

$$= \left(\frac{\ell^\mu}{24}\right)\left(\chi_{\mathbf{1}}^{\mu *}\right)\cdot \mathbf{1}\left(\mathbf{1} + d_{\rho_z}^{m_4}\,\boldsymbol{\rho}_z + d_{R_z}^{m_4}\,\mathbf{R}_z + d_{\tilde{R}_z}^{m_4}\,\tilde{\mathbf{R}}_z\right)\frac{1}{4}$$

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$$\boldsymbol{\rho}_x C_4 = \boldsymbol{\rho}_x\left\{\mathbf{1},\boldsymbol{\rho}_z,\mathbf{R}_z,\tilde{\mathbf{R}}_z\right\} = \left\{\boldsymbol{\rho}_x,\boldsymbol{\rho}_y,\mathbf{i}_4,\mathbf{i}_3\right\} Coset$$

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O characters

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

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

C_4 characters

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

$$\mathbf{r}_1 C_4 = \mathbf{r}_1\left\{\mathbf{1},\boldsymbol{\rho}_z,\mathbf{R}_z,\tilde{\mathbf{R}}_z\right\} = \left\{\mathbf{r}_1,\mathbf{r}_4,\mathbf{i}_1,\mathbf{R}_y\right\} Coset$$

General development of irep projectors $\mathbf{P}^{\mu}_{m_4m_4} = \sum_{g}^{\circ O} \frac{\ell^{\mu}}{\circ O} D^{\mu *}_{m_4m_4}(g)\,\mathbf{g}$ *for subgroup chain* $O \supset D_4 \supset C_4$

$\mathbf{P}^{\mu}_{m_4m_4} = \mathbf{p}^{m_4}\mathbf{P}^{\mu} = \mathbf{P}^{\mu}\mathbf{p}^{m_4}$

(Deriving diagonal irreducible *O*-representation ("irep") components $D^{\mu *}_{m_4m_4}(g)$

$= \sum_{g}^{\circ O} \frac{\ell^{\mu}}{\circ O}(\chi^{\mu *}_{g})\cdot \mathbf{g}\left(\mathbf{p}^{m_4}\right)$

$= \left(\frac{\ell^{\mu}}{24}\right)\left(\chi^{\mu *}_{\mathbf{1}}\right)\cdot \mathbf{1}\left(\mathbf{1} + d^{m_4}_{\rho_z}\boldsymbol{\rho}_z + d^{m_4}_{R_z}\mathbf{R}_z + d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right)\frac{1}{4} \quad = \left(\frac{\ell^{\mu}\chi^{\mu *}_{\mathbf{1}}}{96}\right)\left(1\cdot\mathbf{1} + d^{m_4}_{\rho_z}\boldsymbol{\rho}_z + d^{m_4}_{R_z}\mathbf{R}_z + d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right)$

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$\boldsymbol{\rho}_x C_4 = \boldsymbol{\rho}_x\left\{\mathbf{1},\boldsymbol{\rho}_z,\mathbf{R}_z,\tilde{\mathbf{R}}_z\right\} = \left\{\boldsymbol{\rho}_x,\boldsymbol{\rho}_y,\mathbf{i}_4,\mathbf{i}_3\right\}$ *Coset*

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O characters

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

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

C_4 *characters*

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

+

$\mathbf{r}_1 C_4 = \mathbf{r}_1\left\{\mathbf{1},\boldsymbol{\rho}_z,\mathbf{R}_z,\tilde{\mathbf{R}}_z\right\} = \left\{\mathbf{r}_1,\mathbf{r}_4,\mathbf{i}_1,\mathbf{R}_y\right\}$ *Coset*

General development of irep projectors $\mathbf{P}^{\mu}_{m_4 m_4} = \sum_{g}^{\circ O} \frac{\ell^{\mu}}{\circ O} D^{\mu *}_{m_4 m_4}(g)\, \mathbf{g}$ *for subgroup chain* $O \supset D_4 \supset C_4$

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

(Deriving diagonal irreducible O-representation ("irep") components $D^{\mu *}_{m_4 m_4}(g)$)

$$= \sum_{g}^{\circ O} \frac{\ell^{\mu}}{\circ O}(\chi^{\mu *}_{g}) \cdot \mathbf{g}\left(\mathbf{p}^{m_4}\right)$$

$$= \left(\frac{\ell^{\mu}}{24}\right)\left(\chi^{\mu *}_{\mathbf{1}}\right)\cdot \mathbf{1}\left(\mathbf{1} + d^{m_4}_{\rho_z}\boldsymbol{\rho}_z + d^{m_4}_{R_z}\mathbf{R}_z + d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right)\frac{1}{4} \quad = \left(\frac{\ell^{\mu}\chi^{\mu *}_{\mathbf{1}}}{96}\right)\left(1\cdot\mathbf{1} + d^{m_4}_{\rho_z}\boldsymbol{\rho}_z + d^{m_4}_{R_z}\mathbf{R}_z + d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right)$$

$$+\left(\frac{\ell^{\mu}}{24}\right)\left(\chi^{\mu *}_{\rho_z}\right)\cdot \boldsymbol{\rho}_z\left(\mathbf{1} + d^{m_4}_{\rho_z}\boldsymbol{\rho}_z + d^{m_4}_{R_z}\mathbf{R}_z + d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right)\frac{1}{4}$$

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$$\boldsymbol{\rho}_x C_4 = \boldsymbol{\rho}_x\left\{\mathbf{1}, \boldsymbol{\rho}_z, \mathbf{R}_z, \tilde{\mathbf{R}}_z\right\} = \left\{\boldsymbol{\rho}_x, \boldsymbol{\rho}_y, \mathbf{i}_4, \mathbf{i}_3\right\} Coset$$

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O characters

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

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

C_4 characters

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

$$\mathbf{r}_1 C_4 = \mathbf{r}_1\left\{\mathbf{1}, \boldsymbol{\rho}_z, \mathbf{R}_z, \tilde{\mathbf{R}}_z\right\} = \left\{\mathbf{r}_1, \mathbf{r}_4, \mathbf{i}_1, \mathbf{R}_y\right\} Coset$$

General development of irep projectors $\mathbf{P}^{\mu}_{m_4 m_4} = \sum_g^{\circ O} \frac{\ell^\mu}{\circ O} D^{\mu *}_{m_4 m_4}(g)\,\mathbf{g}$ *for subgroup chain* $O \supset D_4 \supset C_4$

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

(Deriving diagonal irreducible *O*-representation (“irep”) components $D^{\mu *}_{m_4 m_4}(g)$)

$$= \sum_g^{\circ O} \frac{\ell^\mu}{\circ O}(\chi_g^{\mu *})\cdot \mathbf{g}\left(\mathbf{p}^{m_4}\right)$$

$$= \left(\frac{\ell^\mu}{24}\right)\left(\chi_{\mathbf{1}}^{\mu *}\right)\cdot\mathbf{1}\left(\mathbf{1} + d^{m_4}_{\rho_z}\boldsymbol{\rho}_z + d^{m_4}_{R_z}\mathbf{R}_z + d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^\mu \chi_{\mathbf{1}}^{\mu *}}{96}\right)\left(1\cdot\mathbf{1} + d^{m_4}_{\rho_z}\boldsymbol{\rho}_z + d^{m_4}_{R_z}\mathbf{R}_z + d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right)$$

$$+\left(\frac{\ell^\mu}{24}\right)\left(\chi_{\rho_z}^{\mu *}\right)\cdot\boldsymbol{\rho}_z\left(\mathbf{1} + d^{m_4}_{\rho_z}\boldsymbol{\rho}_z + d^{m_4}_{R_z}\mathbf{R}_z + d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^\mu \chi_{\rho_z}^{\mu *}}{96}\right)\left(1\cdot\boldsymbol{\rho}_z + d^{m_4}_{\rho_z}\mathbf{1} + d^{m_4}_{R_z}\tilde{\mathbf{R}}_z + d^{m_4}_{\tilde{R}_z}\mathbf{R}_z\right)$$

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$$\boldsymbol{\rho}_x C_4 = \boldsymbol{\rho}_x\left\{\mathbf{1},\boldsymbol{\rho}_z,\mathbf{R}_z,\tilde{\mathbf{R}}_z\right\} = \left\{\boldsymbol{\rho}_x,\boldsymbol{\rho}_y,\mathbf{i}_4,\mathbf{i}_3\right\} Coset$$

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O characters

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

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

($e^{\frac{2\pi i m_4\cdot p}{4}}$: C_4 characters)

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

$$\mathbf{r}_1 C_4 = \mathbf{r}_1\left\{\mathbf{1},\boldsymbol{\rho}_z,\mathbf{R}_z,\tilde{\mathbf{R}}_z\right\} = \left\{\mathbf{r}_1,\mathbf{r}_4,\mathbf{i}_1,\mathbf{R}_y\right\} Coset$$

General development of irep projectors $\mathbf{P}^{\mu}_{m_4m_4} = \sum_{g}^{\circ O} \frac{\ell^{\mu}}{\circ O} D^{\mu*}_{m_4m_4}(g)\,\mathbf{g}$ *for subgroup chain* O⊃D_4⊃C_4

$$\mathbf{P}^{\mu}_{m_4m_4} = \mathbf{p}^{m_4}\mathbf{P}^{\mu} = \mathbf{P}^{\mu}\mathbf{p}^{m_4}$$

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$$= \sum_{g}^{\circ O} \frac{\ell^{\mu}}{\circ O}(\chi_g^{\mu*})\cdot\mathbf{g}\left(\mathbf{p}^{m_4}\right)$$

$$= \left(\frac{\ell^{\mu}}{24}\right)\left(\chi_{\mathbf{1}}^{\mu*}\right)\cdot\mathbf{1}\left(\mathbf{1}+d^{m_4}_{\rho_z}\boldsymbol{\rho}_z+d^{m_4}_{R_z}\mathbf{R}_z+d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^{\mu}\chi_{\mathbf{1}}^{\mu*}}{96}\right)\left(1\cdot\mathbf{1}+d^{m_4}_{\rho_z}\boldsymbol{\rho}_z+d^{m_4}_{R_z}\mathbf{R}_z+d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right) = \left(\frac{\ell^{\mu}\chi_{\mathbf{1}}^{\mu*}}{96}\right)\left(1\cdot\mathbf{1}+d^{m_4}_{\rho_z}\boldsymbol{\rho}_z+d^{m_4}_{R_z}\mathbf{R}_z+d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right)$$

$$+\left(\frac{\ell^{\mu}}{24}\right)\left(\chi_{\rho_z}^{\mu*}\right)\cdot\boldsymbol{\rho}_z\left(\mathbf{1}+d^{m_4}_{\rho_z}\boldsymbol{\rho}_z+d^{m_4}_{R_z}\mathbf{R}_z+d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^{\mu}\chi_{\rho_z}^{\mu*}}{96}\right)\left(1\cdot\boldsymbol{\rho}_z+d^{m_4}_{\rho_z}\mathbf{1}+d^{m_4}_{R_z}\tilde{\mathbf{R}}_z+d^{m_4}_{\tilde{R}_z}\mathbf{R}_z\right) = \left(\frac{\ell^{\mu}\chi_{\rho_z}^{\mu*}}{96}\right)\left(d^{m_4}_{\rho_z}\mathbf{1}+1\cdot\boldsymbol{\rho}_z+d^{m_4}_{\tilde{R}_z}\mathbf{R}_z+d^{m_4}_{R_z}\tilde{\mathbf{R}}_z\right)$$

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$$\boldsymbol{\rho}_x C_4 = \boldsymbol{\rho}_x\left\{\mathbf{1},\boldsymbol{\rho}_z,\mathbf{R}_z,\tilde{\mathbf{R}}_z\right\} = \left\{\boldsymbol{\rho}_x,\boldsymbol{\rho}_y,\mathbf{i}_4,\mathbf{i}_3\right\} Coset$$

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O characters

$O:\chi^{\mu}_{\mathbf{g}}$	$\mathbf{g=1}$	$\mathbf{r}_{1-4}$ $\tilde{\mathbf{r}}_{1-4}$	$\boldsymbol{\rho}_{xyz}$	$\mathbf{R}_{xyz}$ $\tilde{\mathbf{R}}_{xyz}$	$\mathbf{i}_{1-6}$
$\mu=A_1$	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
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C_4 characters

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

$$\mathbf{r}_1 C_4 = \mathbf{r}_1\left\{\mathbf{1},\boldsymbol{\rho}_z,\mathbf{R}_z,\tilde{\mathbf{R}}_z\right\} = \left\{\mathbf{r}_1,\mathbf{r}_4,\mathbf{i}_1,\mathbf{R}_y\right\} Coset$$

General development of irep projectors $\mathbf{P}^{\mu}_{m_4 m_4} = \sum_{g}^{°O} \frac{\ell^{\mu}}{°O} D^{\mu*}_{m_4 m_4}(g)\, \mathbf{g}$ *for subgroup chain* $O \supset D_4 \supset C_4$

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

(Deriving diagonal irreducible *O*-representation ("irep") components $D^{\mu*}_{m_4 m_4}(g)$)

$$= \sum_{g}^{°O} \frac{\ell^{\mu}}{°O} (\chi_g^{\mu*}) \cdot \mathbf{g}\left(\mathbf{p}^{m_4}\right)$$

$$= \left(\frac{\ell^{\mu}}{24}\right)\left(\chi_{\mathbf{1}}^{\mu*}\right)\cdot\mathbf{1}\left(\mathbf{1} + d^{m_4}_{\rho_z}\boldsymbol{\rho}_z + d^{m_4}_{R_z}\mathbf{R}_z + d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^{\mu}\chi_{\mathbf{1}}^{\mu*}}{96}\right)\left(1\cdot\mathbf{1} + d^{m_4}_{\rho_z}\boldsymbol{\rho}_z + d^{m_4}_{R_z}\mathbf{R}_z + d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right) = \left(\frac{\ell^{\mu}\chi_{\mathbf{1}}^{\mu*}}{96}\right)\left(1\cdot\mathbf{1} + d^{m_4}_{\rho_z}\boldsymbol{\rho}_z + d^{m_4}_{R_z}\mathbf{R}_z + d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right)$$

$$+\left(\frac{\ell^{\mu}}{24}\right)\left(\chi_{\rho_z}^{\mu*}\right)\cdot\boldsymbol{\rho}_z\left(\mathbf{1} + d^{m_4}_{\rho_z}\boldsymbol{\rho}_z + d^{m_4}_{R_z}\mathbf{R}_z + d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^{\mu}\chi_{\rho_z}^{\mu*}}{96}\right)\left(1\cdot\boldsymbol{\rho}_z + d^{m_4}_{\rho_z}\mathbf{1} + d^{m_4}_{R_z}\tilde{\mathbf{R}}_z + d^{m_4}_{\tilde{R}_z}\mathbf{R}_z\right) = \left(\frac{\ell^{\mu}\chi_{\rho_z}^{\mu*}}{96}\right)\left(d^{m_4}_{\rho_z}\mathbf{1} + 1\cdot\boldsymbol{\rho}_z + d^{m_4}_{\tilde{R}_z}\mathbf{R}_z + d^{m_4}_{R_z}\tilde{\mathbf{R}}_z\right)$$

$$+\left(\frac{\ell^{\mu}}{24}\right)\left(\chi_{\mathbf{R}_z}^{\mu*}\right)\cdot\mathbf{R}_z\left(\mathbf{1} + d^{m_4}_{\rho_z}\boldsymbol{\rho}_z + d^{m_4}_{R_z}\mathbf{R}_z + d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right)\frac{1}{4}$$

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$\boldsymbol{\rho}_x C_4 = \boldsymbol{\rho}_x\left\{\mathbf{1},\boldsymbol{\rho}_z,\mathbf{R}_z,\tilde{\mathbf{R}}_z\right\} = \left\{\boldsymbol{\rho}_x,\boldsymbol{\rho}_y,\mathbf{i}_4,\mathbf{i}_3\right\}$ *Coset*

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O characters

$O: \chi^{\mu}_{\mathbf{g}}$	$\mathbf{g}=\mathbf{1}$	$\mathbf{r}_{1-4}$ $\tilde{\mathbf{r}}_{1-4}$	$\boldsymbol{\rho}_{xyz}$	$\mathbf{R}_{xyz}$ $\tilde{\mathbf{R}}_{xyz}$	$\mathbf{i}_{1-6}$
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C_4 characters

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

$\mathbf{r}_1 C_4 = \mathbf{r}_1\left\{\mathbf{1},\boldsymbol{\rho}_z,\mathbf{R}_z,\tilde{\mathbf{R}}_z\right\} = \left\{\mathbf{r}_1,\mathbf{r}_4,\mathbf{i}_1,\mathbf{R}_y\right\}$ *Coset*

General development of irep projectors $\mathbf{P}^{\mu}_{m_4 m_4} = \sum_{g}^{°O} \frac{\ell^{\mu}}{°O} D^{\mu *}_{m_4 m_4}(g)\, \mathbf{g}$ *for subgroup chain* $O \supset D_4 \supset C_4$

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

(Deriving diagonal irreducible O-representation ("irep") components $D^{\mu *}_{m_4 m_4}(g)$)

$= \sum_{g}^{°O} \frac{\ell^{\mu}}{°O} (\chi^{\mu *}_{g}) \cdot \mathbf{g}\left(\mathbf{p}^{m_4}\right)$

$= \left(\frac{\ell^{\mu}}{24}\right)\left(\chi^{\mu *}_{\mathbf{1}}\right)\cdot \mathbf{1}\left(\mathbf{1} + d^{m_4}_{\rho_z}\boldsymbol{\rho}_z + d^{m_4}_{R_z}\mathbf{R}_z + d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^{\mu}\chi^{\mu *}_{\mathbf{1}}}{96}\right)\left(1\cdot \mathbf{1} + d^{m_4}_{\rho_z}\boldsymbol{\rho}_z + d^{m_4}_{R_z}\mathbf{R}_z + d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right) = \left(\frac{\ell^{\mu}\chi^{\mu *}_{\mathbf{1}}}{96}\right)\left(1\cdot \mathbf{1} + d^{m_4}_{\rho_z}\boldsymbol{\rho}_z + d^{m_4}_{R_z}\mathbf{R}_z + d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right)$

$+\left(\frac{\ell^{\mu}}{24}\right)\left(\chi^{\mu *}_{\rho_z}\right)\cdot \boldsymbol{\rho}_z\left(\mathbf{1} + d^{m_4}_{\rho_z}\boldsymbol{\rho}_z + d^{m_4}_{R_z}\mathbf{R}_z + d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^{\mu}\chi^{\mu *}_{\rho_z}}{96}\right)\left(1\cdot \boldsymbol{\rho}_z + d^{m_4}_{\rho_z}\mathbf{1} + d^{m_4}_{R_z}\tilde{\mathbf{R}}_z + d^{m_4}_{\tilde{R}_z}\mathbf{R}_z\right) = \left(\frac{\ell^{\mu}\chi^{\mu *}_{\rho_z}}{96}\right)\left(d^{m_4}_{\rho_z}\mathbf{1} + 1\cdot \boldsymbol{\rho}_z + d^{m_4}_{\tilde{R}_z}\mathbf{R}_z + d^{m_4}_{R_z}\tilde{\mathbf{R}}_z\right)$

$+\left(\frac{\ell^{\mu}}{24}\right)\left(\chi^{\mu *}_{\mathbf{R}_z}\right)\cdot \mathbf{R}_z\left(\mathbf{1} + d^{m_4}_{\rho_z}\boldsymbol{\rho}_z + d^{m_4}_{R_z}\mathbf{R}_z + d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^{\mu}\chi^{\mu *}_{\mathbf{R}_z}}{96}\right)\left(1\cdot \mathbf{R}_z + d^{m_4}_{\rho_z}\tilde{\mathbf{R}}_z + d^{m_4}_{R_z}\boldsymbol{\rho}_z + d^{m_4}_{\tilde{R}_z}\mathbf{1}\right) =$

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$\boldsymbol{\rho}_x C_4 = \boldsymbol{\rho}_x\left\{\mathbf{1},\boldsymbol{\rho}_z,\mathbf{R}_z,\tilde{\mathbf{R}}_z\right\} = \left\{\boldsymbol{\rho}_x,\boldsymbol{\rho}_y,\mathbf{i}_4,\mathbf{i}_3\right\}$ *Coset*

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O characters

$O: \chi^{\mu}_{\mathbf{g}}$	$\mathbf{g}=\mathbf{1}$	$\mathbf{r}_{1-4}$ $\tilde{\mathbf{r}}_{1-4}$	$\boldsymbol{\rho}_{xyz}$	$\mathbf{R}_{xyz}$ $\tilde{\mathbf{R}}_{xyz}$	$\mathbf{i}_{1-6}$
$\mu=A_1$	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
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$\mathbf{p}_{m_4} = \frac{1}{4}\sum_{p=0}^{3} e^{\frac{2\pi i m_4 \cdot p}{4}} \mathbf{R}_z^p = \begin{cases} \mathbf{p}_{0_4} = (\mathbf{1} + \mathbf{R}_z + \rho_z + \tilde{\mathbf{R}}_z)/4 \\ \mathbf{p}_{1_4} = (\mathbf{1} + i\mathbf{R}_z - \rho_z - i\tilde{\mathbf{R}}_z)/4 \\ \mathbf{p}_{2_4} = (\mathbf{1} - \mathbf{R}_z + \rho_z - \tilde{\mathbf{R}}_z)/4 \\ \mathbf{p}_{3_4} = (\mathbf{1} - i\mathbf{R}_z - \rho_z + i\tilde{\mathbf{R}}_z)/4 \end{cases}$

C_4 characters

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

$\mathbf{r}_1 C_4 = \mathbf{r}_1\left\{\mathbf{1},\boldsymbol{\rho}_z,\mathbf{R}_z,\tilde{\mathbf{R}}_z\right\} = \left\{\mathbf{r}_1,\mathbf{r}_4,\mathbf{i}_1,\mathbf{R}_y\right\}$ *Coset*

General development of irep projectors $\mathbf{P}^{\mu}_{m_4 m_4} = \sum_{g}^{\circ O} \frac{\ell^{\mu}}{\circ O} D^{\mu *}_{m_4 m_4}(g)\, \mathbf{g}$ for subgroup chain $O \supset D_4 \supset C_4$

(Deriving diagonal irreducible O-representation ("irep") components $D^{\mu *}_{m_4 m_4}(g)$)

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

$$= \sum_{g}^{\circ O} \frac{\ell^{\mu}}{\circ O} (\chi^{\mu *}_{g}) \cdot \mathbf{g}\left(\mathbf{p}^{m_4}\right)$$

$$= \left(\frac{\ell^{\mu}}{24}\right)\left(\chi^{\mu *}_{\mathbf{1}}\right)\cdot \mathbf{1}\left(\mathbf{1} + d^{m_4}_{\rho_z}\boldsymbol{\rho}_z + d^{m_4}_{R_z}\mathbf{R}_z + d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^{\mu}\chi^{\mu *}_{\mathbf{1}}}{96}\right)\left(1\cdot\mathbf{1} + d^{m_4}_{\rho_z}\boldsymbol{\rho}_z + d^{m_4}_{R_z}\mathbf{R}_z + d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right) = \left(\frac{\ell^{\mu}\chi^{\mu *}_{\mathbf{1}}}{96}\right)\left(1\cdot\mathbf{1} + d^{m_4}_{\rho_z}\boldsymbol{\rho}_z + d^{m_4}_{R_z}\mathbf{R}_z + d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right)$$

$$+\left(\frac{\ell^{\mu}}{24}\right)\left(\chi^{\mu *}_{\rho_z}\right)\cdot \boldsymbol{\rho}_z\left(\mathbf{1} + d^{m_4}_{\rho_z}\boldsymbol{\rho}_z + d^{m_4}_{R_z}\mathbf{R}_z + d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^{\mu}\chi^{\mu *}_{\rho_z}}{96}\right)\left(1\cdot\boldsymbol{\rho}_z + d^{m_4}_{\rho_z}\mathbf{1} + d^{m_4}_{R_z}\tilde{\mathbf{R}}_z + d^{m_4}_{\tilde{R}_z}\mathbf{R}_z\right) = \left(\frac{\ell^{\mu}\chi^{\mu *}_{\rho_z}}{96}\right)\left(d^{m_4}_{\rho_z}\mathbf{1} + 1\cdot\boldsymbol{\rho}_z + d^{m_4}_{\tilde{R}_z}\mathbf{R}_z + d^{m_4}_{R_z}\tilde{\mathbf{R}}_z\right)$$

$$+\left(\frac{\ell^{\mu}}{24}\right)\left(\chi^{\mu *}_{\mathbf{R}_z}\right)\cdot \mathbf{R}_z\left(\mathbf{1} + d^{m_4}_{\rho_z}\boldsymbol{\rho}_z + d^{m_4}_{R_z}\mathbf{R}_z + d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^{\mu}\chi^{\mu *}_{\mathbf{R}_z}}{96}\right)\left(1\cdot\mathbf{R}_z + d^{m_4}_{\rho_z}\tilde{\mathbf{R}}_z + d^{m_4}_{R_z}\boldsymbol{\rho}_z + d^{m_4}_{\tilde{R}_z}\mathbf{1}\right) = \left(\frac{\ell^{\mu}\chi^{\mu *}_{\mathbf{R}_z}}{96}\right)\left(d^{m_4}_{\tilde{R}_z}\mathbf{1} + d^{m_4}_{R_z}\boldsymbol{\rho}_z + 1\cdot\mathbf{R}_z + d^{m_4}_{\rho_z}\tilde{\mathbf{R}}_z\right)$$

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$$\boldsymbol{\rho}_x C_4 = \boldsymbol{\rho}_x\left\{\mathbf{1},\boldsymbol{\rho}_z,\mathbf{R}_z,\tilde{\mathbf{R}}_z\right\} = \left\{\boldsymbol{\rho}_x,\boldsymbol{\rho}_y,\mathbf{i}_4,\mathbf{i}_3\right\} Coset$$

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O characters

$O:\chi^{\mu}_{\mathbf{g}}$	$\mathbf{g}=\mathbf{1}$	$\mathbf{r}_{1-4}$ $\tilde{\mathbf{r}}_{1-4}$	$\boldsymbol{\rho}_{xyz}$	$\mathbf{R}_{xyz}$ $\tilde{\mathbf{R}}_{xyz}$	$\mathbf{i}_{1-6}$
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A_2	1	1	1	-1	-1
E	2	-1	2	0	0
T_1	3	0	-1	1	-1
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$$\mathbf{p}_{m_4} = \frac{1}{4}\sum_{p=0}^{3} \underbrace{e^{\frac{2\pi i m_4 \cdot p}{4}}}_{C_4\ characters} \mathbf{R}^{p}_{z} = \begin{cases} \mathbf{p}_{0_4} = (\mathbf{1}+\mathbf{R}_z+\rho_z+\tilde{\mathbf{R}}_z)/4 \\ \mathbf{p}_{1_4} = (\mathbf{1}+i\mathbf{R}_z-\rho_z-i\tilde{\mathbf{R}}_z)/4 \\ \mathbf{p}_{2_4} = (\mathbf{1}-\mathbf{R}_z+\rho_z-\tilde{\mathbf{R}}_z)/4 \\ \mathbf{p}_{3_4} = (\mathbf{1}-i\mathbf{R}_z-\rho_z+i\tilde{\mathbf{R}}_z)/4 \end{cases}$$

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

$$\mathbf{r}_1 C_4 = \mathbf{r}_1\left\{\mathbf{1},\boldsymbol{\rho}_z,\mathbf{R}_z,\tilde{\mathbf{R}}_z\right\} = \left\{\mathbf{r}_1,\mathbf{r}_4,\mathbf{i}_1,\mathbf{R}_y\right\} Coset$$

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

(Deriving diagonal irreducible O-representation ("irep") components $D^{\mu *}_{m_4 m_4}(g)$)

$$= \sum_{g}^{\circ O} \frac{\ell^{\mu}}{\circ O} (\chi^{\mu *}_{g}) \cdot \mathbf{g}\left(\mathbf{p}^{m_4}\right)$$

$$= \left(\frac{\ell^{\mu}}{24}\right)\left(\chi^{\mu *}_{\mathbf{1}}\right)\cdot \mathbf{1}\left(\mathbf{1} + d^{m_4}_{\rho_z}\boldsymbol{\rho}_z + d^{m_4}_{R_z}\mathbf{R}_z + d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^{\mu}\chi^{\mu *}_{\mathbf{1}}}{96}\right)\left(1\cdot\mathbf{1} + d^{m_4}_{\rho_z}\boldsymbol{\rho}_z + d^{m_4}_{R_z}\mathbf{R}_z + d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right) = \left(\frac{\ell^{\mu}\chi^{\mu *}_{\mathbf{1}}}{96}\right)\left(1\cdot\mathbf{1} + d^{m_4}_{\rho_z}\boldsymbol{\rho}_z + d^{m_4}_{R_z}\mathbf{R}_z + d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right)$$

$$+\left(\frac{\ell^{\mu}}{24}\right)\left(\chi^{\mu *}_{\rho_z}\right)\cdot \boldsymbol{\rho}_z\left(\mathbf{1} + d^{m_4}_{\rho_z}\boldsymbol{\rho}_z + d^{m_4}_{R_z}\mathbf{R}_z + d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^{\mu}\chi^{\mu *}_{\rho_z}}{96}\right)\left(1\cdot\boldsymbol{\rho}_z + d^{m_4}_{\rho_z}\mathbf{1} + d^{m_4}_{R_z}\tilde{\mathbf{R}}_z + d^{m_4}_{\tilde{R}_z}\mathbf{R}_z\right) = \left(\frac{\ell^{\mu}\chi^{\mu *}_{\rho_z}}{96}\right)\left(d^{m_4}_{\rho_z}\mathbf{1} + 1\cdot\boldsymbol{\rho}_z + d^{m_4}_{\tilde{R}_z}\mathbf{R}_z + d^{m_4}_{R_z}\tilde{\mathbf{R}}_z\right)$$

$$+\left(\frac{\ell^{\mu}}{24}\right)\left(\chi^{\mu *}_{\mathbf{R}_z}\right)\cdot \mathbf{R}_z\left(\mathbf{1} + d^{m_4}_{\rho_z}\boldsymbol{\rho}_z + d^{m_4}_{R_z}\mathbf{R}_z + d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^{\mu}\chi^{\mu *}_{\mathbf{R}_z}}{96}\right)\left(1\cdot\mathbf{R}_z + d^{m_4}_{\rho_z}\tilde{\mathbf{R}}_z + d^{m_4}_{R_z}\boldsymbol{\rho}_z + d^{m_4}_{\tilde{R}_z}\mathbf{1}\right) = \left(\frac{\ell^{\mu}\chi^{\mu *}_{\mathbf{R}_z}}{96}\right)\left(d^{m_4}_{\tilde{R}_z}\mathbf{1} + d^{m_4}_{R_z}\boldsymbol{\rho}_z + 1\cdot\mathbf{R}_z + d^{m_4}_{\rho_z}\tilde{\mathbf{R}}_z\right)$$

$$+\left(\frac{\ell^{\mu}}{24}\right)\left(\chi^{\mu *}_{\tilde{\mathbf{R}}_z}\right)\cdot \tilde{\mathbf{R}}_z\left(\mathbf{1} + d^{m_4}_{\rho_z}\boldsymbol{\rho}_z + d^{m_4}_{R_z}\mathbf{R}_z + d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^{\mu}\chi^{\mu *}_{\tilde{\mathbf{R}}_z}}{96}\right)\left(1\cdot\tilde{\mathbf{R}}_z + d^{m_4}_{\rho_z}\mathbf{R}_z + d^{m_4}_{R_z}\mathbf{1} + d^{m_4}_{\tilde{R}_z}\boldsymbol{\rho}_z\right) = \left(\frac{\ell^{\mu}\chi^{\mu *}_{\tilde{\mathbf{R}}_z}}{96}\right)\left(d^{m_4}_{R_z}\mathbf{1} + d^{m_4}_{\tilde{R}_z}\boldsymbol{\rho}_z + d^{m_4}_{\rho_z}\mathbf{R}_z + 1\cdot\tilde{\mathbf{R}}_z\right)$$

$\boldsymbol{\rho}_x C_4 = \boldsymbol{\rho}_x\left\{\mathbf{1},\boldsymbol{\rho}_z,\mathbf{R}_z,\tilde{\mathbf{R}}_z\right\} = \left\{\boldsymbol{\rho}_x,\boldsymbol{\rho}_y,\mathbf{i}_4,\mathbf{i}_3\right\}$ *Coset*

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O characters

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

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

C_4 characters

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

$\mathbf{r}_1 C_4 = \mathbf{r}_1\left\{\mathbf{1},\boldsymbol{\rho}_z,\mathbf{R}_z,\tilde{\mathbf{R}}_z\right\} = \left\{\mathbf{r}_1,\mathbf{r}_4,\mathbf{i}_1,\mathbf{R}_y\right\}$ *Coset*

General development of irep projectors $\mathbf{P}^{\mu}_{m_4 m_4} = \sum_{g}^{\circ O} \frac{\ell^{\mu}}{\circ O} D^{\mu *}_{m_4 m_4}(g)\,\mathbf{g}$ *for subgroup chain* $O \supset D_4 \supset C_4$

(Deriving diagonal irreducible O-representation ("irep") components $D^{\mu *}_{m_4 m_4}(g)$)

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

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$$= \left(\frac{\ell^{\mu}}{24}\right)\left(\chi_{\mathbf{1}}^{\mu *}\right)\cdot \mathbf{1}\left(\mathbf{1} + d_{\rho_z}^{m_4}\boldsymbol{\rho}_z + d_{R_z}^{m_4}\mathbf{R}_z + d_{\tilde{R}_z}^{m_4}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^{\mu}\chi_{\mathbf{1}}^{\mu *}}{96}\right)\left(1\cdot\mathbf{1} + d_{\rho_z}^{m_4}\boldsymbol{\rho}_z + d_{R_z}^{m_4}\mathbf{R}_z + d_{\tilde{R}_z}^{m_4}\tilde{\mathbf{R}}_z\right) = \left(\frac{\ell^{\mu}\chi_{\mathbf{1}}^{\mu *}}{96}\right)\left(1\cdot\mathbf{1} + d_{\rho_z}^{m_4}\boldsymbol{\rho}_z + d_{R_z}^{m_4}\mathbf{R}_z + d_{\tilde{R}_z}^{m_4}\tilde{\mathbf{R}}_z\right)$$

$$+\left(\frac{\ell^{\mu}}{24}\right)\left(\chi_{\rho_z}^{\mu *}\right)\cdot \boldsymbol{\rho}_z\left(\mathbf{1} + d_{\rho_z}^{m_4}\boldsymbol{\rho}_z + d_{R_z}^{m_4}\mathbf{R}_z + d_{\tilde{R}_z}^{m_4}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^{\mu}\chi_{\rho_z}^{\mu *}}{96}\right)\left(1\cdot\boldsymbol{\rho}_z + d_{\rho_z}^{m_4}\mathbf{1} + d_{R_z}^{m_4}\tilde{\mathbf{R}}_z + d_{\tilde{R}_z}^{m_4}\mathbf{R}_z\right) = \left(\frac{\ell^{\mu}\chi_{\rho_z}^{\mu *}}{96}\right)\left(d_{\rho_z}^{m_4}\mathbf{1} + 1\cdot\boldsymbol{\rho}_z + d_{\tilde{R}_z}^{m_4}\mathbf{R}_z + d_{R_z}^{m_4}\tilde{\mathbf{R}}_z\right)$$

$$+\left(\frac{\ell^{\mu}}{24}\right)\left(\chi_{\mathbf{R}_z}^{\mu *}\right)\cdot \mathbf{R}_z\left(\mathbf{1} + d_{\rho_z}^{m_4}\boldsymbol{\rho}_z + d_{R_z}^{m_4}\mathbf{R}_z + d_{\tilde{R}_z}^{m_4}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^{\mu}\chi_{\mathbf{R}_z}^{\mu *}}{96}\right)\left(1\cdot\mathbf{R}_z + d_{\rho_z}^{m_4}\tilde{\mathbf{R}}_z + d_{R_z}^{m_4}\boldsymbol{\rho}_z + d_{\tilde{R}_z}^{m_4}\mathbf{1}\right) = \left(\frac{\ell^{\mu}\chi_{\mathbf{R}_z}^{\mu *}}{96}\right)\left(d_{\tilde{R}_z}^{m_4}\mathbf{1} + d_{R_z}^{m_4}\boldsymbol{\rho}_z + 1\cdot\mathbf{R}_z + d_{\rho_z}^{m_4}\tilde{\mathbf{R}}_z\right)$$

$$+\left(\frac{\ell^{\mu}}{24}\right)\left(\chi_{\tilde{\mathbf{R}}_z}^{\mu *}\right)\cdot \tilde{\mathbf{R}}_z\left(\mathbf{1} + d_{\rho_z}^{m_4}\boldsymbol{\rho}_z + d_{R_z}^{m_4}\mathbf{R}_z + d_{\tilde{R}_z}^{m_4}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^{\mu}\chi_{\tilde{\mathbf{R}}_z}^{\mu *}}{96}\right)\left(1\cdot\tilde{\mathbf{R}}_z + d_{\rho_z}^{m_4}\mathbf{R}_z + d_{R_z}^{m_4}\mathbf{1} + d_{\tilde{R}_z}^{m_4}\boldsymbol{\rho}_z\right) = \left(\frac{\ell^{\mu}\chi_{\tilde{\mathbf{R}}_z}^{\mu *}}{96}\right)\left(d_{R_z}^{m_4}\mathbf{1} + d_{\tilde{R}_z}^{m_4}\boldsymbol{\rho}_z + d_{\rho_z}^{m_4}\mathbf{R}_z + 1\cdot\tilde{\mathbf{R}}_z\right)$$

$$\boldsymbol{\rho}_x C_4 = \boldsymbol{\rho}_x\left\{\mathbf{1},\boldsymbol{\rho}_z,\mathbf{R}_z,\tilde{\mathbf{R}}_z\right\} = \left\{\boldsymbol{\rho}_x,\boldsymbol{\rho}_y,\mathbf{i}_4,\mathbf{i}_3\right\} Coset$$

$$+\left(\frac{\ell^{\mu}}{24}\right)\left(\chi_{\boldsymbol{\rho}_x}^{\mu *}\right)\cdot \boldsymbol{\rho}_x\left(\mathbf{1} + d_{\rho_z}^{m_4}\boldsymbol{\rho}_z + d_{R_z}^{m_4}\mathbf{R}_z + d_{\tilde{R}_z}^{m_4}\tilde{\mathbf{R}}_z\right)\frac{1}{4}$$

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O characters

$O: \chi_{\mathbf{g}}^{\mu}$	$\mathbf{g}=\mathbf{1}$	$\mathbf{r}_{1-4}$ $\tilde{\mathbf{r}}_{1-4}$	$\boldsymbol{\rho}_{xyz}$	$\mathbf{R}_{xyz}$ $\tilde{\mathbf{R}}_{xyz}$	$\mathbf{i}_{1-6}$
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C_4 characters

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

$$\mathbf{r}_1 C_4 = \mathbf{r}_1\left\{\mathbf{1},\boldsymbol{\rho}_z,\mathbf{R}_z,\tilde{\mathbf{R}}_z\right\} = \left\{\mathbf{r}_1,\mathbf{r}_4,\mathbf{i}_1,\mathbf{R}_y\right\} Coset$$

General development of irep projectors $\mathbf{P}^{\mu}_{m_4 m_4} = \sum_g^{\circ O} \frac{\ell^{\mu}}{\circ O} D^{\mu *}_{m_4 m_4}(g)\, \mathbf{g}$ *for subgroup chain* $O \supset D_4 \supset C_4$

(Deriving diagonal irreducible O-representation ("irep") components $D^{\mu *}_{m_4 m_4}(g)$)

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

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$$= \left(\frac{\ell^{\mu}}{24}\right)\left(\chi_{\mathbf{1}}^{\mu *}\right)\cdot \mathbf{1}\left(\mathbf{1} + d^{m_4}_{\rho_z}\boldsymbol{\rho}_z + d^{m_4}_{R_z}\mathbf{R}_z + d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^{\mu}\chi_{\mathbf{1}}^{\mu *}}{96}\right)\left(1\cdot\mathbf{1} + d^{m_4}_{\rho_z}\boldsymbol{\rho}_z + d^{m_4}_{R_z}\mathbf{R}_z + d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right) = \left(\frac{\ell^{\mu}\chi_{\mathbf{1}}^{\mu *}}{96}\right)\left(1\cdot\mathbf{1} + d^{m_4}_{\rho_z}\boldsymbol{\rho}_z + d^{m_4}_{R_z}\mathbf{R}_z + d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right)$$

$$+\left(\frac{\ell^{\mu}}{24}\right)\left(\chi_{\rho_z}^{\mu *}\right)\cdot \boldsymbol{\rho}_z\left(\mathbf{1} + d^{m_4}_{\rho_z}\boldsymbol{\rho}_z + d^{m_4}_{R_z}\mathbf{R}_z + d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^{\mu}\chi_{\rho_z}^{\mu *}}{96}\right)\left(1\cdot\boldsymbol{\rho}_z + d^{m_4}_{\rho_z}\mathbf{1} + d^{m_4}_{R_z}\tilde{\mathbf{R}}_z + d^{m_4}_{\tilde{R}_z}\mathbf{R}_z\right) = \left(\frac{\ell^{\mu}\chi_{\rho_z}^{\mu *}}{96}\right)\left(d^{m_4}_{\rho_z}\mathbf{1} + 1\cdot\boldsymbol{\rho}_z + d^{m_4}_{\tilde{R}_z}\mathbf{R}_z + d^{m_4}_{R_z}\tilde{\mathbf{R}}_z\right)$$

$$+\left(\frac{\ell^{\mu}}{24}\right)\left(\chi_{\mathbf{R}_z}^{\mu *}\right)\cdot \mathbf{R}_z\left(\mathbf{1} + d^{m_4}_{\rho_z}\boldsymbol{\rho}_z + d^{m_4}_{R_z}\mathbf{R}_z + d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^{\mu}\chi_{\mathbf{R}_z}^{\mu *}}{96}\right)\left(1\cdot\mathbf{R}_z + d^{m_4}_{\rho_z}\tilde{\mathbf{R}}_z + d^{m_4}_{R_z}\boldsymbol{\rho}_z + d^{m_4}_{\tilde{R}_z}\mathbf{1}\right) = \left(\frac{\ell^{\mu}\chi_{\mathbf{R}_z}^{\mu *}}{96}\right)\left(d^{m_4}_{\tilde{R}_z}\mathbf{1} + d^{m_4}_{R_z}\boldsymbol{\rho}_z + 1\cdot\mathbf{R}_z + d^{m_4}_{\rho_z}\tilde{\mathbf{R}}_z\right)$$

$$+\left(\frac{\ell^{\mu}}{24}\right)\left(\chi_{\tilde{\mathbf{R}}_z}^{\mu *}\right)\cdot \tilde{\mathbf{R}}_z\left(\mathbf{1} + d^{m_4}_{\rho_z}\boldsymbol{\rho}_z + d^{m_4}_{R_z}\mathbf{R}_z + d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^{\mu}\chi_{\tilde{\mathbf{R}}_z}^{\mu *}}{96}\right)\left(1\cdot\tilde{\mathbf{R}}_z + d^{m_4}_{\rho_z}\mathbf{R}_z + d^{m_4}_{R_z}\mathbf{1} + d^{m_4}_{\tilde{R}_z}\boldsymbol{\rho}_z\right) = \left(\frac{\ell^{\mu}\chi_{\tilde{\mathbf{R}}_z}^{\mu *}}{96}\right)\left(d^{m_4}_{R_z}\mathbf{1} + d^{m_4}_{\tilde{R}_z}\boldsymbol{\rho}_z + d^{m_4}_{\rho_z}\mathbf{R}_z + 1\cdot\tilde{\mathbf{R}}_z\right)$$

$$\boldsymbol{\rho}_x C_4 = \boldsymbol{\rho}_x\left\{\mathbf{1},\boldsymbol{\rho}_z,\mathbf{R}_z,\tilde{\mathbf{R}}_z\right\} = \left\{\boldsymbol{\rho}_x,\boldsymbol{\rho}_y,\mathbf{i}_4,\mathbf{i}_3\right\}\mathit{Coset}$$

$$+\left(\frac{\ell^{\mu}}{24}\right)\left(\chi_{\rho_x}^{\mu *}\right)\cdot \boldsymbol{\rho}_x\left(\mathbf{1} + d^{m_4}_{\rho_z}\boldsymbol{\rho}_z + d^{m_4}_{R_z}\mathbf{R}_z + d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^{\mu}\chi_{\rho_x}^{\mu *}}{96}\right)\left(1\cdot\boldsymbol{\rho}_x + d^{m_4}_{\rho_z}\boldsymbol{\rho}_y + d^{m_4}_{R_z}\mathbf{i}_4 + d^{m_4}_{\tilde{R}_z}\mathbf{i}_3\right) =$$

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O characters

$O:\chi^{\mu}_{\mathbf{g}}$	$\mathbf{g}=\mathbf{1}$	$\mathbf{r}_{1-4}$ $\tilde{\mathbf{r}}_{1-4}$	$\boldsymbol{\rho}_{xyz}$	$\mathbf{R}_{xyz}$ $\tilde{\mathbf{R}}_{xyz}$	$\mathbf{i}_{1-6}$
$\mu=A_1$	1	1	1	1	1
A_2	1	1	1	-1	-1
E	2	-1	2	0	0
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$$\mathbf{p}_{m_4} = \frac{1}{4}\sum_{p=0}^{3} e^{\frac{2\pi i m_4 \cdot p}{4}}\mathbf{R}_z^p = \begin{cases} \mathbf{p}_{0_4} = (\mathbf{1}+\mathbf{R}_z+\rho_z+\tilde{\mathbf{R}}_z)/4 \\ \mathbf{p}_{1_4} = (\mathbf{1}+i\mathbf{R}_z-\rho_z-i\tilde{\mathbf{R}}_z)/4 \\ \mathbf{p}_{2_4} = (\mathbf{1}-\mathbf{R}_z+\rho_z-\tilde{\mathbf{R}}_z)/4 \\ \mathbf{p}_{3_4} = (\mathbf{1}-i\mathbf{R}_z-\rho_z+i\tilde{\mathbf{R}}_z)/4 \end{cases}$$

C_4 characters

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$$= \sum_{g}^{\circ O} \frac{\ell^{\mu}}{\circ O}(\chi_g^{\mu*})\cdot\mathbf{g}\left(\mathbf{p}^{m_4}\right)$$

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$$+\left(\frac{\ell^{\mu}}{24}\right)\left(\chi_{\rho_z}^{\mu*}\right)\cdot\boldsymbol{\rho}_z\left(\mathbf{1}+d^{m_4}_{\rho_z}\boldsymbol{\rho}_z+d^{m_4}_{R_z}\mathbf{R}_z+d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^{\mu}\chi_{\rho_z}^{\mu*}}{96}\right)\left(1\cdot\boldsymbol{\rho}_z+d^{m_4}_{\rho_z}\mathbf{1}+d^{m_4}_{R_z}\tilde{\mathbf{R}}_z+d^{m_4}_{\tilde{R}_z}\mathbf{R}_z\right) = \left(\frac{\ell^{\mu}\chi_{\rho_z}^{\mu*}}{96}\right)\left(d^{m_4}_{\rho_z}\mathbf{1}+1\cdot\boldsymbol{\rho}_z+d^{m_4}_{\tilde{R}_z}\mathbf{R}_z+d^{m_4}_{R_z}\tilde{\mathbf{R}}_z\right)$$

$$+\left(\frac{\ell^{\mu}}{24}\right)\left(\chi_{\mathbf{R}_z}^{\mu*}\right)\cdot\mathbf{R}_z\left(\mathbf{1}+d^{m_4}_{\rho_z}\boldsymbol{\rho}_z+d^{m_4}_{R_z}\mathbf{R}_z+d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^{\mu}\chi_{\mathbf{R}_z}^{\mu*}}{96}\right)\left(1\cdot\mathbf{R}_z+d^{m_4}_{\rho_z}\tilde{\mathbf{R}}_z+d^{m_4}_{R_z}\boldsymbol{\rho}_z+d^{m_4}_{\tilde{R}_z}\mathbf{1}\right) = \left(\frac{\ell^{\mu}\chi_{\mathbf{R}_z}^{\mu*}}{96}\right)\left(d^{m_4}_{\tilde{R}_z}\mathbf{1}+d^{m_4}_{R_z}\boldsymbol{\rho}_z+1\cdot\mathbf{R}_z+d^{m_4}_{\rho_z}\tilde{\mathbf{R}}_z\right)$$

$$+\left(\frac{\ell^{\mu}}{24}\right)\left(\chi_{\tilde{\mathbf{R}}_z}^{\mu*}\right)\cdot\tilde{\mathbf{R}}_z\left(\mathbf{1}+d^{m_4}_{\rho_z}\boldsymbol{\rho}_z+d^{m_4}_{R_z}\mathbf{R}_z+d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^{\mu}\chi_{\tilde{\mathbf{R}}_z}^{\mu*}}{96}\right)\left(1\cdot\tilde{\mathbf{R}}_z+d^{m_4}_{\rho_z}\mathbf{R}_z+d^{m_4}_{R_z}\mathbf{1}+d^{m_4}_{\tilde{R}_z}\boldsymbol{\rho}_z\right) = \left(\frac{\ell^{\mu}\chi_{\tilde{\mathbf{R}}_z}^{\mu*}}{96}\right)\left(d^{m_4}_{R_z}\mathbf{1}+d^{m_4}_{\tilde{R}_z}\boldsymbol{\rho}_z+d^{m_4}_{\rho_z}\mathbf{R}_z+1\cdot\tilde{\mathbf{R}}_z\right)$$

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O characters

$O:\chi^{\mu}_{\mathbf{g}}$	$\mathbf{g}=\mathbf{1}$	$\mathbf{r}_{1-4}$ $\tilde{\mathbf{r}}_{1-4}$	$\boldsymbol{\rho}_{xyz}$	$\mathbf{R}_{xyz}$ $\tilde{\mathbf{R}}_{xyz}$	$\mathbf{i}_{1-6}$
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C_4 characters

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

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General development of irep projectors $\mathbf{P}^{\mu}_{m_4 m_4} = \sum_g^{\circ O} \frac{\ell^{\mu}}{\circ O} D^{\mu *}_{m_4 m_4}(g)\,\mathbf{g}$ *for subgroup chain* $O \supset D_4 \supset C_4$

(Deriving diagonal irreducible O-representation ("irep") components $D^{\mu *}_{m_4 m_4}(g)$)

$$\mathbf{P}^{\mu}_{m_4 m_4} = \mathbf{p}^{m_4}\mathbf{P}^{\mu} = \mathbf{P}^{\mu}\mathbf{p}^{m_4} = \sum_g^{\circ O} \frac{\ell^{\mu}}{\circ O}(\chi_g^{\mu *})\cdot \mathbf{g}\left(\mathbf{p}^{m_4}\right)$$

$$= \left(\frac{\ell^{\mu}}{24}\right)\left(\chi_{\mathbf{1}}^{\mu *}\right)\cdot\mathbf{1}\left(\mathbf{1}+d_{\rho_z}^{m_4}\boldsymbol{\rho}_z+d_{R_z}^{m_4}\mathbf{R}_z+d_{\tilde{R}_z}^{m_4}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^{\mu}\chi_{\mathbf{1}}^{\mu *}}{96}\right)\left(1\cdot\mathbf{1}+d_{\rho_z}^{m_4}\boldsymbol{\rho}_z+d_{R_z}^{m_4}\mathbf{R}_z+d_{\tilde{R}_z}^{m_4}\tilde{\mathbf{R}}_z\right) = \left(\frac{\ell^{\mu}\chi_{\mathbf{1}}^{\mu *}}{96}\right)\left(1\cdot\mathbf{1}+d_{\rho_z}^{m_4}\boldsymbol{\rho}_z+d_{R_z}^{m_4}\mathbf{R}_z+d_{\tilde{R}_z}^{m_4}\tilde{\mathbf{R}}_z\right)$$

$$+\left(\frac{\ell^{\mu}}{24}\right)\left(\chi_{\rho_z}^{\mu *}\right)\cdot\boldsymbol{\rho}_z\left(\mathbf{1}+d_{\rho_z}^{m_4}\boldsymbol{\rho}_z+d_{R_z}^{m_4}\mathbf{R}_z+d_{\tilde{R}_z}^{m_4}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^{\mu}\chi_{\rho_z}^{\mu *}}{96}\right)\left(1\cdot\boldsymbol{\rho}_z+d_{\rho_z}^{m_4}\mathbf{1}+d_{R_z}^{m_4}\tilde{\mathbf{R}}_z+d_{\tilde{R}_z}^{m_4}\mathbf{R}_z\right) = \left(\frac{\ell^{\mu}\chi_{\rho_z}^{\mu *}}{96}\right)\left(d_{\rho_z}^{m_4}\mathbf{1}+1\cdot\boldsymbol{\rho}_z+d_{\tilde{R}_z}^{m_4}\mathbf{R}_z+d_{R_z}^{m_4}\tilde{\mathbf{R}}_z\right)$$

$$+\left(\frac{\ell^{\mu}}{24}\right)\left(\chi_{\mathbf{R}_z}^{\mu *}\right)\cdot\mathbf{R}_z\left(\mathbf{1}+d_{\rho_z}^{m_4}\boldsymbol{\rho}_z+d_{R_z}^{m_4}\mathbf{R}_z+d_{\tilde{R}_z}^{m_4}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^{\mu}\chi_{\mathbf{R}_z}^{\mu *}}{96}\right)\left(1\cdot\mathbf{R}_z+d_{\rho_z}^{m_4}\tilde{\mathbf{R}}_z+d_{R_z}^{m_4}\boldsymbol{\rho}_z+d_{\tilde{R}_z}^{m_4}\mathbf{1}\right) = \left(\frac{\ell^{\mu}\chi_{\mathbf{R}_z}^{\mu *}}{96}\right)\left(d_{\tilde{R}_z}^{m_4}\mathbf{1}+d_{R_z}^{m_4}\boldsymbol{\rho}_z+1\cdot\mathbf{R}_z+d_{\rho_z}^{m_4}\tilde{\mathbf{R}}_z\right)$$

$$+\left(\frac{\ell^{\mu}}{24}\right)\left(\chi_{\tilde{\mathbf{R}}_z}^{\mu *}\right)\cdot\tilde{\mathbf{R}}_z\left(\mathbf{1}+d_{\rho_z}^{m_4}\boldsymbol{\rho}_z+d_{R_z}^{m_4}\mathbf{R}_z+d_{\tilde{R}_z}^{m_4}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^{\mu}\chi_{\tilde{\mathbf{R}}_z}^{\mu *}}{96}\right)\left(1\cdot\tilde{\mathbf{R}}_z+d_{\rho_z}^{m_4}\mathbf{R}_z+d_{R_z}^{m_4}\mathbf{1}+d_{\tilde{R}_z}^{m_4}\boldsymbol{\rho}_z\right) = \left(\frac{\ell^{\mu}\chi_{\tilde{\mathbf{R}}_z}^{\mu *}}{96}\right)\left(d_{R_z}^{m_4}\mathbf{1}+d_{\tilde{R}_z}^{m_4}\boldsymbol{\rho}_z+d_{\rho_z}^{m_4}\mathbf{R}_z+1\cdot\tilde{\mathbf{R}}_z\right)$$

$\boldsymbol{\rho}_x C_4 = \boldsymbol{\rho}_x\left\{\mathbf{1},\boldsymbol{\rho}_z,\mathbf{R}_z,\tilde{\mathbf{R}}_z\right\} = \left\{\boldsymbol{\rho}_x,\boldsymbol{\rho}_y,\mathbf{i}_4,\mathbf{i}_3\right\}$ *Coset*

$$+\left(\frac{\ell^{\mu}}{24}\right)\left(\chi_{\rho_x}^{\mu *}\right)\cdot\boldsymbol{\rho}_x\left(\mathbf{1}+d_{\rho_z}^{m_4}\boldsymbol{\rho}_z+d_{R_z}^{m_4}\mathbf{R}_z+d_{\tilde{R}_z}^{m_4}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^{\mu}\chi_{\rho_x}^{\mu *}}{96}\right)\left(1\cdot\boldsymbol{\rho}_x+d_{\rho_z}^{m_4}\boldsymbol{\rho}_y+d_{R_z}^{m_4}\mathbf{i}_4+d_{\tilde{R}_z}^{m_4}\mathbf{i}_3\right) = \left(\frac{\ell^{\mu}\chi_{\rho_x}^{\mu *}}{96}\right)\left(1\cdot\boldsymbol{\rho}_x+d_{\rho_z}^{m_4}\boldsymbol{\rho}_y+d_{R_z}^{m_4}\mathbf{i}_4+d_{\tilde{R}_z}^{m_4}\mathbf{i}_3\right)$$

$$+\left(\frac{\ell^{\mu}}{24}\right)\left(\chi_{\rho_y}^{\mu *}\right)\cdot\boldsymbol{\rho}_y\left(\mathbf{1}+d_{\rho_z}^{m_4}\boldsymbol{\rho}_z+d_{R_z}^{m_4}\mathbf{R}_z+d_{\tilde{R}_z}^{m_4}\tilde{\mathbf{R}}_z\right)\frac{1}{4}$$

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O characters

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

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

C_4 *characters*

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

$\mathbf{r}_1 C_4 = \mathbf{r}_1\left\{\mathbf{1},\boldsymbol{\rho}_z,\mathbf{R}_z,\tilde{\mathbf{R}}_z\right\} = \left\{\mathbf{r}_1,\mathbf{r}_4,\mathbf{i}_1,\mathbf{R}_y\right\}$ *Coset*

General development of irep projectors $\mathbf{P}^{\mu}_{m_4 m_4} = \sum_g^{\circ O} \frac{\ell^\mu}{{}^\circ O} D^{\mu *}_{m_4 m_4}(g)\,\mathbf{g}$ *for subgroup chain* $O \supset D_4 \supset C_4$

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$$= \sum_g^{\circ O} \frac{\ell^\mu}{{}^\circ O}(\chi_g^{\mu *})\cdot \mathbf{g}\left(\mathbf{p}^{m_4}\right)$$

$$= \left(\frac{\ell^\mu}{24}\right)\left(\chi_{\mathbf{1}}^{\mu *}\right)\cdot \mathbf{1}\left(\mathbf{1} + d^{m_4}_{\rho_z}\boldsymbol{\rho}_z + d^{m_4}_{R_z}\mathbf{R}_z + d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^\mu \chi_{\mathbf{1}}^{\mu *}}{96}\right)\left(1\cdot\mathbf{1} + d^{m_4}_{\rho_z}\boldsymbol{\rho}_z + d^{m_4}_{R_z}\mathbf{R}_z + d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right) = \left(\frac{\ell^\mu \chi_{\mathbf{1}}^{\mu *}}{96}\right)\left(1\cdot\mathbf{1} + d^{m_4}_{\rho_z}\boldsymbol{\rho}_z + d^{m_4}_{R_z}\mathbf{R}_z + d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right)$$

$$+\left(\frac{\ell^\mu}{24}\right)\left(\chi_{\rho_z}^{\mu *}\right)\cdot \boldsymbol{\rho}_z\left(\mathbf{1} + d^{m_4}_{\rho_z}\boldsymbol{\rho}_z + d^{m_4}_{R_z}\mathbf{R}_z + d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^\mu \chi_{\rho_z}^{\mu *}}{96}\right)\left(1\cdot\boldsymbol{\rho}_z + d^{m_4}_{\rho_z}\mathbf{1} + d^{m_4}_{R_z}\tilde{\mathbf{R}}_z + d^{m_4}_{\tilde{R}_z}\mathbf{R}_z\right) = \left(\frac{\ell^\mu \chi_{\rho_z}^{\mu *}}{96}\right)\left(d^{m_4}_{\rho_z}\mathbf{1} + 1\cdot\boldsymbol{\rho}_z + d^{m_4}_{\tilde{R}_z}\mathbf{R}_z + d^{m_4}_{R_z}\tilde{\mathbf{R}}_z\right)$$

$$+\left(\frac{\ell^\mu}{24}\right)\left(\chi_{\mathbf{R}_z}^{\mu *}\right)\cdot \mathbf{R}_z\left(\mathbf{1} + d^{m_4}_{\rho_z}\boldsymbol{\rho}_z + d^{m_4}_{R_z}\mathbf{R}_z + d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^\mu \chi_{\mathbf{R}_z}^{\mu *}}{96}\right)\left(1\cdot\mathbf{R}_z + d^{m_4}_{\rho_z}\tilde{\mathbf{R}}_z + d^{m_4}_{R_z}\boldsymbol{\rho}_z + d^{m_4}_{\tilde{R}_z}\mathbf{1}\right) = \left(\frac{\ell^\mu \chi_{\mathbf{R}_z}^{\mu *}}{96}\right)\left(d^{m_4}_{\tilde{R}_z}\mathbf{1} + d^{m_4}_{R_z}\boldsymbol{\rho}_z + 1\cdot\mathbf{R}_z + d^{m_4}_{\rho_z}\tilde{\mathbf{R}}_z\right)$$

$$+\left(\frac{\ell^\mu}{24}\right)\left(\chi_{\tilde{\mathbf{R}}_z}^{\mu *}\right)\cdot \tilde{\mathbf{R}}_z\left(\mathbf{1} + d^{m_4}_{\rho_z}\boldsymbol{\rho}_z + d^{m_4}_{R_z}\mathbf{R}_z + d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^\mu \chi_{\tilde{\mathbf{R}}_z}^{\mu *}}{96}\right)\left(1\cdot\tilde{\mathbf{R}}_z + d^{m_4}_{\rho_z}\mathbf{R}_z + d^{m_4}_{R_z}\mathbf{1} + d^{m_4}_{\tilde{R}_z}\boldsymbol{\rho}_z\right) = \left(\frac{\ell^\mu \chi_{\tilde{\mathbf{R}}_z}^{\mu *}}{96}\right)\left(d^{m_4}_{R_z}\mathbf{1} + d^{m_4}_{\tilde{R}_z}\boldsymbol{\rho}_z + d^{m_4}_{\rho_z}\mathbf{R}_z + 1\cdot\tilde{\mathbf{R}}_z\right)$$

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$$+\left(\frac{\ell^\mu}{24}\right)\left(\chi_{\rho_x}^{\mu *}\right)\cdot \boldsymbol{\rho}_x\left(\mathbf{1} + d^{m_4}_{\rho_z}\boldsymbol{\rho}_z + d^{m_4}_{R_z}\mathbf{R}_z + d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^\mu \chi_{\rho_x}^{\mu *}}{96}\right)\left(1\cdot\boldsymbol{\rho}_x + d^{m_4}_{\rho_z}\boldsymbol{\rho}_y + d^{m_4}_{R_z}\mathbf{i}_4 + d^{m_4}_{\tilde{R}_z}\mathbf{i}_3\right) = \left(\frac{\ell^\mu \chi_{\rho_x}^{\mu *}}{96}\right)\left(1\cdot\boldsymbol{\rho}_x + d^{m_4}_{\rho_z}\boldsymbol{\rho}_y + d^{m_4}_{R_z}\mathbf{i}_4 + d^{m_4}_{\tilde{R}_z}\mathbf{i}_3\right)$$

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C_4 *characters*

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$$+\left(\frac{\ell^{\mu}}{24}\right)\left(\chi_{\rho_z}^{\mu *}\right)\cdot \boldsymbol{\rho}_z\left(\mathbf{1} + d_{\rho_z}^{m4}\boldsymbol{\rho}_z + d_{R_z}^{m4}\mathbf{R}_z + d_{\tilde{R}_z}^{m4}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^{\mu}\chi_{\rho_z}^{\mu *}}{96}\right)\left(1\cdot\boldsymbol{\rho}_z + d_{\rho_z}^{m4}\mathbf{1} + d_{R_z}^{m4}\tilde{\mathbf{R}}_z + d_{\tilde{R}_z}^{m4}\mathbf{R}_z\right) = \left(\frac{\ell^{\mu}\chi_{\rho_z}^{\mu *}}{96}\right)\left(d_{\rho_z}^{m4}\mathbf{1} + 1\cdot\boldsymbol{\rho}_z + d_{\tilde{R}_z}^{m4}\mathbf{R}_z + d_{R_z}^{m4}\tilde{\mathbf{R}}_z\right)$$

$$+\left(\frac{\ell^{\mu}}{24}\right)\left(\chi_{\mathbf{R}_z}^{\mu *}\right)\cdot \mathbf{R}_z\left(\mathbf{1} + d_{\rho_z}^{m4}\boldsymbol{\rho}_z + d_{R_z}^{m4}\mathbf{R}_z + d_{\tilde{R}_z}^{m4}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^{\mu}\chi_{\mathbf{R}_z}^{\mu *}}{96}\right)\left(1\cdot\mathbf{R}_z + d_{\rho_z}^{m4}\tilde{\mathbf{R}}_z + d_{R_z}^{m4}\boldsymbol{\rho}_z + d_{\tilde{R}_z}^{m4}\mathbf{1}\right) = \left(\frac{\ell^{\mu}\chi_{\mathbf{R}_z}^{\mu *}}{96}\right)\left(d_{\tilde{R}_z}^{m4}\mathbf{1} + d_{R_z}^{m4}\boldsymbol{\rho}_z + 1\cdot\mathbf{R}_z + d_{\rho_z}^{m4}\tilde{\mathbf{R}}_z\right)$$

$$+\left(\frac{\ell^{\mu}}{24}\right)\left(\chi_{\tilde{\mathbf{R}}_z}^{\mu *}\right)\cdot \tilde{\mathbf{R}}_z\left(\mathbf{1} + d_{\rho_z}^{m4}\boldsymbol{\rho}_z + d_{R_z}^{m4}\mathbf{R}_z + d_{\tilde{R}_z}^{m4}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^{\mu}\chi_{\tilde{\mathbf{R}}_z}^{\mu *}}{96}\right)\left(1\cdot\tilde{\mathbf{R}}_z + d_{\rho_z}^{m4}\mathbf{R}_z + d_{R_z}^{m4}\mathbf{1} + d_{\tilde{R}_z}^{m4}\boldsymbol{\rho}_z\right) = \left(\frac{\ell^{\mu}\chi_{\tilde{\mathbf{R}}_z}^{\mu *}}{96}\right)\left(d_{R_z}^{m4}\mathbf{1} + d_{\tilde{R}_z}^{m4}\boldsymbol{\rho}_z + d_{\rho_z}^{m4}\mathbf{R}_z + 1\cdot\tilde{\mathbf{R}}_z\right)$$

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$\mathbf{r}_1 C_4 = \mathbf{r}_1\left\{\mathbf{1},\boldsymbol{\rho}_z,\mathbf{R}_z,\tilde{\mathbf{R}}_z\right\} = \left\{\mathbf{r}_1,\mathbf{r}_4,\mathbf{i}_1,\mathbf{R}_y\right\}$ *Coset*

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$$+ \left(\frac{\ell^{\mu}}{24}\right)\left(\chi^{\mu *}_{\rho_z}\right)\cdot\boldsymbol{\rho}_z\left(\mathbf{1} + d^{m_4}_{\rho_z}\boldsymbol{\rho}_z + d^{m_4}_{R_z}\mathbf{R}_z + d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^{\mu}\chi^{\mu *}_{\rho_z}}{96}\right)\left(1\cdot\boldsymbol{\rho}_z + d^{m_4}_{\rho_z}\mathbf{1} + d^{m_4}_{R_z}\tilde{\mathbf{R}}_z + d^{m_4}_{\tilde{R}_z}\mathbf{R}_z\right) = \left(\frac{\ell^{\mu}\chi^{\mu *}_{\rho_z}}{96}\right)\left(d^{m_4}_{\rho_z}\mathbf{1} + 1\cdot\boldsymbol{\rho}_z + d^{m_4}_{\tilde{R}_z}\mathbf{R}_z + d^{m_4}_{R_z}\tilde{\mathbf{R}}_z\right)$$

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$$+ \left(\frac{\ell^{\mu}}{24}\right)\left(\chi^{\mu *}_{\tilde{\mathbf{R}}_z}\right)\cdot\tilde{\mathbf{R}}_z\left(\mathbf{1} + d^{m_4}_{\rho_z}\boldsymbol{\rho}_z + d^{m_4}_{R_z}\mathbf{R}_z + d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^{\mu}\chi^{\mu *}_{\tilde{\mathbf{R}}_z}}{96}\right)\left(1\cdot\tilde{\mathbf{R}}_z + d^{m_4}_{\rho_z}\mathbf{R}_z + d^{m_4}_{R_z}\mathbf{1} + d^{m_4}_{\tilde{R}_z}\boldsymbol{\rho}_z\right) = \left(\frac{\ell^{\mu}\chi^{\mu *}_{\tilde{\mathbf{R}}_z}}{96}\right)\left(d^{m_4}_{R_z}\mathbf{1} + d^{m_4}_{\tilde{R}_z}\boldsymbol{\rho}_z + d^{m_4}_{\rho_z}\mathbf{R}_z + 1\cdot\tilde{\mathbf{R}}_z\right)$$

$$\boldsymbol{\rho}_x C_4 = \boldsymbol{\rho}_x\left\{\mathbf{1},\boldsymbol{\rho}_z,\mathbf{R}_z,\tilde{\mathbf{R}}_z\right\} = \left\{\boldsymbol{\rho}_x,\boldsymbol{\rho}_y,\mathbf{i}_4,\mathbf{i}_3\right\} \textit{Coset}$$

$$+ \left(\frac{\ell^{\mu}}{24}\right)\left(\chi^{\mu *}_{\rho_x}\right)\cdot\boldsymbol{\rho}_x\left(\mathbf{1} + d^{m_4}_{\rho_z}\boldsymbol{\rho}_z + d^{m_4}_{R_z}\mathbf{R}_z + d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^{\mu}\chi^{\mu *}_{\rho_x}}{96}\right)\left(1\cdot\boldsymbol{\rho}_x + d^{m_4}_{\rho_z}\boldsymbol{\rho}_y + d^{m_4}_{R_z}\mathbf{i}_4 + d^{m_4}_{\tilde{R}_z}\mathbf{i}_3\right) = \left(\frac{\ell^{\mu}\chi^{\mu *}_{\rho_x}}{96}\right)\left(1\cdot\boldsymbol{\rho}_x + d^{m_4}_{\rho_z}\boldsymbol{\rho}_y + d^{m_4}_{R_z}\mathbf{i}_4 + d^{m_4}_{\tilde{R}_z}\mathbf{i}_3\right)$$

$$+ \left(\frac{\ell^{\mu}}{24}\right)\left(\chi^{\mu *}_{\rho_y}\right)\cdot\boldsymbol{\rho}_y\left(\mathbf{1} + d^{m_4}_{\rho_z}\boldsymbol{\rho}_z + d^{m_4}_{R_z}\mathbf{R}_z + d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^{\mu}\chi^{\mu *}_{\rho_y}}{96}\right)\left(1\cdot\boldsymbol{\rho}_y + d^{m_4}_{\rho_z}\boldsymbol{\rho}_x + d^{m_4}_{R_z}\mathbf{i}_3 + d^{m_4}_{\tilde{R}_z}\mathbf{i}_4\right) = \left(\frac{\ell^{\mu}\chi^{\mu *}_{\rho_y}}{96}\right)\left(d^{m_4}_{\rho_z}\boldsymbol{\rho}_x + 1\cdot\boldsymbol{\rho}_y + d^{m_4}_{\tilde{R}_z}\mathbf{i}_4 + d^{m_4}_{R_z}\mathbf{i}_3\right)$$

$$+ \left(\frac{\ell^{\mu}}{24}\right)\left(\chi^{\mu *}_{\mathbf{i}_4}\right)\cdot\mathbf{i}_4\left(\mathbf{1} + d^{m_4}_{\rho_z}\boldsymbol{\rho}_z + d^{m_4}_{R_z}\mathbf{R}_z + d^{m_4}_{\tilde{R}_z}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^{\mu}\chi^{\mu *}_{\mathbf{i}_4}}{96}\right)\left(1\cdot\mathbf{i}_4 + d^{m_4}_{\rho_z}\mathbf{i}_3 + d^{m_4}_{R_z}\boldsymbol{\rho}_y + d^{m_4}_{\tilde{R}_z}\boldsymbol{\rho}_x\right) = \left(\frac{\ell^{\mu}\chi^{\mu *}_{\mathbf{i}_4}}{96}\right)\left(d^{m_4}_{\tilde{R}_z}\boldsymbol{\rho}_x + d^{m_4}_{R_z}\boldsymbol{\rho}_y + 1\cdot\mathbf{i}_4 + d^{m_4}_{\rho_z}\mathbf{i}_3\right)$$

$$+$$

$$\mathbf{r}_1 C_4 = \mathbf{r}_1\left\{\mathbf{1},\boldsymbol{\rho}_z,\mathbf{R}_z,\tilde{\mathbf{R}}_z\right\} = \left\{\mathbf{r}_1,\mathbf{r}_4,\mathbf{i}_1,\mathbf{R}_y\right\} \textit{Coset}$$

General development of irep projectors $\mathbf{P}^{\mu}_{m_4 m_4} = \sum_{g}^{\circ O} \frac{\ell^{\mu}}{\circ O} D^{\mu *}_{m_4 m_4}(g)\, \mathbf{g}$ *for subgroup chain* $O \supset D_4 \supset C_4$

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

(Deriving diagonal irreducible O-representation ("irep") components $D^{\mu *}_{m_4 m_4}(g)$)

$$= \sum_{g}^{\circ O} \frac{\ell^{\mu}}{\circ O} (\chi_g^{\mu *}) \cdot \mathbf{g}\left(\mathbf{p}^{m_4}\right)$$

$$= \left(\frac{\ell^{\mu}}{24}\right)\left(\chi_{\mathbf{1}}^{\mu *}\right)\cdot \mathbf{1}\left(\mathbf{1} + d_{\rho_z}^{m_4}\boldsymbol{\rho}_z + d_{R_z}^{m_4}\mathbf{R}_z + d_{\tilde{R}_z}^{m_4}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^{\mu}\chi_{\mathbf{1}}^{\mu *}}{96}\right)\left(1\cdot\mathbf{1} + d_{\rho_z}^{m_4}\boldsymbol{\rho}_z + d_{R_z}^{m_4}\mathbf{R}_z + d_{\tilde{R}_z}^{m_4}\tilde{\mathbf{R}}_z\right) = \left(\frac{\ell^{\mu}\chi_{\mathbf{1}}^{\mu *}}{96}\right)\left(1\cdot\mathbf{1} + d_{\rho_z}^{m_4}\boldsymbol{\rho}_z + d_{R_z}^{m_4}\mathbf{R}_z + d_{\tilde{R}_z}^{m_4}\tilde{\mathbf{R}}_z\right)$$

$$+\left(\frac{\ell^{\mu}}{24}\right)\left(\chi_{\rho_z}^{\mu *}\right)\cdot \boldsymbol{\rho}_z\left(\mathbf{1} + d_{\rho_z}^{m_4}\boldsymbol{\rho}_z + d_{R_z}^{m_4}\mathbf{R}_z + d_{\tilde{R}_z}^{m_4}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^{\mu}\chi_{\rho_z}^{\mu *}}{96}\right)\left(1\cdot\boldsymbol{\rho}_z + d_{\rho_z}^{m_4}\mathbf{1} + d_{R_z}^{m_4}\tilde{\mathbf{R}}_z + d_{\tilde{R}_z}^{m_4}\mathbf{R}_z\right) = \left(\frac{\ell^{\mu}\chi_{\rho_z}^{\mu *}}{96}\right)\left(d_{\rho_z}^{m_4}\mathbf{1} + 1\cdot\boldsymbol{\rho}_z + d_{\tilde{R}_z}^{m_4}\mathbf{R}_z + d_{R_z}^{m_4}\tilde{\mathbf{R}}_z\right)$$

$$+\left(\frac{\ell^{\mu}}{24}\right)\left(\chi_{\mathbf{R}_z}^{\mu *}\right)\cdot \mathbf{R}_z\left(\mathbf{1} + d_{\rho_z}^{m_4}\boldsymbol{\rho}_z + d_{R_z}^{m_4}\mathbf{R}_z + d_{\tilde{R}_z}^{m_4}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^{\mu}\chi_{\mathbf{R}_z}^{\mu *}}{96}\right)\left(1\cdot\mathbf{R}_z + d_{\rho_z}^{m_4}\tilde{\mathbf{R}}_z + d_{R_z}^{m_4}\boldsymbol{\rho}_z + d_{\tilde{R}_z}^{m_4}\mathbf{1}\right) = \left(\frac{\ell^{\mu}\chi_{\mathbf{R}_z}^{\mu *}}{96}\right)\left(d_{\tilde{R}_z}^{m_4}\mathbf{1} + d_{R_z}^{m_4}\boldsymbol{\rho}_z + 1\cdot\mathbf{R}_z + d_{\rho_z}^{m_4}\tilde{\mathbf{R}}_z\right)$$

$$+\left(\frac{\ell^{\mu}}{24}\right)\left(\chi_{\tilde{\mathbf{R}}_z}^{\mu *}\right)\cdot \tilde{\mathbf{R}}_z\left(\mathbf{1} + d_{\rho_z}^{m_4}\boldsymbol{\rho}_z + d_{R_z}^{m_4}\mathbf{R}_z + d_{\tilde{R}_z}^{m_4}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^{\mu}\chi_{\tilde{\mathbf{R}}_z}^{\mu *}}{96}\right)\left(1\cdot\tilde{\mathbf{R}}_z + d_{\rho_z}^{m_4}\mathbf{R}_z + d_{R_z}^{m_4}\mathbf{1} + d_{\tilde{R}_z}^{m_4}\boldsymbol{\rho}_z\right) = \left(\frac{\ell^{\mu}\chi_{\tilde{\mathbf{R}}_z}^{\mu *}}{96}\right)\left(d_{R_z}^{m_4}\mathbf{1} + d_{\tilde{R}_z}^{m_4}\boldsymbol{\rho}_z + d_{\rho_z}^{m_4}\mathbf{R}_z + 1\cdot\tilde{\mathbf{R}}_z\right)$$

$\boldsymbol{\rho}_x C_4 = \boldsymbol{\rho}_x\left\{\mathbf{1},\boldsymbol{\rho}_z,\mathbf{R}_z,\tilde{\mathbf{R}}_z\right\} = \left\{\boldsymbol{\rho}_x,\boldsymbol{\rho}_y,\mathbf{i}_4,\mathbf{i}_3\right\} Coset$

$$+\left(\frac{\ell^{\mu}}{24}\right)\left(\chi_{\rho_x}^{\mu *}\right)\cdot \boldsymbol{\rho}_x\left(\mathbf{1} + d_{\rho_z}^{m_4}\boldsymbol{\rho}_z + d_{R_z}^{m_4}\mathbf{R}_z + d_{\tilde{R}_z}^{m_4}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^{\mu}\chi_{\rho_x}^{\mu *}}{96}\right)\left(1\cdot\boldsymbol{\rho}_x + d_{\rho_z}^{m_4}\boldsymbol{\rho}_y + d_{R_z}^{m_4}\mathbf{i}_4 + d_{\tilde{R}_z}^{m_4}\mathbf{i}_3\right) = \left(\frac{\ell^{\mu}\chi_{\rho_x}^{\mu *}}{96}\right)\left(1\cdot\boldsymbol{\rho}_x + d_{\rho_z}^{m_4}\boldsymbol{\rho}_y + d_{R_z}^{m_4}\mathbf{i}_4 + d_{\tilde{R}_z}^{m_4}\mathbf{i}_3\right)$$

$$+\left(\frac{\ell^{\mu}}{24}\right)\left(\chi_{\rho_y}^{\mu *}\right)\cdot \boldsymbol{\rho}_y\left(\mathbf{1} + d_{\rho_z}^{m_4}\boldsymbol{\rho}_z + d_{R_z}^{m_4}\mathbf{R}_z + d_{\tilde{R}_z}^{m_4}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^{\mu}\chi_{\rho_y}^{\mu *}}{96}\right)\left(1\cdot\boldsymbol{\rho}_y + d_{\rho_z}^{m_4}\boldsymbol{\rho}_x + d_{R_z}^{m_4}\mathbf{i}_3 + d_{\tilde{R}_z}^{m_4}\mathbf{i}_4\right) = \left(\frac{\ell^{\mu}\chi_{\rho_y}^{\mu *}}{96}\right)\left(d_{\rho_z}^{m_4}\boldsymbol{\rho}_x + 1\cdot\boldsymbol{\rho}_y + d_{\tilde{R}_z}^{m_4}\mathbf{i}_4 + d_{R_z}^{m_4}\mathbf{i}_3\right)$$

$$+\left(\frac{\ell^{\mu}}{24}\right)\left(\chi_{\mathbf{i}_4}^{\mu *}\right)\cdot \mathbf{i}_4\left(\mathbf{1} + d_{\rho_z}^{m_4}\boldsymbol{\rho}_z + d_{R_z}^{m_4}\mathbf{R}_z + d_{\tilde{R}_z}^{m_4}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^{\mu}\chi_{\mathbf{i}_4}^{\mu *}}{96}\right)\left(1\cdot\mathbf{i}_4 + d_{\rho_z}^{m_4}\mathbf{i}_3 + d_{R_z}^{m_4}\boldsymbol{\rho}_y + d_{\tilde{R}_z}^{m_4}\boldsymbol{\rho}_x\right) = \left(\frac{\ell^{\mu}\chi_{\mathbf{i}_4}^{\mu *}}{96}\right)\left(d_{\tilde{R}_z}^{m_4}\boldsymbol{\rho}_x + d_{R_z}^{m_4}\boldsymbol{\rho}_y + 1\cdot\mathbf{i}_4 + d_{\rho_z}^{m_4}\mathbf{i}_3\right)$$

$$+\left(\frac{\ell^{\mu}}{24}\right)\left(\chi_{\mathbf{i}_3}^{\mu *}\right)\cdot \mathbf{i}_3\left(\mathbf{1} + d_{\rho_z}^{m_4}\boldsymbol{\rho}_z + d_{R_z}^{m_4}\mathbf{R}_z + d_{\tilde{R}_z}^{m_4}\tilde{\mathbf{R}}_z\right)\frac{1}{4} = \left(\frac{\ell^{\mu}\chi_{\mathbf{i}_3}^{\mu *}}{96}\right)\left(1\cdot\mathbf{i}_3 + d_{\rho_z}^{m_4}\mathbf{i}_4 + d_{R_z}^{m_4}\mathbf{1} + d_{\tilde{R}_z}^{m_4}\boldsymbol{\rho}_y\right) = \left(\frac{\ell^{\mu}\chi_{\mathbf{i}_3}^{\mu *}}{96}\right)\left(d_{R_z}^{m_4}\boldsymbol{\rho}_x + d_{\tilde{R}_z}^{m_4}\boldsymbol{\rho}_y + d_{\rho_z}^{m_4}\mathbf{i}_4 + 1\cdot\mathbf{i}_3\right)$$

$\mathbf{r}_1 C_4 = \mathbf{r}_1\left\{\mathbf{1},\boldsymbol{\rho}_z,\mathbf{R}_z,\tilde{\mathbf{R}}_z\right\} = \left\{\mathbf{r}_1,\mathbf{r}_4,\mathbf{i}_1,\mathbf{R}_y\right\} Coset$ *etc. etc.*

General development of irep projectors $\mathbf{P}^{\mu}_{m_4 m_4} = \sum_{g}^{°O} \frac{\ell^{\mu}}{°O} D^{\mu*}_{m_4 m_4}(g)\,\mathbf{g}$ *for subgroup chain* $O \supset D_4 \supset C_4$

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

(Deriving diagonal irreducible O-representation ("irep") components $D^{\mu*}_{m_4 m_4}(g)$)

$$= \sum_{g}^{°O} \frac{\ell^{\mu}}{°O}(\chi_g^{\mu*})\cdot\mathbf{g}\cdot\left(\mathbf{p}_{m_4}\right) = \sum_{g}^{°O} \frac{\ell^{\mu}}{4°O}(\chi_g^{\mu*})\cdot\mathbf{g}\cdot\left(d_1^{m_4}\mathbf{1} + d_{\rho_z}^{m_4}\rho_z + d_{\mathbf{R}_z}^{m_4}\mathbf{R}_z + d_{\tilde{\mathbf{R}}_z}^{m_4}\tilde{\mathbf{R}}_z\right)$$

O characters $\chi^{\mu}_{\mathbf{g}}$

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

$$\mathbf{p}_{m_4} = \frac{1}{4}\sum_{p=0}^{3} \underbrace{e^{\frac{2\pi i\, m_4 \cdot p}{4}}}_{C_4 \text{ characters}} \mathbf{R}_z^{p} = \begin{cases} \mathbf{p}_{0_4} = (\mathbf{1}+\mathbf{R}_z+\rho_z+\tilde{\mathbf{R}}_z)/4 \\ \mathbf{p}_{1_4} = (\mathbf{1}+i\mathbf{R}_z-\rho_z-i\tilde{\mathbf{R}}_z)/4 \\ \mathbf{p}_{2_4} = (\mathbf{1}-\mathbf{R}_z+\rho_z-\tilde{\mathbf{R}}_z)/4 \\ \mathbf{p}_{3_4} = (\mathbf{1}-i\mathbf{R}_z-\rho_z+i\tilde{\mathbf{R}}_z)/4 \end{cases}$$

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

Coset array that helps sum character products for O projector splitting

	$\mathbf{1}$	ρ_z	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$
$\ell\chi\,\mathbf{1}$	$\mathbf{1}$	ρ_z	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$
$\ell\chi\,\rho_z$	ρ_z	$\mathbf{1}$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$
$\ell\chi\,\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$	$\mathbf{1}$	ρ_z
$\ell\chi\,\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$	ρ_z	$\mathbf{1}$

	ρ_x	ρ_y	$\mathbf{i}_4$	$\mathbf{i}_3$
$\ell\chi\,\rho_x$	$\mathbf{1}$	ρ_z	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$
$\ell\chi\,\rho_y$	ρ_z	$\mathbf{1}$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$
$\ell\chi\,\mathbf{i}_4$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$	$\mathbf{1}$	ρ_z
$\ell\chi\,\mathbf{i}_3$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$	ρ_z	$\mathbf{1}$

	$\mathbf{r}_1$	$\mathbf{r}_4$	$\mathbf{i}_1$	$\mathbf{R}_y$
$\ell\chi\,\mathbf{r}_1$	$\mathbf{1}$	ρ_z	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$
$\ell\chi\,\mathbf{r}_4$	ρ_z	$\mathbf{1}$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$
$\ell\chi\,\mathbf{i}_1$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$	$\mathbf{1}$	ρ_z
$\ell\chi\,\mathbf{R}_y$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$	ρ_z	$\mathbf{1}$

	$\mathbf{r}_2$	$\mathbf{r}_3$	$\mathbf{i}_2$	$\tilde{\mathbf{R}}_y$
$\ell\chi\,\mathbf{r}_2$	$\mathbf{1}$	ρ_z	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$
$\ell\chi\,\mathbf{r}_3$	ρ_z	$\mathbf{1}$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$
$\ell\chi\,\mathbf{i}_2$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$	$\mathbf{1}$	ρ_z
$\ell\chi\,\tilde{\mathbf{R}}_y$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$	ρ_z	$\mathbf{1}$

	$\tilde{\mathbf{r}}_1$	$\tilde{\mathbf{r}}_3$	$\tilde{\mathbf{R}}_x$	$\mathbf{i}_6$
$\ell\chi\,\tilde{\mathbf{r}}_1$	$\mathbf{1}$	ρ_z	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$
$\ell\chi\,\tilde{\mathbf{r}}_3$	ρ_z	$\mathbf{1}$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$
$\ell\chi\,\tilde{\mathbf{R}}_x$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$	$\mathbf{1}$	ρ_z
$\ell\chi\,\mathbf{i}_6$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$	ρ_z	$\mathbf{1}$

	$\tilde{\mathbf{r}}_2$	$\tilde{\mathbf{r}}_4$	$\mathbf{R}_x$	$\mathbf{i}_5$
$\ell\chi\,\tilde{\mathbf{r}}_2$	$\mathbf{1}$	ρ_z	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$
$\ell\chi\,\tilde{\mathbf{r}}_4$	ρ_z	$\mathbf{1}$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$
$\ell\chi\,\mathbf{R}_x$	$\tilde{\mathbf{R}}_z$	$\mathbf{R}_z$	$\mathbf{1}$	ρ_z
$\ell\chi\,\mathbf{i}_5$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_z$	ρ_z	$\mathbf{1}$

General development of irep projectors $\mathbf{P}^{\mu}_{m_4 m_4} = \sum_{g}^{\circ O} \frac{\ell^{\mu}}{\circ O} D^{\mu *}_{m_4 m_4}(g)\,\mathbf{g}$ *for subgroup chain* $O \supset D_4 \supset C_4$

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

(Deriving diagonal irreducible O-representation ("irep") components $D^{\mu *}_{m_4 m_4}(g)$)

$$= \sum_{g}^{\circ O} \frac{\ell^{\mu}}{\circ O}(\chi^{\mu *}_{g}) \cdot \mathbf{g} \cdot \left(\mathbf{p}_{m_4}\right) = \sum_{g}^{\circ O} \frac{\ell^{\mu}}{4 \circ O}(\chi^{\mu *}_{g}) \cdot \mathbf{g} \cdot \left(d_1^{m_4}\mathbf{1} + d^{m_4}_{\rho_z}\boldsymbol{\rho}_z + d^{m_4}_{\mathbf{R}_z}\mathbf{R}_z + d^{m_4}_{\tilde{\mathbf{R}}_z}\tilde{\mathbf{R}}_z\right)$$

O characters $\chi^{\mu}_{\mathbf{g}}$

$O:\chi^{\mu}_{\mathbf{g}}$	$\mathbf{g}=\mathbf{1}$	$\mathbf{r}^{p}_{1-4}$	$\boldsymbol{\rho}_{xyz}$	$\mathbf{R}^{p}_{xyz}$	$\mathbf{i}_{1-6}$
$\mu=A_1$	1	1	1	1	1
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$$\mathbf{p}_{m_4} = \frac{1}{4}\sum_{p=0}^{3} e^{\frac{2\pi i m_4 \cdot p}{4}} \mathbf{R}^{p}_{z} = \begin{cases} \mathbf{p}_{0_4} = (\mathbf{1}+\mathbf{R}_z+\rho_z+\tilde{\mathbf{R}}_z)/4 \\ \mathbf{p}_{1_4} = (\mathbf{1}+i\mathbf{R}_z-\rho_z-i\tilde{\mathbf{R}}_z)/4 \\ \mathbf{p}_{2_4} = (\mathbf{1}-\mathbf{R}_z+\rho_z-\tilde{\mathbf{R}}_z)/4 \\ \mathbf{p}_{3_4} = (\mathbf{1}-i\mathbf{R}_z-\rho_z+i\tilde{\mathbf{R}}_z)/4 \end{cases}$$

C_4 characters $d^{m_4}_{R^p} = e^{\frac{2\pi i m_4 \cdot p}{4}}$

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

$$= \tfrac{\ell^\mu}{96}\chi^{\mu*}_{\mathbf{1}}(1,d^{m4}_{\rho_z},d^{m4}_{R_z},d^{m4}_{\tilde{R}_z}) + \tfrac{\ell^\mu}{96}\chi^{\mu*}_{\rho_x}(1,d^{m4}_{\rho_z},d^{m4}_{R_z},d^{m4}_{\tilde{R}_z}) + \tfrac{\ell^\mu}{96}\chi^{\mu*}_{\mathbf{r}_1}(1,d^{m4}_{\rho_z},d^{m4}_{R_z},d^{m4}_{\tilde{R}_z}) + \tfrac{\ell^\mu}{96}\chi^{\mu*}_{\mathbf{r}_2}(1,d^{m4}_{\rho_z},d^{m4}_{R_z},d^{m4}_{\tilde{R}_z}) + \tfrac{\ell^\mu}{96}\chi^{\mu*}_{\tilde{\mathbf{r}}_1}(1,d^{m4}_{\rho_z},d^{m4}_{R_z},d^{m4}_{\tilde{R}_z}) + \tfrac{\ell^\mu}{96}\chi^{\mu*}_{\tilde{\mathbf{r}}_2}(1,d^{m4}_{\rho_z},d^{m4}_{R_z},d^{m4}_{\tilde{R}_z})$$

$$+ \tfrac{\ell^\mu}{96}\chi^{\mu*}_{\rho_z}(d^{m4}_{\rho_z},1,d^{m4}_{\tilde{R}_z},d^{m4}_{R_z}) + \tfrac{\ell^\mu}{96}\chi^{\mu*}_{\rho_y}(d^{m4}_{\rho_z},1,d^{m4}_{\tilde{R}_z},d^{m4}_{R_z}) + \tfrac{\ell^\mu}{96}\chi^{\mu*}_{\mathbf{r}_4}(d^{m4}_{\rho_z},1,d^{m4}_{\tilde{R}_z},d^{m4}_{R_z}) + \tfrac{\ell^\mu}{96}\chi^{\mu*}_{\mathbf{r}_3}(d^{m4}_{\rho_z},1,d^{m4}_{\tilde{R}_z},d^{m4}_{R_z}) + \tfrac{\ell^\mu}{96}\chi^{\mu*}_{\tilde{\mathbf{r}}_3}(d^{m4}_{\rho_z},1,d^{m4}_{\tilde{R}_z},d^{m4}_{R_z}) + \tfrac{\ell^\mu}{96}\chi^{\mu*}_{\tilde{\mathbf{r}}_4}(d^{m4}_{\rho_z},1,d^{m4}_{\tilde{R}_z},d^{m4}_{R_z})$$

$$+ \tfrac{\ell^\mu}{96}\chi^{\mu*}_{\mathbf{R}_z}(d^{m4}_{\tilde{R}_z},d^{m4}_{R_z},1,d^{m4}_{\rho_z}) + \tfrac{\ell^\mu}{96}\chi^{\mu*}_{\mathbf{i}_4}(d^{m4}_{\tilde{R}_z},d^{m4}_{R_z},1,d^{m4}_{\rho_z}) + \tfrac{\ell^\mu}{96}\chi^{\mu*}_{\mathbf{i}_1}(d^{m4}_{\tilde{R}_z},d^{m4}_{R_z},1,d^{m4}_{\rho_z}) + \tfrac{\ell^\mu}{96}\chi^{\mu*}_{\mathbf{i}_2}(d^{m4}_{\tilde{R}_z},d^{m4}_{R_z},1,d^{m4}_{\rho_z}) + \tfrac{\ell^\mu}{96}\chi^{\mu*}_{\tilde{\mathbf{R}}_x}(d^{m4}_{\tilde{R}_z},d^{m4}_{R_z},1,d^{m4}_{\rho_z}) + \tfrac{\ell^\mu}{96}\chi^{\mu*}_{\mathbf{R}_x}(d^{m4}_{\tilde{R}_z},d^{m4}_{R_z},1,d^{m4}_{\rho_z})$$

$$+ \tfrac{\ell^\mu}{96}\chi^{\mu*}_{\tilde{\mathbf{R}}_z}(d^{m4}_{R_z},d^{m4}_{\tilde{R}_z},d^{m4}_{\rho_z},1) + \tfrac{\ell^\mu}{96}\chi^{\mu*}_{\mathbf{i}_3}(d^{m4}_{R_z},d^{m4}_{\tilde{R}_z},d^{m4}_{\rho_z},1) + \tfrac{\ell^\mu}{96}\chi^{\mu*}_{\mathbf{R}_y}(d^{m4}_{R_z},d^{m4}_{\tilde{R}_z},d^{m4}_{\rho_z},1) + \tfrac{\ell^\mu}{96}\chi^{\mu*}_{\tilde{\mathbf{R}}_y}(d^{m4}_{R_z},d^{m4}_{\tilde{R}_z},d^{m4}_{\rho_z},1) + \tfrac{\ell^\mu}{96}\chi^{\mu*}_{\mathbf{i}_6}(d^{m4}_{R_z},d^{m4}_{\tilde{R}_z},d^{m4}_{\rho_z},1) + \tfrac{\ell^\mu}{96}\chi^{\mu*}_{\mathbf{i}_5}(d^{m4}_{R_z},d^{m4}_{\tilde{R}_z},d^{m4}_{\rho_z},1)$$

Each of 24 columns is a sum of 4 products $\frac{\ell^\mu}{96}\chi^{\mu*}_{\mathbf{g}} d^{m4}_{\rho_p}$ that gives coefficient $? = \frac{\ell^{\mu}}{\circ O} D^{\mu *}_{m_4 m_4}(g)$ of $\mathbf{P}^{\mu}_{m_4 m_4}$

$$\tfrac{1}{96}(\underline{?}\mathbf{1} + \underline{?}\boldsymbol{\rho}_z + \underline{?}\mathbf{R}_z + \underline{?}\tilde{\mathbf{R}}_z \;+ \underline{?}\boldsymbol{\rho}_x + \underline{?}\boldsymbol{\rho}_y + \underline{?}\mathbf{i}_4 + \underline{?}\mathbf{i}_3 \;+ \underline{?}\mathbf{r}_1 + \underline{?}\mathbf{r}_4 + \underline{?}\mathbf{i}_1 + \underline{?}\mathbf{R}_y \;+ \underline{?}\mathbf{r}_2 + \underline{?}\mathbf{r}_3 + \underline{?}\mathbf{i}_2 + \underline{?}\tilde{\mathbf{R}}_y \;+ \underline{?}\tilde{\mathbf{r}}_1 + \underline{?}\tilde{\mathbf{r}}_3 + \underline{?}\tilde{\mathbf{R}}_x + \underline{?}\mathbf{i}_6 \;+ \underline{?}\tilde{\mathbf{r}}_2 + \underline{?}\tilde{\mathbf{r}}_4 + \underline{?}\mathbf{R}_x + \underline{?}\mathbf{i}_5)$$

This $\mathbf{P}^{\mu}_{m_4 m_4}$-sum is in order of left cosets $\mathbf{g}\cdot C_4$ of C_4 in O. (Examples follow.)

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

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William G. Harter - University of Arkansas

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Review Octahedral $O_h\supset O$ group operator structure

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- *$O\supset D_4\supset C_4$ subgroup chain splitting*
- *$O\supset D_4\supset D_2$ subgroup chain splitting (nOrmal D_2 vs. unOrmal D_2)*
- *$O_h\supset O\supset D_4\supset C_{4v}$ and $O_h\supset O\supset D_4\supset C_{4v}\supset C_{2v}$ subgroup splitting*

Splitting O class projectors $\mathbf{P}^{\mu}$ into irreducible projectors $\mathbf{P}^{\mu}_{m_4m_4}$ for $O\supset C_4$

- *Left-cosets and coefficient arrays*

Development of irreducible projectors $\mathbf{P}^{\mu}_{m_4m_4}$ and representations $D^{\mu}_{m_4m_4}$

- *Calculating $\mathbf{P}^{E}_{0_40_4}$, $\mathbf{P}^{E}_{2_42_4}$, $\mathbf{P}^{T_1}_{0_40_4}$, $\mathbf{P}^{T_1}_{1_41_4}$, $\mathbf{P}^{T_2}_{2_42_4}$, $\mathbf{P}^{T_2}_{1_41_4}$, Collected $\mathbf{P}_{mm}$ results Table*

$O\supset C_4$ induced representation $0_4(C_4)\uparrow O \sim A_1\oplus T_1\oplus E$ and spectral analysis examples

- *Elementary induced representation $0_4(C_4)\uparrow O$*
- *Projection reduction of induced representation $0_4(C_4)\uparrow O$*
- *Introduction to ortho-complete eigenvalue-parameter relations*
  - *Examples in SF_6 spectroscopy*

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

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

O characters

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$4,\ 4,\ 4,\ 4, \qquad 4,\ 4,\ 4,\ 4, \qquad -2,-2,-2,-2, \qquad -2,-2,-2,-2, \qquad -2,-2,-2,-2, \qquad -2,-2,-2,-2,$$

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

Coset-factored sum:

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

Broken-class-ordered sum:

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

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

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

O characters

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

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

C_4 characters

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

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

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

$$\mathbf{1}C_4=\mathbf{1}\{\mathbf{1},\boldsymbol{\rho}_z,\mathbf{R}_z,\tilde{\mathbf{R}}_z\}\quad \boldsymbol{\rho}_xC_4=\{\boldsymbol{\rho}_x,\boldsymbol{\rho}_y,\mathbf{i}_4,\mathbf{i}_3\}\quad \mathbf{r}_1C_4=\{\mathbf{r}_1,\mathbf{r}_4,\mathbf{i}_1,\mathbf{R}_y\}\quad \mathbf{r}_2C_4=\{\mathbf{r}_2,\mathbf{r}_3,\mathbf{i}_2,\tilde{\mathbf{R}}_y\}\quad \tilde{\mathbf{r}}_1C_4=\{\tilde{\mathbf{r}}_1,\tilde{\mathbf{r}}_3,\tilde{\mathbf{R}}_x,\mathbf{i}_6\}\quad \tilde{\mathbf{r}}_2C_4=\{\tilde{\mathbf{r}}_2,\tilde{\mathbf{r}}_4,\mathbf{R}_x,\mathbf{i}_5\}$$

$$=\tfrac{1}{48}\chi^{E}_{\mathbf{1}}(1,d^{2_4}_{\rho_z},d^{2_4}_{R_z},d^{2_4}_{\tilde{R}_z}) +\tfrac{1}{48}\chi^{E}_{\rho_x}(1,d^{2_4}_{\rho_z},d^{2_4}_{R_z},d^{2_4}_{\tilde{R}_z}) +\tfrac{1}{48}\chi^{E}_{\mathbf{r}_1}(1,d^{2_4}_{\rho_z},d^{2_4}_{R_z},d^{2_4}_{\tilde{R}_z}) +\tfrac{1}{48}\chi^{E}_{\mathbf{r}_2}(1,d^{2_4}_{\rho_z},d^{2_4}_{R_z},d^{2_4}_{\tilde{R}_z}) +\tfrac{1}{48}\chi^{E}_{\tilde{\mathbf{r}}_1}(1,d^{2_4}_{\rho_z},d^{2_4}_{R_z},d^{2_4}_{\tilde{R}_z}) +\tfrac{1}{48}\chi^{E}_{\tilde{\mathbf{r}}_2}(1,d^{2_4}_{\rho_z},d^{2_4}_{R_z},d^{2_4}_{\tilde{R}_z})$$

$$+\tfrac{1}{48}\chi^{E}_{\rho_z}(d^{2_4}_{\rho_z},1,d^{2_4}_{\tilde{R}_z},d^{2_4}_{R_z}) +\tfrac{1}{48}\chi^{E}_{\rho_y}(d^{2_4}_{\rho_z},1,d^{2_4}_{\tilde{R}_z},d^{2_4}_{R_z}) +\tfrac{1}{48}\chi^{E}_{\mathbf{r}_4}(d^{2_4}_{\rho_z},1,d^{2_4}_{\tilde{R}_z},d^{2_4}_{R_z}) +\tfrac{1}{48}\chi^{E}_{\mathbf{r}_3}(d^{2_4}_{\rho_z},1,d^{2_4}_{\tilde{R}_z},d^{2_4}_{R_z}) +\tfrac{1}{48}\chi^{E}_{\tilde{\mathbf{r}}_3}(d^{2_4}_{\rho_z},1,d^{2_4}_{\tilde{R}_z},d^{2_4}_{R_z}) +\tfrac{1}{48}\chi^{E}_{\tilde{\mathbf{r}}_4}(d^{2_4}_{\rho_z},1,d^{2_4}_{\tilde{R}_z},d^{2_4}_{R_z})$$

$$+\tfrac{1}{48}\chi^{E}_{\mathbf{R}_z}(d^{2_4}_{\tilde{R}_z},d^{2_4}_{R_z},1,d^{2_4}_{\rho_z}) +\tfrac{1}{48}\chi^{E}_{\mathbf{i}_4}(d^{2_4}_{\tilde{R}_z},d^{2_4}_{R_z},1,d^{2_4}_{\rho_z}) +\tfrac{1}{48}\chi^{E}_{\mathbf{i}_1}(d^{2_4}_{\tilde{R}_z},d^{2_4}_{R_z},1,d^{2_4}_{\rho_z}) +\tfrac{1}{48}\chi^{E}_{\mathbf{i}_2}(d^{2_4}_{\tilde{R}_z},d^{2_4}_{R_z},1,d^{2_4}_{\rho_z}) +\tfrac{1}{48}\chi^{E}_{\tilde{\mathbf{R}}_x}(d^{2_4}_{\tilde{R}_z},d^{2_4}_{R_z},1,d^{2_4}_{\rho_z}) +\tfrac{1}{48}\chi^{E}_{\mathbf{R}_x}(d^{2_4}_{\tilde{R}_z},d^{2_4}_{R_z},1,d^{2_4}_{\rho_z})$$

$$+\tfrac{1}{48}\chi^{E}_{\tilde{\mathbf{R}}_z}(d^{2_4}_{R_z},d^{2_4}_{\tilde{R}_z},d^{2_4}_{\rho_z},1) +\tfrac{1}{48}\chi^{E}_{\mathbf{i}_3}(d^{2_4}_{R_z},d^{2_4}_{\tilde{R}_z},d^{2_4}_{\rho_z},1) +\tfrac{1}{48}\chi^{E}_{\mathbf{R}_y}(d^{2_4}_{R_z},d^{2_4}_{\tilde{R}_z},d^{2_4}_{\rho_z},1) +\tfrac{1}{48}\chi^{E}_{\tilde{\mathbf{R}}_y}(d^{2_4}_{R_z},d^{2_4}_{\tilde{R}_z},d^{2_4}_{\rho_z},1) +\tfrac{1}{48}\chi^{E}_{\mathbf{i}_6}(d^{2_4}_{R_z},d^{2_4}_{\tilde{R}_z},d^{2_4}_{\rho_z},1) +\tfrac{1}{48}\chi^{E}_{\mathbf{i}_5}(d^{2_4}_{R_z},d^{2_4}_{\tilde{R}_z},d^{2_4}_{\rho_z},1)$$

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

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

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

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

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

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

Coset-factored sum:

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

Broken-class-ordered sum:

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

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3.07.18 class 16.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Discrete symmetry subgroups of $O(3)\supset$(Octahedral $O_h\supset O$): Deriving $D^{(\alpha)}$-matrices defined by subgroup-chains $O\supset D_4\supset C_4$, $O\supset D_4\supset D_2$, and $O\supset D_3\supset C_3$ applications to IR spectra of SF_6

Review Octahedral $O_h\supset O$ group operator structure

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Comparison of $O\supset D_4\supset C_4$ and $O\supset D_4\supset D_2$ correlations and level/projector splitting

- *$O\supset D_4\supset C_4$ subgroup chain splitting*
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- *$O_h\supset O\supset D_4\supset C_{4v}$ and $O_h\supset O\supset D_4\supset C_{4v}\supset C_{2v}$ subgroup splitting*

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- *Left-cosets and coefficient arrays*

Development of irreducible projectors $\mathbf{P}^{\mu}_{m_4m_4}$ and representations $D^{\mu}_{m_4m_4}$

- *Calculating $\mathbf{P}^{E}_{0_40_4}$, $\mathbf{P}^{E}_{2_42_4}$, $\mathbf{P}^{T_1}_{0_40_4}$, $\mathbf{P}^{T_1}_{1_41_4}$, $\mathbf{P}^{T_2}_{2_42_4}$, $\mathbf{P}^{T_2}_{1_41_4}$, Collected $\mathbf{P}_{mm}$ results Table*

$O\supset C_4$ induced representation $0_4(C_4)\uparrow O \sim A_1\oplus T_1\oplus E$ and spectral analysis examples

- *Elementary induced representation $0_4(C_4)\uparrow O$*
- *Projection reduction of induced representation $0_4(C_4)\uparrow O$*
- *Introduction to ortho-complete eigenvalue-parameter relations*
  - *Examples in SF_6 spectroscopy*

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

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

O characters

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

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

C_4 characters

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Coset-factored sum:

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

Broken-class-ordered sum:

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

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3.07.18 class 16.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

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  - *Examples in SF_6 spectroscopy*

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

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

O characters

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

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

C_4 characters

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

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

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

$$\mathbf{1}C_4=\mathbf{1}\{\mathbf{1},\boldsymbol{\rho}_z,\mathbf{R}_z,\tilde{\mathbf{R}}_z\}\quad \boldsymbol{\rho}_xC_4=\{\boldsymbol{\rho}_x,\boldsymbol{\rho}_y,\mathbf{i}_4,\mathbf{i}_3\}\quad \mathbf{r}_1C_4=\{\mathbf{r}_1,\mathbf{r}_4,\mathbf{i}_1,\mathbf{R}_y\}\quad \mathbf{r}_2C_4=\{\mathbf{r}_2,\mathbf{r}_3,\mathbf{i}_2,\tilde{\mathbf{R}}_y\}\quad \tilde{\mathbf{r}}_1C_4=\{\tilde{\mathbf{r}}_1,\tilde{\mathbf{r}}_3,\tilde{\mathbf{R}}_x,\mathbf{i}_6\}\quad \tilde{\mathbf{r}}_2C_4=\{\tilde{\mathbf{r}}_2,\tilde{\mathbf{r}}_4,\mathbf{R}_x,\mathbf{i}_5\}$$

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

$$+\tfrac{1}{32}\chi^{T_1}_{\rho_z}(d^{1_4}_{\rho_z},1,d^{1_4}_{\tilde R_z},d^{1_4}_{R_z}) +\tfrac{1}{32}\chi^{T_1}_{\boldsymbol{\rho}_y}(d^{1_4}_{\rho_z},1,d^{1_4}_{\tilde R_z},d^{1_4}_{R_z}) +\tfrac{1}{32}\chi^{T_1}_{\mathbf{r}_4}(d^{1_4}_{\rho_z},1,d^{1_4}_{\tilde R_z},d^{1_4}_{R_z}) +\tfrac{1}{32}\chi^{T_1}_{\mathbf{r}_3}(d^{1_4}_{\rho_z},1,d^{1_4}_{\tilde R_z},d^{1_4}_{R_z}) +\tfrac{1}{32}\chi^{T_1}_{\tilde{\mathbf{r}}_3}(d^{1_4}_{\rho_z},1,d^{1_4}_{\tilde R_z},d^{1_4}_{R_z}) +\tfrac{1}{32}\chi^{T_1}_{\tilde{\mathbf{r}}_4}(d^{1_4}_{\rho_z},1,d^{1_4}_{\tilde R_z},d^{1_4}_{R_z})$$

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

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

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

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

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

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

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

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

Coset-factored sum:

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

Broken-class-ordered sum:

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

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3.07.18 class 16.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Discrete symmetry subgroups of O(3)⊃(Octahedral O_h⊃O): Deriving $D^{(\alpha)}$-matrices defined by subgroup-chains $O \supset D_4 \supset C_4$, $O \supset D_4 \supset D_2$, and $O \supset D_3 \supset C_3$ applications to IR spectra of SF_6

Review Octahedral $O_h \supset O$ *group operator structure*

Review Octahedral $O_h \supset O \supset D_4 \supset C_4$ *subgroup chain correlations*

Comparison of $O \supset D_4 \supset C_4$ *and* $O \supset D_4 \supset D_2$ *correlations and level/projector splitting*

- $O \supset D_4 \supset C_4$ *subgroup chain splitting*
- $O \supset D_4 \supset D_2$ *subgroup chain splitting (nOrmal* D_2 *vs. unOrmal* D_2*)*
- $O_h \supset O \supset D_4 \supset C_{4v}$ *and* $O_h \supset O \supset D_4 \supset C_{4v} \supset C_{2v}$ *subgroup splitting*

Splitting O class projectors $\mathbf{P}^{\mu}$ *into irreducible projectors* $\mathbf{P}^{\mu}_{m_4 m_4}$ *for* $O \supset C_4$

- *Left-cosets and coefficient arrays*

➡ *Development of irreducible projectors* $\mathbf{P}^{\mu}_{m_4 m_4}$ *and representations* $D^{\mu}_{m_4 m_4}$

- ➡ *Calculating* $\mathbf{P}^{E}_{0_4 0_4}$, $\mathbf{P}^{E}_{2_4 2_4}$, $\mathbf{P}^{T_1}_{0_4 0_4}$, $\mathbf{P}^{T_1}_{1_4 1_4}$, $\mathbf{P}^{T_2}_{2_4 2_4}$ ⬆, $\mathbf{P}^{T_2}_{1_4 1_4}$, *Collected* $\mathbf{P}_{mm}$ *results Table*

$O \supset C_4$ *induced representation* $0_4(C_4)\uparrow O \sim A_1 \oplus T_1 \oplus E$ *and spectral analysis examples*

- *Elementary induced representation* $0_4(C_4)\uparrow O$
- *Projection reduction of induced representation* $0_4(C_4)\uparrow O$
- *Introduction to ortho-complete eigenvalue-parameter relations*
  - *Examples in* SF_6 *spectroscopy*

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

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

O characters

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

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

C_4 characters

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

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

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

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

$$=\tfrac{1}{32}\chi^{T_2}_{\mathbf{1}}(1,d^{2_4}_{\rho_z},d^{2_4}_{R_z},d^{2_4}_{\tilde R_z})+\tfrac{1}{32}\chi^{T_2}_{\rho_x}(1,d^{2_4}_{\rho_z},d^{2_4}_{R_z},d^{2_4}_{\tilde R_z})+\tfrac{1}{32}\chi^{T_2}_{\mathbf{r}_1}(1,d^{2_4}_{\rho_z},d^{2_4}_{R_z},d^{2_4}_{\tilde R_z})+\tfrac{1}{32}\chi^{T_2}_{\mathbf{r}_2}(1,d^{2_4}_{\rho_z},d^{2_4}_{R_z},d^{2_4}_{\tilde R_z})+\tfrac{1}{32}\chi^{T_2}_{\tilde{\mathbf{r}}_1}(1,d^{2_4}_{\rho_z},d^{2_4}_{R_z},d^{2_4}_{\tilde R_z})+\tfrac{1}{32}\chi^{T_2}_{\tilde{\mathbf{r}}_2}(1,d^{2_4}_{\rho_z},d^{2_4}_{R_z},d^{2_4}_{\tilde R_z})$$

$$+\tfrac{1}{32}\chi^{T_2}_{\rho_z}(d^{2_4}_{\rho_z},1,d^{2_4}_{\tilde R_z},d^{2_4}_{R_z})+\tfrac{1}{32}\chi^{T_2}_{\rho_y}(d^{2_4}_{\rho_z},1,d^{2_4}_{\tilde R_z},d^{2_4}_{R_z})+\tfrac{1}{32}\chi^{T_2}_{\mathbf{r}_4}(d^{2_4}_{\rho_z},1,d^{2_4}_{\tilde R_z},d^{2_4}_{R_z})+\tfrac{1}{32}\chi^{T_2}_{\mathbf{r}_3}(d^{2_4}_{\rho_z},1,d^{2_4}_{\tilde R_z},d^{2_4}_{R_z})+\tfrac{1}{32}\chi^{T_2}_{\tilde{\mathbf{r}}_3}(d^{2_4}_{\rho_z},1,d^{2_4}_{\tilde R_z},d^{2_4}_{R_z})+\tfrac{1}{32}\chi^{T_2}_{\tilde{\mathbf{r}}_4}(d^{2_4}_{\rho_z},1,d^{2_4}_{\tilde R_z},d^{2_4}_{R_z})$$

$$+\tfrac{1}{32}\chi^{T_2}_{\mathbf{R}_z}(d^{2_4}_{\tilde R_z},d^{2_4}_{R_z},1,d^{2_4}_{\rho_z})+\tfrac{1}{32}\chi^{T_2}_{\mathbf{i}_4}(d^{2_4}_{\tilde R_z},d^{2_4}_{R_z},1,d^{2_4}_{\rho_z})+\tfrac{1}{32}\chi^{T_2}_{\mathbf{i}_1}(d^{2_4}_{\tilde R_z},d^{2_4}_{R_z},1,d^{2_4}_{\rho_z})+\tfrac{1}{32}\chi^{T_2}_{\mathbf{i}_2}(d^{2_4}_{\tilde R_z},d^{2_4}_{R_z},1,d^{2_4}_{\rho_z})+\tfrac{1}{32}\chi^{T_2}_{\tilde{\mathbf{R}}_x}(d^{2_4}_{\tilde R_z},d^{2_4}_{R_z},1,d^{2_4}_{\rho_z})+\tfrac{1}{32}\chi^{T_2}_{\mathbf{R}_x}(d^{2_4}_{\tilde R_z},d^{2_4}_{R_z},1,d^{2_4}_{\rho_z})$$

$$+\tfrac{1}{32}\chi^{T_2}_{\tilde{\mathbf{R}}_z}(d^{2_4}_{R_z},d^{2_4}_{\tilde R_z},d^{2_4}_{\rho_z},1)+\tfrac{1}{32}\chi^{T_2}_{\mathbf{i}_3}(d^{2_4}_{R_z},d^{2_4}_{\tilde R_z},d^{2_4}_{\rho_z},1)+\tfrac{1}{32}\chi^{T_2}_{\mathbf{R}_y}(d^{2_4}_{R_z},d^{2_4}_{\tilde R_z},d^{2_4}_{\rho_z},1)+\tfrac{1}{32}\chi^{T_2}_{\tilde{\mathbf{R}}_y}(d^{2_4}_{R_z},d^{2_4}_{\tilde R_z},d^{2_4}_{\rho_z},1)+\tfrac{1}{32}\chi^{T_2}_{\mathbf{i}_6}(d^{2_4}_{R_z},d^{2_4}_{\tilde R_z},d^{2_4}_{\rho_z},1))+\tfrac{1}{32}\chi^{T_2}_{\mathbf{i}_5}(d^{2_4}_{R_z},d^{2_4}_{\tilde R_z},d^{2_4}_{\rho_z},1)$$

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

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

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

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

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

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

Coset-factored sum:

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

Broken-class-ordered sum:

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

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3.07.18 class 16.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

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Discrete symmetry subgroups of O(3)$\supset$(Octahedral $O_h\supset$O): Deriving $D^{(\alpha)}$-matrices defined by subgroup-chains $O\supset D_4\supset C_4$, $O\supset D_4\supset D_2$, and $O\supset D_3\supset C_3$ applications to IR spectra of SF_6

Review Octahedral $O_h\supset$O group operator structure

Review Octahedral $O_h\supset O\supset D_4\supset C_4$ subgroup chain correlations

Comparison of $O\supset D_4\supset C_4$ and $O\supset D_4\supset D_2$ correlations and level/projector splitting

- *$O\supset D_4\supset C_4$ subgroup chain splitting*
- *$O\supset D_4\supset D_2$ subgroup chain splitting (nOrmal D_2 vs. unOrmal D_2)*
- *$O_h\supset O\supset D_4\supset C_{4v}$ and $O_h\supset O\supset D_4\supset C_{4v}\supset C_{2v}$ subgroup splitting*

Splitting O class projectors $\mathbf{P}^{\mu}$ into irreducible projectors $\mathbf{P}^{\mu}_{m_4m_4}$ for $O\supset C_4$

- *Left-cosets and coefficient arrays*

Development of irreducible projectors $\mathbf{P}^{\mu}_{m_4m_4}$ and representations $D^{\mu}_{m_4m_4}$

- *Calculating $\mathbf{P}^{E}_{0_40_4}$, $\mathbf{P}^{E}_{2_42_4}$, $\mathbf{P}^{T_1}_{0_40_4}$, $\mathbf{P}^{T_1}_{1_41_4}$, $\mathbf{P}^{T_2}_{2_42_4}$, $\mathbf{P}^{T_2}_{1_41_4}$, Collected $\mathbf{P}_{mm}$ results Table*

$O\supset C_4$ induced representation $0_4(C_4)\uparrow O \sim A_1\oplus T_1\oplus E$ and spectral analysis examples

- *Elementary induced representation $0_4(C_4)\uparrow O$*
- *Projection reduction of induced representation $0_4(C_4)\uparrow O$*
- *Introduction to ortho-complete eigenvalue-parameter relations*
  - *Examples in SF_6 spectroscopy*

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

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

O characters

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

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

C_4 characters

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

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

$$= \sum_{g}^{\circ O}\frac{\ell^{T_2}}{\circ O}(\chi^{T_2}_g)\cdot\mathbf{g}\cdot(\mathbf{p}_{1_4}) = \sum_{g}^{\circ O}\frac{3}{96}(\chi^{T_2}_g)\cdot\mathbf{g}\cdot(1\cdot\mathbf{1}-1\cdot\rho_z+i\cdot\mathbf{R}_z-i\cdot\tilde{\mathbf{R}}_z)$$

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

$$=\tfrac{1}{32}\chi^{T_2}_{\mathbf{1}}(1,d^{1_4}_{\rho_z},d^{1_4}_{R_z},d^{1_4}_{\tilde{R}_z}) +\tfrac{1}{32}\chi^{T_2}_{\rho_x}(1,d^{1_4}_{\rho_z},d^{1_4}_{R_z},d^{1_4}_{\tilde{R}_z}) +\tfrac{1}{32}\chi^{T_2}_{\mathbf{r}_1}(1,d^{1_4}_{\rho_z},d^{1_4}_{R_z},d^{1_4}_{\tilde{R}_z}) +\tfrac{1}{32}\chi^{T_2}_{\mathbf{r}_2}(1,d^{1_4}_{\rho_z},d^{1_4}_{R_z},d^{1_4}_{\tilde{R}_z}) +\tfrac{1}{32}\chi^{T_2}_{\tilde{\mathbf{r}}_1}(1,d^{1_4}_{\rho_z},d^{1_4}_{R_z},d^{1_4}_{\tilde{R}_z}) +\tfrac{1}{32}\chi^{T_2}_{\tilde{\mathbf{r}}_2}(1,d^{1_4}_{\rho_z},d^{1_4}_{R_z},d^{1_4}_{\tilde{R}_z})$$

$$+\tfrac{1}{32}\chi^{T_2}_{\rho_z}(d^{1_4}_{\rho_z},1,d^{1_4}_{\tilde{R}_z},d^{1_4}_{R_z}) +\tfrac{1}{32}\chi^{T_2}_{\rho_y}(d^{1_4}_{\rho_z},1,d^{1_4}_{\tilde{R}_z},d^{1_4}_{R_z}) +\tfrac{1}{32}\chi^{T_2}_{\mathbf{r}_4}(d^{1_4}_{\rho_z},1,d^{1_4}_{\tilde{R}_z},d^{1_4}_{R_z}) +\tfrac{1}{32}\chi^{T_2}_{\mathbf{r}_3}(d^{1_4}_{\rho_z},1,d^{1_4}_{\tilde{R}_z},d^{1_4}_{R_z}) +\tfrac{1}{32}\chi^{T_2}_{\tilde{\mathbf{r}}_3}(d^{1_4}_{\rho_z},1,d^{1_4}_{\tilde{R}_z},d^{1_4}_{R_z}) +\tfrac{1}{32}\chi^{T_2}_{\tilde{\mathbf{r}}_4}(d^{1_4}_{\rho_z},1,d^{1_4}_{\tilde{R}_z},d^{1_4}_{R_z})$$

$$+\tfrac{1}{32}\chi^{T_2}_{\mathbf{R}_z}(d^{1_4}_{\tilde{R}_z},d^{1_4}_{R_z},1,d^{1_4}_{\rho_z}) +\tfrac{1}{32}\chi^{T_2}_{\mathbf{i}_4}(d^{1_4}_{\tilde{R}_z},d^{1_4}_{R_z},1,d^{1_4}_{\rho_z}) +\tfrac{1}{32}\chi^{T_2}_{\mathbf{i}_1}(d^{1_4}_{\tilde{R}_z},d^{1_4}_{R_z},1,d^{1_4}_{\rho_z}) +\tfrac{1}{32}\chi^{T_2}_{\mathbf{i}_2}(d^{1_4}_{\tilde{R}_z},d^{1_4}_{R_z},1,d^{1_4}_{\rho_z}) +\tfrac{1}{32}\chi^{T_2}_{\tilde{\mathbf{R}}_x}(d^{1_4}_{\tilde{R}_z},d^{1_4}_{R_z},1,d^{1_4}_{\rho_z}) +\tfrac{1}{32}\chi^{T_2}_{\mathbf{R}_x}(d^{1_4}_{\tilde{R}_z},d^{1_4}_{R_z},1,d^{1_4}_{\rho_z})$$

$$+\tfrac{1}{32}\chi^{T_2}_{\tilde{\mathbf{R}}_z}(d^{1_4}_{R_z},d^{1_4}_{\tilde{R}_z},d^{1_4}_{\rho_z},1) +\tfrac{1}{32}\chi^{T_2}_{\mathbf{i}_3}(d^{1_4}_{R_z},d^{1_4}_{\tilde{R}_z},d^{1_4}_{\rho_z},1) +\tfrac{1}{32}\chi^{T_2}_{\mathbf{R}_y}(d^{1_4}_{R_z},d^{1_4}_{\tilde{R}_z},d^{1_4}_{\rho_z},1) +\tfrac{1}{32}\chi^{T_2}_{\tilde{\mathbf{R}}_y}(d^{1_4}_{R_z},d^{1_4}_{\tilde{R}_z},d^{1_4}_{\rho_z},1) +\tfrac{1}{32}\chi^{T_2}_{\mathbf{i}_6}(d^{1_4}_{R_z},d^{1_4}_{\tilde{R}_z},d^{1_4}_{\rho_z},1) +\tfrac{1}{32}\chi^{T_2}_{\mathbf{i}_5}(d^{1_4}_{R_z},d^{1_4}_{\tilde{R}_z},d^{1_4}_{\rho_z},1)$$

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

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

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

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

$+4,-4,4i,-4i,\qquad 0,0,0,0,\qquad -2i,2i,2,-2,\qquad -2i,2i,2,-2,\qquad 2i,-2i,-2,2,\qquad 2i,-2i,-2,2.$

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

Coset-factored sum:

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

Broken-class-ordered sum:

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

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Discrete symmetry subgroups of O(3)⊃(Octahedral O_h⊃O): Deriving $D^{(\alpha)}$-matrices defined by subgroup-chains $O \supset D_4 \supset C_4$, $O \supset D_4 \supset D_2$, and $O \supset D_3 \supset C_3$ applications to IR spectra of SF_6

Review Octahedral $O_h \supset O$ group operator structure

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- *$O \supset D_4 \supset C_4$ subgroup chain splitting*
- *$O \supset D_4 \supset D_2$ subgroup chain splitting (nOrmal D_2 vs. unOrmal D_2)*
- *$O_h \supset O \supset D_4 \supset C_{4v}$ and $O_h \supset O \supset D_4 \supset C_{4v} \supset C_{2v}$ subgroup splitting*

Splitting O class projectors $\mathbf{P}^{\mu}$ into irreducible projectors $\mathbf{P}^{\mu}_{m_4 m_4}$ for $O \supset C_4$

- *Left-cosets and coefficient arrays*

Development of irreducible projectors $\mathbf{P}^{\mu}_{m_4 m_4}$ and representations $D^{\mu}_{m_4 m_4}$

- *Calculating $\mathbf{P}^{E}_{0_4 0_4}$, $\mathbf{P}^{E}_{2_4 2_4}$, $\mathbf{P}^{T_1}_{0_4 0_4}$, $\mathbf{P}^{T_1}_{1_4 1_4}$, $\mathbf{P}^{T_2}_{2_4 2_4}$, $\mathbf{P}^{T_2}_{1_4 1_4}$, Collected $\mathbf{P}_{mm}$ results Table*

$O \supset C_4$ induced representation $0_4(C_4)\uparrow O \sim A_1 \oplus T_1 \oplus E$ and spectral analysis examples

- *Elementary induced representation $0_4(C_4)\uparrow O$*
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- *Introduction to ortho-complete eigenvalue-parameter relations*
  - *Examples in SF_6 spectroscopy*

$O\supset C_4$	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

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

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

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

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

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

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

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

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

$\mathbf{P}^{(\alpha)}_{n_4 n_4}(O\supset C_4)$	**1**	$r_1r_2\tilde{r}_3\tilde{r}_4$	$\tilde{r}_1\tilde{r}_2r_3r_4$	$\rho_x\rho_y$	ρ_z	$R_x\tilde{R}_xR_y\tilde{R}_y$	R_z	$\tilde{R}_z$	$i_1i_2i_5i_6$	i_3i_4
$24\cdot\mathbf{P}^{A_1}_{0_40_4}$	1	1	1	1	1	1	1	1	1	1
$24\cdot\mathbf{P}^{A_2}_{2_42_4}$	1	1	1	1	1	-1	-1	-1	-1	-1
$12\cdot\mathbf{P}^{E}_{0_40_4}$	1	$-\frac{1}{2}$	$-\frac{1}{2}$	1	1	$-\frac{1}{2}$	1	1	$-\frac{1}{2}$	1
$12\cdot\mathbf{P}^{E}_{2_42_4}$	1	$-\frac{1}{2}$	$-\frac{1}{2}$	1	1	$+\frac{1}{2}$	-1	-1	$+\frac{1}{2}$	-1
$8\cdot\mathbf{P}^{T_1}_{1_41_4}$	1	$-\frac{i}{2}$	$+\frac{i}{2}$	0	-1	$+\frac{1}{2}$	$-i$	$+i$	$-\frac{1}{2}$	0
$8\cdot\mathbf{P}^{T_1}_{3_43_4}$	1	$+\frac{i}{2}$	$-\frac{i}{2}$	0	-1	$+\frac{1}{2}$	$+i$	$-i$	$-\frac{1}{2}$	0
$8\cdot\mathbf{P}^{T_1}_{0_40_4}$	1	0	0	-1	1	0	1	1	0	-1
$8\cdot\mathbf{P}^{T_2}_{1_41_4}$	1	$+\frac{i}{2}$	$-\frac{i}{2}$	0	-1	$-\frac{1}{2}$	$-i$	$+i$	$+\frac{1}{2}$	0
$8\cdot\mathbf{P}^{T_2}_{3_43_4}$	1	$-\frac{i}{2}$	$+\frac{i}{2}$	0	-1	$-\frac{1}{2}$	$+i$	$-i$	$+\frac{1}{2}$	0
$8\cdot\mathbf{P}^{T_2}_{2_42_4}$	1	0	0	-1	1	0	-1	-1	0	1

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

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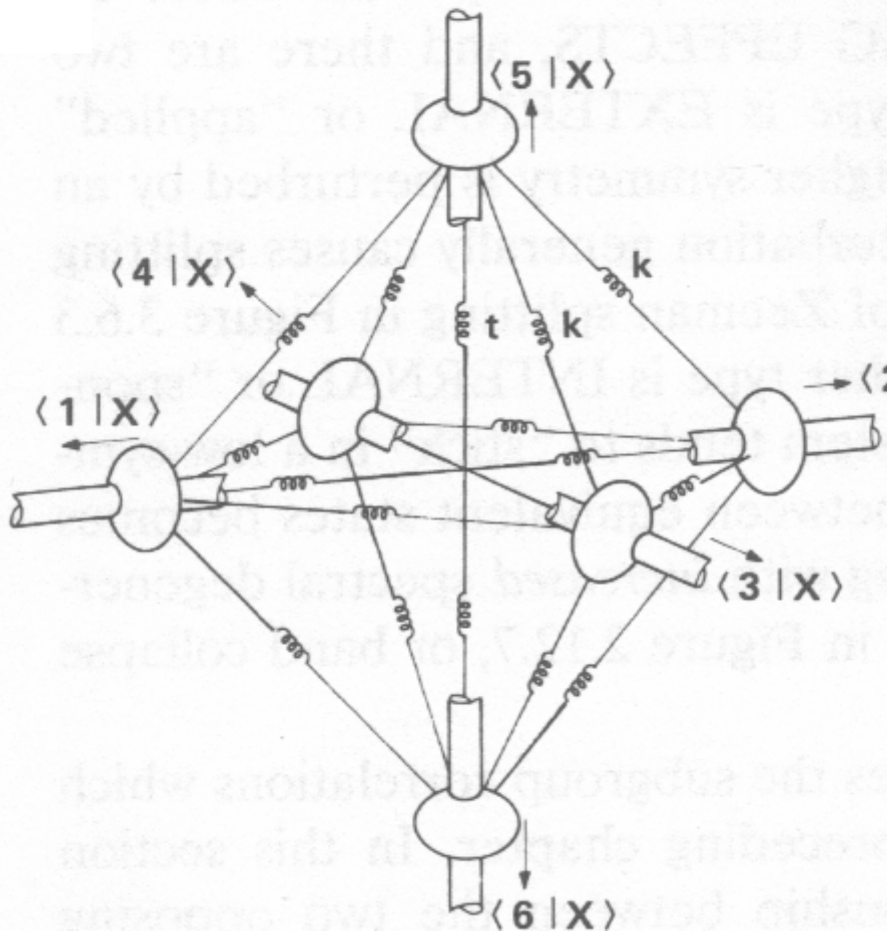
  - *Examples from SF_6 model spectroscopy*

O⊃C_4 *induced representation* $0_4\uparrow O\sim A_1\oplus T_1\oplus E$ *and spectral analysis examples*



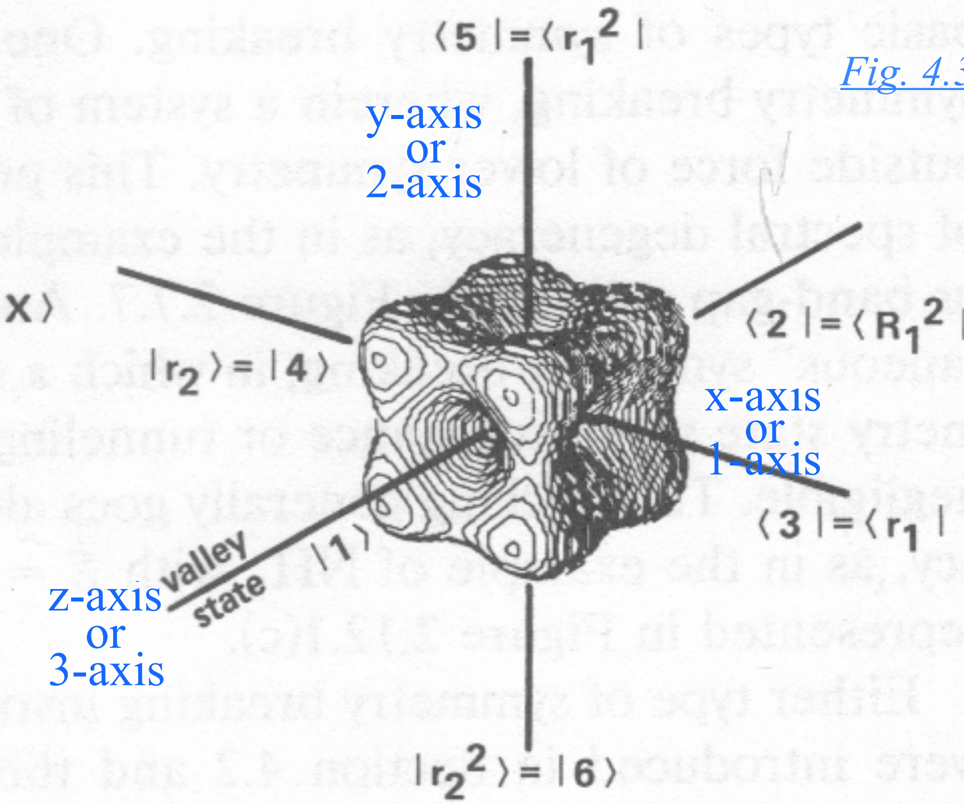


Fig. 4.3.1 PSDS

Solve XY_6 radial vibration **K**=**a**-*matrix*

$$
\begin{pmatrix}
\langle 1|\mathbf{a}|1\rangle & \langle 1|\mathbf{a}|2\rangle & \cdots & \langle 1|\mathbf{a}|6\rangle \\
\langle 2|\mathbf{a}|1\rangle & \langle 2|\mathbf{a}|2\rangle & \cdots & \langle 2|\mathbf{a}|6\rangle \\
\cdot & & & \\
\cdot & h = 2k+t, & & \\
\cdot & s = k/2 & & \\
\langle 6|\mathbf{a}|1\rangle & \langle 6|\mathbf{a}|2\rangle & \cdots & \langle y|\mathbf{a}|6\rangle
\end{pmatrix}
=
\begin{pmatrix}
h & t & s & s & s & s \\
t & h & s & s & s & s \\
s & s & h & t & s & s \\
s & s & t & h & s & s \\
s & s & s & s & h & t \\
s & s & s & s & t & h
\end{pmatrix},
$$

Solve SF_6 J-tunneling Hamiltonian **H**

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

O⊃C_4 *induced representation* $0_4\uparrow O \sim A_1 \oplus T_1 \oplus E$ *and spectral analysis examples*

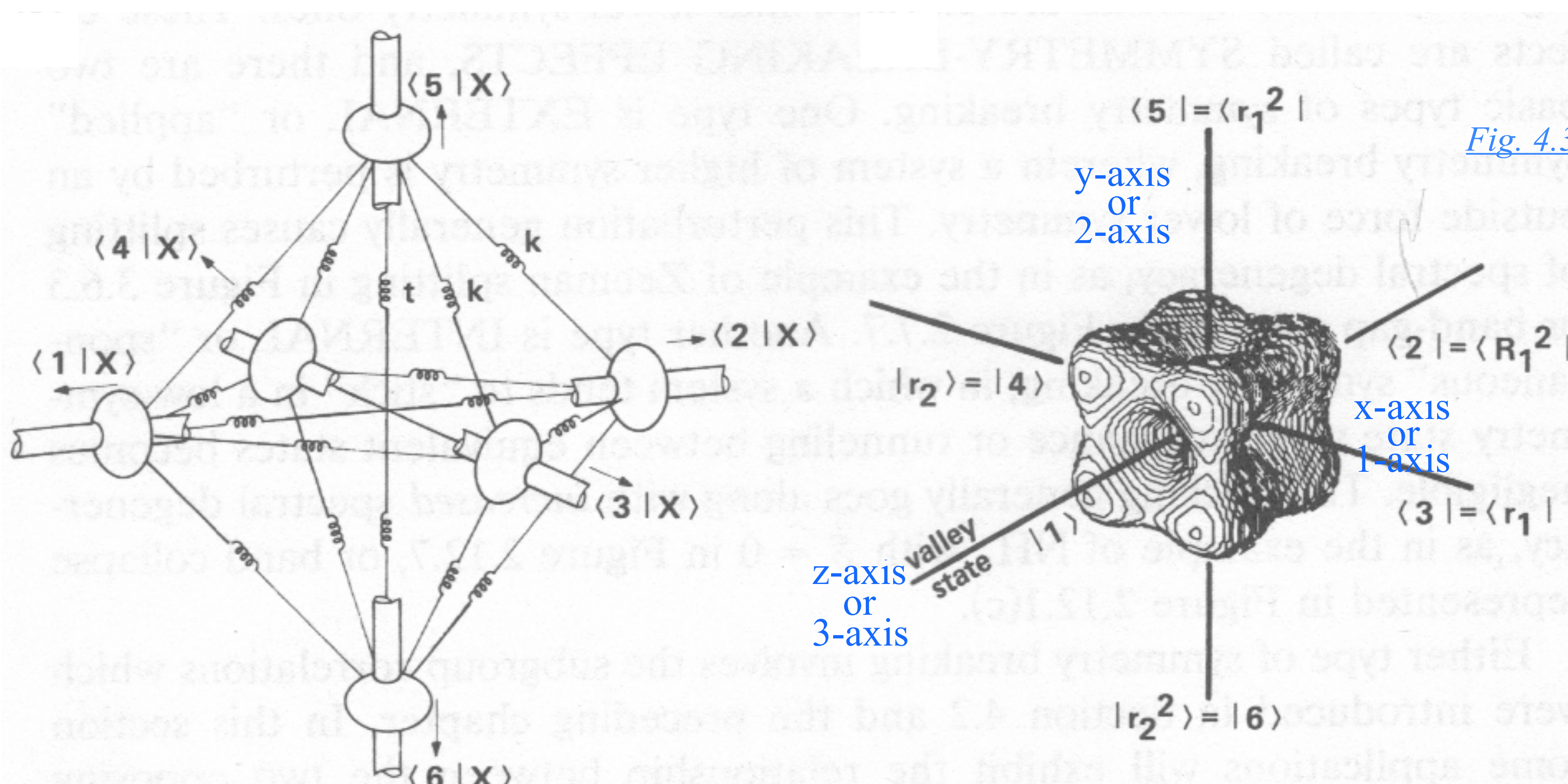


Fig. 4.3.1 PSDS

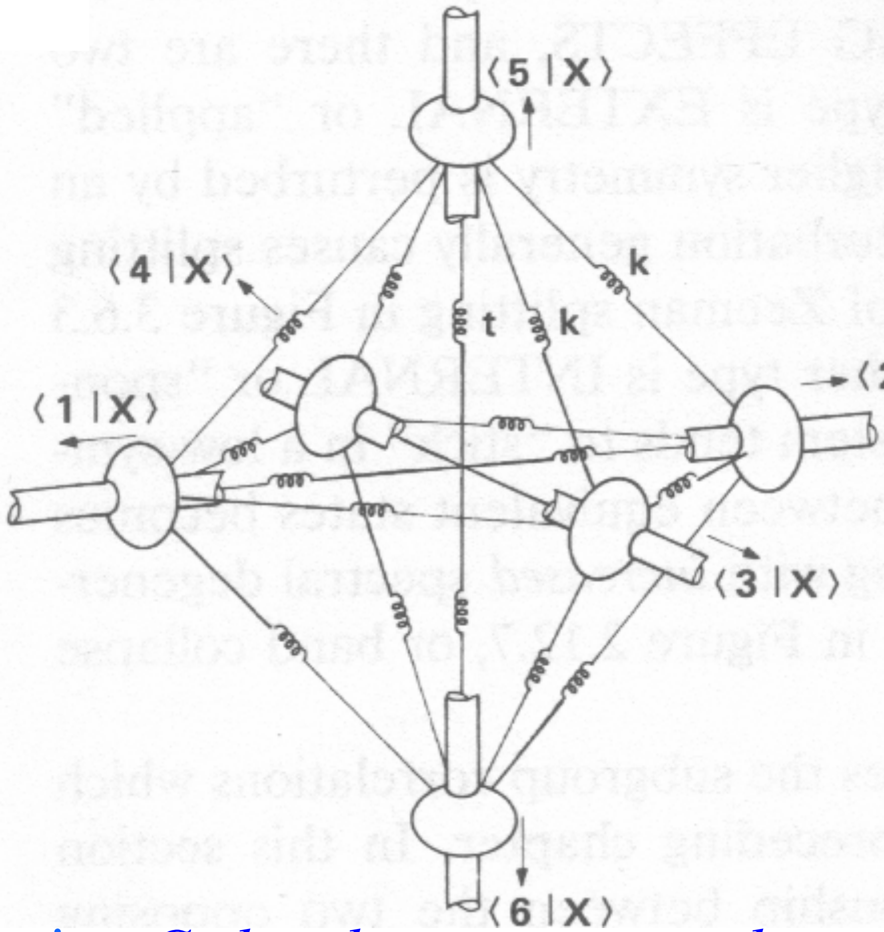
Assuming *C_4-local symmetry conditions* for $|\mathbf{1}\rangle$ state

$$|1\rangle = \mathbf{1}|1\rangle = R_3|1\rangle = R_3^2|1\rangle = R_3^3|1\rangle$$

O operators (Two notations: Older *Princ.of Symm.Dynamics and Spectra.* *and Newer* *Int.J.Mol.Sci)*

PSDS:	$\mathbf{1}$	$\mathbf{r}_1$	$\mathbf{r}_2$	$\mathbf{r}_3$	$\mathbf{r}_4$	$\mathbf{r}_1^2$	$\mathbf{r}_2^2$	$\mathbf{r}_3^2$	$\mathbf{r}_4^2$	$\mathbf{R}_1^2$	$\mathbf{R}_2^2$	$\mathbf{R}_3^2$	$\mathbf{R}_1$	$\mathbf{R}_2$	$\mathbf{R}_3$	$\mathbf{R}_1^3$	$\mathbf{R}_2^3$	$\mathbf{R}_3^3$	$\mathbf{i}_1$	$\mathbf{i}_2$	$\mathbf{i}_3$	$\mathbf{i}_4$	$\mathbf{i}_5$	$\mathbf{i}_6$
IJMS:	$\mathbf{1}$	$\mathbf{r}_1$	$\mathbf{r}_2$	$\mathbf{r}_3$	$\mathbf{r}_4$	$\tilde{\mathbf{r}}_1$	$\tilde{\mathbf{r}}_2$	$\tilde{\mathbf{r}}_3$	$\tilde{\mathbf{r}}_4$	ρ_x	ρ_y	ρ_z	$\mathbf{R}_x$	$\mathbf{R}_y$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_x$	$\tilde{\mathbf{R}}_y$	$\tilde{\mathbf{R}}_z$	$\mathbf{i}_1$	$\mathbf{i}_2$	$\mathbf{i}_3$	$\mathbf{i}_4$	$\mathbf{i}_5$	$\mathbf{i}_6$

O⊃C_4 induced representation $0_4\uparrow O\sim A_1\oplus T_1\oplus E$ and spectral analysis examples



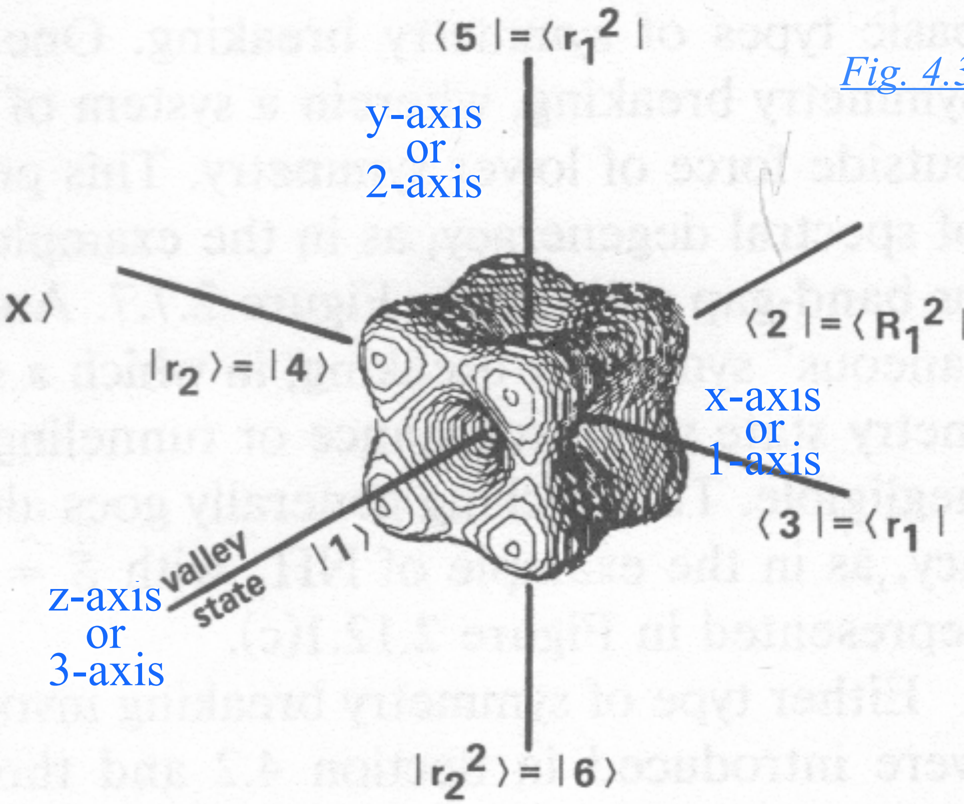


Fig. 4.3.1 PSDS

Assuming *C_4-local symmetry conditions* for $|\mathbf{1}\rangle$ state

$$|1\rangle = \mathbf{1}|1\rangle = R_3|1\rangle = R_3^2|1\rangle = R_3^3|1\rangle$$

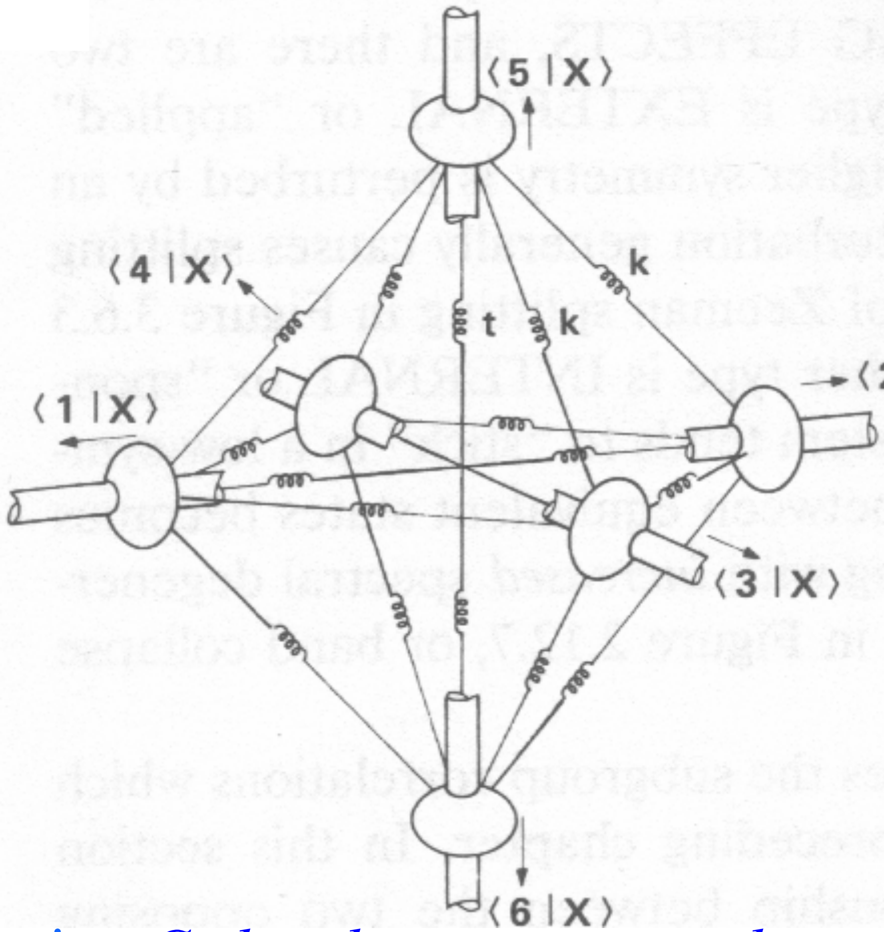
Using *C_4-local symmetry projector* equations $P^A \equiv P^{0_4} = (\mathbf{1} + R_3 + R_3^2 + R_3^3)/4$

$$|1\rangle = P^{0_4}|1\rangle = (\mathbf{1} + R_3 + R_3^2 + R_3^3)|1\rangle/4.$$

O operators (Two notations: Older Princ.of Symm.Dynamics and Spectra. *and Newer* Int.J.Mol.Sci*)*

PSDS:	$\mathbf{1}$	$\mathbf{r}_1$	$\mathbf{r}_2$	$\mathbf{r}_3$	$\mathbf{r}_4$	$\mathbf{r}_1^2$	$\mathbf{r}_2^2$	$\mathbf{r}_3^2$	$\mathbf{r}_4^2$	$\mathbf{R}_1^2$	$\mathbf{R}_2^2$	$\mathbf{R}_3^2$	$\mathbf{R}_1$	$\mathbf{R}_2$	$\mathbf{R}_3$	$\mathbf{R}_1^3$	$\mathbf{R}_2^3$	$\mathbf{R}_3^3$	$\mathbf{i}_1$	$\mathbf{i}_2$	$\mathbf{i}_3$	$\mathbf{i}_4$	$\mathbf{i}_5$	$\mathbf{i}_6$
IJMS:	$\mathbf{1}$	$\mathbf{r}_1$	$\mathbf{r}_2$	$\mathbf{r}_3$	$\mathbf{r}_4$	$\tilde{\mathbf{r}}_1$	$\tilde{\mathbf{r}}_2$	$\tilde{\mathbf{r}}_3$	$\tilde{\mathbf{r}}_4$	ρ_x	ρ_y	ρ_z	$\mathbf{R}_x$	$\mathbf{R}_y$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_x$	$\tilde{\mathbf{R}}_y$	$\tilde{\mathbf{R}}_z$	$\mathbf{i}_1$	$\mathbf{i}_2$	$\mathbf{i}_3$	$\mathbf{i}_4$	$\mathbf{i}_5$	$\mathbf{i}_6$

$O\supset C_4$ *induced representation* $0_4\uparrow O\sim A_1\oplus T_1\oplus E$ *and spectral analysis examples*



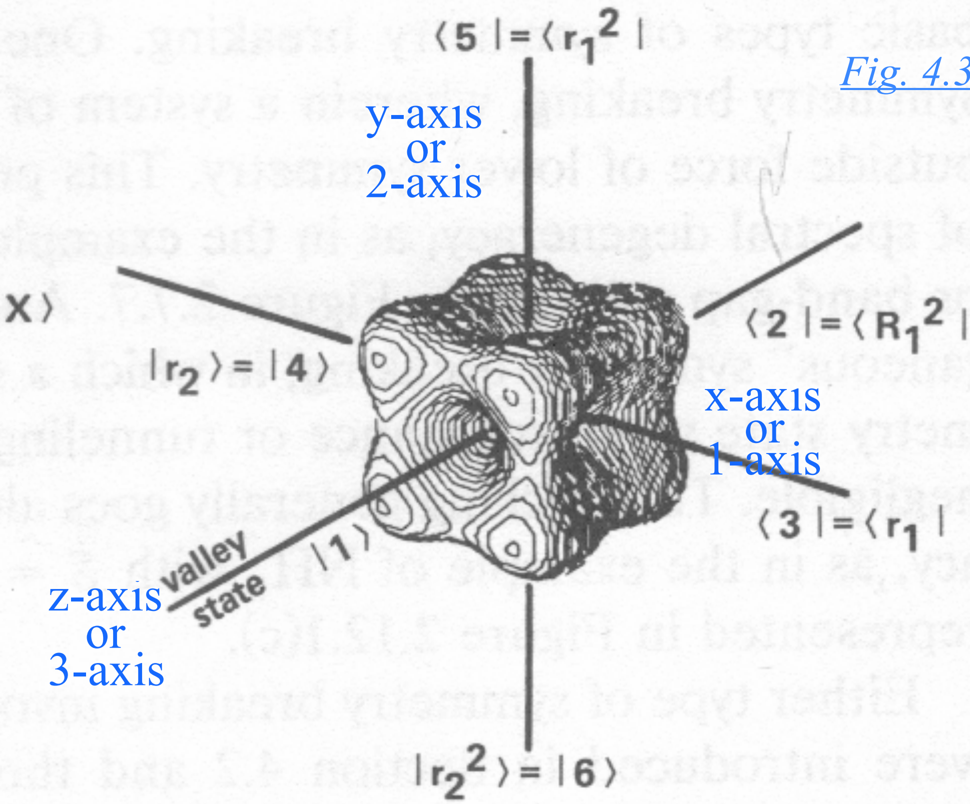


Fig. 4.3.1 PSDS

Assuming *C_4-local symmetry conditions* for $|\mathbf{1}\rangle$ state

$$|1\rangle = \mathbf{1}|1\rangle = R_3|1\rangle = R_3^2|1\rangle = R_3^3|1\rangle$$

Using *C_4-local symmetry projector equations* $P^A \equiv P^{0_4} = (\mathbf{1} + R_3 + R_3^2 + R_3^3)/4$

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O operators (Two notations: Older Princ.of Symm.Dynamics and Spectra. *and Newer* Int.J.Mol.Sci*)*

PSDS:	$\mathbf{1}$	$\mathbf{r}_1$	$\mathbf{r}_2$	$\mathbf{r}_3$	$\mathbf{r}_4$	$\mathbf{r}_1^2$	$\mathbf{r}_2^2$	$\mathbf{r}_3^2$	$\mathbf{r}_4^2$	$\mathbf{R}_1^2$	$\mathbf{R}_2^2$	$\mathbf{R}_3^2$	$\mathbf{R}_1$	$\mathbf{R}_2$	$\mathbf{R}_3$	$\mathbf{R}_1^3$	$\mathbf{R}_2^3$	$\mathbf{R}_3^3$	$\mathbf{i}_1$	$\mathbf{i}_2$	$\mathbf{i}_3$	$\mathbf{i}_4$	$\mathbf{i}_5$	$\mathbf{i}_6$
IJMS:	$\mathbf{1}$	$\mathbf{r}_1$	$\mathbf{r}_2$	$\mathbf{r}_3$	$\mathbf{r}_4$	$\tilde{\mathbf{r}}_1$	$\tilde{\mathbf{r}}_2$	$\tilde{\mathbf{r}}_3$	$\tilde{\mathbf{r}}_4$	ρ_x	ρ_y	ρ_z	$\mathbf{R}_x$	$\mathbf{R}_y$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_x$	$\tilde{\mathbf{R}}_y$	$\tilde{\mathbf{R}}_z$	$\mathbf{i}_1$	$\mathbf{i}_2$	$\mathbf{i}_3$	$\mathbf{i}_4$	$\mathbf{i}_5$	$\mathbf{i}_6$

$O\supset C_4$ *induced representation* $0_4\uparrow O\sim A_1\oplus T_1\oplus E$ *and spectral analysis examples*

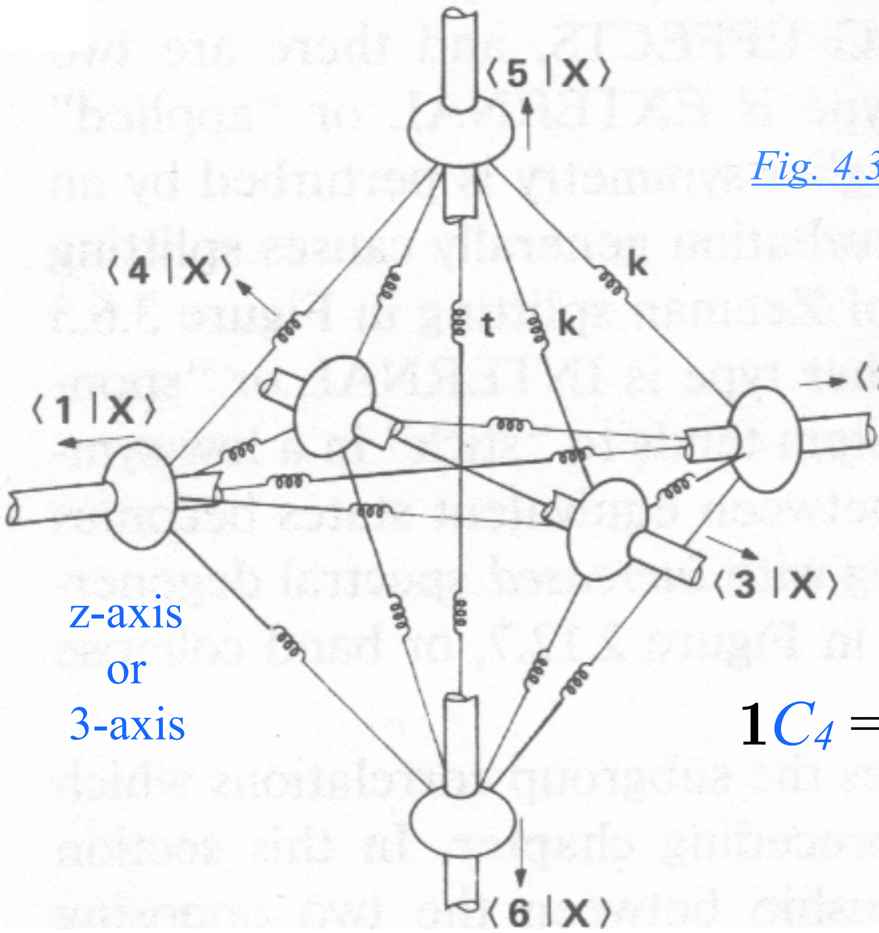
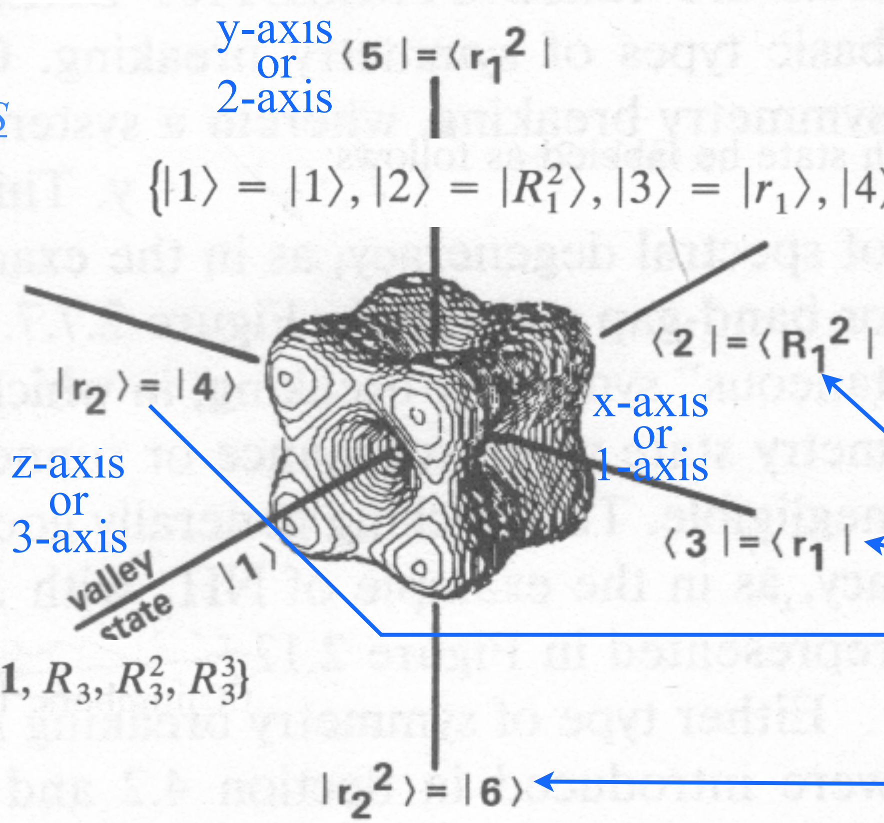


Fig. 4.3.1 PSDS

$\{|1\rangle = |1\rangle, |2\rangle = |R_1^2\rangle, |3\rangle = |r_1\rangle, |4\rangle = |r_2\rangle, |5\rangle = |r_1^2\rangle, |6\rangle = |r_2^2\rangle$



$\mathbf{1}C_4 = C_4 = \{\mathbf{1}, R_3, R_3^2, R_3^3\}$

Thus we label states by left *cosets* $\mathbf{r}_\ell C_4$ *of Local* C_4

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$r_2(\mathbf{1}, R_3, R_3^2, R_3^3) = (r_2, i_2, r_3, R_2^3),$

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IJMS:	$\mathbf{1}$	$\mathbf{r}_1$	$\mathbf{r}_2$	$\mathbf{r}_3$	$\mathbf{r}_4$	$\tilde{\mathbf{r}}_1$	$\tilde{\mathbf{r}}_2$	$\tilde{\mathbf{r}}_3$	$\tilde{\mathbf{r}}_4$	ρ_x	ρ_y	ρ_z	$\mathbf{R}_x$	$\mathbf{R}_y$	$\mathbf{R}_z$	$\tilde{\mathbf{R}}_x$	$\tilde{\mathbf{R}}_y$	$\tilde{\mathbf{R}}_z$	$\mathbf{i}_1$	$\mathbf{i}_2$	$\mathbf{i}_3$	$\mathbf{i}_4$	$\mathbf{i}_5$	$\mathbf{i}_6$

$O \supset C_4$ induced representation $0_4 \uparrow O \sim A_1 \oplus T_1 \oplus E$ and spectral analysis examples

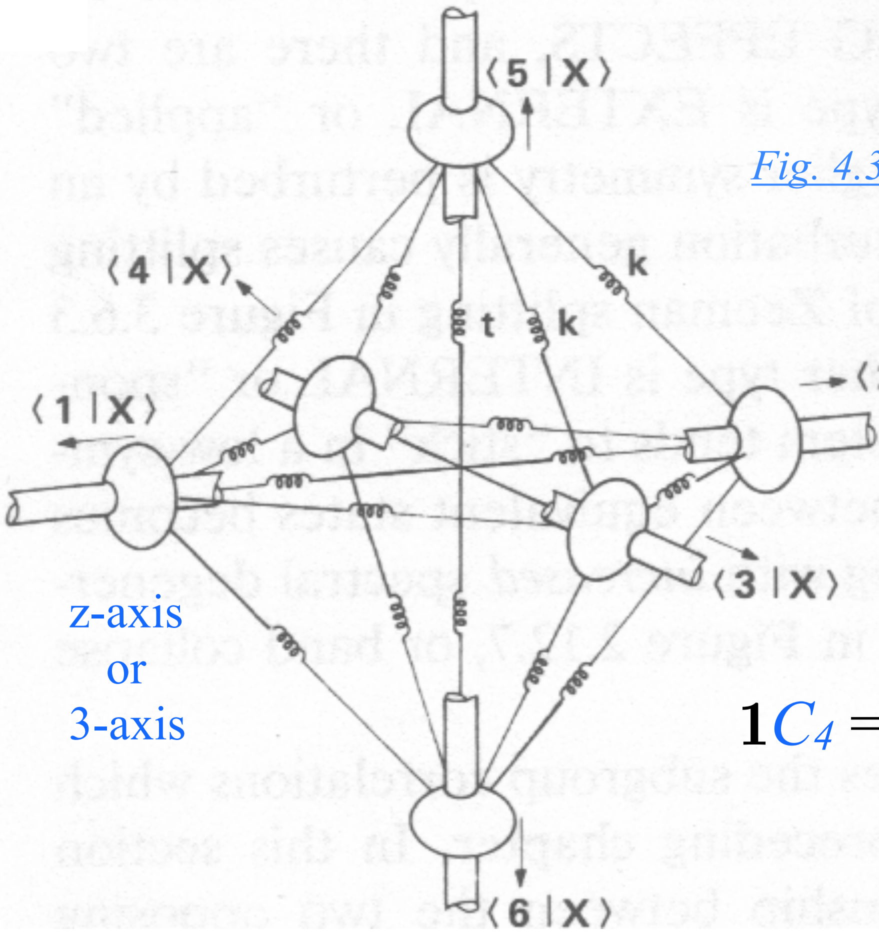
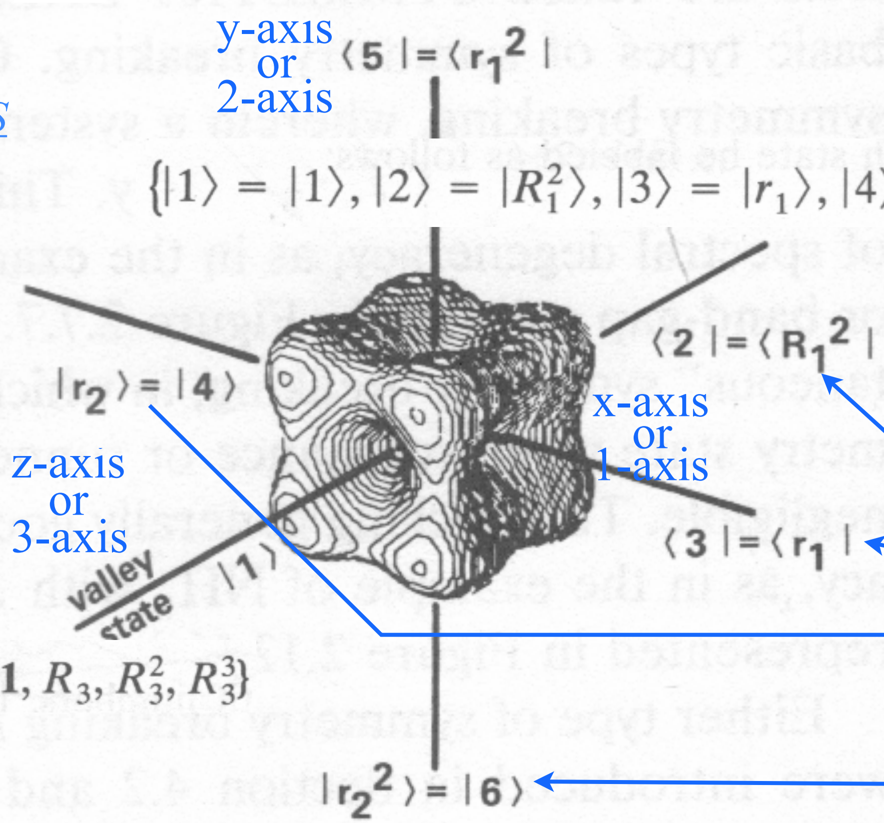


Fig. 4.3.1 PSDS



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$$r_2(1, R_3, R_3^2, R_3^3) = (r_2, i_2, r_3, R_2^3),$$

$$r_1^2(1, R_3, R_3^2, R_3^3) = (r_1^2, R_1^3, r_3^2, i_6),$$

$$r_2^2(1, R_3, R_3^2, R_3^3) = (r_2^2, R_1, r_4^2, i_5),$$

Compare to IJMS cosets on pages 25 -60:

Switch columns 1 with 2

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

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

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

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

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

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

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AMOP reference links on page 2

3.07.18 class 16.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Discrete symmetry subgroups of O(3)⊃(Octahedral O_h⊃O): Deriving $D^{(\alpha)}$-matrices defined by subgroup-chains $O\supset D_4\supset C_4$, $O\supset D_4\supset D_2$, and $O\supset D_3\supset C_3$ applications to IR spectra of SF_6

Review Octahedral $O_h\supset O$ group operator structure

Review Octahedral $O_h\supset O\supset D_4\supset C_4$ subgroup chain correlations

Comparison of $O\supset D_4\supset C_4$ and $O\supset D_4\supset D_2$ correlations and level/projector splitting

- *$O\supset D_4\supset C_4$ subgroup chain splitting*
- *$O\supset D_4\supset D_2$ subgroup chain splitting (nOrmal D_2 vs. unOrmal D_2)*
- *$O_h\supset O\supset D_4\supset C_{4v}$ and $O_h\supset O\supset D_4\supset C_{4v}\supset C_{2v}$ subgroup splitting*

Splitting O class projectors $\mathbf{P}^{\mu}$ into irreducible projectors $\mathbf{P}^{\mu}_{m_4m_4}$ for $O\supset C_4$

- *Left-cosets and coefficient arrays*

Development of irreducible projectors $\mathbf{P}^{\mu}_{m_4m_4}$ and representations $D^{\mu}_{m_4m_4}$

- *Calculating $\mathbf{P}^{E}_{0_40_4}$, $\mathbf{P}^{E}_{2_42_4}$, $\mathbf{P}^{T_1}_{0_40_4}$, $\mathbf{P}^{T_1}_{1_41_4}$, $\mathbf{P}^{T_2}_{2_42_4}$, $\mathbf{P}^{T_2}_{1_41_4}$, Collected $\mathbf{P}_{mm}$ results Table*

$O\supset C_4$ induced representation $0_4(C_4)\uparrow O \sim A_1\oplus T_1\oplus E$ and spectral analysis examples

- *Elementary induced representation $0_4(C_4)\uparrow O$*
- *Projection reduction of induced representation $0_4(C_4)\uparrow O$*
- *Introduction to ortho-complete eigenvalue-parameter relations*
  - *Examples from SF_6 model spectroscopy*

Elementary induced representation $0_4(C_4)\uparrow O$

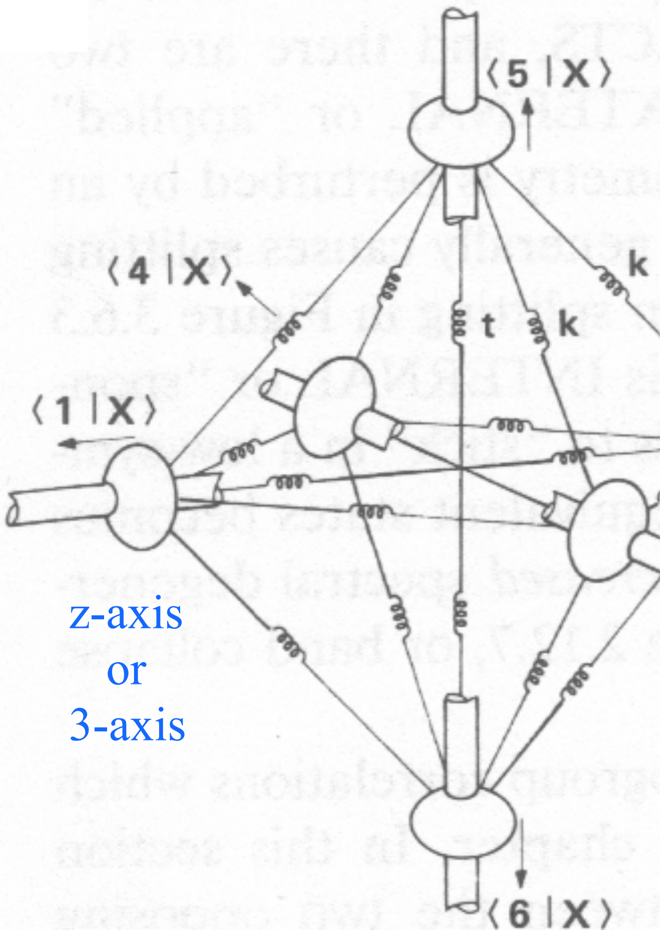
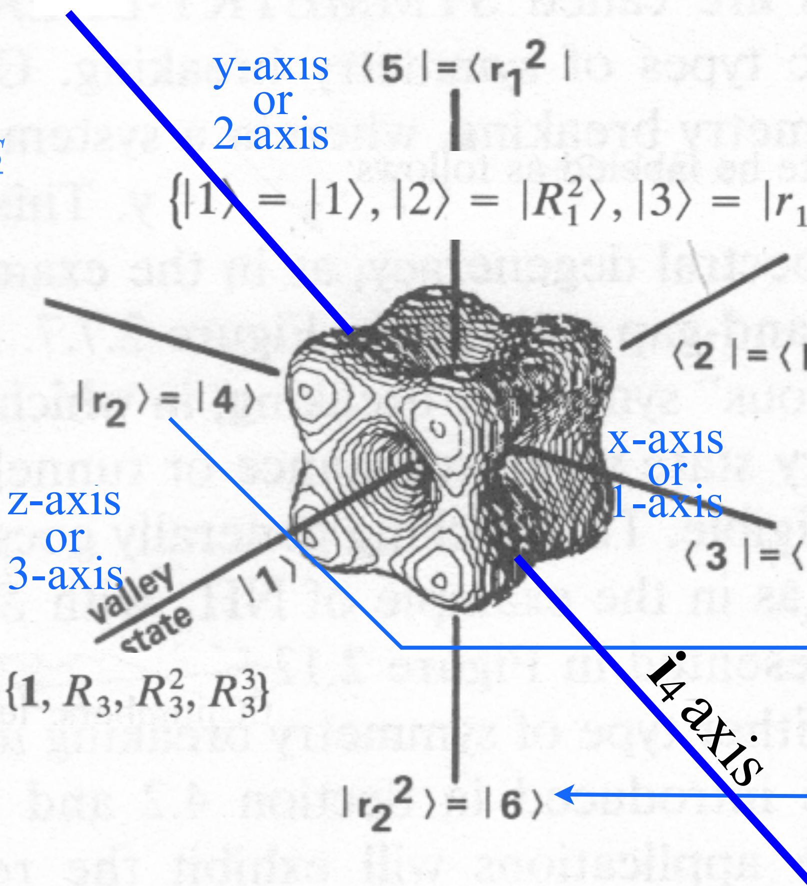


Fig. 4.3.1 PSDS



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This "coset-basis" spans a *scalar* $0_4(C_4)$ *induced representation* $0_4(C_4)\uparrow O$

$$\begin{array}{llllll}
\mathbf{i}_4|1\rangle=\mathbf{i}_4|1\rangle, & \mathbf{i}_4|2\rangle=\mathbf{i}_4\mathbf{R}_1^2|1\rangle, & \mathbf{i}_4|3\rangle=\mathbf{i}_4\mathbf{r}_1|1\rangle, & \mathbf{i}_4|4\rangle=\mathbf{i}_4\mathbf{r}_2|1\rangle, & \mathbf{i}_4|5\rangle=\mathbf{i}_4\mathbf{r}_1^2|1\rangle, & \mathbf{i}_4|6\rangle=\mathbf{i}_4\mathbf{r}_2^2|1\rangle. \\
=\mathbf{R}_1^2|1\rangle, & =\mathbf{R}_3^3|1\rangle, & =\mathbf{i}_5|1\rangle, & =\mathbf{i}_6|1\rangle, & =\mathbf{i}_2|1\rangle, & =\mathbf{i}_1|1\rangle. \\
=|2\rangle, & =|1\rangle, & =|6\rangle, & =|5\rangle, & =|4\rangle, & =|3\rangle.
\end{array}$$

Elementary induced representation $0_4(C_4)\uparrow O$

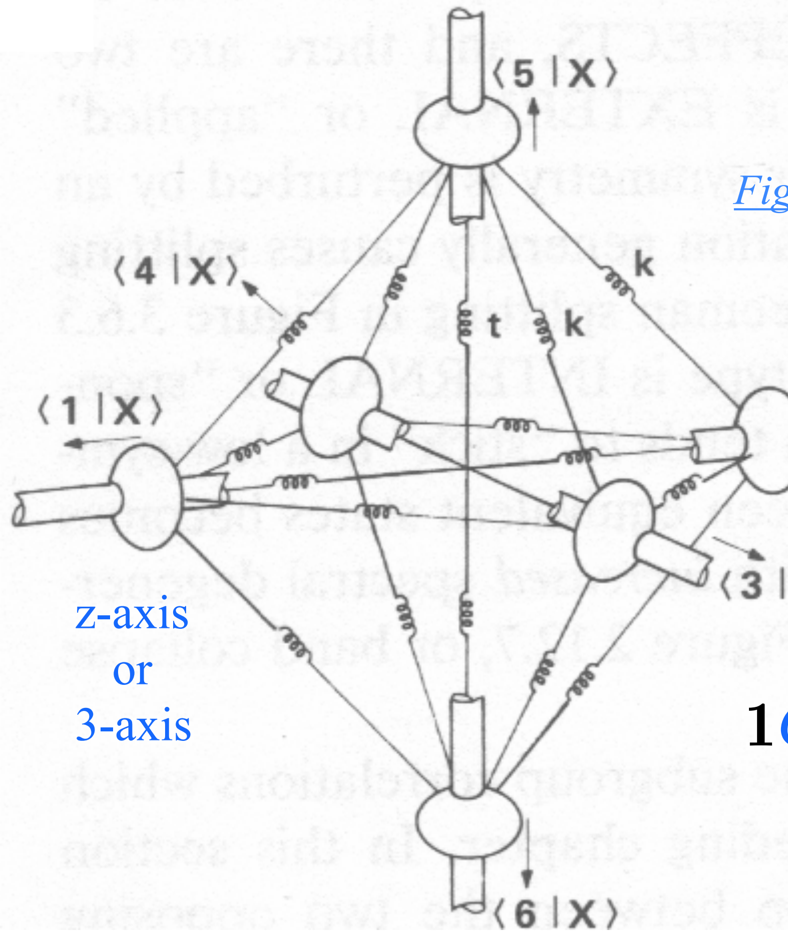
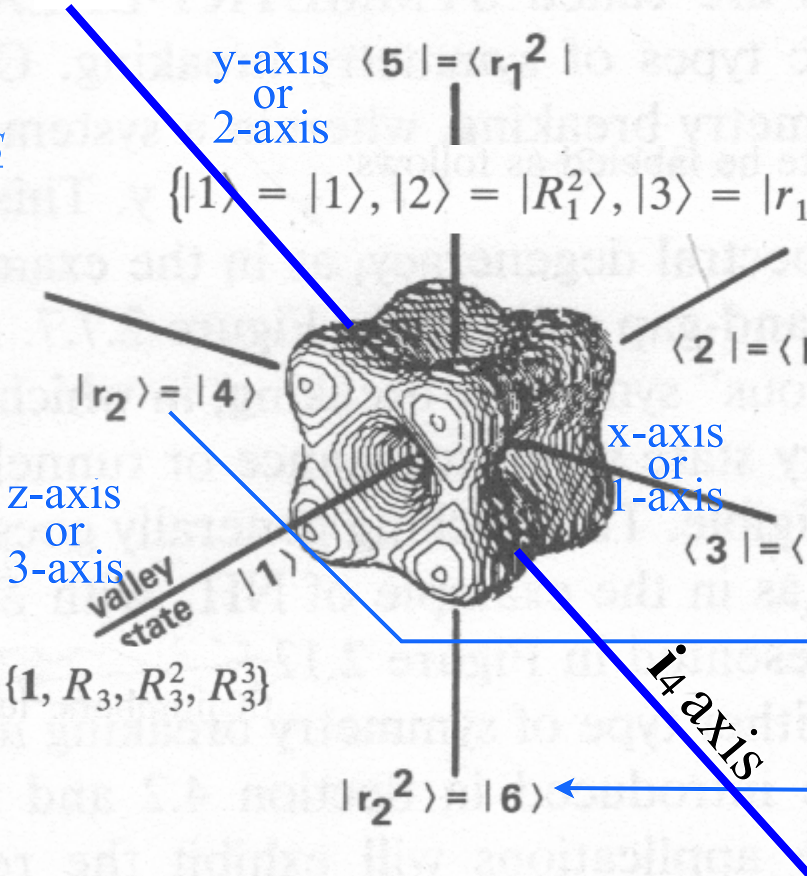


Fig. 4.3.1 PSDS



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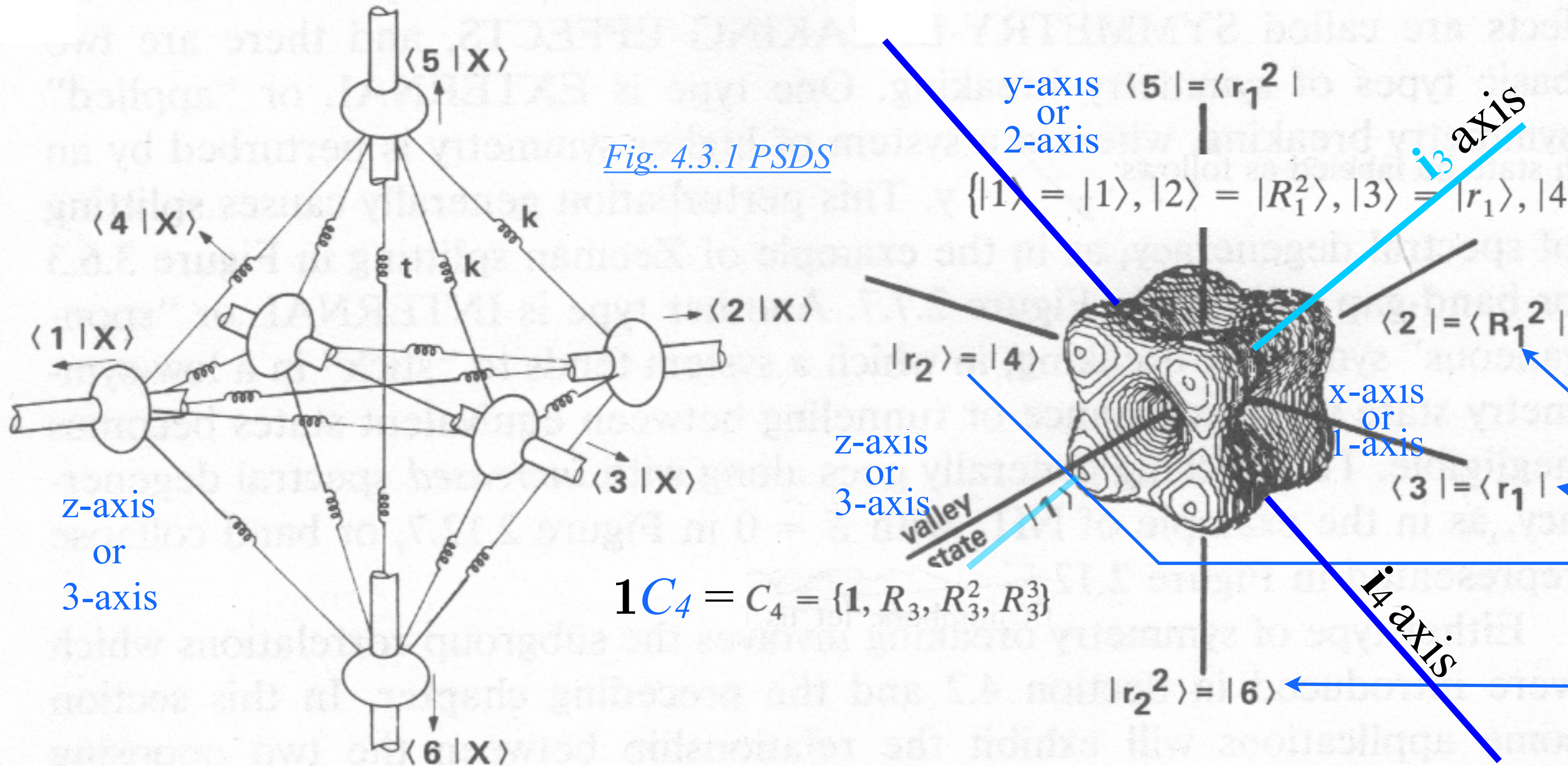
=|2\rangle, & =|1\rangle, & =|6\rangle, & =|5\rangle, & =|4\rangle, & =|3\rangle.
\end{array}$$

For example here is $0_4(C_4)$ *induced representation* $0_4(C_4)\uparrow O(\mathbf{i}_4)$

$$\mathscr{I}^{0_4\uparrow O}(\mathbf{i}_4)=\begin{pmatrix}
\langle 1|\mathbf{i}_4|1\rangle & \langle 1|\mathbf{i}_4|2\rangle & \cdots & \langle 1|\mathbf{i}_4|6\rangle \\
\langle 2|\mathbf{i}_4|1\rangle & \langle 2|\mathbf{i}_4|2\rangle & & \vdots \\
\vdots & & & \vdots \\
\langle 6|\mathbf{i}_4|1\rangle & \langle 6|\mathbf{i}_4|2\rangle & & \langle 1|\mathbf{i}_4|6\rangle
\end{pmatrix}
=
\begin{array}{c|cccccc}
 & |1\rangle & |2\rangle & |3\rangle & |4\rangle & |5\rangle & |6\rangle \\ \hline
\langle 1| & \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\
\langle 2| & 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\
\langle 3| & \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\
\langle 4| & \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\
\langle 5| & \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\
\langle 6| & \cdot & \cdot & 1 & \cdot & \cdot & \cdot
\end{array}$$

Elementary induced representation $0_4(C_4)\uparrow O$



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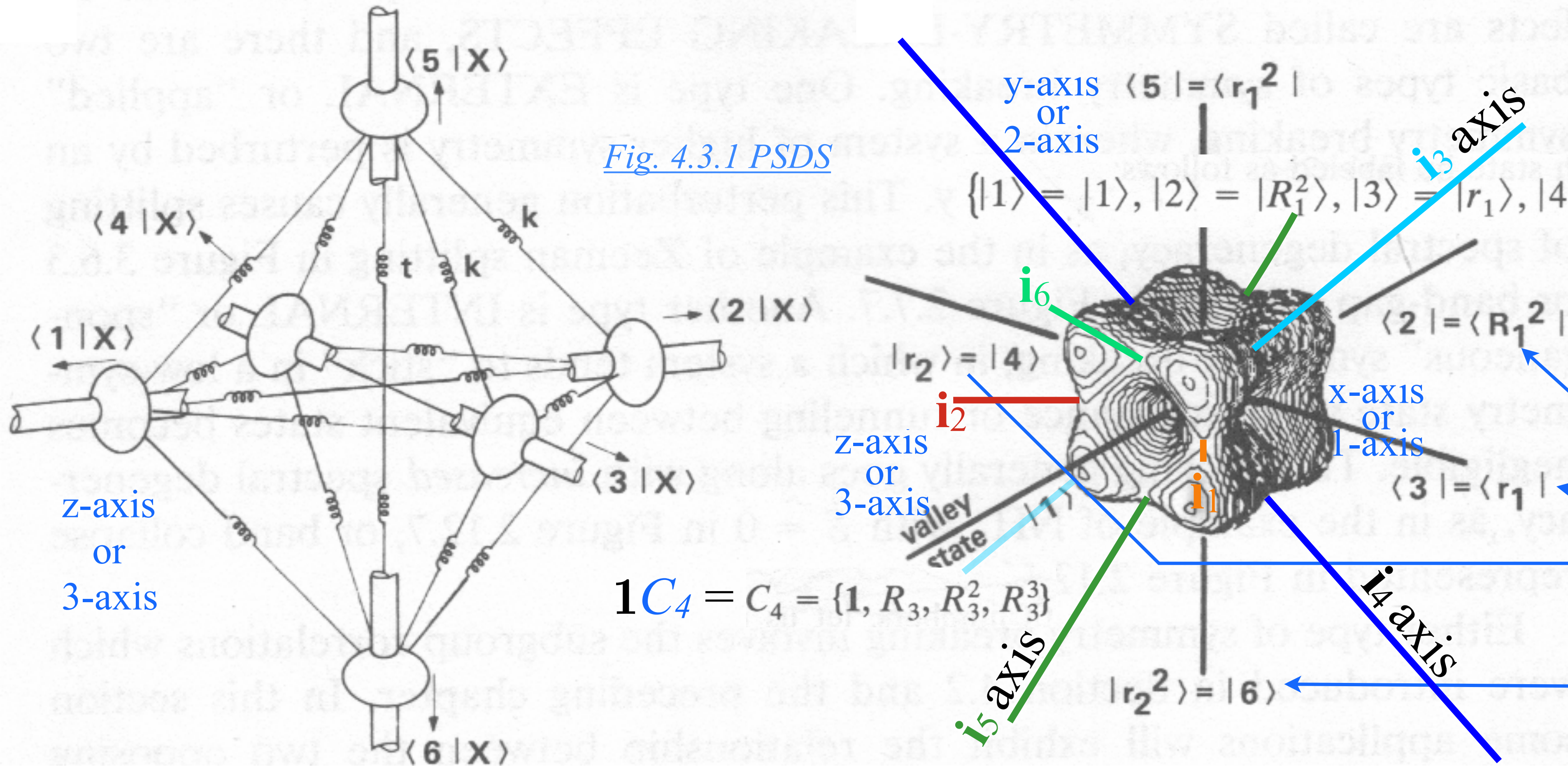
$$=|2\rangle,\quad =|1\rangle,\quad =|6\rangle,\quad =|5\rangle,\quad =|4\rangle,\quad =|3\rangle.$$

For example here is $0_4(C_4)$ *induced representation* $0_4(C_4)\uparrow O(\mathbf{i}_4)$ *and* $0_4(C_4)\uparrow O(\mathbf{i}_3)$

$$\mathscr{I}^{0_4\uparrow O}(\mathbf{i}_4)=\begin{pmatrix} \langle 1|\mathbf{i}_4|1\rangle & \langle 1|\mathbf{i}_4|2\rangle & \cdots & \langle 1|\mathbf{i}_4|6\rangle \\ \langle 2|\mathbf{i}_4|1\rangle & \langle 2|\mathbf{i}_4|2\rangle & & \vdots \\ \vdots & & & \vdots \\ \langle 6|\mathbf{i}_4|1\rangle & \langle 6|\mathbf{i}_4|2\rangle & & \langle 1|\mathbf{i}_4|6\rangle \end{pmatrix} = \begin{array}{c|cccccc} & |1\rangle & |2\rangle & |3\rangle & |4\rangle & |5\rangle & |6\rangle \\ \hline \langle 1| & \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \langle 2| & 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \langle 3| & \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \langle 4| & \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \langle 5| & \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \langle 6| & \cdot & \cdot & 1 & \cdot & \cdot & \cdot \end{array}$$

$$\mathscr{I}^{0_4\uparrow O}(\mathbf{i}_3)=\begin{pmatrix} \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \end{pmatrix}$$

Elementary induced representation $0_4(C_4)\uparrow O$



Thus we label states by left *cosets* $\mathbf{r}_\ell C_4$ *of Local* C_4

$$\mathbf{1}C_4 = C_4 = \{\mathbf{1}, R_3, R_3^2, R_3^3\}$$

$$R_1^2(\mathbf{1}, R_3, R_3^2, R_3^3) = (R_1^2, i_4, R_2^2, i_3),$$
$$r_1(\mathbf{1}, R_3, R_3^2, R_3^3) = (r_1, i_1, r_4, R_2),$$
$$r_2(\mathbf{1}, R_3, R_3^2, R_3^3) = (r_2, i_2, r_3, R_2^3),$$
$$r_1^2(\mathbf{1}, R_3, R_3^2, R_3^3) = (r_1^2, R_1^3, r_3^2, i_6),$$
$$r_2^2(\mathbf{1}, R_3, R_3^2, R_3^3) = (r_2^2, R_1, r_4^2, i_5),$$

Here is $0_4(C_4)$ *induced representation* $\mathscr{I}^{0_4\uparrow O}(\mathbf{I_i})$ *of a linear combination of* **i**-*class rotations*

$$\mathbf{I_i} = i_1\mathbf{i_1} + i_2\mathbf{i_2} + i_3\mathbf{i_3} + i_4\mathbf{i_4} + i_5\mathbf{i_5} + i_6\mathbf{i_6}$$

$\mathscr{I}^{0_4\uparrow O}(\mathbf{I_i}) =$

	$\vert 1\rangle$	$\vert 2\rangle$	$\vert 3\rangle$	$\vert 4\rangle$	$\vert 5\rangle$	$\vert 6\rangle$
$\langle 1\vert$	1	i_3+i_4	i_1	i_2	i_6	i_5
$\langle 2\vert$	i_3+i_4	1	i_2	i_1	i_5	i_6
$\langle 3\vert$	i_1	i_2	1	i_5+i_6	i_3	i_4
$\langle 4\vert$	i_2	i_1	i_5+i_6	1	i_4	i_3
$\langle 5\vert$	i_6	i_5	i_3	i_4	1	i_1+i_2
$\langle 6\vert$	i_5	i_6	i_4	i_3	i_1+i_2	1

$$\mathscr{I}^{0_4\uparrow O}(\mathbf{i}_3) = \begin{pmatrix} \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \end{pmatrix}$$

AMOP reference links on page 2

3.07.18 class 16.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Discrete symmetry subgroups of $O(3)\supset$(Octahedral $O_h\supset O$): Deriving $D^{(\alpha)}$-matrices defined by subgroup-chains $O\supset D_4\supset C_4$, $O\supset D_4\supset D_2$, and $O\supset D_3\supset C_3$ applications to IR spectra of SF_6

Review Octahedral $O_h\supset O$ group operator structure

Review Octahedral $O_h\supset O\supset D_4\supset C_4$ subgroup chain correlations

Comparison of $O\supset D_4\supset C_4$ and $O\supset D_4\supset D_2$ correlations and level/projector splitting

- *$O\supset D_4\supset C_4$ subgroup chain splitting*
- *$O\supset D_4\supset D_2$ subgroup chain splitting (nOrmal D_2 vs. unOrmal D_2)*
- *$O_h\supset O\supset D_4\supset C_{4v}$ and $O_h\supset O\supset D_4\supset C_{4v}\supset C_{2v}$ subgroup splitting*

Splitting O class projectors $\mathbf{P}^\mu$ into irreducible projectors $\mathbf{P}^\mu_{m_4m_4}$ for $O\supset C_4$

- *Left-cosets and coefficient arrays*

Development of irreducible projectors $\mathbf{P}^\mu_{m_4m_4}$ and representations $D^\mu_{m_4m_4}$

- *Calculating $\mathbf{P}^E_{0_40_4}$, $\mathbf{P}^E_{2_42_4}$, $\mathbf{P}^{T_1}_{0_40_4}$, $\mathbf{P}^{T_1}_{1_41_4}$, $\mathbf{P}^{T_2}_{2_42_4}$, $\mathbf{P}^{T_2}_{1_41_4}$, Collected $\mathbf{P}_{mm}$ results Table*

➡ *$O\supset C_4$ induced representation $0_4(C_4)\uparrow O \sim A_1\oplus T_1\oplus E$ and spectral analysis examples*

- *Elementary induced representation $0_4(C_4)\uparrow O$*
- ➡ *Projection reduction of induced representation $0_4(C_4)\uparrow O$*
- *Introduction to ortho-complete eigenvalue-parameter relations*
  - *Examples from SF_6 model spectroscopy*

Projection reduction of induced representation $0_4(C_4)\uparrow O$

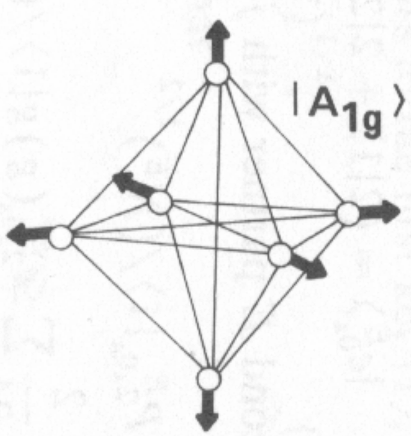
Scalar A_1 eigenket

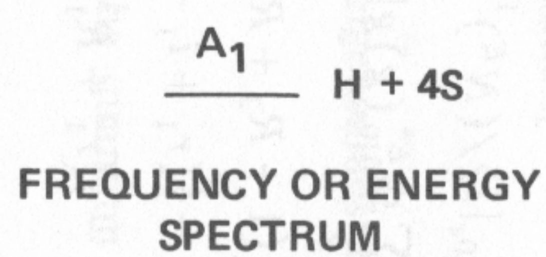
$$\left|e^{A_1}_{0_4 0_4}\right\rangle = \mathbf{P}^{A_1}_{0_4 0_4}\left|1\right\rangle / \sqrt{N^{A_1}}$$

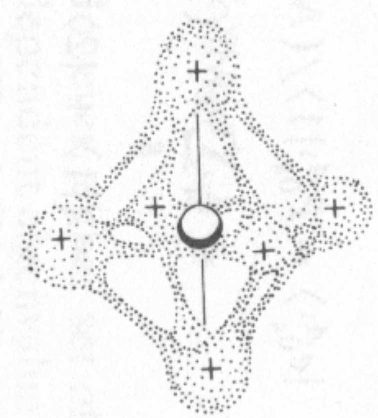
$$= \frac{1}{24}\sum_{p=1}^{24} D^{A_1 *}_{0_4 0_4}(g_p)\,\mathbf{g}_p\left|1\right\rangle / \sqrt{N^{A_1}}$$

$$= \left(\left|1\right\rangle + \left|2\right\rangle + \left|3\right\rangle + \left|4\right\rangle + \left|5\right\rangle + \left|6\right\rangle\right)/\sqrt{6}$$

$$\left|e^{A_1}_{0_4 0_4}\right\rangle = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} \frac{1}{\sqrt{6}}$$







$$\left|e^{A_1}_{0_4 0_4}\right\rangle = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} \frac{1}{\sqrt{6}}$$

Projection reduction of induced representation $0_4(C_4)\uparrow O$

Scalar A_1 eigenket 0_40_4

$$\left|e^{A_1}_{0_40_4}\right\rangle = \mathbf{P}^{A_1}_{0_40_4}\left|1\right\rangle/\sqrt{N^{A_1}}$$
$$= \frac{1}{24}\sum_{p=1}^{24} D^{A_1 *}_{0_40_4}(g_p)\,\mathbf{g}_p\left|1\right\rangle/\sqrt{N^{A_1}}$$
$$= \left(\left|1\right\rangle+\left|2\right\rangle+\left|3\right\rangle+\left|4\right\rangle+\left|5\right\rangle+\left|6\right\rangle\right)/\sqrt{6}$$

Tensor E-eigenket 0_40_4

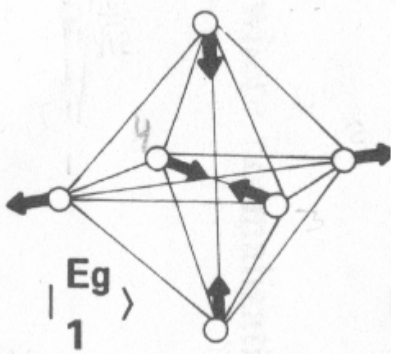
Diagonal (idempotent) Projector $\mathbf{P}^{\mu}_{jj}$

From p.49-50:

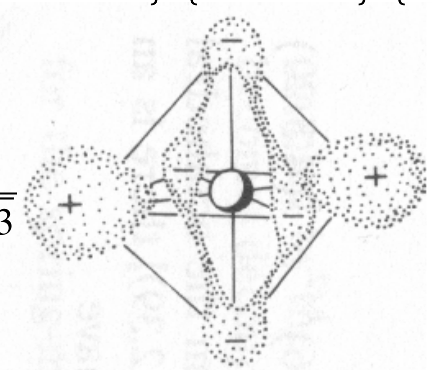
$$\left|e^{E}_{0_40_4}\right\rangle = \mathbf{P}^{E}_{0_40_4}\left|1\right\rangle/\sqrt{N^{E}}$$
$$= \frac{2}{24}\sum_{p=1}^{24} D^{E *}_{0_40_4}(g_p)\,\mathbf{g}_p\left|1\right\rangle/\sqrt{N^{E}}$$
$$= \left(\left|1\right\rangle+\left|2\right\rangle-\tfrac{1}{2}\left|3\right\rangle-\tfrac{1}{2}\left|4\right\rangle-\tfrac{1}{2}\left|5\right\rangle-\tfrac{1}{2}\left|6\right\rangle\right)/\sqrt{3}$$

$$\mathbf{P}^{E}_{0_40_4} = \tfrac{1}{12}[(1)\cdot\mathbf{1}\mathbf{p}_{0_4}+(1)\cdot\boldsymbol{\rho}_x\mathbf{p}_{0_4}+(-\tfrac{1}{2})\cdot\mathbf{r}_1\mathbf{p}_{0_4}+(-\tfrac{1}{2})\cdot\mathbf{r}_2\mathbf{p}_{0_4}+(-\tfrac{1}{2})\cdot\tilde{\mathbf{r}}_1\mathbf{p}_{0_4}+(-\tfrac{1}{2})\cdot\tilde{\mathbf{r}}_2\mathbf{p}_{0_4}]$$
$$\{\mathbf{1},\boldsymbol{\rho}_z,\mathbf{R}_z,\tilde{\mathbf{R}}_z\}\ \{\boldsymbol{\rho}_x,\boldsymbol{\rho}_y,\mathbf{i}_3,\mathbf{i}_4\}\ \{\mathbf{r}_1,\mathbf{r}_4,\mathbf{i}_1,\mathbf{R}_y\}\ \{\mathbf{r}_2,\mathbf{r}_3,\mathbf{i}_2,\tilde{\mathbf{R}}_y\}\ \{\tilde{\mathbf{r}}_1,\tilde{\mathbf{r}}_3,\tilde{\mathbf{R}}_x,\mathbf{i}_6\}\ \{\tilde{\mathbf{r}}_2,\tilde{\mathbf{r}}_4,\mathbf{R}_x,\mathbf{i}_5\}$$

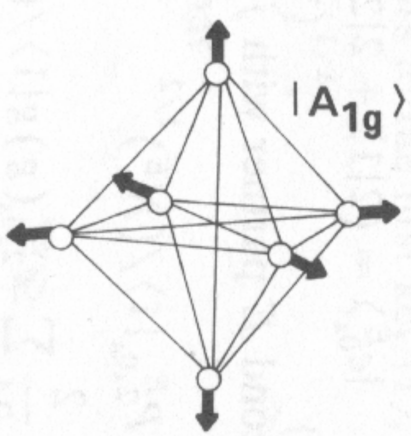
$$\left|e^{E}_{0_40_4}\right\rangle = \begin{pmatrix}2\\2\\-1\\-1\\-1\\-1\end{pmatrix}\frac{1}{2\sqrt{3}}$$

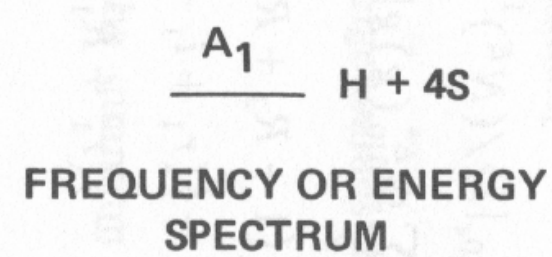


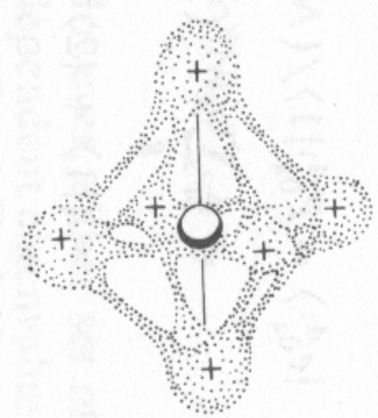
$$\left|e^{E}_{0_40_4}\right\rangle = \begin{pmatrix}2\\2\\-1\\-1\\-1\\-1\end{pmatrix}\frac{1}{2\sqrt{3}}$$



$$\left|e^{A_1}_{0_40_4}\right\rangle = \begin{pmatrix}1\\1\\1\\1\\1\\1\end{pmatrix}\frac{1}{\sqrt{6}}$$







$$\left|e^{A_1}_{0_40_4}\right\rangle = \begin{pmatrix}1\\1\\1\\1\\1\\1\end{pmatrix}\frac{1}{\sqrt{6}}$$

Projection reduction of induced representation $0_4(C_4)\uparrow O$

Scalar A_1 eigenket $0_4 0_4$

$$\left|e^{A_1}_{0_4 0_4}\right\rangle = \mathbf{P}^{A_1}_{0_4 0_4}\left|1\right\rangle / \sqrt{N^{A_1}}$$
$$= \frac{1}{24}\sum_{p=1}^{24} D^{A_1 *}_{0_4 0_4}(g_p)\,\mathbf{g}_p\left|1\right\rangle / \sqrt{N^{A_1}}$$
$$= \left(\left|1\right\rangle + \left|2\right\rangle + \left|3\right\rangle + \left|4\right\rangle + \left|5\right\rangle + \left|6\right\rangle\right)/\sqrt{6}$$

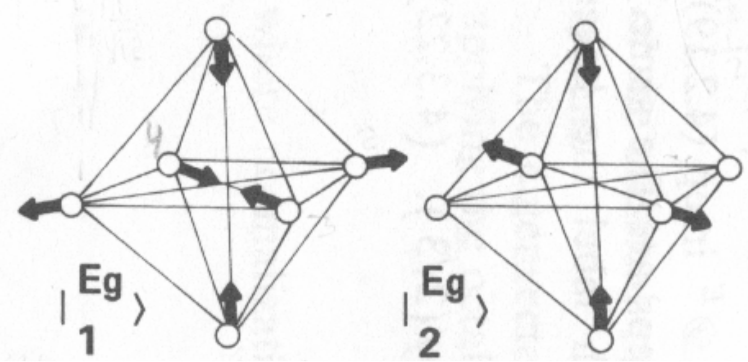
Off-Diagonal (nilpotent) Projector $\mathbf{P}^{\mu}{}_{jk}$

Derived next lectures

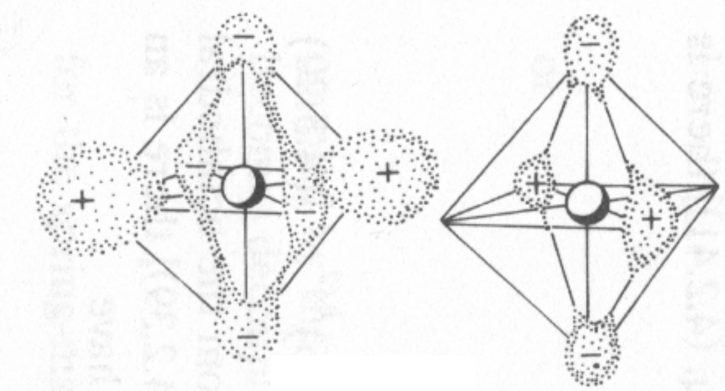
Tensor E-eigenket $2_4 0_4$

$$\left|e^{E}_{2_4 0_4}\right\rangle = \mathbf{P}^{E}_{2_4 0_4}\left|1\right\rangle / \sqrt{N^{E}}$$
$$= \frac{2}{24}\sum_{p=1}^{24} D^{E *}_{2_4 0_4}(g_p)\,\mathbf{g}_p\left|1\right\rangle / \sqrt{N^{E}}$$
$$= \left(\left|3\right\rangle + \left|4\right\rangle - \left|5\right\rangle - \left|6\right\rangle\right)/2$$

$$\left|e^{E}_{0_4 0_4}\right\rangle = \begin{pmatrix} 2 \\ 2 \\ -1 \\ -1 \\ -1 \\ -1 \end{pmatrix} \frac{1}{2\sqrt{3}}$$

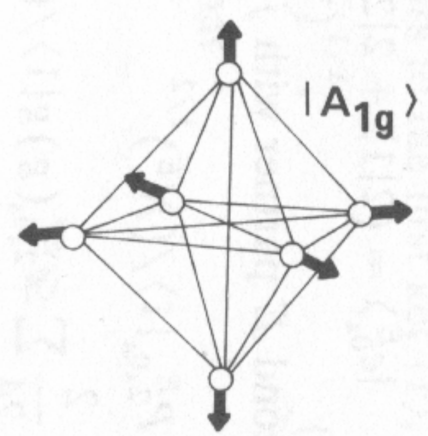


E



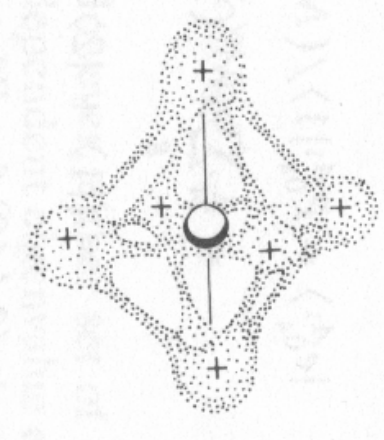
$$\left|e^{E}_{2_4 0_4}\right\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 1 \\ -1 \\ -1 \end{pmatrix} \frac{1}{2}$$

$$\left|e^{A_1}_{0_4 0_4}\right\rangle = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} \frac{1}{\sqrt{6}}$$



A_1

FREQUENCY OR ENERGY SPECTRUM



$$\left|e^{A_1}_{0_4 0_4}\right\rangle = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} \frac{1}{\sqrt{6}}$$

Projection reduction of induced representation $0_4(C_4)\uparrow O$

Scalar A_1 eigenket 0_40_4

$$\left|e^{A_1}_{0_40_4}\right\rangle = \mathbf{P}^{A_1}_{0_40_4}\left|1\right\rangle/\sqrt{N^{A_1}}$$
$$= \frac{1}{24}\sum_{p=1}^{24} D^{A_1 *}_{0_40_4}(g_p)\,\mathbf{g}_p\left|1\right\rangle/\sqrt{N^{A_1}}$$
$$= \left(\left|1\right\rangle+\left|2\right\rangle+\left|3\right\rangle+\left|4\right\rangle+\left|5\right\rangle+\left|6\right\rangle\right)/\sqrt{6}$$

Diagonal (idempotent) Projector $\mathbf{P}^{\mu}_{jj}$

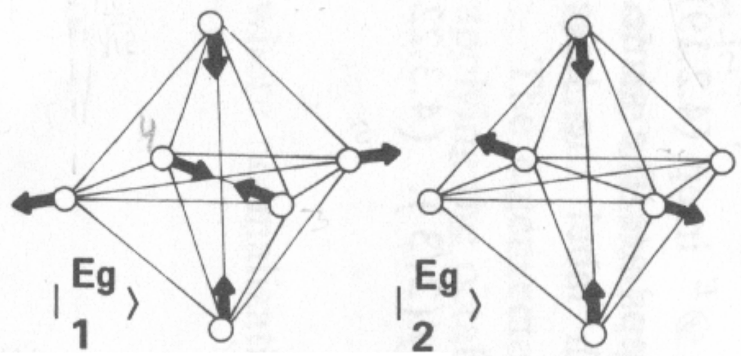
From p.53:

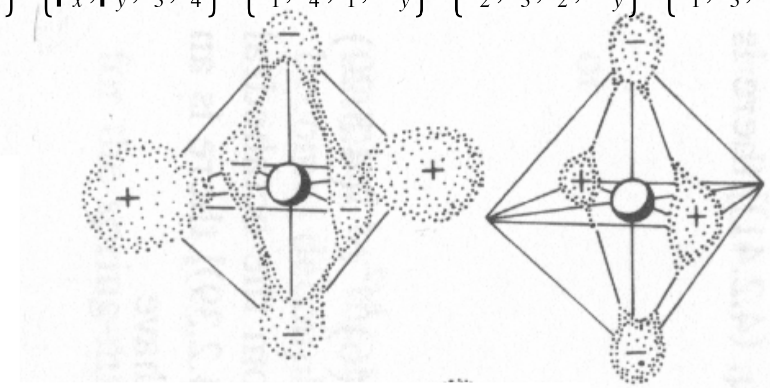
Vector T_1-eigenket 0_40_4

$$\left|e^{T_1}_{0_40_4}\right\rangle = \mathbf{P}^{T_1}_{0_40_4}\left|1\right\rangle/\sqrt{N^{T_1}}$$
$$= \frac{1}{24}\sum_{p=1}^{24} D^{T_1 *}_{0_40_4}(g_p)\,\mathbf{g}_p\left|1\right\rangle/\sqrt{N^{T_1}}$$
$$= \left(\left|1\right\rangle-\left|2\right\rangle+0+0+0+0\right)/\sqrt{2}$$

$$\mathbf{P}^{T_1}_{0_40_4} = \tfrac{1}{8}\left[(1)\cdot\mathbf{1p}_{0_4} + (-1)\cdot\rho_x\mathbf{p}_{0_4} + (0)\cdot\mathbf{r}_1\mathbf{p}_{0_4} + (0)\cdot\mathbf{r}_2\mathbf{p}_{0_4} + (0)\cdot\tilde{\mathbf{r}}_1\mathbf{p}_{0_4} + (0)\cdot\tilde{\mathbf{r}}_2\mathbf{p}_{0_4}\right]$$
$$\{\mathbf{1},\rho_z,\mathbf{R}_z,\tilde{\mathbf{R}}_z\}\ \{\rho_x,\rho_y,\mathbf{i}_3,\mathbf{i}_4\}\ \{\mathbf{r}_1,\mathbf{r}_4,\mathbf{i}_1,\mathbf{R}_y\}\ \{\mathbf{r}_2,\mathbf{r}_3,\mathbf{i}_2,\tilde{\mathbf{R}}_y\}\ \{\tilde{\mathbf{r}}_1,\tilde{\mathbf{r}}_3,\tilde{\mathbf{R}}_x,\mathbf{i}_6\}\ \{\tilde{\mathbf{r}}_2,\tilde{\mathbf{r}}_4,\mathbf{R}_x,\mathbf{i}_5\}$$

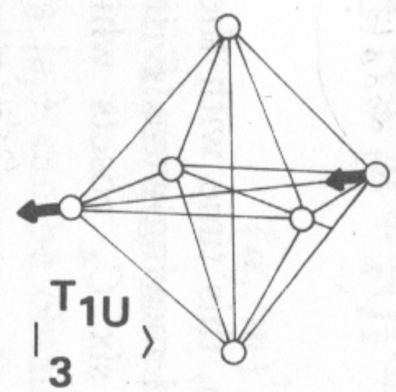
$$\left|e^{E}_{0_40_4}\right\rangle = \begin{pmatrix}2\\2\\-1\\-1\\-1\\-1\end{pmatrix}\frac{1}{2\sqrt{3}}$$



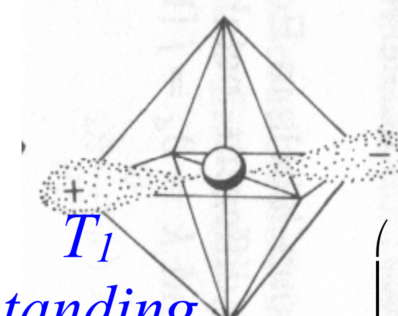


$$\left|e^{E}_{2_40_4}\right\rangle = \begin{pmatrix}0\\0\\1\\1\\-1\\-1\end{pmatrix}\frac{1}{2}$$

E



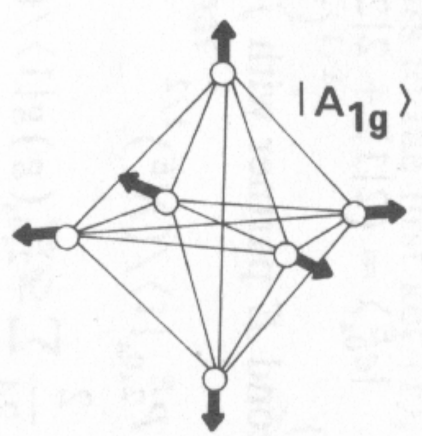
T_1



T_1 standing wave $0_4=z$

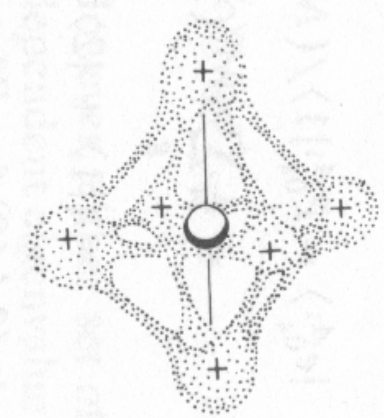
$$\left|{}^{T_1}_{0_40_4}\right\rangle = \begin{pmatrix}1\\-1\\0\\0\\0\\0\end{pmatrix}\frac{1}{\sqrt{2}}$$

$$\left|e^{A_1}_{0_40_4}\right\rangle = \begin{pmatrix}1\\1\\1\\1\\1\\1\end{pmatrix}\frac{1}{\sqrt{6}}$$



A_1

FREQUENCY OR ENERGY SPECTRUM



$$\left|e^{A_1}_{0_40_4}\right\rangle = \begin{pmatrix}1\\1\\1\\1\\1\\1\end{pmatrix}\frac{1}{\sqrt{6}}$$

Projection reduction of induced representation $0_4(C_4)\uparrow O$

Scalar A_1 eigenket 0_40_4

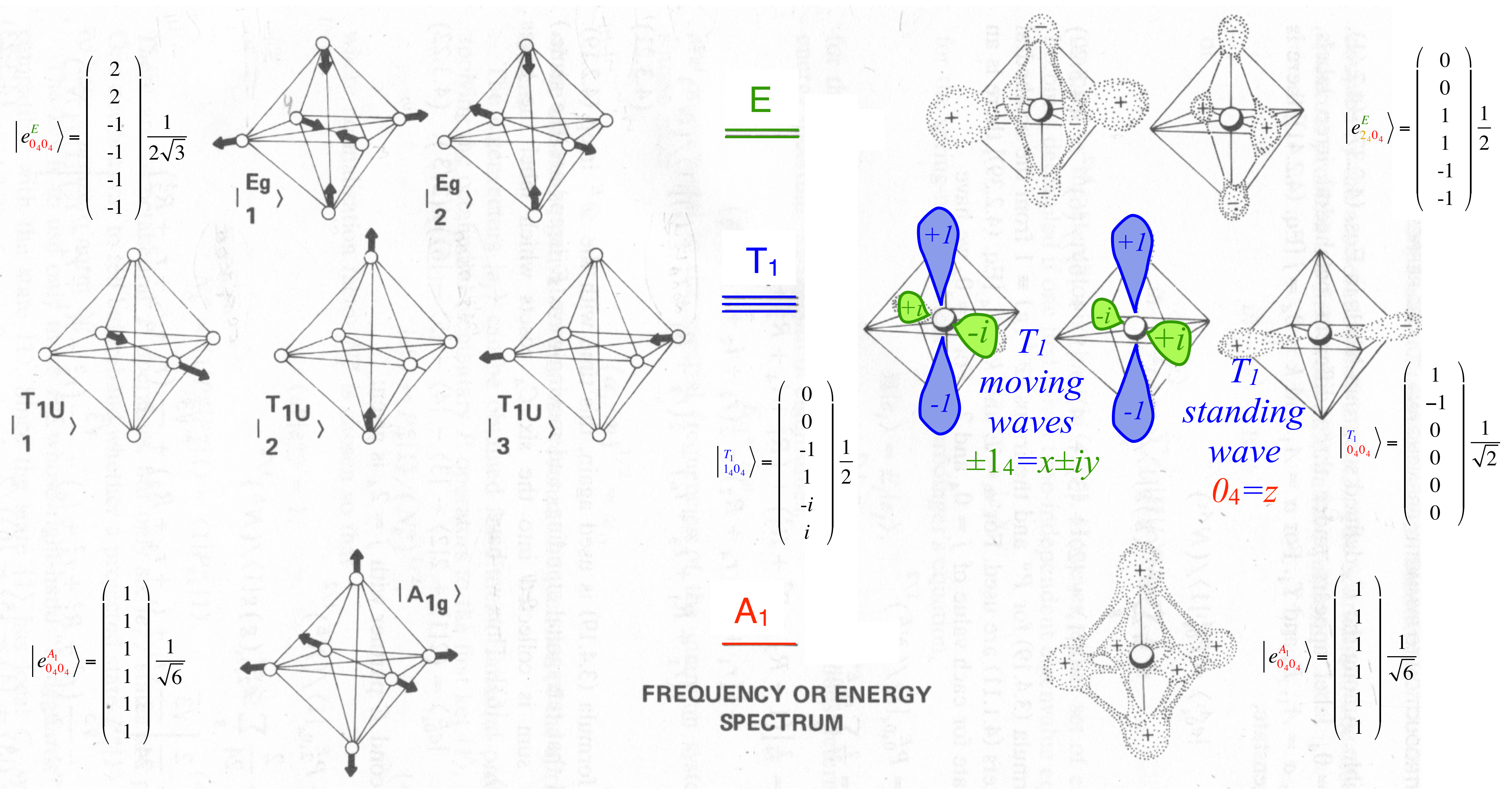
$$\left|e^{A_1}_{0_40_4}\right\rangle = \mathbf{P}^{A_1}_{0_40_4}\left|1\right\rangle / \sqrt{N^{A_1}}$$
$$= \frac{1}{24}\sum_{p=1}^{24} D^{A_1 *}_{0_40_4}(g_p)\,\mathbf{g}_p\left|1\right\rangle / \sqrt{N^{A_1}}$$
$$= \left(\left|1\right\rangle+\left|2\right\rangle+\left|3\right\rangle+\left|4\right\rangle+\left|5\right\rangle+\left|6\right\rangle\right)/\sqrt{6}$$

Off-Diagonal (nilpotent) Projector $\mathbf{P}^{\mu}{}_{jk}$

Derived next lectures

Vector T_1-eigenket $\pm 1_40_4$ and 0_40_4

$$\left|e^{T_1}_{\pm 1_40_4}\right\rangle = \mathbf{P}^{T_1}_{1_40_4}\left|1\right\rangle / \sqrt{N^{T_1}}$$
$$= \frac{1}{24}\sum_{p=1}^{24} D^{T_1 *}_{\pm 1_40_4}(g_p)\,\mathbf{g}_p\left|1\right\rangle / \sqrt{N^{T_1}}$$
$$= \left(0+0+\left|3\right\rangle+\left|4\right\rangle \pm i\left|5\right\rangle \pm i\left|6\right\rangle\right)/2$$



Projection reduction of induced representation $0_4(C_4)\uparrow O$

Tunneling T (next-neighbor) is too "Tiny" to contribute to E^{α}

$$E^{A_1} = H + T + 4S,$$
$$E^{T_1} = H - T,$$
$$E^{E} = H + T - 2S,$$

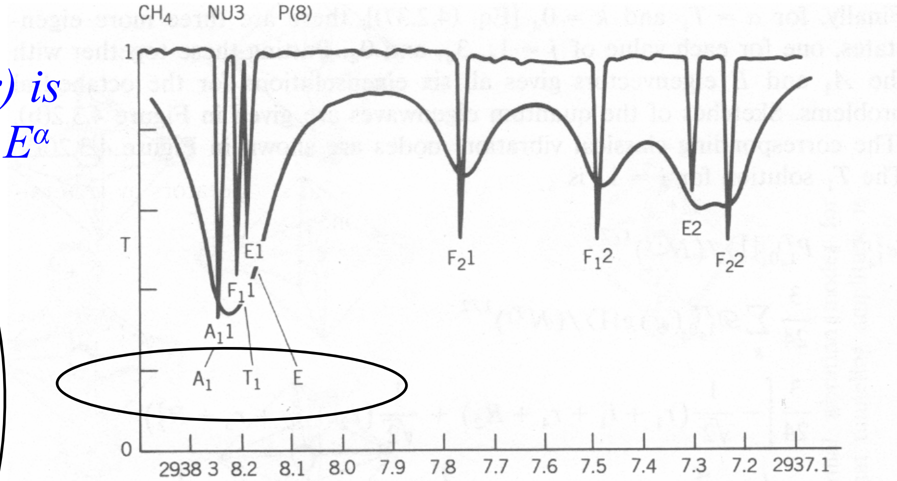
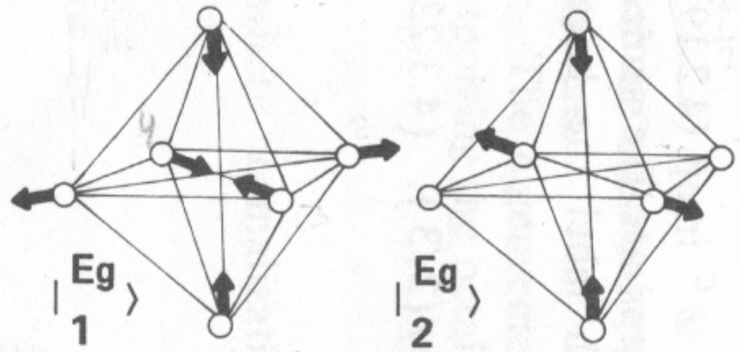


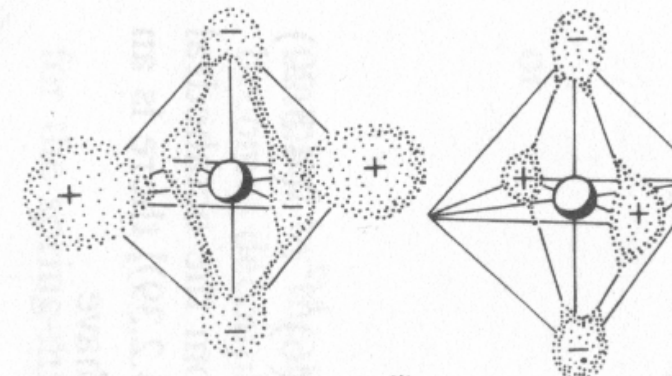
Figure 4.3.3 Evidence of an (A_1T_1E) spectral cluster in methane laser spectra. (Courtesy of Dr. Allan Pine, MIT Lincoln Laboratories, from *Journal of Optical Society of America* **66**, 97 (1976)). The ordering and approximate spacing of the A_1T_1 and E lines is consistent with that of Figure 4.3.2.

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

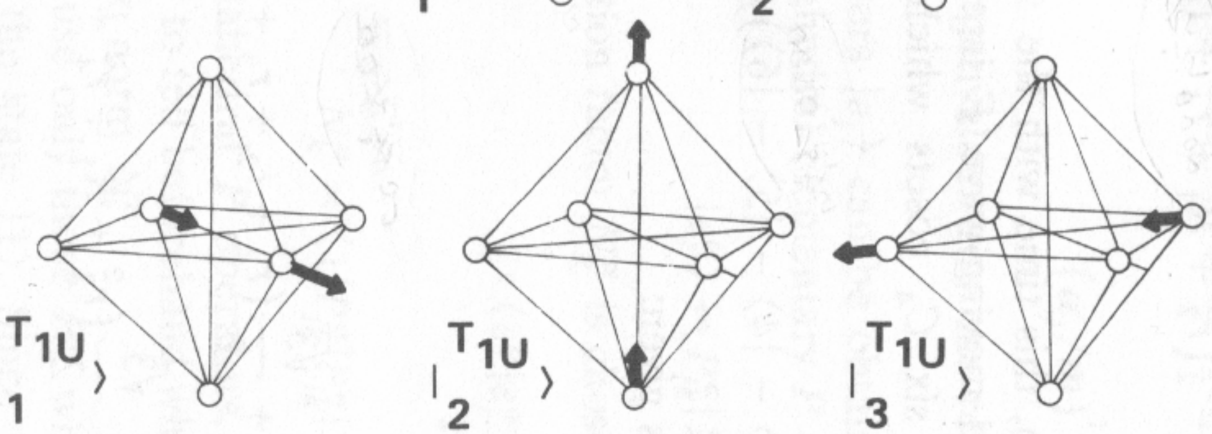
$$\left|{}^{E}_{0_40_4}\right\rangle = \begin{pmatrix} 2 \\ 2 \\ -1 \\ -1 \\ -1 \\ -1 \end{pmatrix} \frac{1}{2\sqrt{3}}$$



Eg ═ H − 2S

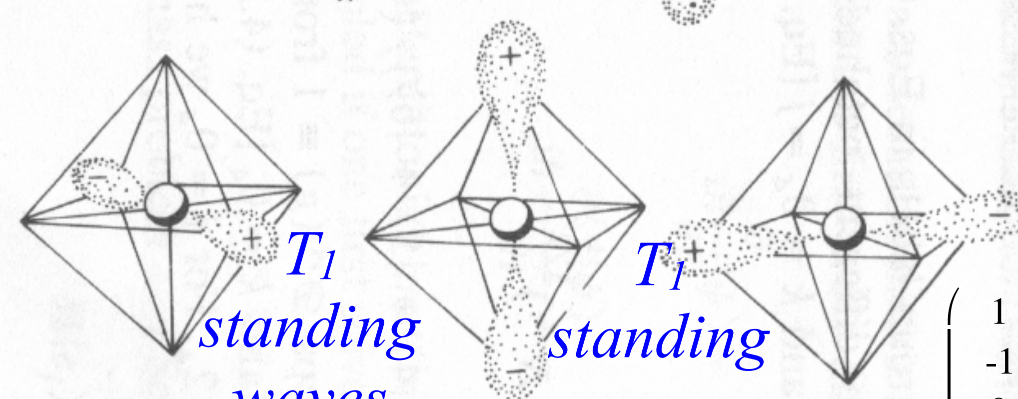


$$\left|{}^{E}_{2_40_4}\right\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 1 \\ -1 \\ -1 \end{pmatrix} \frac{1}{2}$$



T1u ≡ H

$$\left|{}^{T_1}_{1_40_4}\right\rangle = \begin{pmatrix} 0 \\ 0 \\ -1 \\ 1 \\ -i \\ i \end{pmatrix} \frac{1}{2}$$

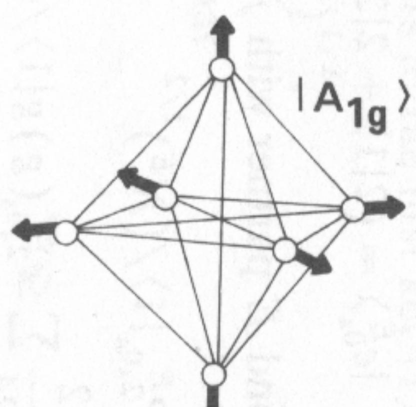


T_1 standing waves x and y

T_1 standing wave 0_4=z

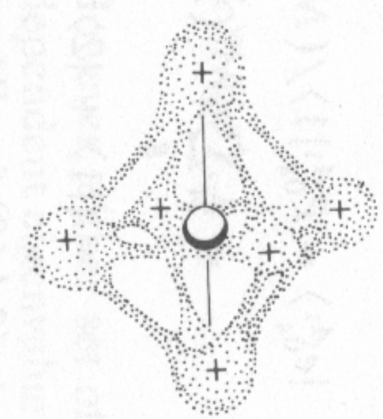
$$\left|{}^{T_1}_{0_40_4}\right\rangle = \begin{pmatrix} 1 \\ -1 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \frac{1}{\sqrt{2}}$$

$$\left|e^{A_1}_{0_40_4}\right\rangle = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} \frac{1}{\sqrt{6}}$$



A1g — H + 4S

FREQUENCY OR ENERGY SPECTRUM



$$\left|e^{A_1}_{0_40_4}\right\rangle = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} \frac{1}{\sqrt{6}}$$

Projection reduction of induced representation $0_4(C_4)\uparrow O$

Tunneling T (next-neighbor) is too "Tiny" to contribute to E^{α}

$$E^{A_1} = H + T + 4S,$$
$$E^{T_1} = H - T,$$
$$E^{E} = H + T - 2S$$

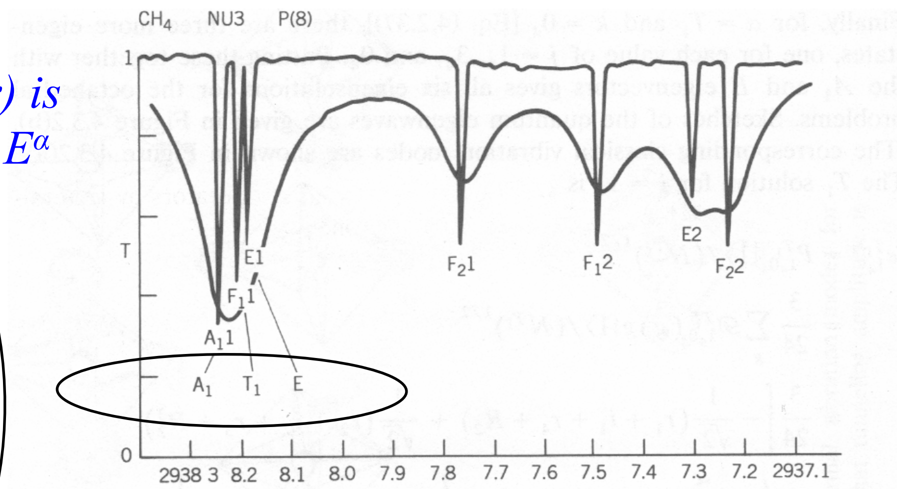


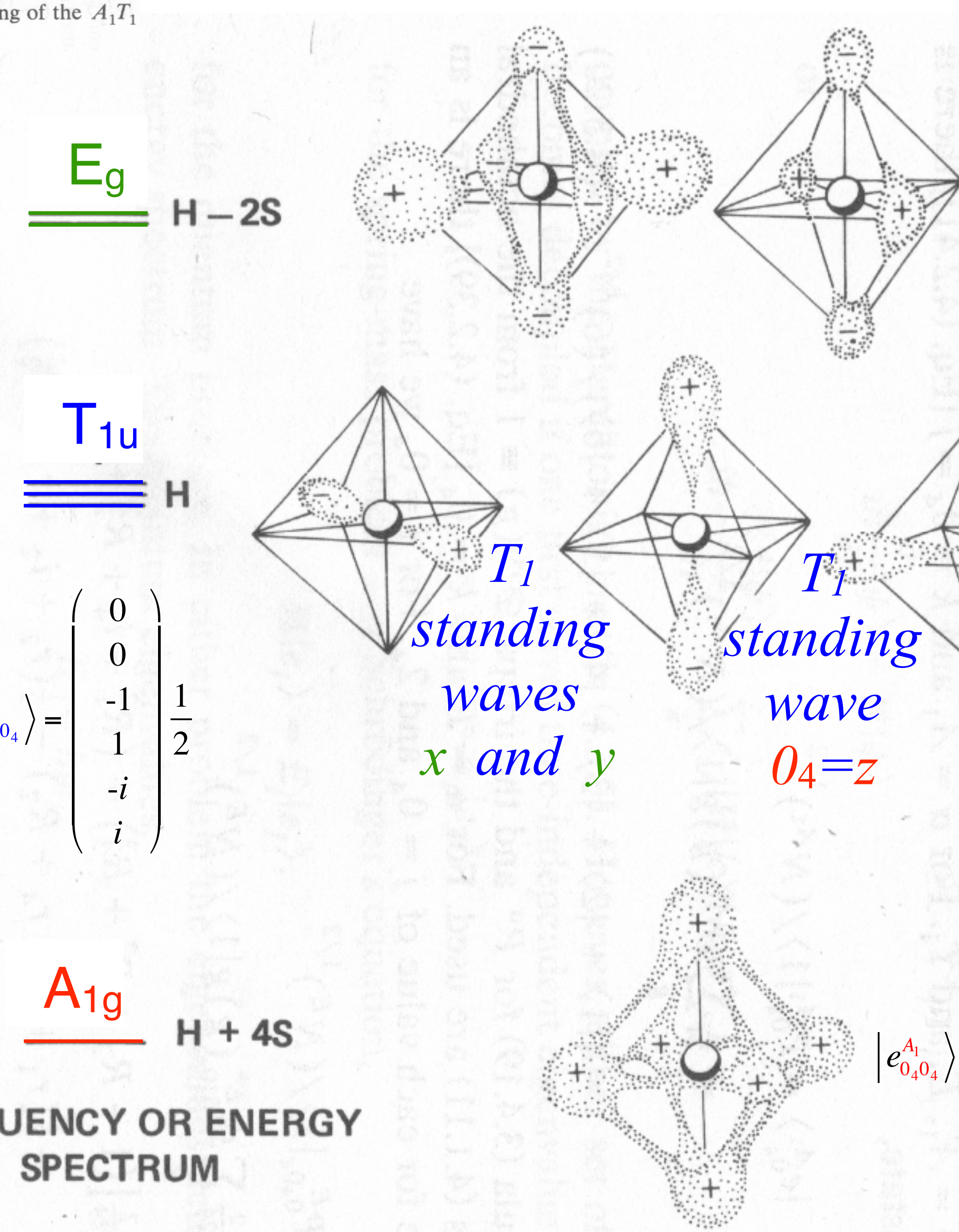
Figure 4.3.3 Evidence of an (A_1T_1E) spectral cluster in methane laser spectra. (Courtesy of Dr. Allan Pine, MIT Lincoln Laboratories, from *Journal of Optical Society of America* **66**, 97 (1976)). The ordering and approximate spacing of the A_1T_1 and E lines is consistent with that of Figure 4.3.2.

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

$O_h \supset D_{4h} \supset C_{4v} \supset C_{2v}$ subgroup splitting

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

Labels correct u or g parity!



$$\left|{}^{E}_{2_4 0_4}\right\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 1 \\ -1 \\ -1 \end{pmatrix} \frac{1}{2}$$

$$\left|{}^{T_1}_{1_4 0_4}\right\rangle = \begin{pmatrix} 0 \\ 0 \\ -1 \\ 1 \\ -i \\ i \end{pmatrix} \frac{1}{2}$$

$$\left|{}^{T_1}_{0_4 0_4}\right\rangle = \begin{pmatrix} 1 \\ -1 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \frac{1}{\sqrt{2}}$$

$$\left|e^{A_1}_{0_4 0_4}\right\rangle = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} \frac{1}{\sqrt{6}}$$

AMOP reference links on page 2

3.07.18 class 16.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Discrete symmetry subgroups of O(3)⊃(Octahedral O_h⊃O): Deriving $D^{(\alpha)}$-matrices defined by subgroup-chains $O \supset D_4 \supset C_4$, $O \supset D_4 \supset D_2$, and $O \supset D_3 \supset C_3$ applications to IR spectra of SF_6

Review Octahedral O_h⊃O group operator structure

Review Octahedral $O_h \supset O \supset D_4 \supset C_4$ subgroup chain correlations

Comparison of $O \supset D_4 \supset C_4$ and $O \supset D_4 \supset D_2$ correlations and level/projector splitting

- *$O \supset D_4 \supset C_4$ subgroup chain splitting*
- *$O \supset D_4 \supset D_2$ subgroup chain splitting (nOrmal D_2 vs. unOrmal D_2)*
- *$O_h \supset O \supset D_4 \supset C_{4v}$ and $O_h \supset O \supset D_4 \supset C_{4v} \supset C_{2v}$ subgroup splitting*

Splitting O class projectors $\mathbf{P}^{\mu}$ into irreducible projectors $\mathbf{P}^{\mu}_{m_4 m_4}$ for $O \supset C_4$

- *Left-cosets and coefficient arrays*

Development of irreducible projectors $\mathbf{P}^{\mu}_{m_4 m_4}$ and representations $D^{\mu}_{m_4 m_4}$

- *Calculating $\mathbf{P}^{E}_{0_4 0_4}$, $\mathbf{P}^{E}_{2_4 2_4}$, $\mathbf{P}^{T_1}_{0_4 0_4}$, $\mathbf{P}^{T_1}_{1_4 1_4}$, $\mathbf{P}^{T_2}_{2_4 2_4}$, $\mathbf{P}^{T_2}_{1_4 1_4}$, Collected $\mathbf{P}_{mm}$ results Table*

$O \supset C_4$ induced representation $0_4(C_4)\uparrow O \sim A_1 \oplus T_1 \oplus E$ and spectral analysis examples

- *Elementary induced representation $0_4(C_4)\uparrow O$*
- *Projection reduction of induced representation $0_4(C_4)\uparrow O$*
- *Introduction to ortho-complete eigenvalue-parameter relations*
  - *Examples from SF_6 model spectroscopy*

$\ell^{A_1} = 1$
$\ell^{A_2} = 1$
$\ell^{E} = 2$
$\ell^{T_1} = 3$
$\ell^{T_2} = 3$

Example: $G=O$

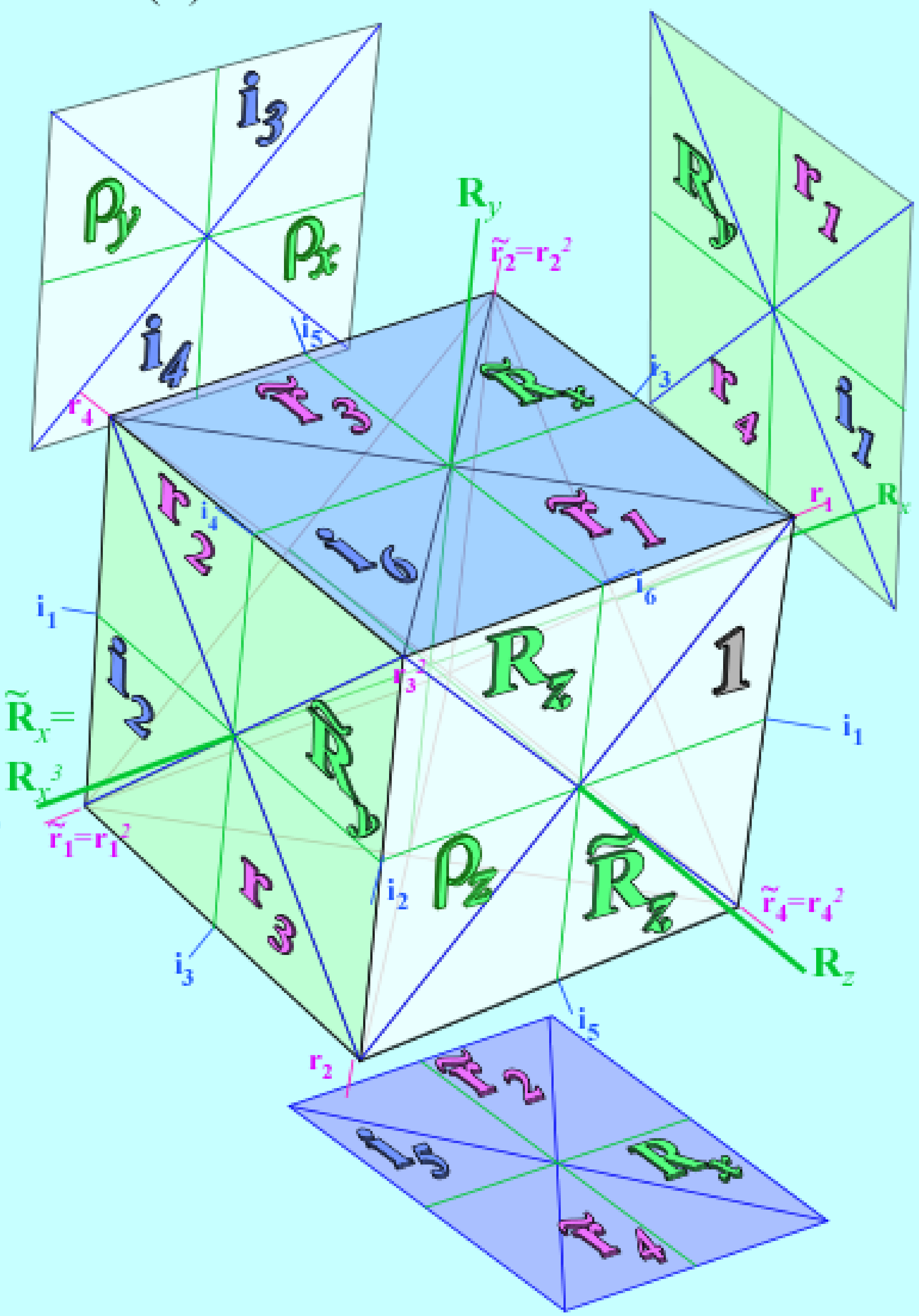
Cubic-Octahedral Group O

Centrum: $\kappa(O)=\Sigma_{(\alpha)} (\ell^{\alpha})^0 = 1^0+1^0+2^0+3^0+3^0=5$

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

Order: $^o(O)=\Sigma_{(\alpha)} (\ell^{\alpha})^0 = 1^2+1^2+2^2+3^2+3^2=24$

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



$O \supset C_4$

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

$O \supset C_3$

	$(0)_3$	$(1)_3$	$(2)_3=(-1)_3$
A_1	1	•	•
A_2	1	•	•
E	•	1	1
T_1	1	1	1
T_2	1	1	1

$O\supset C_4$	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

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

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

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

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

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

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

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

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

$\mathbf{P}^{(\alpha)}_{n_4 n_4}(O\supset C_4)$	$\mathbf{1}$	$r_1r_2\tilde{r}_3\tilde{r}_4$	$\tilde{r}_1\tilde{r}_2r_3r_4$	$\rho_x\rho_y$	ρ_z	$R_x\tilde{R}_xR_y\tilde{R}_y$	R_z	$\tilde{R}_z$	$i_1i_2i_5i_6$	i_3i_4
$24\cdot\mathbf{P}^{A_1}_{0_4 0_4}$	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

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

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

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

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

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

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

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

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

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

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

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

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

next nearest neighbor   *next-next nearest neighbor*

The $0_4\uparrow$ cluster

i_{1256} split   *i_{34} split*

$\mathbf{P}^{A_1}_{0_40_4}$ — +1

$\mathbf{P}^{T_1}_{0_40_4}$ — 0

$\mathbf{P}^{E}_{0_40_4}$ — −1/2

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

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

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

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

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

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

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

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

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

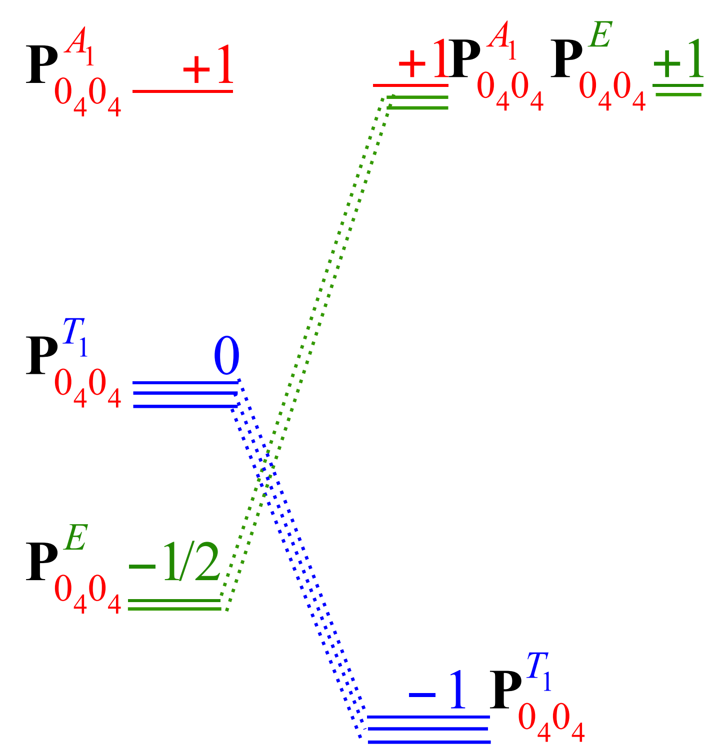
$$\mathbf{p}_{m_4} = \begin{cases} \mathbf{p}_{0_4} = (\mathbf{1}+\mathbf{R}_z+\rho_z+\tilde{\mathbf{R}}_z)/4 \\ \mathbf{p}_{1_4} = (\mathbf{1}+i\mathbf{R}_z-\rho_z-i\tilde{\mathbf{R}}_z)/4 \\ \mathbf{p}_{2_4} = (\mathbf{1}-\mathbf{R}_z+\rho_z-\tilde{\mathbf{R}}_z)/4 \\ \mathbf{p}_{3_4} = (\mathbf{1}-i\mathbf{R}_z-\rho_z+i\tilde{\mathbf{R}}_z)/4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

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

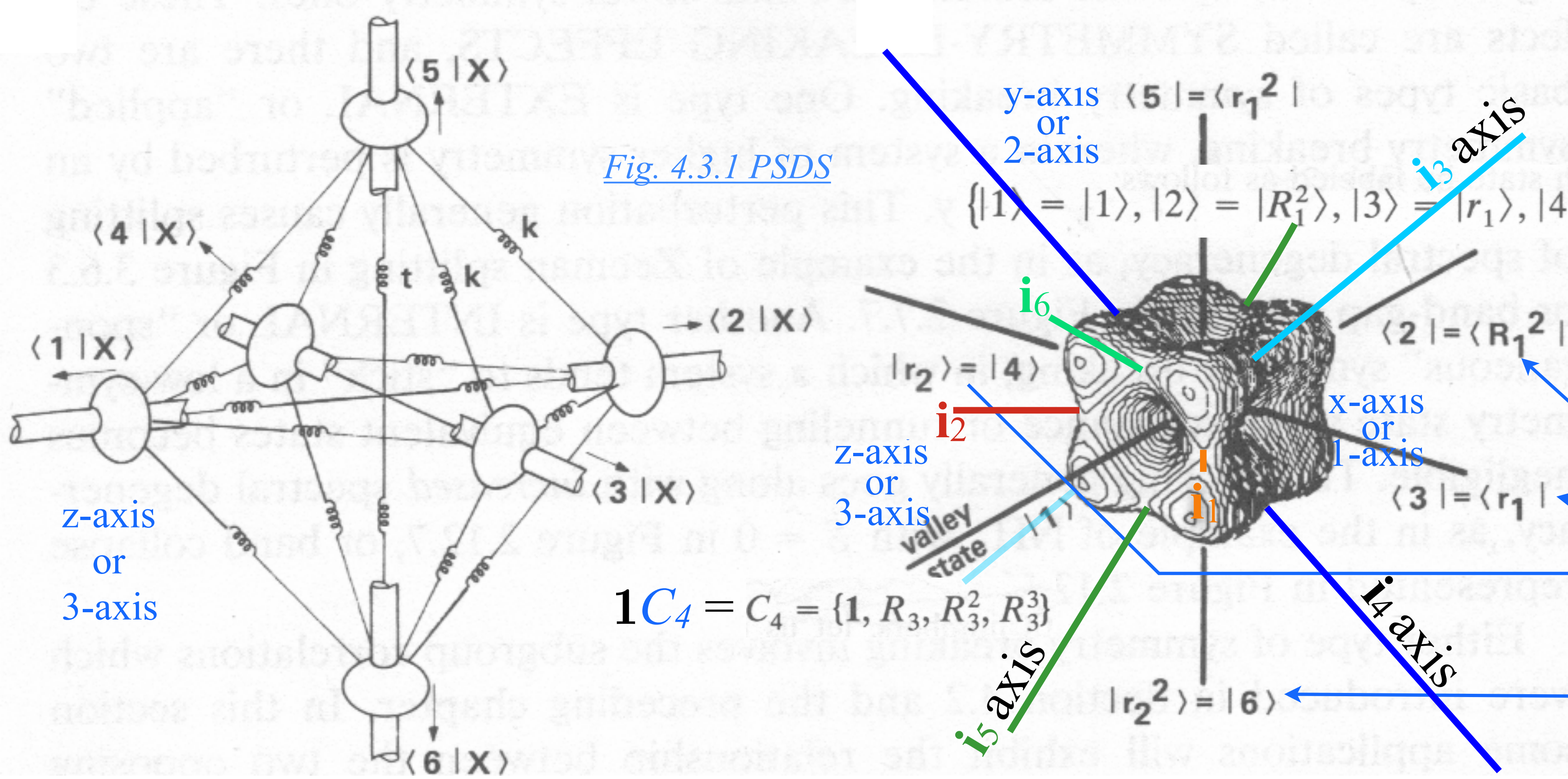
next nearest neighbor — *next-next nearest neighbor*

The $0_4\uparrow$ cluster

i_{16} split — *i_{34} split*



Elementary induced representation $0_4(C_4)\uparrow O$



Thus we label states by left *cosets* $\mathbf{r}_\ell C_4$ *of Local* C_4

$\mathbf{1}C_4 = C_4 = \{\mathbf{1}, R_3, R_3^2, R_3^3\}$

$R_1^2(\mathbf{1}, R_3, R_3^2, R_3^3) = (R_1^2, i_4, R_2^2, i_3),$

$r_1(\mathbf{1}, R_3, R_3^2, R_3^3) = (r_1, i_1, r_4, R_2),$

$r_2(\mathbf{1}, R_3, R_3^2, R_3^3) = (r_2, i_2, r_3, R_2^3),$

$r_1^2(\mathbf{1}, R_3, R_3^2, R_3^3) = (r_1^2, R_1^3, r_3^2, i_6),$

$r_2^2(\mathbf{1}, R_3, R_3^2, R_3^3) = (r_2^2, R_1, r_4^2, i_5),$

Here is $0_4(C_4)$ *induced representation* $\mathscr{I}^{0_4\uparrow O}(\mathbf{I_i})$ *of a linear combination of* **i**-*class rotations*

$$\mathbf{I_i} = i_1\mathbf{i_1} + i_2\mathbf{i_2} + i_3\mathbf{i_3} + i_4\mathbf{i_4} + i_5\mathbf{i_5} + i_6\mathbf{i_6} \longrightarrow \mathbf{I_i} = i_{34}(\mathbf{i_3} + \mathbf{i_4}) + i_{16}(\mathbf{i_1} + \mathbf{i_2} + \mathbf{i_5} + \mathbf{i_6})$$

$\mathscr{I}^{0_4\uparrow O}(\mathbf{I_i}) =$

	$\|1\rangle$	$\|2\rangle$	$\|3\rangle$	$\|4\rangle$	$\|5\rangle$	$\|6\rangle$
$\langle 1\|$	1	i_3+i_4	i_1	i_2	i_6	i_5
$\langle 2\|$	i_3+i_4	1	i_2	i_1	i_5	i_6
$\langle 3\|$	i_1	i_2	1	i_5+i_6	i_3	i_4
$\langle 4\|$	i_2	i_1	i_5+i_6	1	i_4	i_3
$\langle 5\|$	i_6	i_5	i_3	i_4	1	i_1+i_2
$\langle 6\|$	i_5	i_6	i_4	i_3	i_1+i_2	1

Let: $i_3 = i_{34} = i_4$

and/or: $i_{16} = i_1 = i_2 = i_5 = i_6$

	$\|1\rangle$	$\|2\rangle$	$\|3\rangle$	$\|4\rangle$	$\|5\rangle$	$\|6\rangle$
$\langle 1\|$	1	$2i_{34}$	i_{16}	i_{16}	i_{16}	i_{16}
$\langle 2\|$	$2i_{34}$	1	i_{16}	i_{16}	i_{16}	i_{16}
$\langle 3\|$	i_{16}	i_{16}	1	$2i_{16}$	i_{34}	i_{34}
$\langle 4\|$	i_{16}	i_{16}	$2i_{16}$	1	i_{34}	i_{34}
$\langle 5\|$	i_{16}	i_{16}	i_{34}	i_{34}	1	$2i_{16}$
$\langle 6\|$	i_{16}	i_{16}	i_{34}	i_{34}	$2i_{16}$	1

Review Octahedral $O_h \supset O$ *group operator structure*
Review Octahedral $O_h \supset O \supset D_4 \supset C_4$ *subgroup chain correlations*

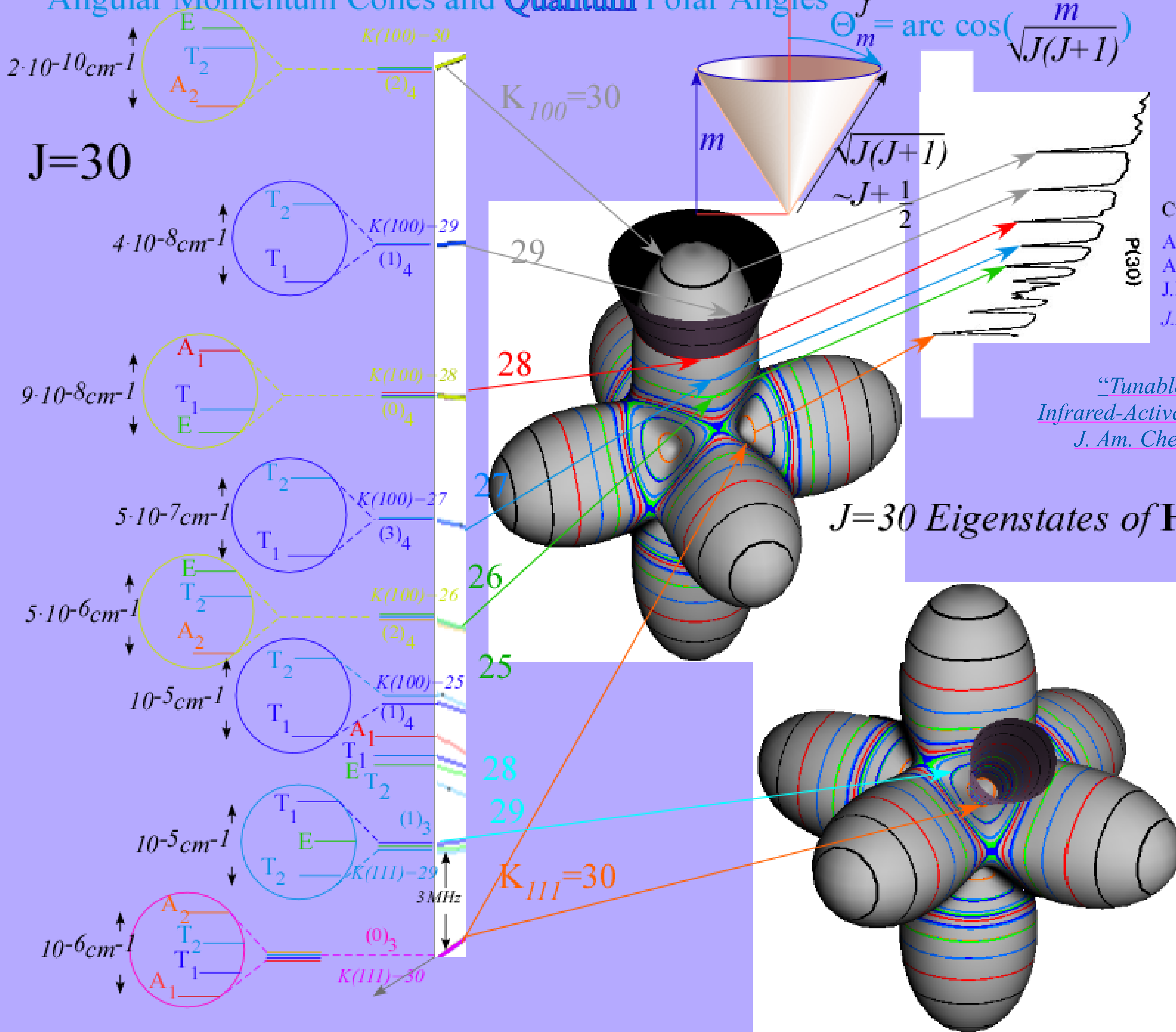
Comparison of $O \supset D_4 \supset C_4$ *and* $O \supset D_4 \supset D_2$ *correlations and level/projector splitting*
- $O \supset D_4 \supset C_4$ *subgroup chain splitting*
- $O \supset D_4 \supset D_2$ *subgroup chain splitting (nOrmal* D_2 *vs. unOrmal* D_2*)*
- $O_h \supset O \supset D_4 \supset C_{4v}$ *and* $O_h \supset O \supset D_4 \supset C_{4v} \supset C_{2v}$ *subgroup splitting*

Splitting O *class projectors* $\mathbf{P}^{\mu}$ *into irreducible projectors* $\mathbf{P}^{\mu}_{m_4 m_4}$ *for* $O \supset C_4$
- *Development of irreducible projectors* $\mathbf{P}^{\mu}_{m_4 m_4}$ *and representations* $D^{\mu}_{m_4 m_4}$
- *Calculating* $\mathbf{P}^{E}_{0_4 0_4}$, $\mathbf{P}^{E}_{2_4 2_4}$, $\mathbf{P}^{T_1}_{0_4 0_4}$, $\mathbf{P}^{T_1}_{1_4 1_4}$, $\mathbf{P}^{T_2}_{2_4 2_4}$, $\mathbf{P}^{T_2}_{1_4 1_4}$,

$O \supset C_4$ *induced representation* $0_4(C_4)\uparrow O \sim A_1 \oplus T_1 \oplus E$ *and spectral analysis examples*
- *Elementary induced representation* $0_4(C_4)\uparrow O$
- *Projection reduction of induced representation* $0_4(C_4)\uparrow O$
- *Introduction to ortho-complete eigenvalue-parameter relations*
  - *Examples in* SF_6 *spectroscopy*

Angular Momentum Cones and Quantum Polar Angles

$$\Theta_m^J = \arccos\left(\frac{m}{\sqrt{J(J+1)}}\right)$$



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)*

"Tunable Laser Spectra of the Infrared-Active Fundamentals of Cubane" J. Am. Chem. Soc. 106, 891 (1984)

J=30 Eigenstates of $\mathbf{H}=B\mathbf{J}^2+T^{[4]}$

	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

$1\,(1,\rho_z,R_z,\tilde{R}_z)$, $\rho_x(1,\rho_z,R_z,\tilde{R}_z)$, $r_1(1,\rho_z,R_z,\tilde{R}_z)$, $r_2(1,\rho_z,R_z,\tilde{R}_z)$, $\tilde{r}_1(1,\rho_z,R_z,\tilde{R}_z)$, $\tilde{r}_2(1,\rho_z,R_z,\tilde{R}_z)$

$\rho_z(\rho_z,1,\tilde{R}_z,R_z)$, $\rho_y(\rho_z,1,\tilde{R}_z,R_z)$, $r_4(\rho_z,1,\tilde{R}_z,R_z)$, $r_3(\rho_z,1,\tilde{R}_z,R_z)$, $\tilde{r}_3(\rho_z,1,\tilde{R}_z,R_z)$, $\tilde{r}_4(\rho_z,1,\tilde{R}_z,R_z)$

$R_z(\tilde{R}_z,R_z,1,\rho_z)$, $i_4(\tilde{R}_z,R_z,1,\rho_z)$, $i_1(\tilde{R}_z,R_z,1,\rho_z)$, $i_2(\tilde{R}_z,R_z,1,\rho_z)$, $\tilde{R}_x(\tilde{R}_z,R_z,1,\rho_z)$, $R_x(\tilde{R}_z,R_z,1,\rho_z)$

$\tilde{R}_z(R_z,\tilde{R}_z,\rho_z,1)$, $i_3(R_z,\tilde{R}_z,\rho_z,1)$, $R_y(R_z,\tilde{R}_z,\rho_z,1)$, $\tilde{R}_y(R_z,\tilde{R}_z,\rho_z,1)$, $i_6(R_z,\tilde{R}_z,\rho_z,1)$, $i_5(R_z,\tilde{R}_z,\rho_z,1)$