Group Theory in Quantum Mechanics

Lecture 20 *(4.11.13)*

Octahedral-tetrahedral $O\sim T_d$ representations and spectra

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

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*

Simplest $O_h \supset O \supset D_4 \supset C_4$ *spectral analysis problems*

- *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 expression*

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*

Simplest $O_h \supset O \supset D_4 \supset C_4$ *spectral analysis problems*

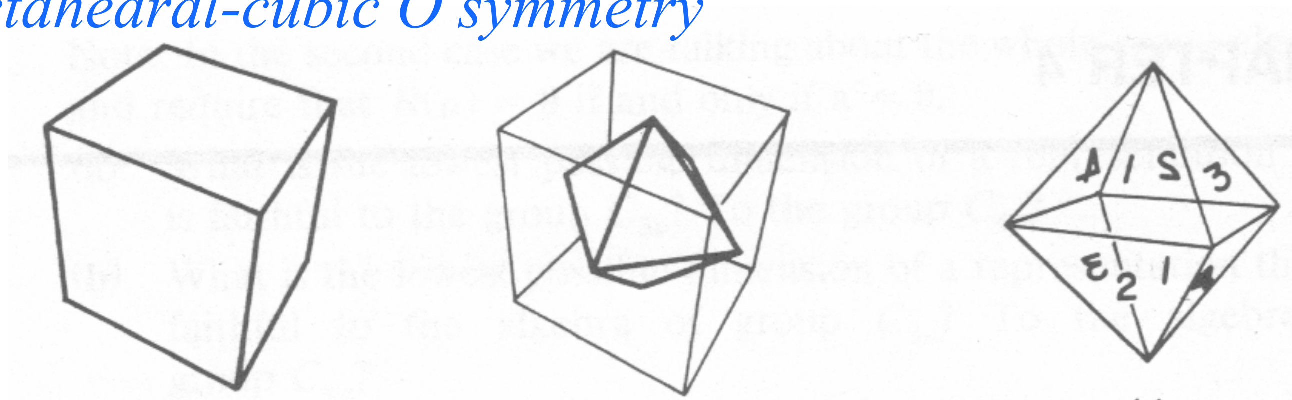
Elementary induced representation $0_4(C_4)\uparrow O$

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

Introduction to ortho-complete eigenvalue expression

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

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

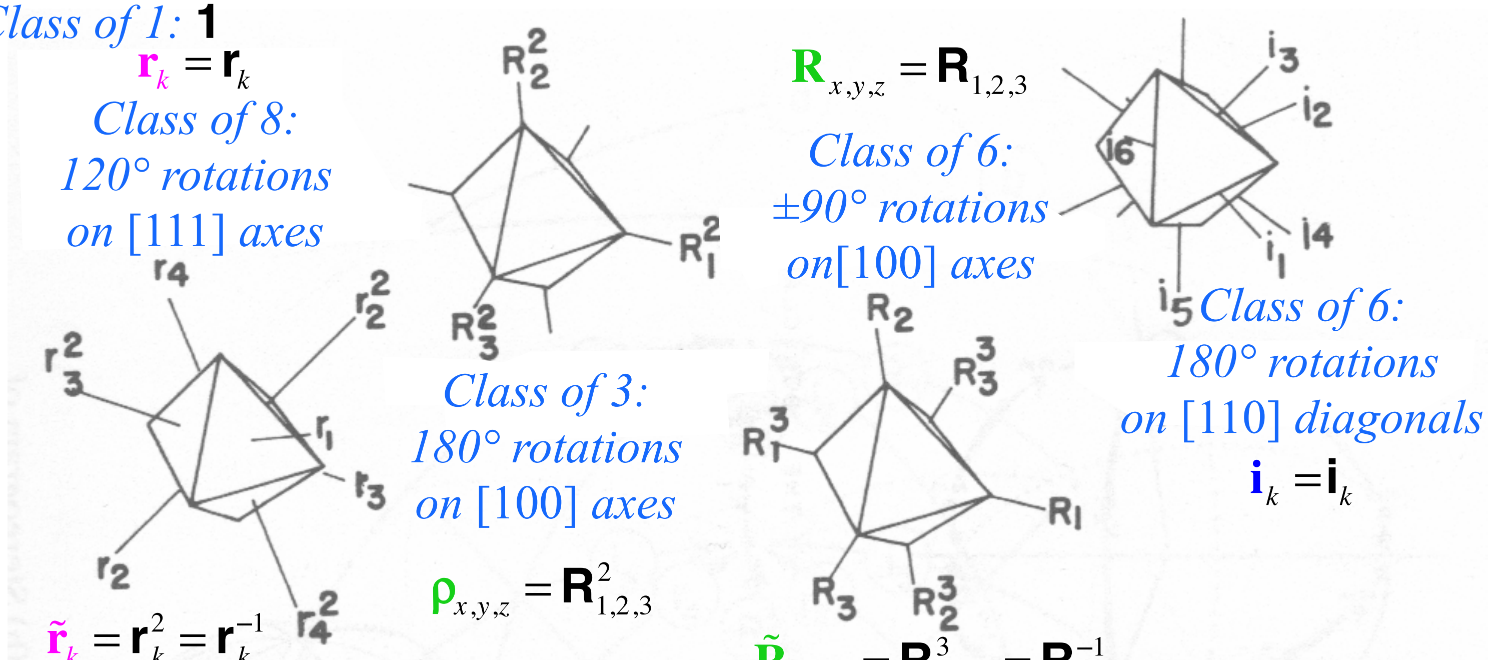
$\mathbf{R}_{x,y,z} = \mathbf{R}_{1,2,3}$

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

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

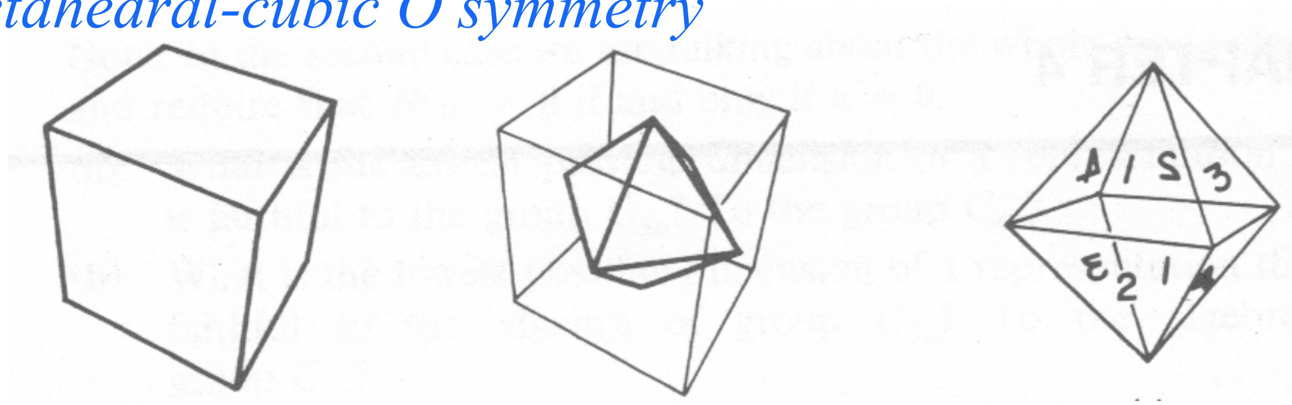
Class of 6: 180° rotations on [110] diagonals

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



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

Octahedral-cubic O symmetry



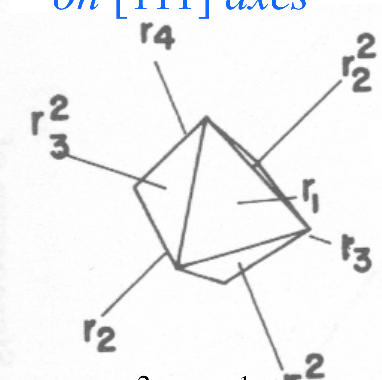
Order °O=6 hexahedron squares · 4 pts =24
=8 octahedron triangles · 3 pts =24
=12 lines · 2 pts =24 positions

Octahedral group O operations

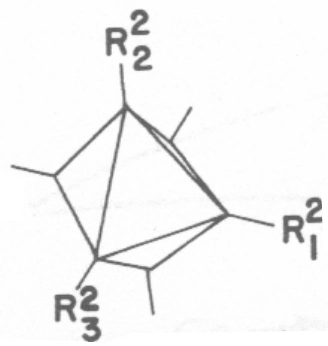
Class of 1: $\mathbf{1}$

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

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



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

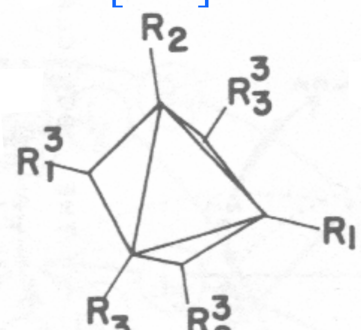


Class of 3:
180° rotations
on [100] axes

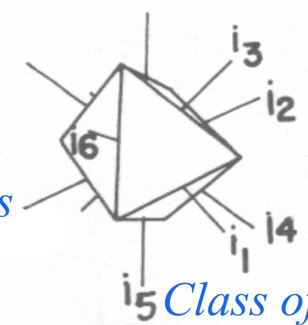
$\rho_{x,y,z} = \mathbf{R}^2_{1,2,3}$

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

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

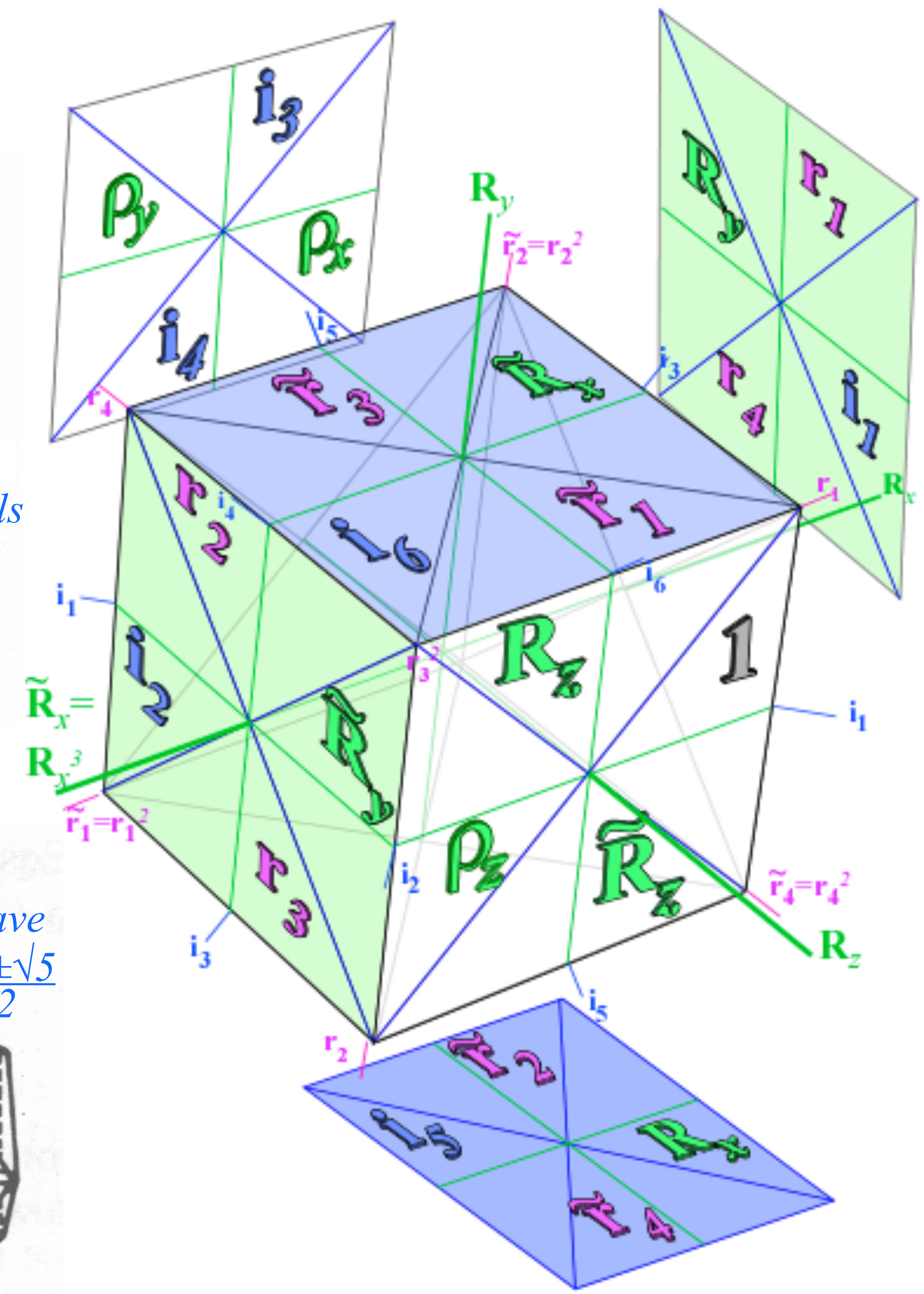


$\tilde{\mathbf{R}}_{x,y,z} = \mathbf{R}^3_{1,2,3} = \mathbf{R}^{-1}_{1,2,3}$

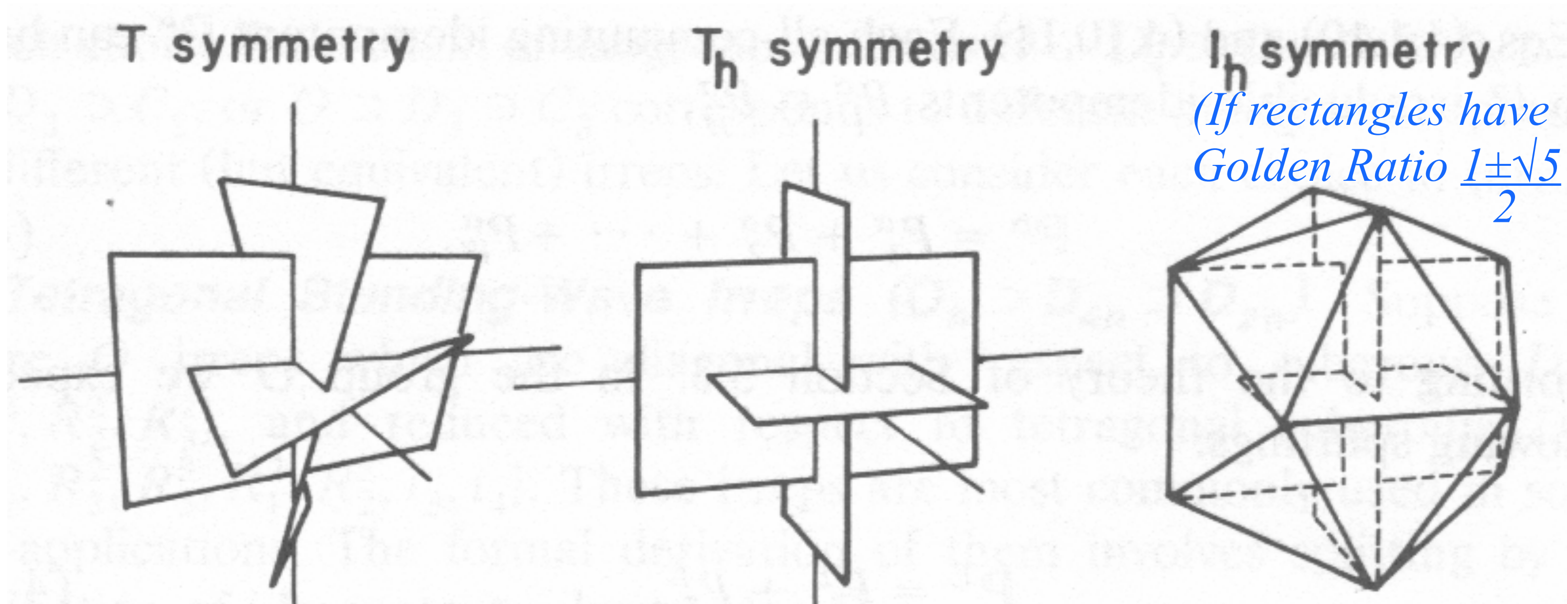


Class of 6:
180° rotations
on [110] diagonals

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



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 $O_h \supset T_h \supset T$

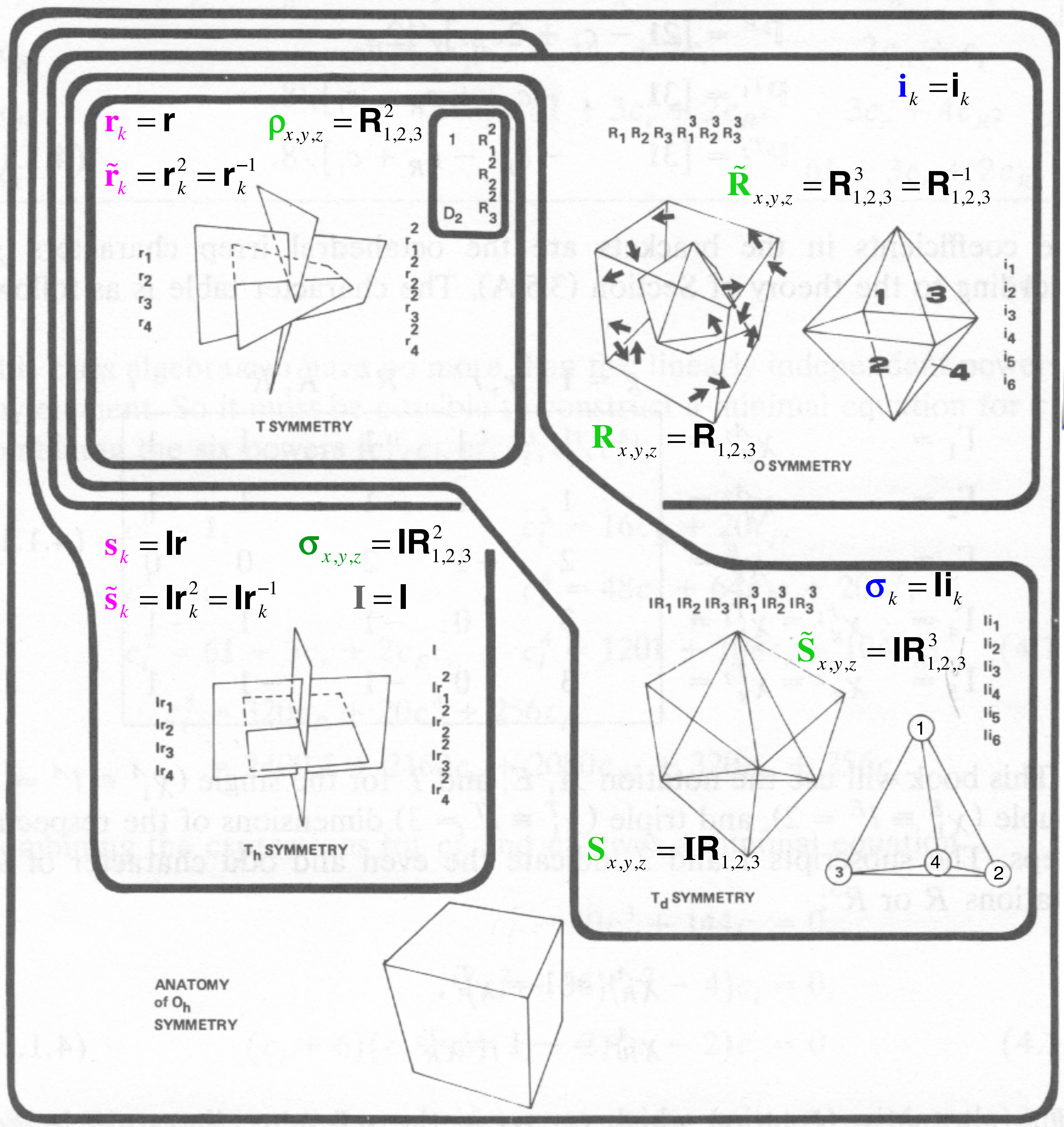
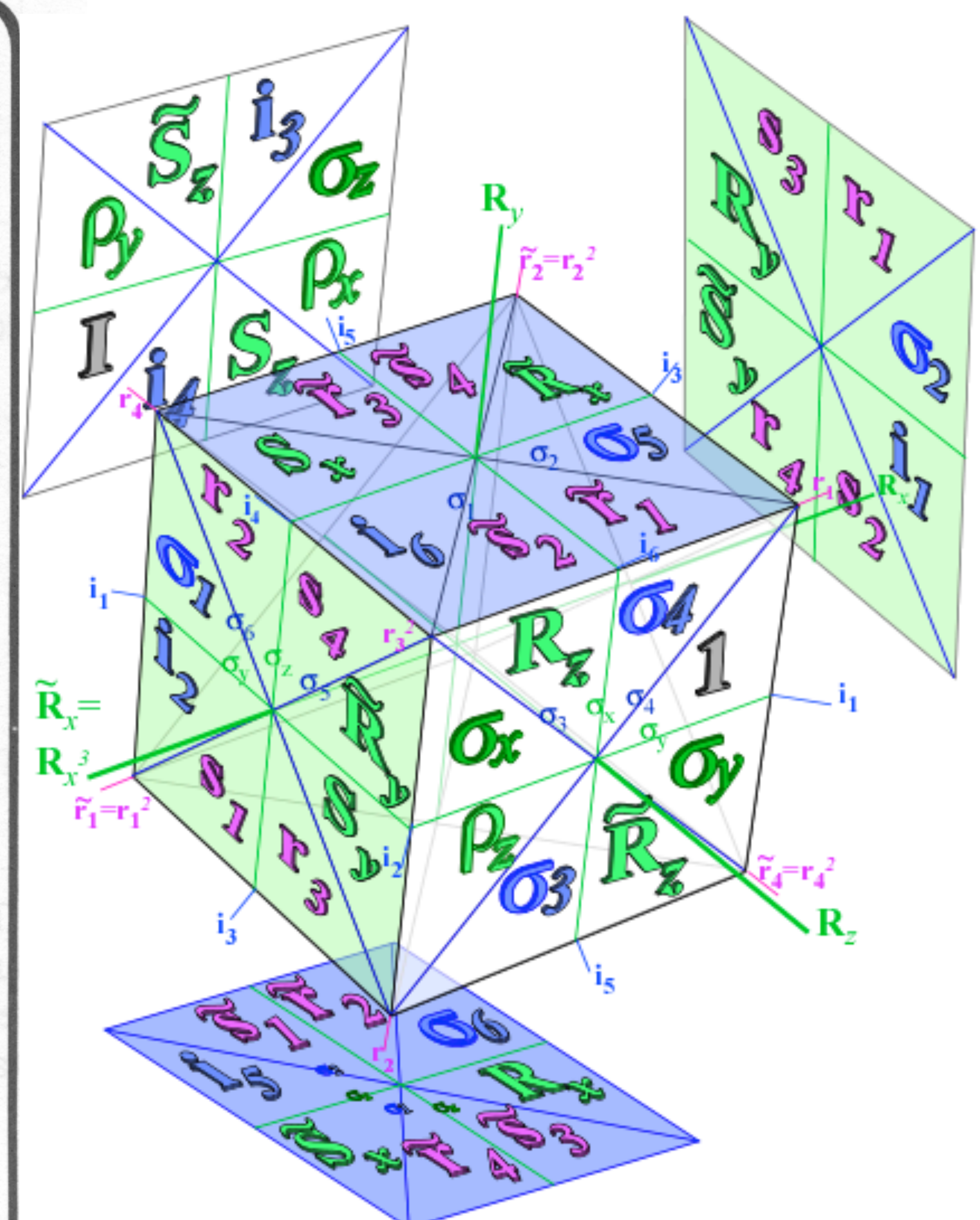
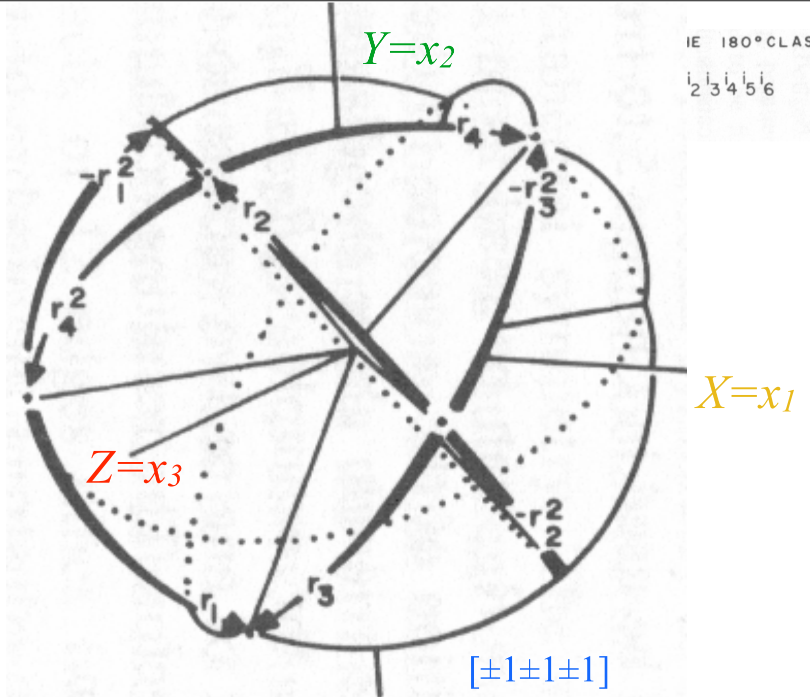
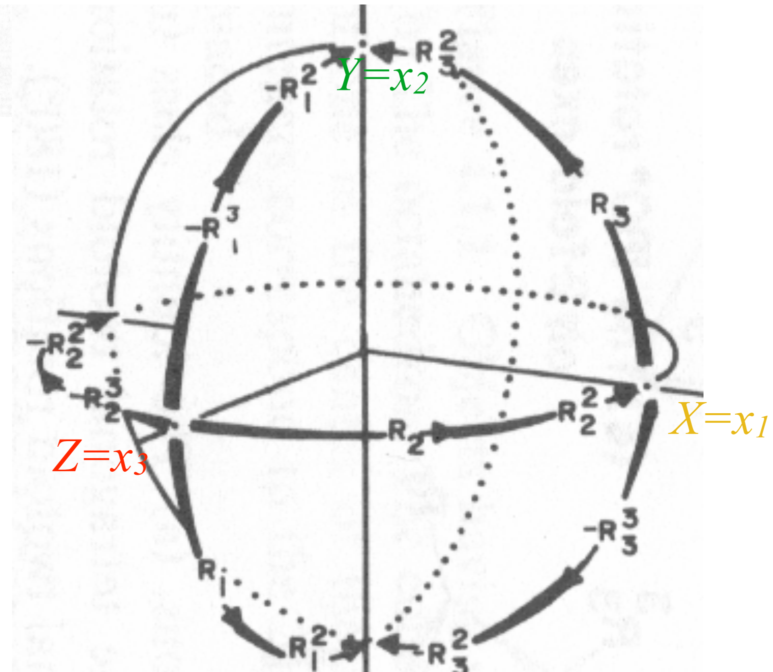


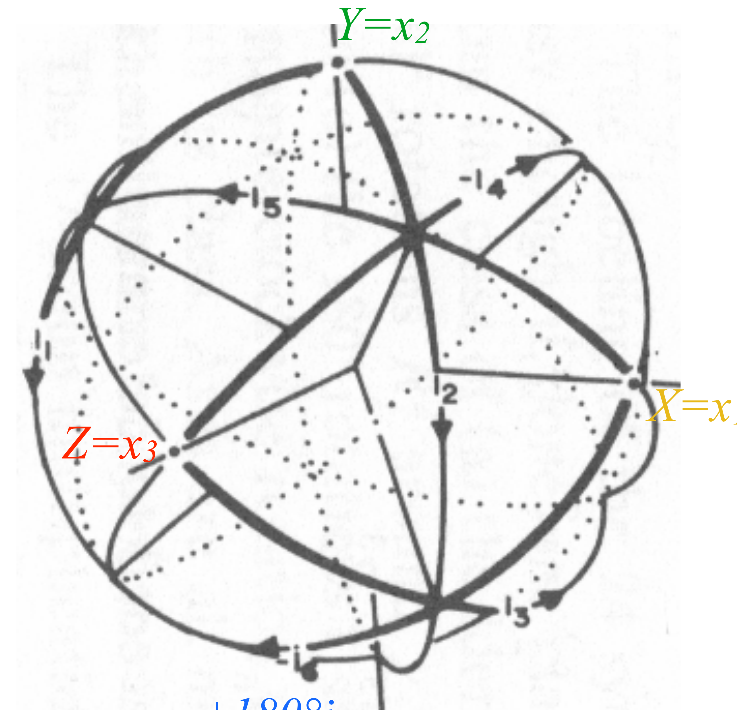
Figure 4.1.5 The full octahedral group (O_h) and four non-Abelian subgroups T, T_h, T_d, and O. The Abelian D_2 subgroup of T is indicated also.

Fig. 4.1.5 from Principles of Symmetry, Dynamics and Spectroscopy









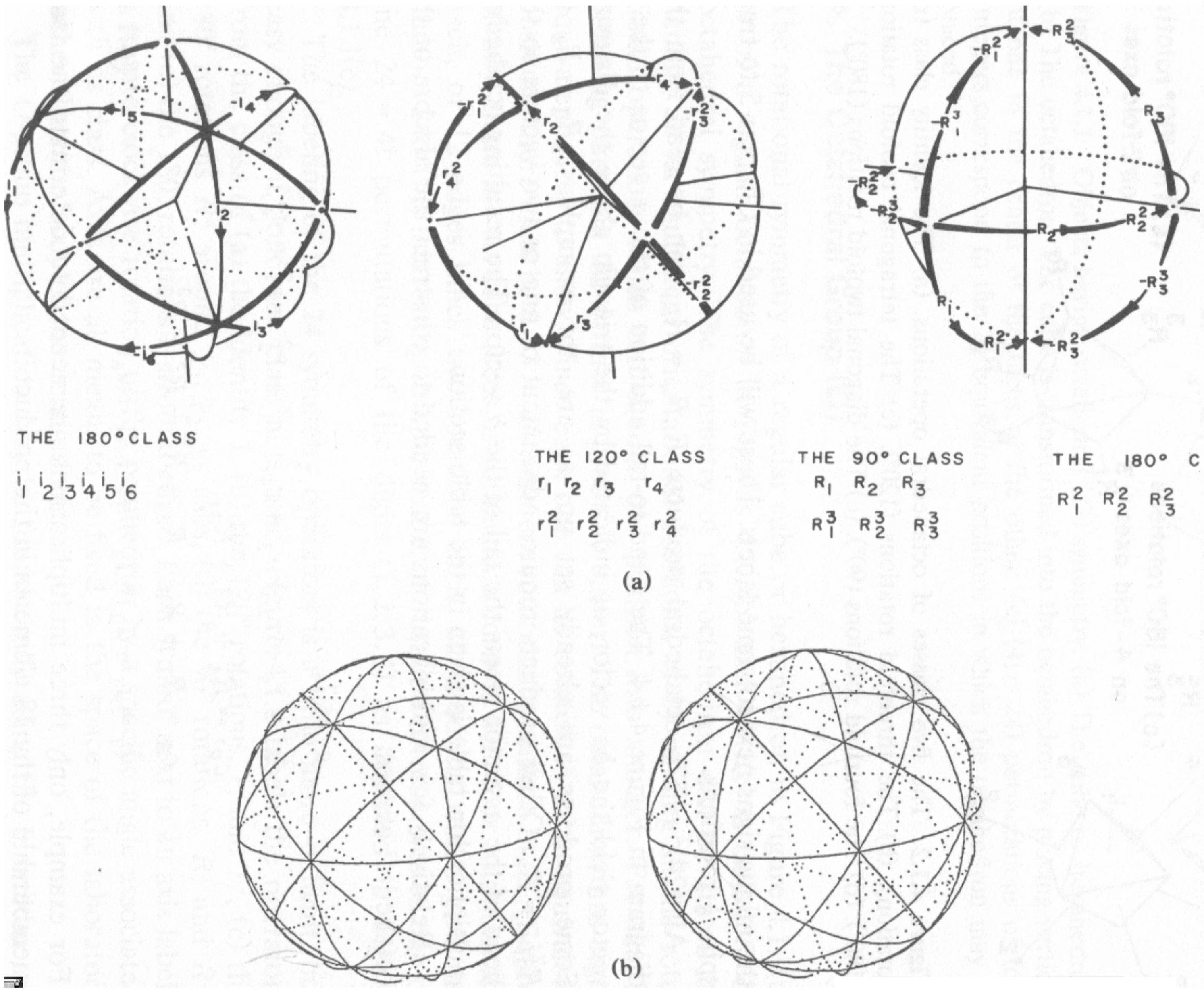
+120°   -120°   ±180° XYZ   +90° XYZ   -90° XYZ   ±180° i_k

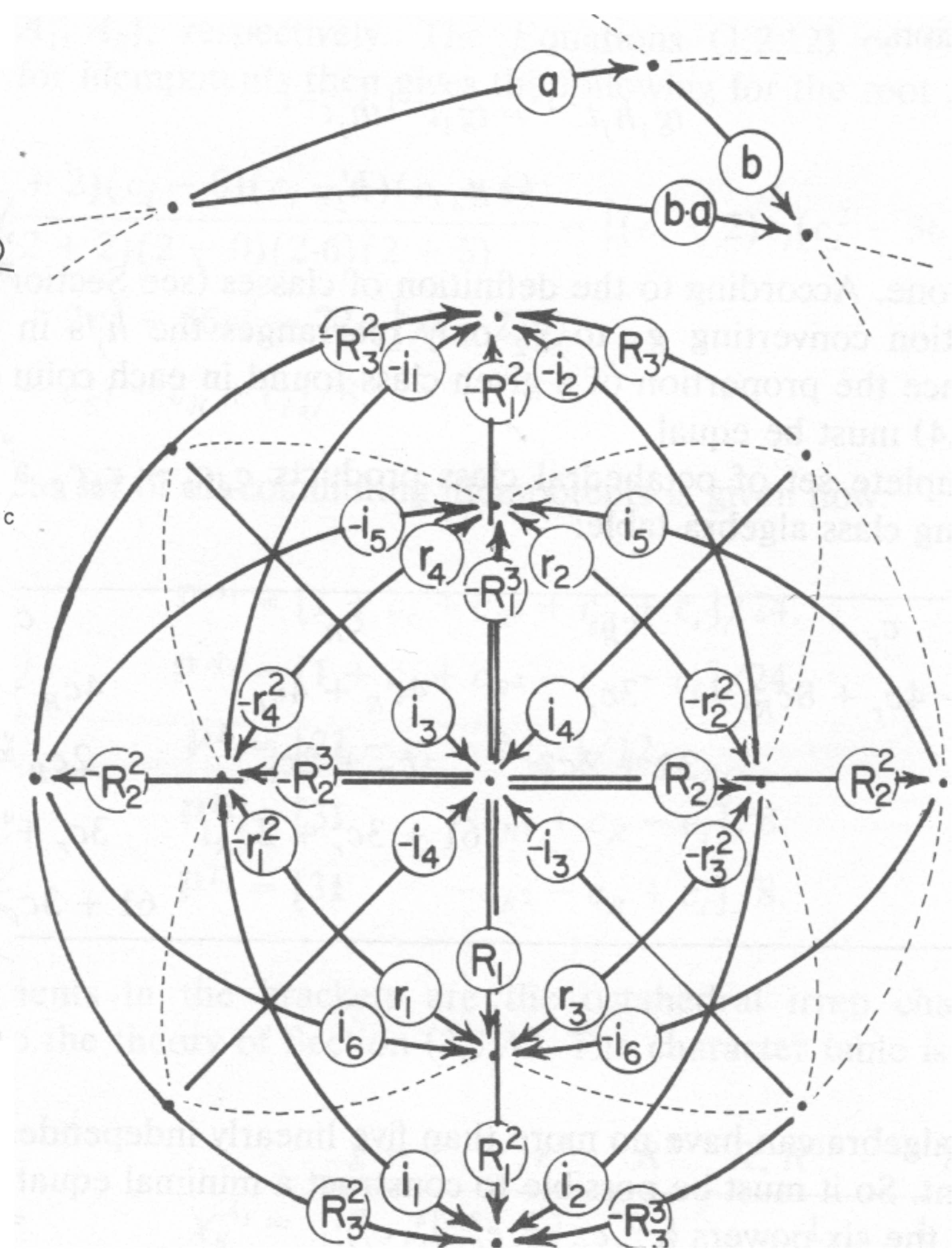
$[1\,1\,1][\bar{1}\,\bar{1}\,1][1\,\bar{1}\,\bar{1}][\bar{1}\,1\,\bar{1}]$ $[\bar{1}\,\bar{1}\,\bar{1}][1\,1\,\bar{1}][\bar{1}\,1\,1][1\,\bar{1}\,1]$ $[1\,0\,0][0\,1\,0][0\,0\,1]$ $[1\,0\,0][0\,1\,0][0\,0\,1]$ $[\bar{1}\,0\,0][0\,\bar{1}\,0][0\,0\,\bar{1}]$ $[1\,0\,1][1\,0\,\bar{1}][1\,1\,0]$ $[1\,\bar{1}\,0]$ $[0\,1\,\bar{1}]$ $[0\,1\,1]$

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

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

Octahedral O and spin-O⊂U(2) rotation nomogram from Fig. 4.1.3-4 Principles of Symmetry, Dynamics and Spectroscopy





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*

Simplest $O_h \supset O \supset D_4 \supset C_4$ *spectral analysis problems*

- *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 expression*

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

$\chi^\mu_g(O)$	$\mathbf{g=1}$	$\mathbf{r}_{1...4}$	180° ρ_{xyz}	90° $\mathbf{R}_{xyz}$	180° $\mathbf{i}_{1...6}$
A_1	1	$\cancel{1}$	1	1	1
A_2	1	$\cancel{1}$	1	−1	−1
E	2	$\cancel{-1}$	2	0	0
T_1	3	$\cancel{0}$	−1	1	−1
T_2	3	$\cancel{0}$	−1	−1	1

$O \downarrow D_4$ subduction

D_4: $\mathbf{1}, \rho_{z180°}, \mathbf{R}_{z\pm 90°}, \rho_{z180°}, \mathbf{i}_{3,4}$

$A_1(O)\downarrow D_4 = 1, \ 1, \ 1, \ 1, \ 1 .$

$A_2(O)\downarrow D_4 = 1, \ 1, \ -1, \ 1, \ -1 .$

$E(O)\downarrow D_4 = 2, \ 2, \ 0, \ 2, \ 0 .$

$T_2(O)\downarrow D_4 = 3, \ -1, \ 1, \ -1, \ -1 .$

$T_2(O)\downarrow D_4 = 3, \ -1, \ -1, \ -1, \ 1 .$

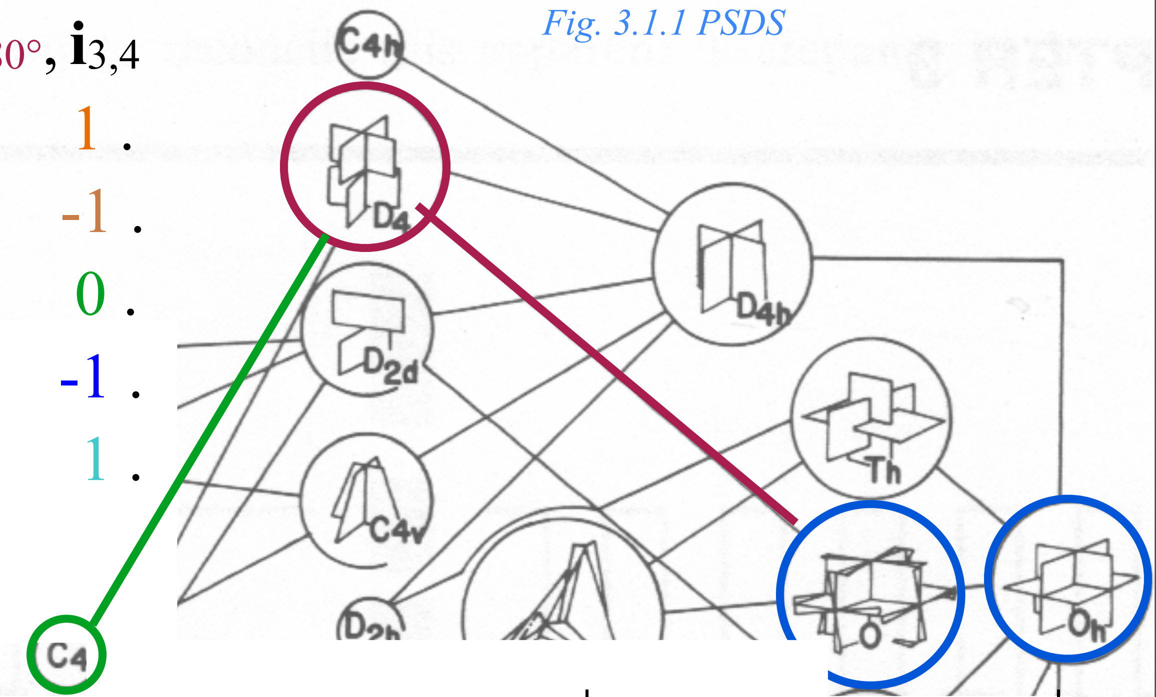


Fig. 3.1.1 PSDS

$\chi^\mu_g(D_4)$	$\mathbf{g=1}$	$\rho_{z180°}$	$\mathbf{R}_{z\pm 90°}$	$\rho_{x,y180°}$	$\mathbf{i}_{3,4}$
A_1	1	1	1	$\cancel{1}$	$\cancel{1}$
B_1	1	1	−1	$\cancel{1}$	$\cancel{-1}$
A_2	1	1	1	$\cancel{-1}$	$\cancel{-1}$
B_2	1	1	−1	$\cancel{-1}$	$\cancel{1}$
E	2	−2	0	$\cancel{0}$	$\cancel{0}$

$D_4 \downarrow C_4$ subduction

$\mathbf{1}, \mathbf{R}_{z+90°}, \rho_{z180°}, \mathbf{R}_{z-90°}$

$A_1(D_4)\downarrow C_4 = 1, \ 1, \ 1, \ 1. \quad =(0)_4$

$B_1(D_4)\downarrow C_4 = 1, \ -1, \ 1, \ -1. \quad =(2)_4$

$A_2(D_4)\downarrow C_4 = 1, \ 1, \ 1, \ 1. \quad =(0)_4$

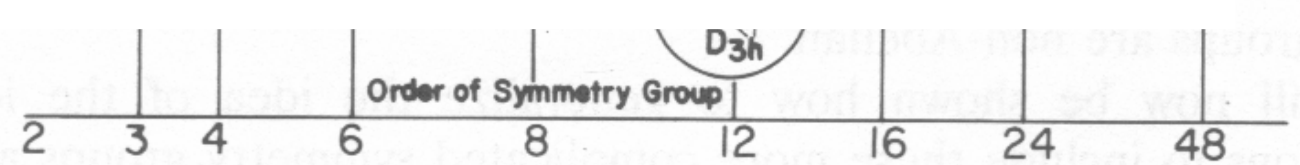
$B_2(D_4)\downarrow C_4 = 1, \ -1, \ 1, \ -1. \quad =(2)_4$

$E(D_4)\downarrow C_4 = 2, \ 0, \ -2, \ 0. \quad =(1)_4 \oplus (3)_4$

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

$\chi^\mu_g(C_4)$	$\mathbf{g=1}$	$\mathbf{R}_{z+90°}$	$\mathbf{R}_{z+180°}$	$\mathbf{R}_{z-90°}$
$(0)_4$	1	1	1	1
$(1)_4$	1	i	−1	$-i$
$(2)_4$	1	−1	1	−1
$(3)_4$	1	$-i$	−1	i

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



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

$\chi^\mu_g(O)$	$\mathbf{g=1}$	$\mathbf{r}_{1\ldots4}$	180° ρ_{xyz}	90° $\mathbf{R}_{xyz}$	180° $\mathbf{i}_{1\ldots6}$
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

$O\downarrow D_4$ subduction

D_4: $\mathbf{1}, \rho_{z180°}, \mathbf{R}_{z\pm90°}, \rho_{z180°}, \mathbf{i}_{3,4}$

$A_1(O)\downarrow D_4 = 1,\ 1,\ 1,\ 1,\ 1\ .$

$A_2(O)\downarrow D_4 = 1,\ 1,\ -1,\ 1,\ -1\ .$

$E(O)\downarrow D_4 = 2,\ 2,\ 0,\ 2,\ 0\ .$

$T_2(O)\downarrow D_4 = 3,\ -1,\ 1,\ -1,\ -1\ .$

$T_2(O)\downarrow D_4 = 3,\ -1,\ -1,\ -1,\ 1\ .$

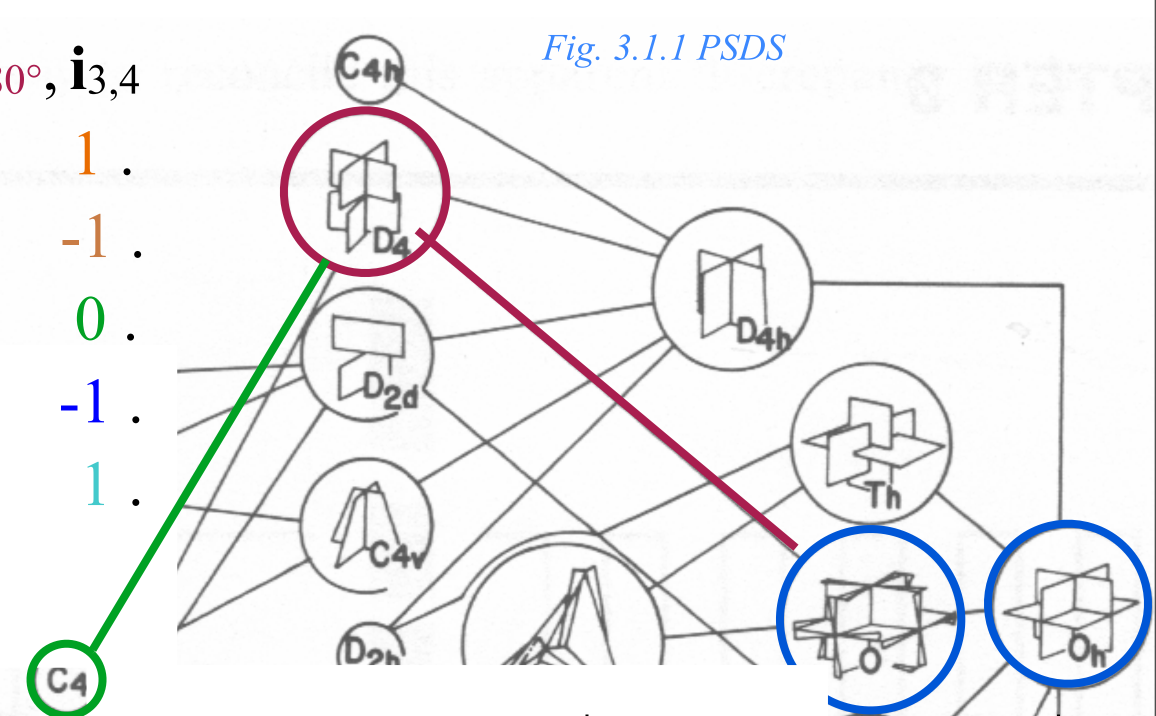


Fig. 3.1.1 PSDS

$\chi^\mu_g(D_4)$	$\mathbf{g=1}$	$\rho_{z180°}$	$\mathbf{R}_{z\pm90°}$	$\rho_{x,y180°}$	$\mathbf{i}_{3,4}$
A_1	1	1	1	1	1
B_1	1	1	−1	1	−1
A_2	1	1	1	−1	−1
B_2	1	1	−1	−1	1
E	2	−2	0	0	0

$D_4\downarrow C_4$ subduction

$\mathbf{1}, \mathbf{R}_{z+90°}, \rho_{z180°}, \mathbf{R}_{z-90°}$

$A_1(D_4)\downarrow C_4 = 1,\ 1,\ 1,\ 1. \quad =(0)_4$

$B_1(D_4)\downarrow C_4 = 1,\ -1,\ 1,\ -1. \quad =(2)_4$

$A_2(D_4)\downarrow C_4 = 1,\ 1,\ 1,\ 1. \quad =(0)_4$

$B_2(D_4)\downarrow C_4 = 1,\ -1,\ 1,\ -1. \quad =(2)_4$

$E(D_4)\downarrow C_4 = 2,\ 0,\ -2,\ 0\ . \quad =(1)_4\oplus(3)_4$

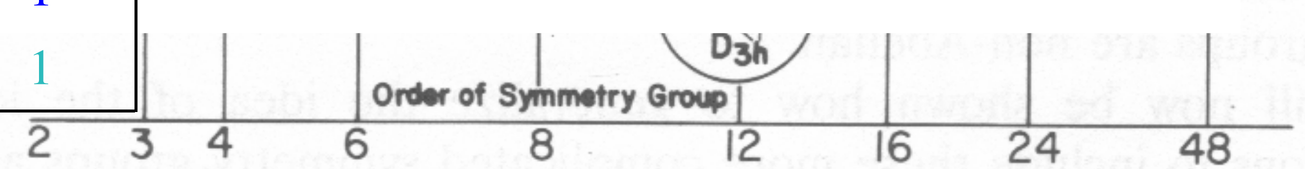
$O\downarrow D_4$	A_1	B_1	A_2	B_2	E
A_1	1	·	·	·	·
A_2	·	1	·	·	·
E	1	1	·	·	·
T_1	·	·	1	·	1
T_2	·	·	·	1	1

$\chi^\mu_g(C_4)$	$\mathbf{g=1}$	$\mathbf{R}_{z+90°}$	$\mathbf{R}_{z+180°}$	$\mathbf{R}_{z-90°}$
$(0)_4$	1	1	1	1
$(1)_4$	1	i	−1	$-i$
$(2)_4$	1	−1	1	−1
$(3)_4$	1	$-i$	−1	i

$O\downarrow C_4$ subduction

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

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



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

$\chi^{\mu}_{g}(O)$	$\mathbf{g=1}$	$\mathbf{r}_{1...4}$	180° ρ_{xyz}	90° $\mathbf{R}_{xyz}$	180° $\mathbf{i}_{1...6}$
A_1	1	1	1	1	1
A_2	1	1	1	−1	−1
E	2	−1	2	0	0
T_1	3	0	−1	1	−1
T_2	3	0	−1	−1	1

$O\downarrow D_4$ subduction

D_4: $\mathbf{1}, \rho_{z180°}, \mathbf{R}_{z\pm 90°}, \rho_{z180°}, \mathbf{i}_{3,4}$

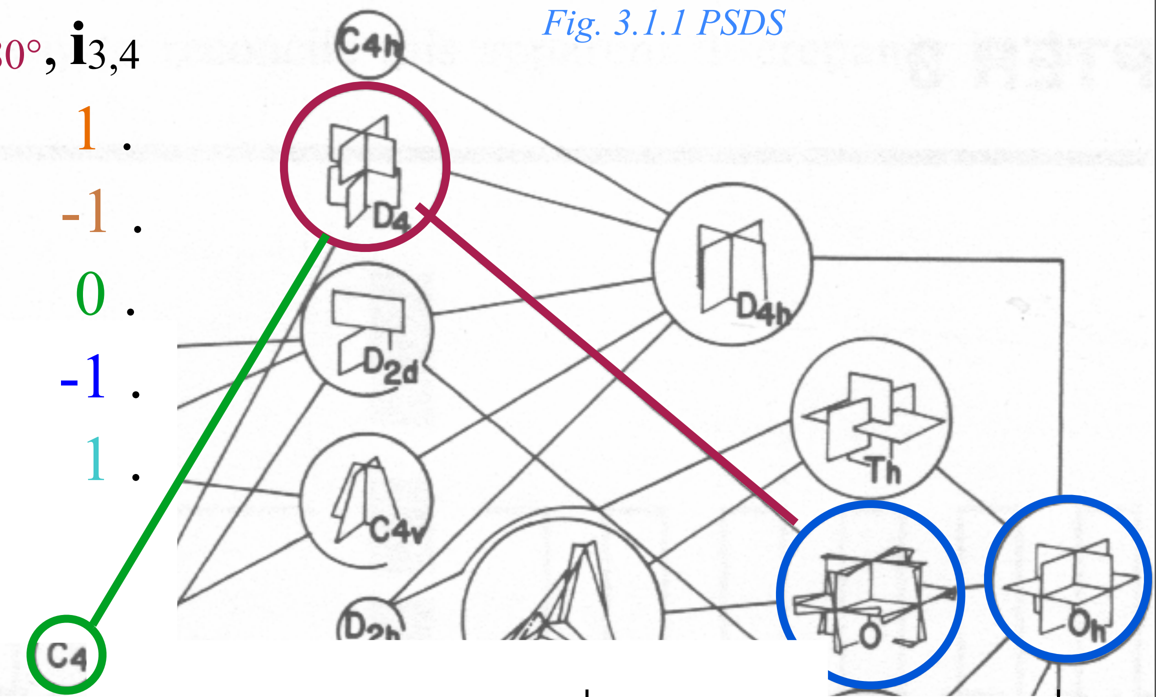
$A_1(O)\downarrow D_4 = 1,\ 1,\ 1,\ 1,\ 1\ .$

$A_2(O)\downarrow D_4 = 1,\ 1,\ -1,\ 1,\ -1\ .$

$E(O)\downarrow D_4 = 2,\ 2,\ 0,\ 2,\ 0\ .$

$T_2(O)\downarrow D_4 = 3,\ -1,\ 1,\ -1,\ -1\ .$

$T_2(O)\downarrow D_4 = 3,\ -1,\ -1,\ -1,\ 1\ .$



$\chi^{\mu}_{g}(D_4)$	$\mathbf{g=1}$	$\rho_{z180°}$	$\mathbf{R}_{z\pm 90°}$	$\rho_{x,y180°}$	$\mathbf{i}_{3,4}$
A_1	1	1	1	1	1
B_1	1	1	−1	1	−1
A_2	1	1	1	−1	−1
B_2	1	1	−1	−1	1
E	2	−2	0	0	0

$D_4\downarrow C_4$ subduction

$\mathbf{1}, \mathbf{R}_{z+90°}, \rho_{z180°}, \mathbf{R}_{z-90°}$

$A_1(D_4)\downarrow C_4 = 1,\ 1,\ 1,\ 1. \quad =(0)_4$

$B_1(D_4)\downarrow C_4 = 1,\ -1,\ 1,\ -1. \quad =(2)_4$

$A_2(D_4)\downarrow C_4 = 1,\ 1,\ 1,\ 1. \quad =(0)_4$

$B_2(D_4)\downarrow C_4 = 1,\ -1,\ 1,\ -1. \quad =(2)_4$

$E(D_4)\downarrow C_4 = 2,\ 0,\ -2,\ 0\ . \quad =(1)_4 \oplus (3)_4$

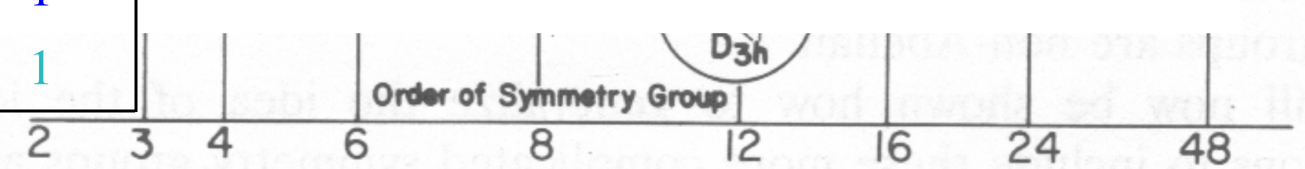
$O\downarrow D_4$	A_1	B_1	A_2	B_2	E
A_1	1	·	·	·	·
A_2	·	1	·	·	·
E	1	1	·	·	·
T_1	·	·	1	·	1
T_2	·	·	·	1	1

$\chi^{\mu}_{g}(C_4)$	$\mathbf{g=1}$	$\mathbf{R}_{z+90°}$	$\mathbf{R}_{z+180°}$	$\mathbf{R}_{z-90°}$
$(0)_4$	1	1	1	1
$(1)_4$	1	i	−1	$-i$
$(2)_4$	1	−1	1	−1
$(3)_4$	1	$-i$	−1	i

$O\downarrow C_4$ subduction

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

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



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

$\chi^{\mu}_{g}(O)$	$\mathbf{g}=\mathbf{1}$	$\mathbf{r}_{1\ldots4}$	$180°$ ρ_{xyz}	$90°$ $\mathbf{R}_{xyz}$	$180°$ $\mathbf{i}_{1\ldots6}$
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

$O\downarrow D_4$ subduction

D_4: $\mathbf{1}, \rho_{z180°}, \mathbf{R}_{z\pm90°}, \rho_{z180°}, \mathbf{i}_{3,4}$

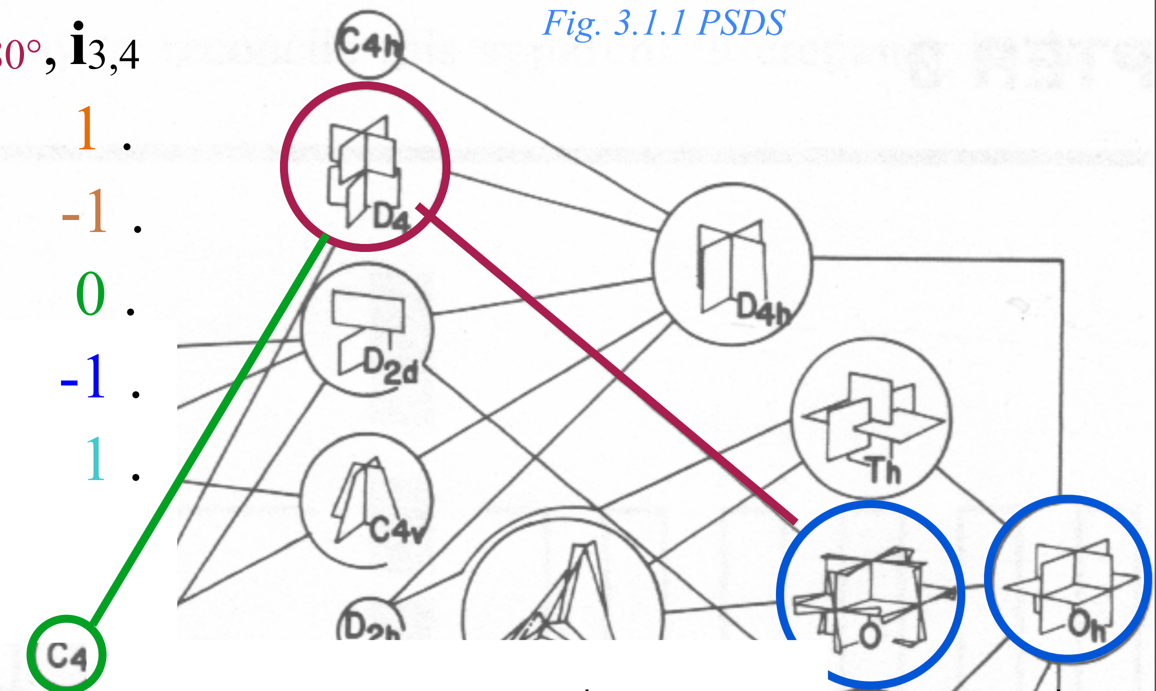
$A_1(O)\downarrow D_4 = 1,\ 1,\ 1,\ 1,\ 1.$

$A_2(O)\downarrow D_4 = 1,\ 1,\ -1,\ 1,\ -1.$

$E(O)\downarrow D_4 = 2,\ 2,\ 0,\ 2,\ 0.$

$T_2(O)\downarrow D_4 = 3,\ -1,\ 1,\ -1,\ -1.$

$T_2(O)\downarrow D_4 = 3,\ -1,\ -1,\ -1,\ 1.$



$\chi^{\mu}_{g}(D_4)$	$\mathbf{g}=\mathbf{1}$	$\rho_{z180°}$	$\mathbf{R}_{z\pm90°}$	$\rho_{x,y180°}$	$\mathbf{i}_{3,4}$
A_1	1	1	1	1	1
B_1	1	1	−1	1	−1
A_2	1	1	1	−1	−1
B_2	1	1	−1	−1	1
E	2	−2	0	0	0

$D_4\downarrow C_4$ subduction

$\mathbf{1}, \mathbf{R}_{z+90°}, \rho_{z180°}, \mathbf{R}_{z-90°}$

$A_1(D_4)\downarrow C_4 = 1,\ 1,\ 1,\ 1. \quad =(0)_4$

$B_1(D_4)\downarrow C_4 = 1,\ -1,\ 1,\ -1. \quad =(2)_4$

$A_2(D_4)\downarrow C_4 = 1,\ 1,\ 1,\ 1. \quad =(0)_4$

$B_2(D_4)\downarrow C_4 = 1,\ -1,\ 1,\ -1. \quad =(2)_4$

$E(D_4)\downarrow C_4 = 2,\ 0,\ -2,\ 0. \quad =(1)_4\oplus(3)_4$

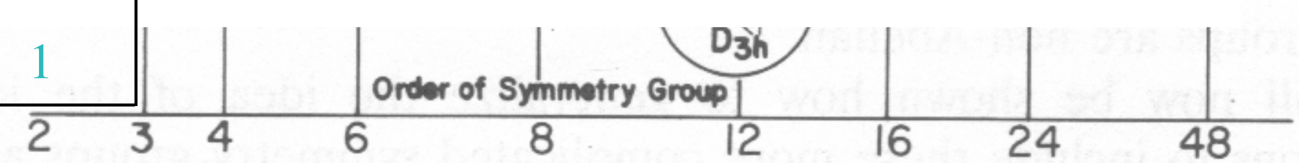
$O\downarrow D_4$	A_1	B_1	A_2	B_2	E
A_1	1	·	·	·	·
A_2	·	1	·	·	·
E	1	1	·	·	·
T_1	·	·	1	·	1
T_2	·	·	·	1	1

$\chi^{\mu}_{g}(C_4)$	$\mathbf{g}=\mathbf{1}$	$\mathbf{R}_{z+90°}$	$\mathbf{R}_{z+180°}$	$\mathbf{R}_{z-90°}$
$(0)_4$	1	1	1	1
$(1)_4$	1	i	−1	$-i$
$(2)_4$	1	−1	1	−1
$(3)_4$	1	$-i$	−1	i

$O\downarrow C_4$ subduction

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

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



Octahedral O⊃D₄⊃C₄ subgroup correlations

$\chi^{\mu}_{g}(O)$	$\mathbf{g=1}$	$\mathbf{r}_{1\ldots4}$	$\boldsymbol{\rho}_{xyz}$ (180°)	$\mathbf{R}_{xyz}$ (90°)	$\mathbf{i}_{1\ldots6}$ (180°)
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↓D₄ subduction

D_4: $\mathbf{1}, \rho_{z180°}, \mathbf{R}_{z\pm90°}, \rho_{z180°}, \mathbf{i}_{3,4}$

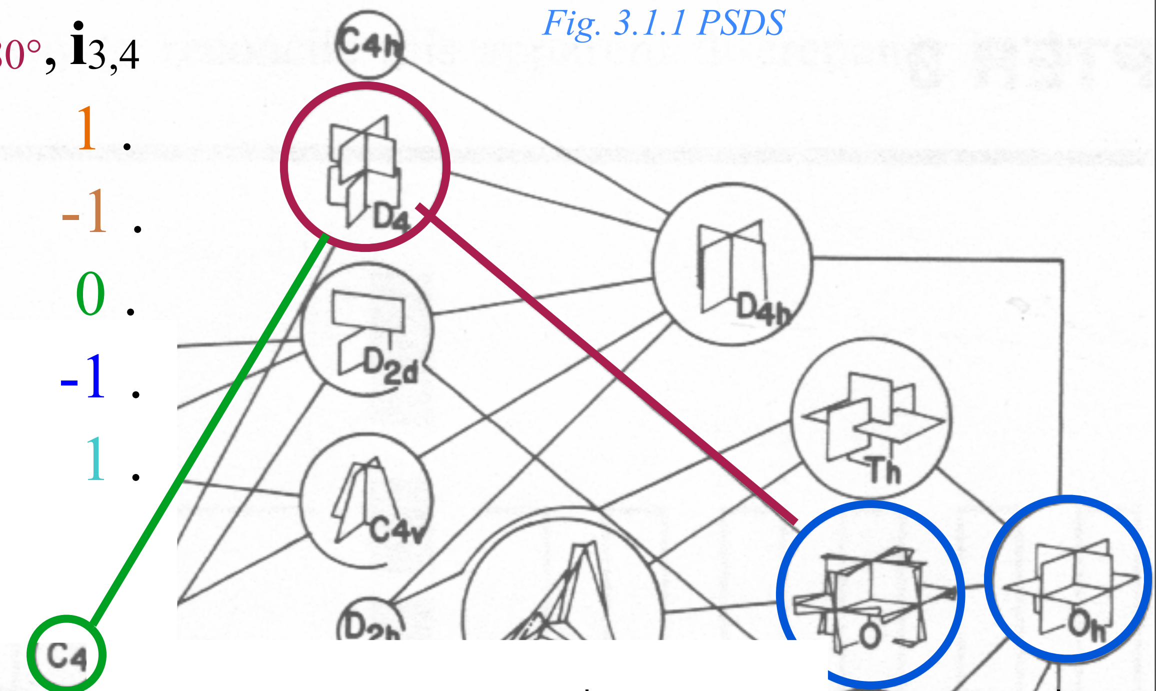
$A_1(O)\downarrow D_4 = 1,\ 1,\ 1,\ 1,\ 1.$

$A_2(O)\downarrow D_4 = 1,\ 1,\ -1,\ 1,\ -1.$

$E(O)\downarrow D_4 = 2,\ 2,\ 0,\ 2,\ 0.$

$T_2(O)\downarrow D_4 = 3,\ -1,\ 1,\ -1,\ -1.$

$T_2(O)\downarrow D_4 = 3,\ -1,\ -1,\ -1,\ 1.$



$\chi^{\mu}_{g}(D_4)$	$\mathbf{g=1}$	$\boldsymbol{\rho}_{z180°}$	$\mathbf{R}_{z\pm90°}$	$\boldsymbol{\rho}_{x,y180°}$	$\mathbf{i}_{3,4}$
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

D₄↓C₄ subduction

$\mathbf{1}, \mathbf{R}_{z+90°}, \rho_{z180°}, \mathbf{R}_{z-90°}$

$A_1(D_4)\downarrow C_4 = 1,\ 1,\ 1,\ 1. \quad =(0)_4$

$B_1(D_4)\downarrow C_4 = 1,\ -1,\ 1,\ -1. \quad =(2)_4$

$A_2(D_4)\downarrow C_4 = 1,\ 1,\ 1,\ 1. \quad =(0)_4$

$B_2(D_4)\downarrow C_4 = 1,\ -1,\ 1,\ -1. \quad =(2)_4$

$E(D_4)\downarrow C_4 = 2,\ 0,\ -2,\ 0. \quad =(1)_4\oplus(3)_4$

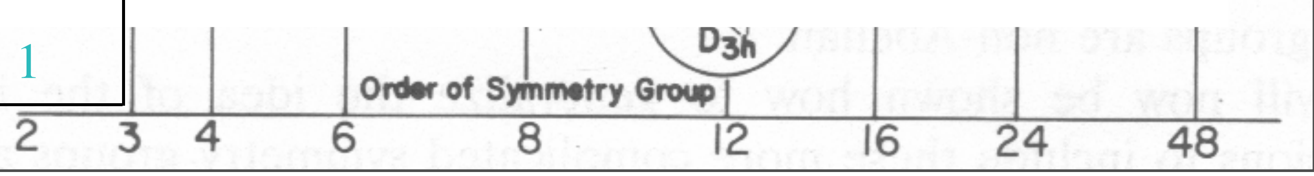
$O\downarrow D_4$	A_1	B_1	A_2	B_2	E
A_1	1	·	·	·	·
A_2	·	1	·	·	·
E	1	1	·	·	·
T_1	·	·	1	·	1
T_2	·	·	·	1	1

$\chi^{\mu}_{g}(C_4)$	$\mathbf{g=1}$	$\mathbf{R}_{z+90°}$	$\mathbf{R}_{z+180°}$	$\mathbf{R}_{z-90°}$
$(0)_4$	1	1	1	1
$(1)_4$	1	i	−1	$-i$
$(2)_4$	1	−1	1	−1
$(3)_4$	1	$-i$	−1	i

O↓C₄ subduction

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

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



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

$\chi^{\mu}_{g}(O)$	$g=1$	$r_{1\ldots4}$	180° ρ_{xyz}	90° R_{xyz}	180° $i_{1\ldots6}$
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

$O\downarrow D_4$ subduction

D_4: $\mathbf{1}, \rho_{z180°}, R_{z\pm90°}, \rho_{z180°}, \mathbf{i}_{3,4}$

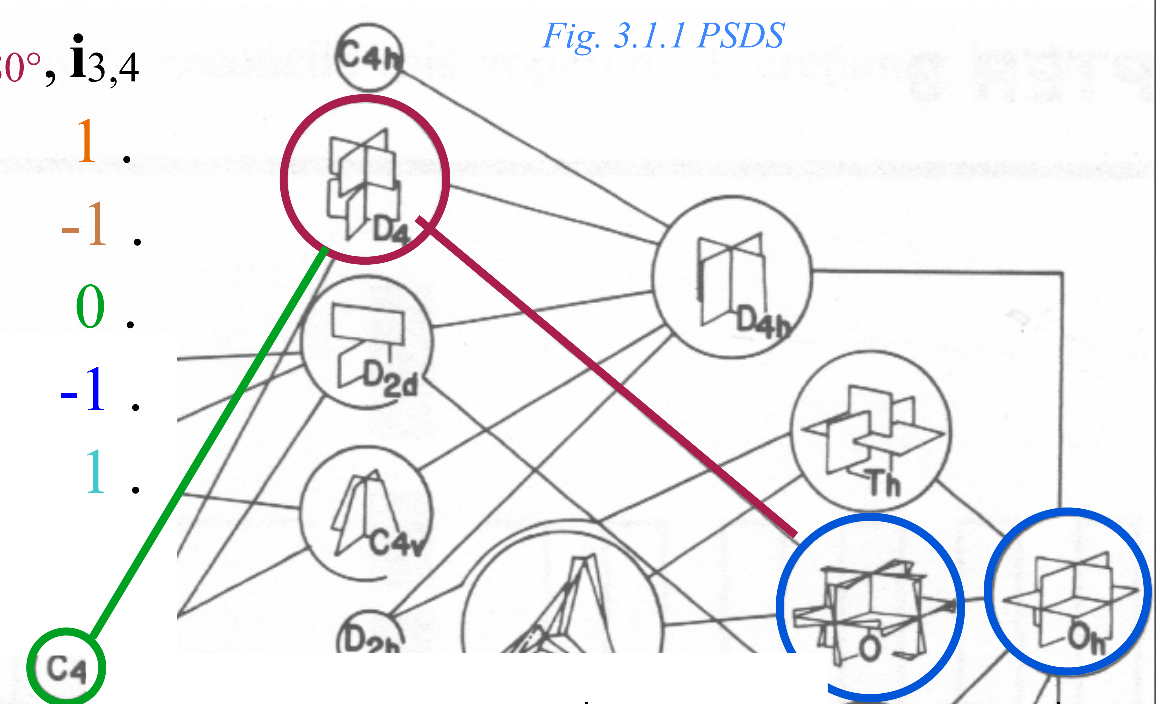
$A_1(O)\downarrow D_4 = 1,\ 1,\ 1,\ 1,\ 1\ .$

$A_2(O)\downarrow D_4 = 1,\ 1,\ -1,\ 1,\ -1\ .$

$E(O)\downarrow D_4 = 2,\ 2,\ 0,\ 2,\ 0\ .$

$T_2(O)\downarrow D_4 = 3,\ -1,\ 1,\ -1,\ -1\ .$

$T_2(O)\downarrow D_4 = 3,\ -1,\ -1,\ -1,\ 1\ .$



$\chi^{\mu}_{g}(D_4)$	$g=1$	$\rho_{z180°}$	$R_{z\pm90°}$	$\rho_{x,y180°}$	$i_{3,4}$
A_1	1	1	1	1	1
B_1	1	1	−1	1	−1
A_2	1	1	1	−1	−1
B_2	1	1	−1	−1	1
E	2	−2	0	0	0

$D_4\downarrow C_4$ subduction

$\mathbf{1},\ R_{z+90°},\ \rho_{z180°},\ R_{z-90°}$

$A_1(D_4)\downarrow C_4 = 1,\ 1,\ 1,\ 1. \quad =(0)_4$

$B_1(D_4)\downarrow C_4 = 1,\ -1,\ 1,\ -1. \quad =(2)_4$

$A_2(D_4)\downarrow C_4 = 1,\ 1,\ 1,\ 1. \quad =(0)_4$

$B_2(D_4)\downarrow C_4 = 1,\ -1,\ 1,\ -1. \quad =(2)_4$

$E(D_4)\downarrow C_4 = 2,\ 0,\ -2,\ 0\ . \quad =(1)_4\oplus(3)_4$

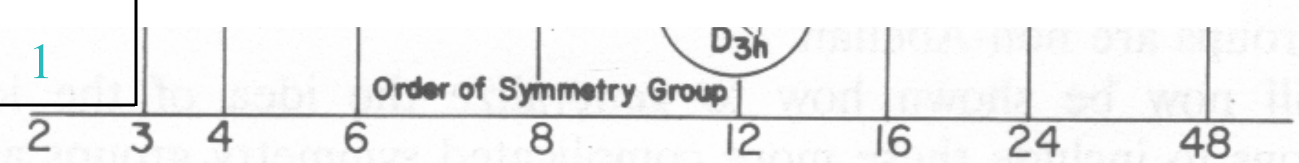
$O\downarrow D_4$	A_1	B_1	A_2	B_2	E
A_1	1	·	·	·	·
A_2	·	1	·	·	·
E	1	1	·	·	·
T_1	·	·	1	·	1
T_2	·	·	·	1	1

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

$O\downarrow C_4$ subduction

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

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



Octahedral O⊃D₄⊃C₄ subgroup correlations

$\chi^{\mu}_{g}(O)$	$\mathbf{g=1}$	$\mathbf{r}_{1\ldots4}$	180° $\boldsymbol{\rho}_{xyz}$	90° $\mathbf{R}_{xyz}$	180° $\mathbf{i}_{1\ldots6}$
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↓D₄ subduction

D_4: $\mathbf{1}, \rho_{z180°}, \mathbf{R}_{z\pm90°}, \rho_{z180°}, \mathbf{i}_{3,4}$

$A_1(O)\downarrow D_4 = 1,\ 1,\ 1,\ 1,\ 1.$

$A_2(O)\downarrow D_4 = 1,\ 1,\ -1,\ 1,\ -1.$

$E(O)\downarrow D_4 = 2,\ 2,\ 0,\ 2,\ 0.$

$T_2(O)\downarrow D_4 = 3,\ -1,\ 1,\ -1,\ -1.$

$T_2(O)\downarrow D_4 = 3,\ -1,\ -1,\ -1,\ 1.$

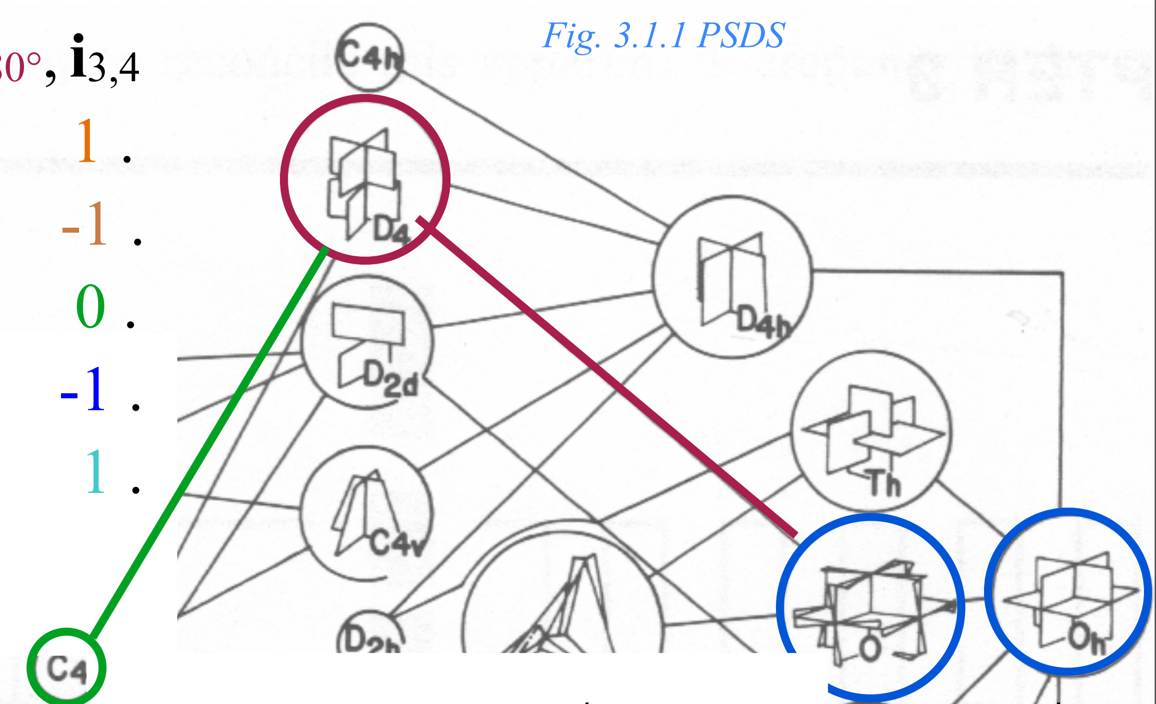


Fig. 3.1.1 PSDS

$\chi^{\mu}_{g}(D_4)$	$\mathbf{g=1}$	$\boldsymbol{\rho}_{z180°}$	$\mathbf{R}_{z\pm90°}$	$\boldsymbol{\rho}_{x,y180°}$	$\mathbf{i}_{3,4}$
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

D₄↓C₄ subduction

$\mathbf{1}, \mathbf{R}_{z+90°}, \rho_{z180°}, \mathbf{R}_{z-90°}$

$A_1(D_4)\downarrow C_4 = 1,\ 1,\ 1,\ 1. \quad =(0)_4$

$B_1(D_4)\downarrow C_4 = 1,\ -1,\ 1,\ -1. \quad =(2)_4$

$A_2(D_4)\downarrow C_4 = 1,\ 1,\ 1,\ 1. \quad =(0)_4$

$B_2(D_4)\downarrow C_4 = 1,\ -1,\ 1,\ -1. \quad =(2)_4$

$E(D_4)\downarrow C_4 = 2,\ 0,\ -2,\ 0. \quad =(1)_4\oplus(3)_4$

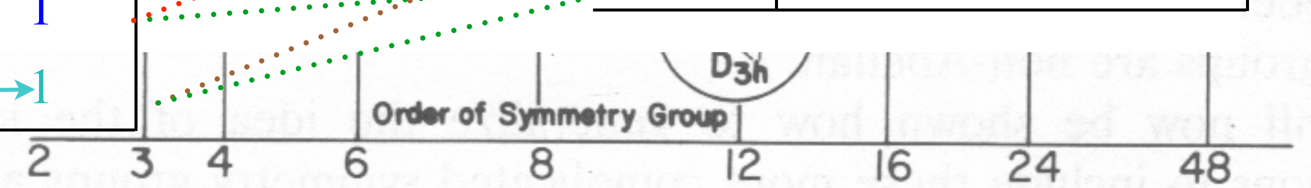
$O\downarrow D_4$	A_1	B_1	A_2	B_2	E
A_1	1	·	·	·	·
A_2	·	1	·	·	·
E	1	1	·	·	·
T_1	·	·	1	·	1
T_2	·	·	·	1	1

$\chi^{\mu}_{g}(C_4)$	$\mathbf{g=1}$	$\mathbf{R}_{z+90°}$	$\mathbf{R}_{z+180°}$	$\mathbf{R}_{z-90°}$
$(0)_4$	1	1	1	1
$(1)_4$	1	i	−1	$-i$
$(2)_4$	1	−1	1	−1
$(3)_4$	1	$-i$	−1	i

O↓C₄ subduction

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

$D_4\downarrow C_4$	0_4	1_4	2_4	$3_4=\bar{1}_4$
A_1	1	·	·	·
B_1	·	·	1	·
A_2	1	·	·	·
B_2	·	·	→1	·
E	·	→1	·	→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*

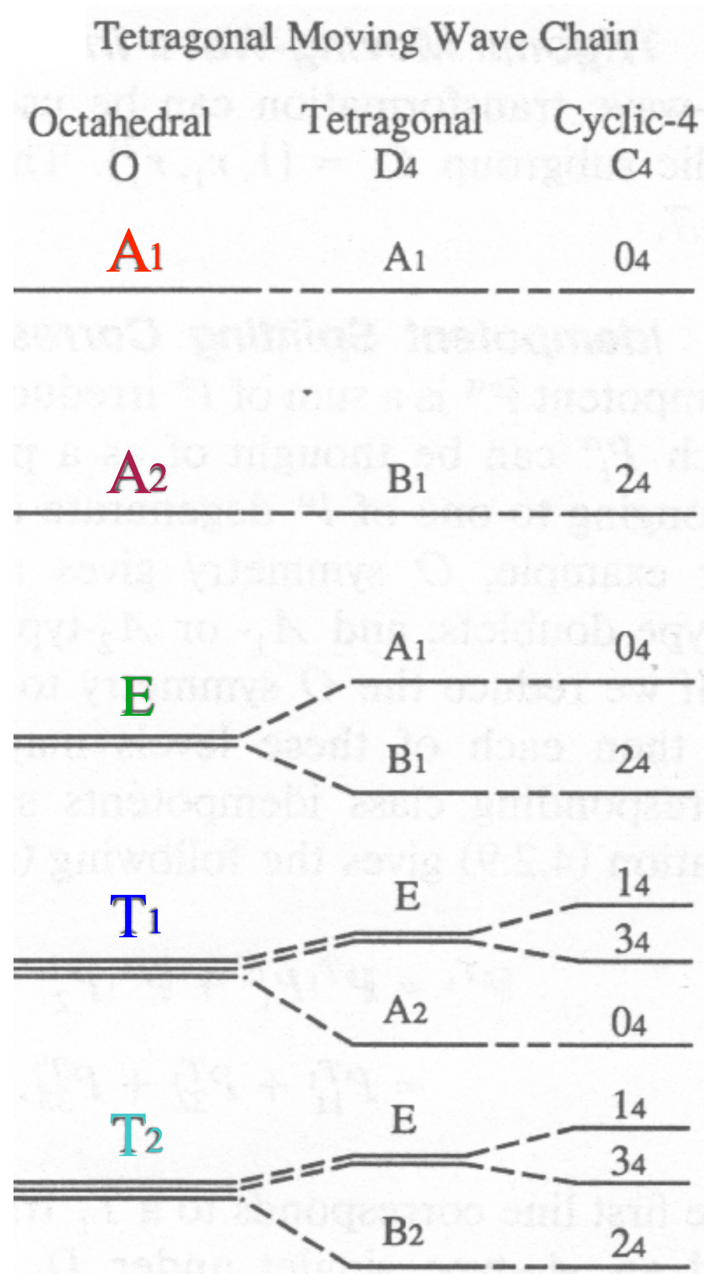
- $O \supset D_4 \supset C_4$ *subgroup chain splitting*
- $O \supset D_4 \supset D_2$ *subgroup chain splitting (nOrmal* D_2 *vs. unOrmal* D_2*)*
- $O_h \supset O \supset D_4 \supset C_{4v}$ *and* $O_h \supset O \supset D_4 \supset C_{4v} \supset C_{2v}$ *subgroup splitting*

Simplest $O_h \supset O \supset D_4 \supset C_4$ *spectral analysis problems*

- *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 expression*

$O \supset D_4 \supset C_4$ 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

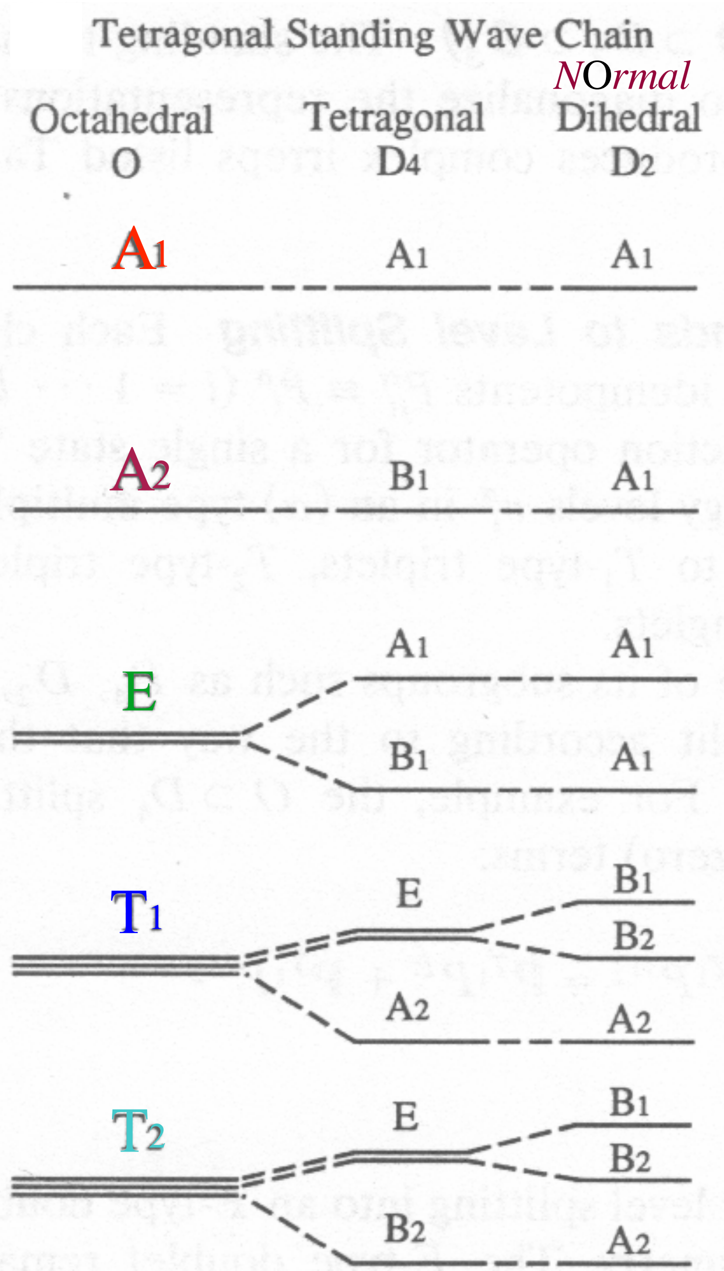
O	$\mathbf{1}$	$\mathbf{r}$ ($\mathbf{r},\tilde{\mathbf{r}}_i$)	$\mathbf{R}^2$ (ρ_{xyz})	$\mathbf{R}^3$ ($\mathbf{R},\tilde{\mathbf{R}}_{xyz}$)	$\mathbf{i}_k$
A_1	1	1	1	1	1
A_2	1	1	1	-1	-1
E	2	-1	2	0	0
T_1	3	0	-1	1	-1
T_2	3	0	-1	-1	1

$-1_4 =$

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

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

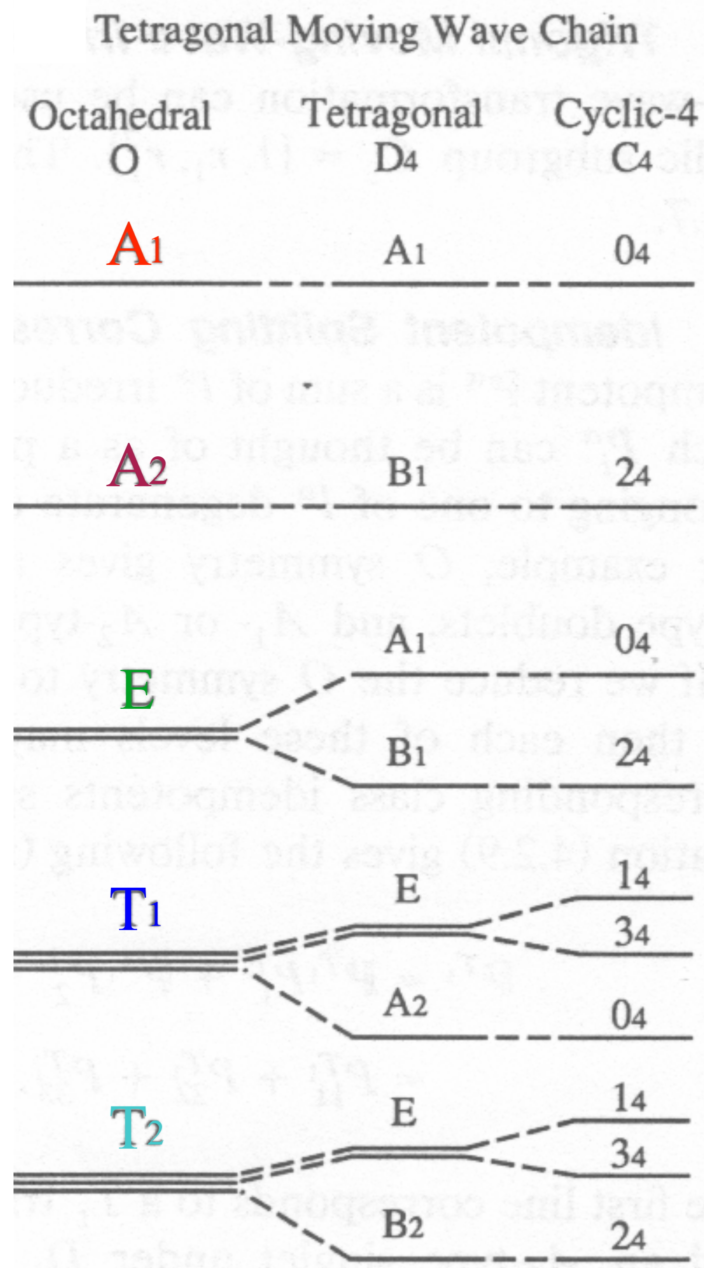
$O \supset D_4 \supset D_2$ level splitting



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

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



D_2^{Nm}	$\{\mathbf{1},$	$\mathbf{R}_z^2,$	$\mathbf{R}_x^2,$	$\mathbf{R}_y^2\}$
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	$\mathbf{1}$	$\mathbf{r}$	$\mathbf{R}^2$	$\mathbf{R}^3$	$\mathbf{i}_k$
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

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

$-1_4 =$

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

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

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

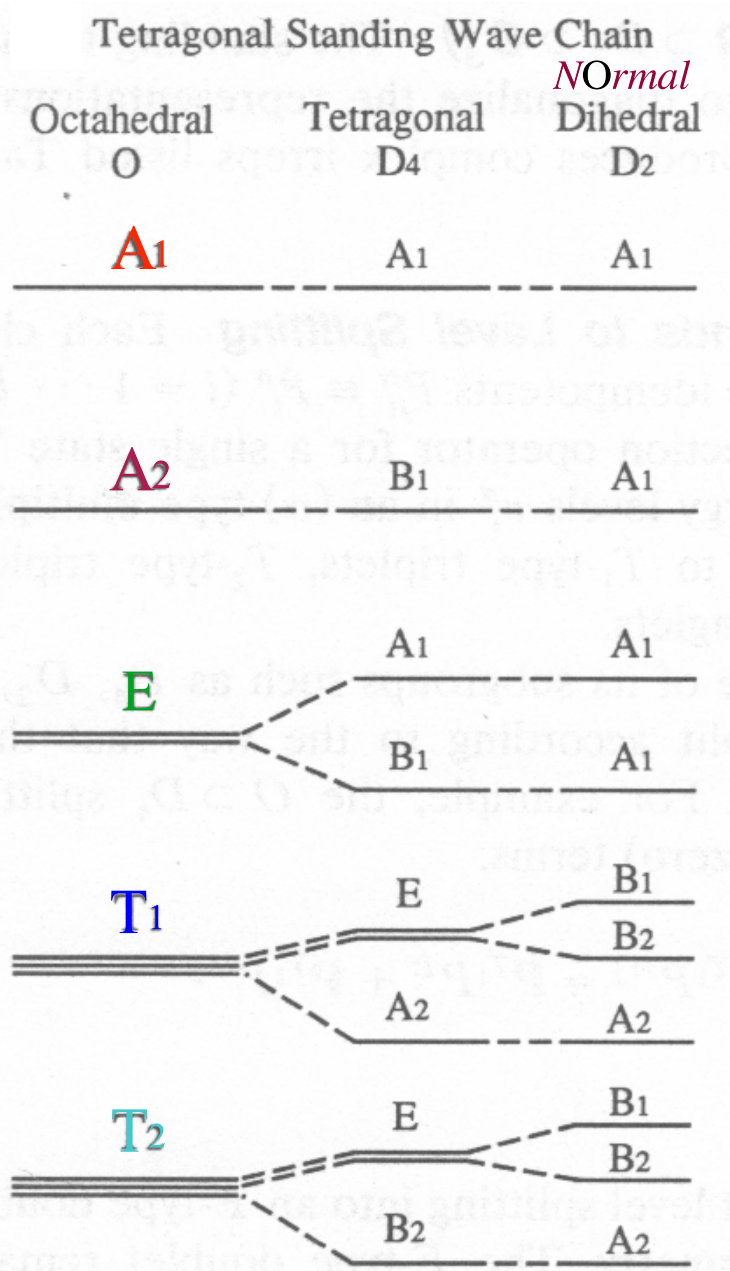
Comparison of $O \supset D_4 \supset C_4$ *and* $O \supset D_4 \supset D_2$ *correlations and level/projector splitting*

- $O \supset D_4 \supset C_4$ *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*

Simplest $O_h \supset O \supset D_4 \supset C_4$ *spectral analysis problems*

- *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 expression*

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



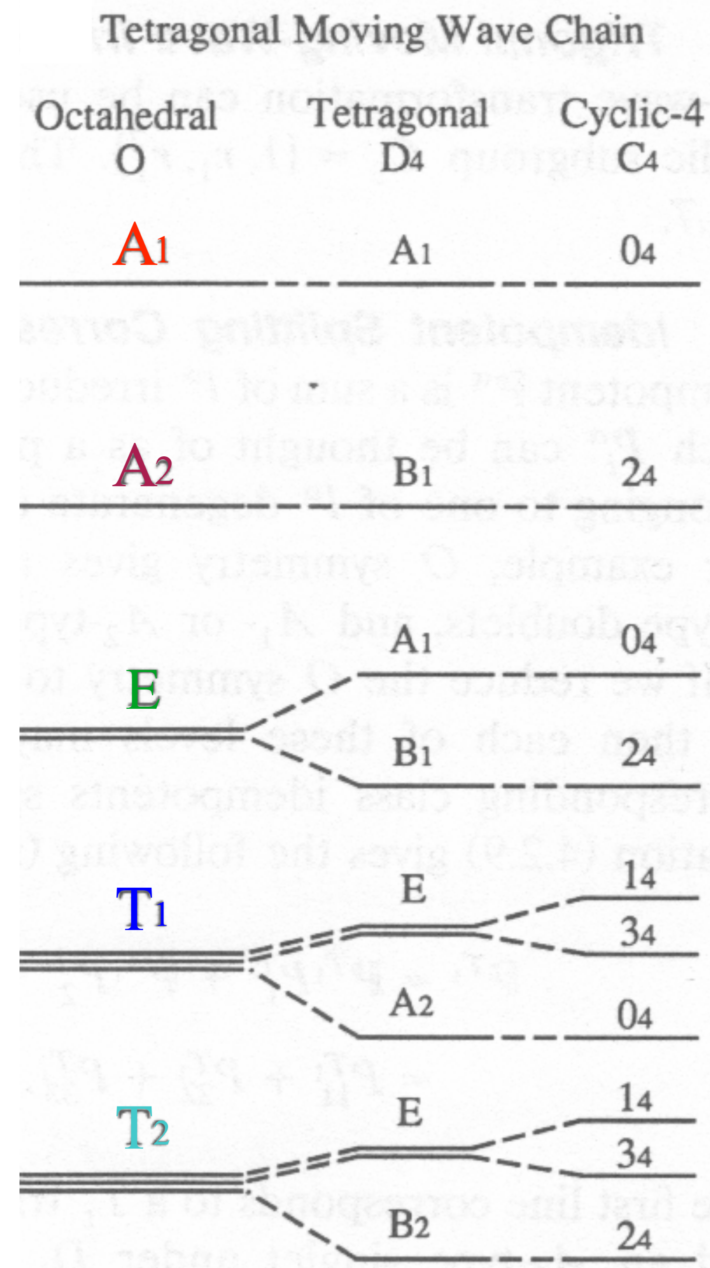
D_4	$\mathbf{1}$	ρ_z	$\mathbf{R}_z$	$\rho_{x,y}$	$\mathbf{i}_{3,4}$
A_1	1	1	1	1	1
B_1	1	1	-1	1	-1
A_2	1	1	1	-1	-1
B_2	1	1	-1	-1	1
E	2	-2	0	0	0

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

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

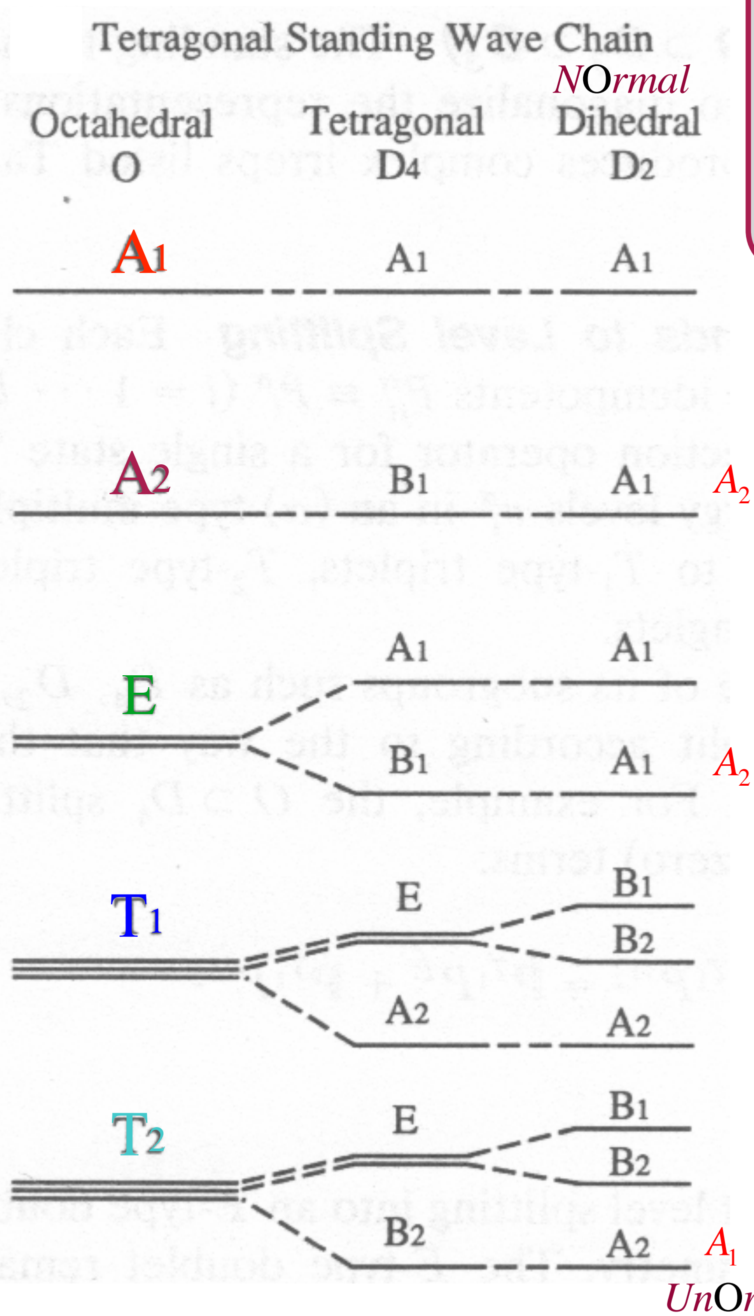
$O \downarrow D_2$	A_1	B_1	A_2	B_2
A_1	1	·	·	·
A_2	1	·	·	·
E	2	·	·	·
T_1	·	1	1	1
T_2	·	1	1	1

$O \downarrow D_4$	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

$-1_4 =$

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

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



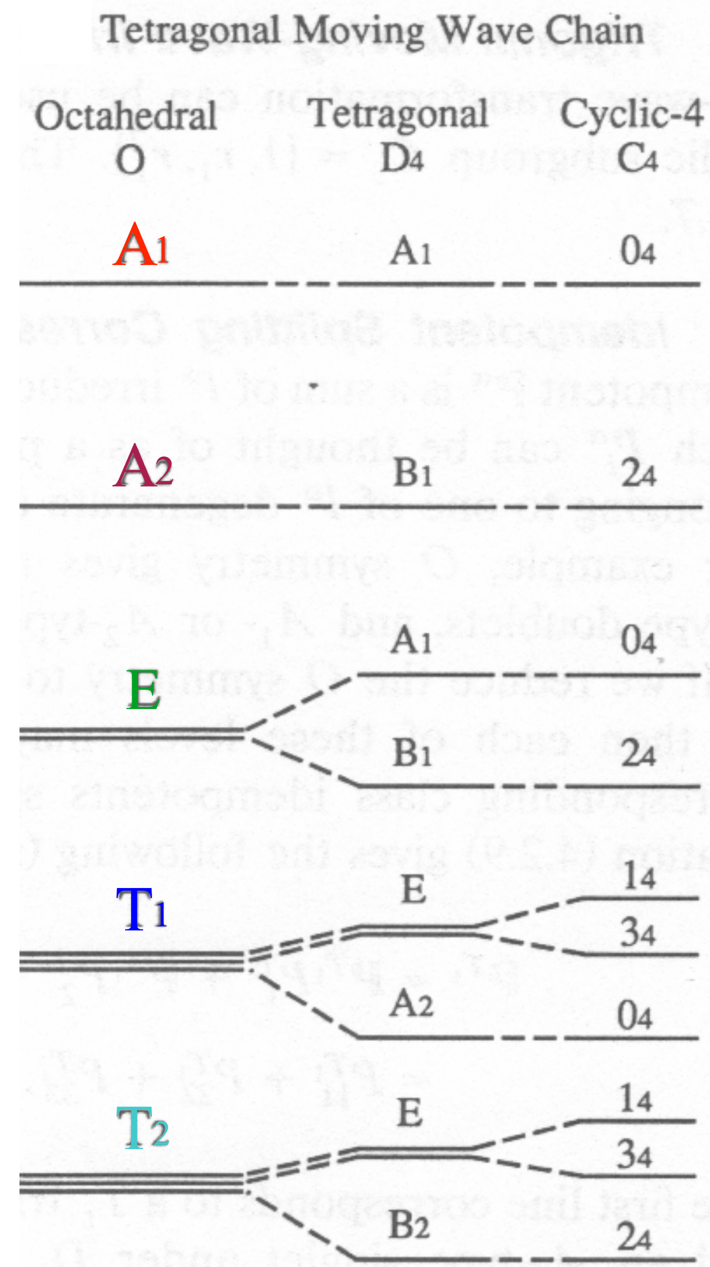
D_4	$\mathbf{1}$	ρ_z	$\mathbf{R}_z$	$\rho_{x,y}$	$\mathbf{i}_{3,4}$
A_1	1	1	1	1	1
B_1	1	1	-1	1	-1
A_2	1	1	1	-1	-1
B_2	1	1	-1	-1	1
E	2	-2	0	0	0

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

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

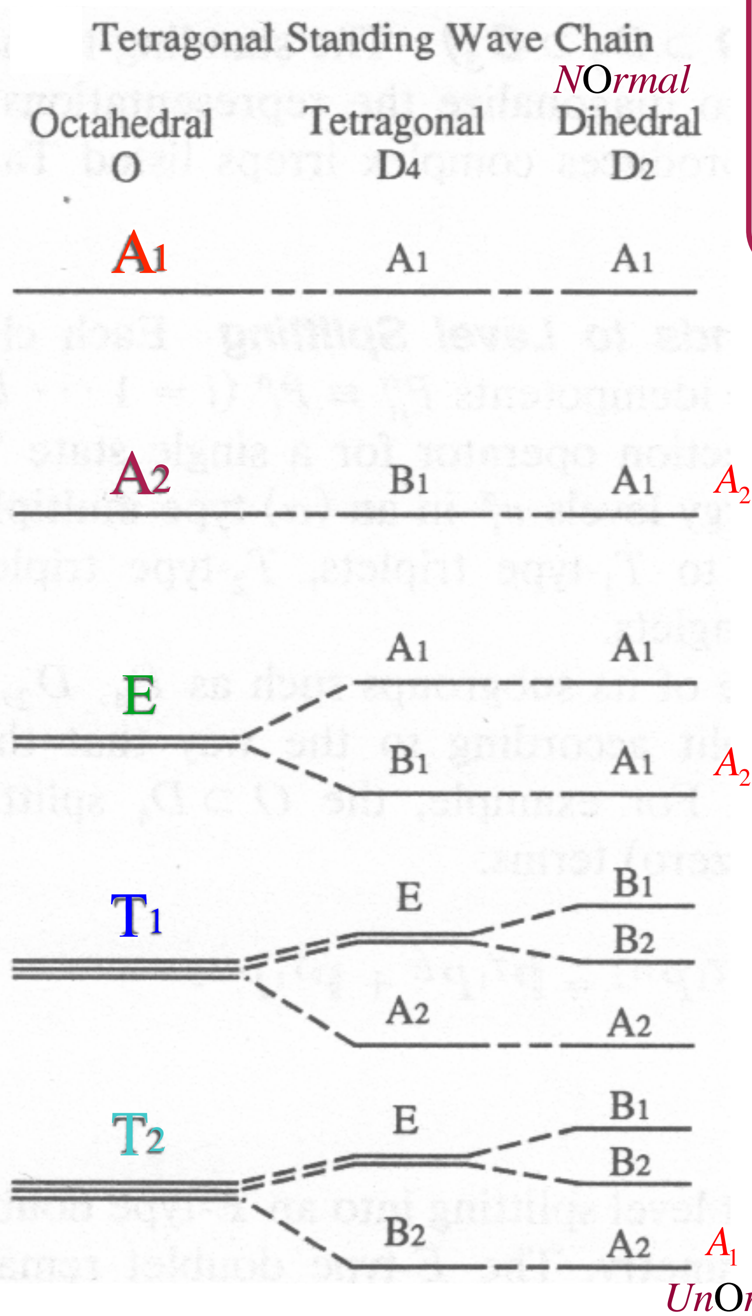
$O \downarrow D_2$	A_1	B_1	A_2	B_2
A_1	1	·	·	·
A_2	1	·	·	·
E	2	·	·	·
T_1	·	1	1	1
T_2	·	1	1	1

$O \downarrow D_4$	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

$-1_4 =$

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

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



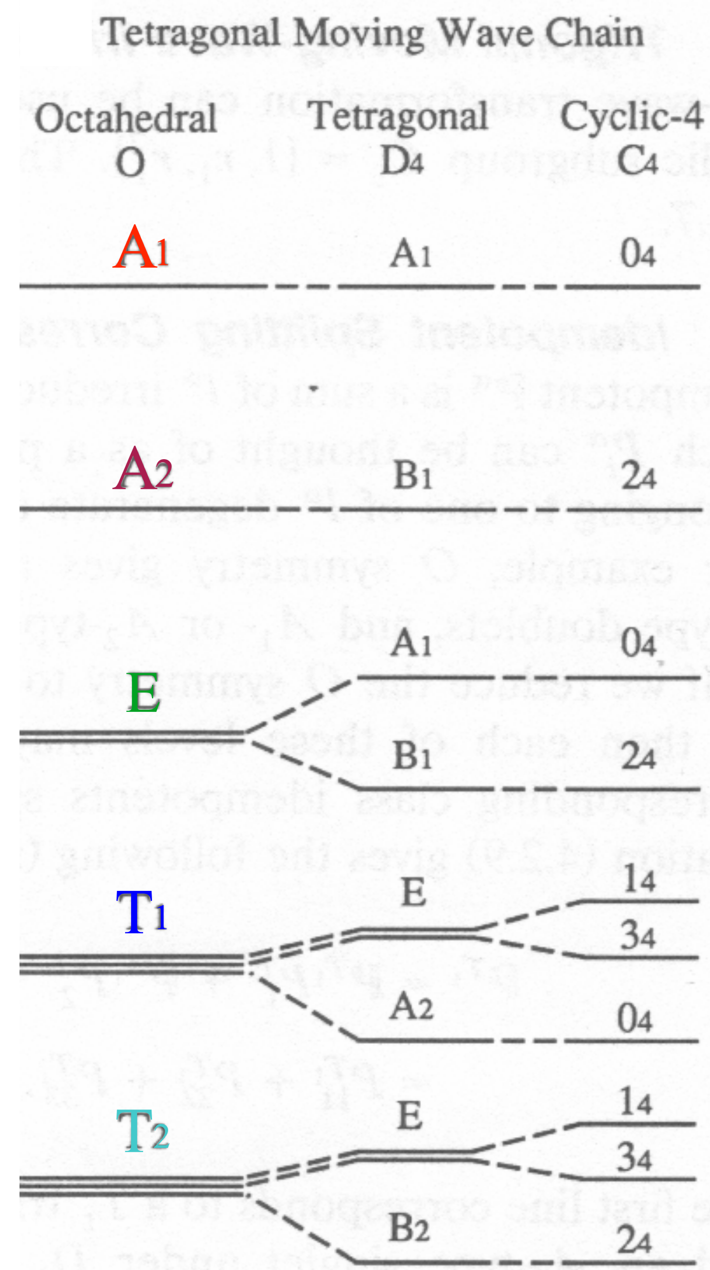
D_4	**1**	ρ_z	$\mathbf{R}_z$	$\rho_{x,y}$	$\mathbf{i}_{3,4}$
A_1	1	1	1	1	1
B_1	1	1	-1	1	-1
A_2	1	1	1	-1	-1
B_2	1	1	-1	-1	1
E	2	-2	0	0	0

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

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

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 $D_2 = \{1, \mathbf{R}_3^2, \mathbf{R}_1^2, \mathbf{R}_2^2\}$ *UnOrmal* $D_2 = \{1, \mathbf{R}_3^2, \mathbf{i}_3, \mathbf{i}_4\}$

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

$-1_4 =$

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

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*

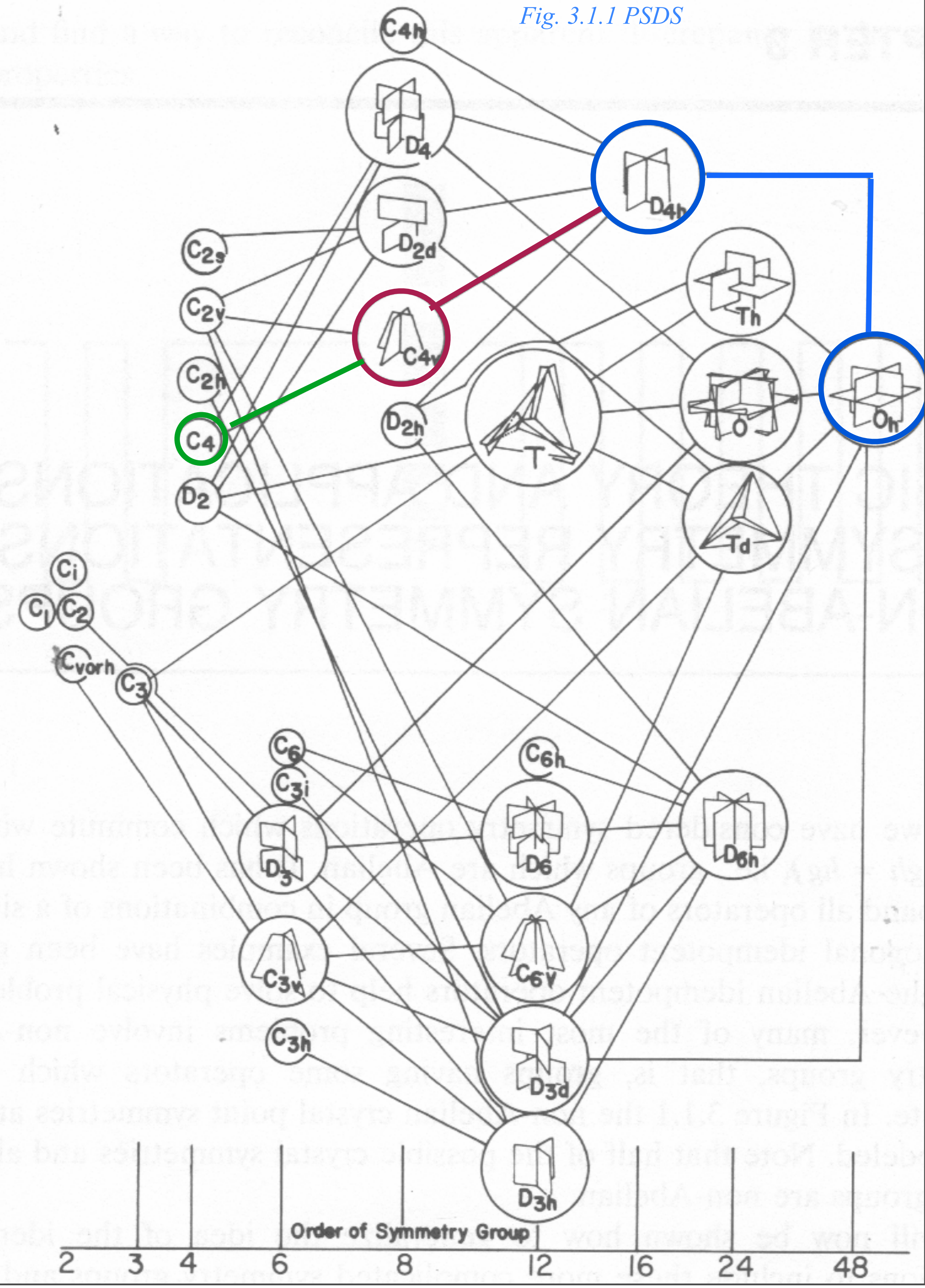
Simplest $O_h \supset O \supset D_4 \supset C_4$ *spectral analysis problems*

- *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 expression*

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

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

Fig. 3.1.1 PSDS



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

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

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

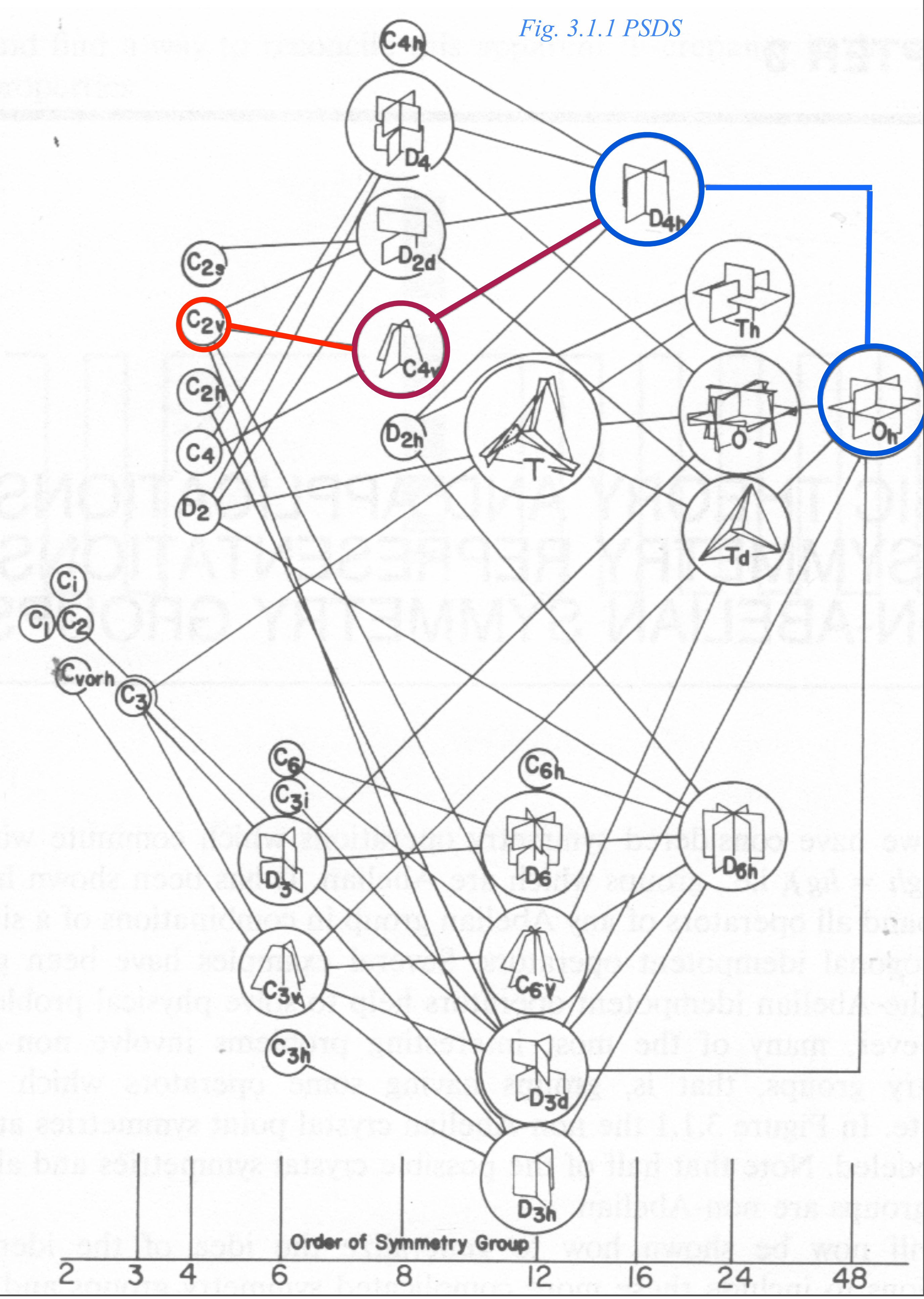


Fig. 3.1.1 PSDS

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*

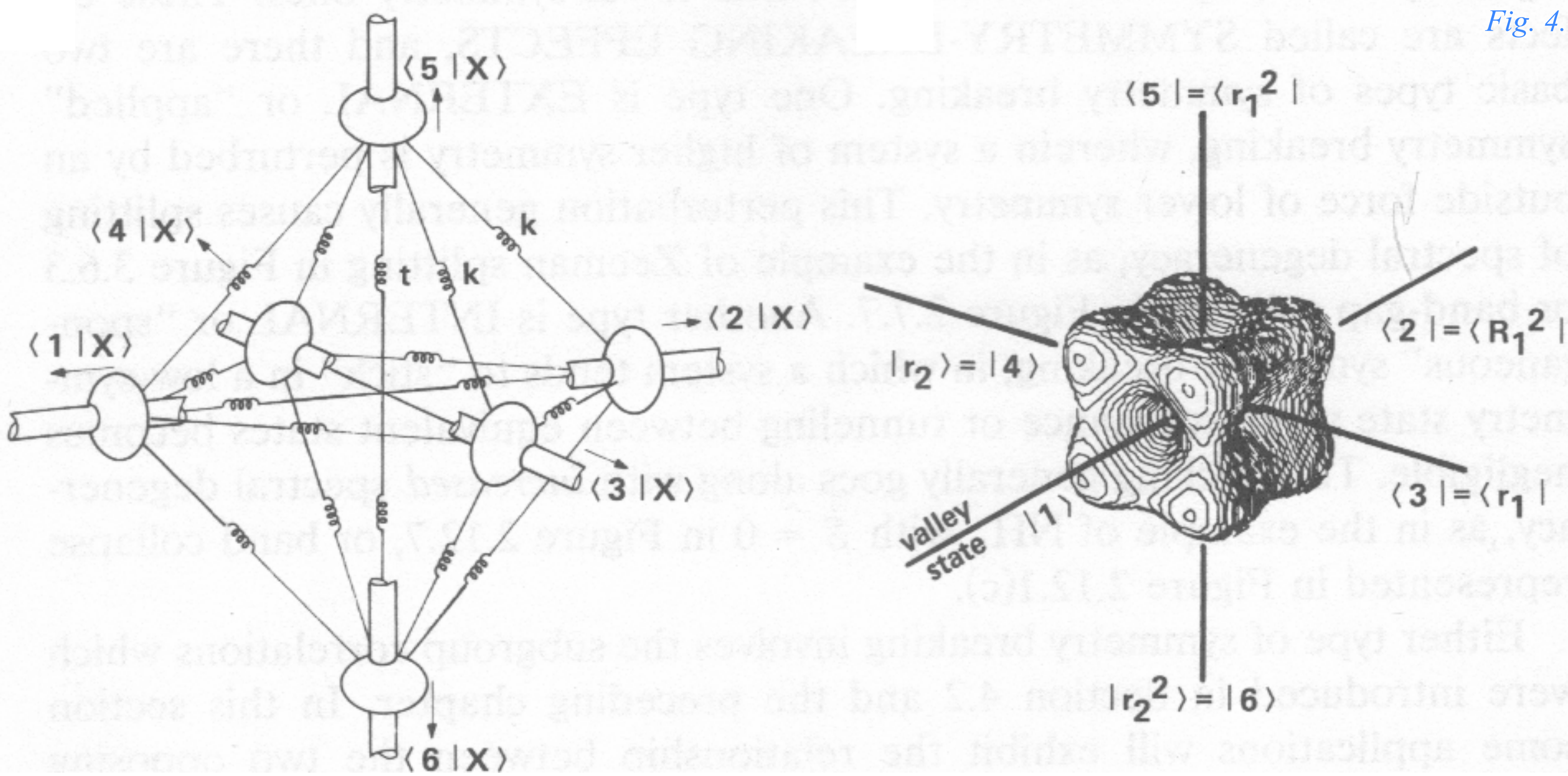
- $O \supset D_4 \supset C_4$ *subgroup chain splitting*
- $O \supset D_4 \supset D_2$ *subgroup chain splitting (nOrmal* D_2 *vs. unOrmal* D_2*)*
- $O_h \supset O \supset D_4 \supset C_{4v}$ *and* $O_h \supset O \supset D_4 \supset C_{4v} \supset C_{2v}$ *subgroup splitting*

Simplest $O_h \supset O \supset D_4 \supset C_4$ *spectral analysis problems*

- *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 expression*

Simplest $O_h \supset O \supset D_4 \supset C_4$ *spectral analysis problems*

Fig. 4.3.1 PSDS



Solve XY_6 *radial vibration* $\mathbf{K}=\mathbf{a}$*-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* $\mathbf{H}$

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

Simplest $O_h \supset O \supset D_4 \supset C_4$ *spectral analysis problems*

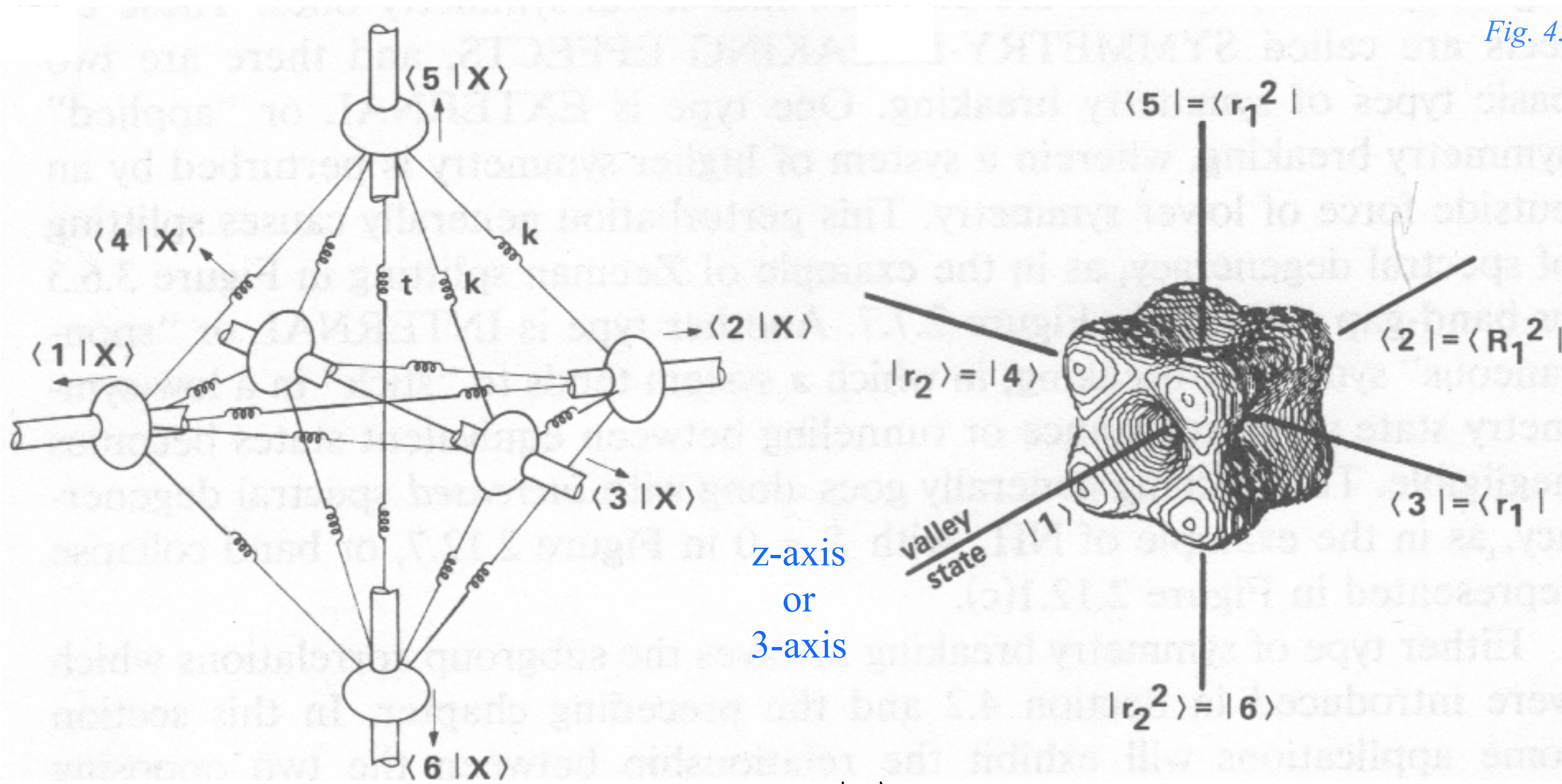


Fig. 4.3.1 PSDS

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)

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

Simplest $O_h \supset O \supset D_4 \supset C_4$ *spectral analysis problems*

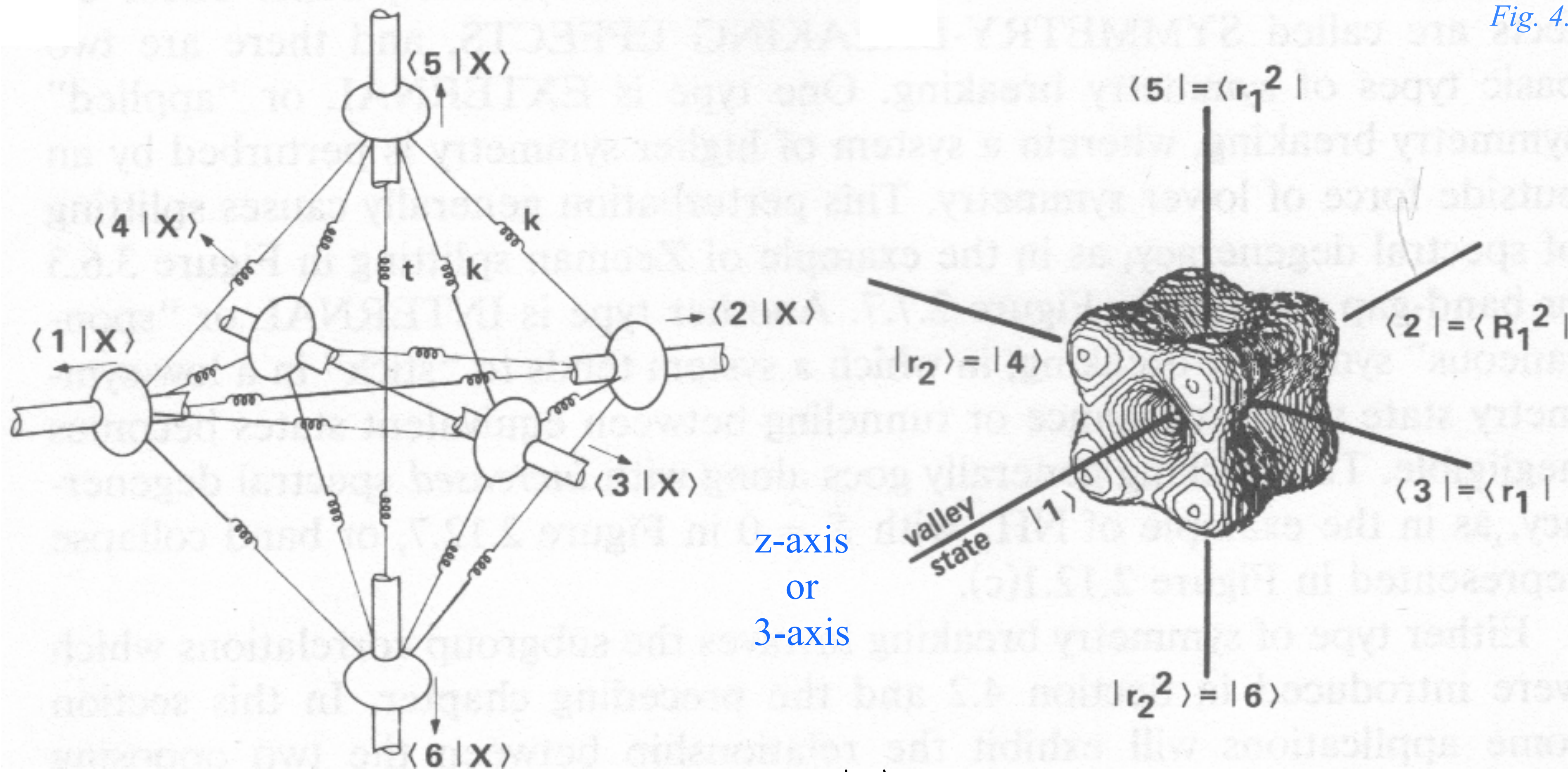


Fig. 4.3.1 PSDS

Assuming *C₄-local symmetry conditions* for $|\mathbf{1}\rangle$ state

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

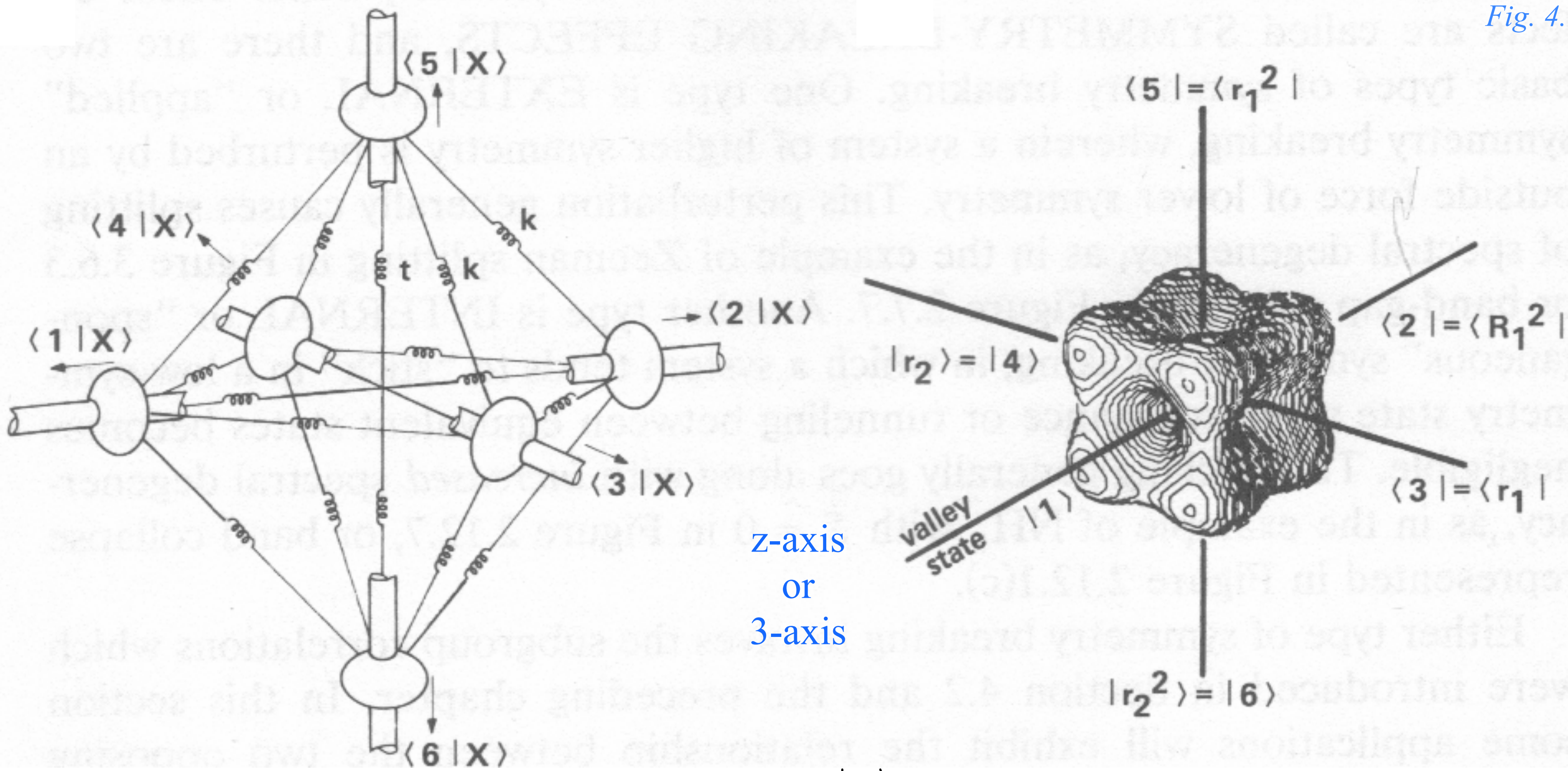
Using *C₄-local symmetry projector* equations $P^A \equiv P^{0_4} = (\mathbf{1} + R_3 + R_3^2 + R_3^3)/4.$

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

O operators (Two notations)

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

Simplest $O_h \supset O \supset D_4 \supset C_4$ *spectral analysis problems*



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

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

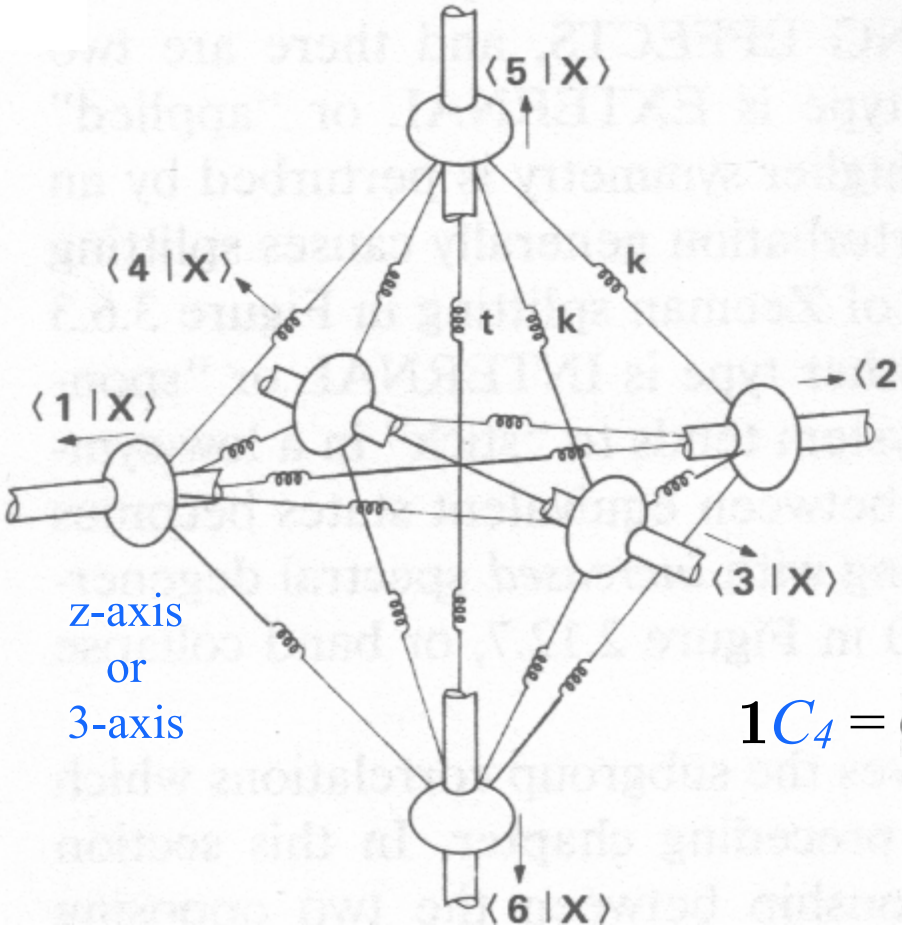
These apply to all six $|\mathbf{g}\rangle = \mathbf{g}|\mathbf{1}\rangle$-base states. $|g\rangle = |gR_3\rangle = |gR_3^2\rangle = |gR_3^3\rangle$

$$|g\rangle = g|1\rangle = gR_3|1\rangle = gR_3^2|1\rangle = gR_3^3|1\rangle$$

O operators (Two notations)

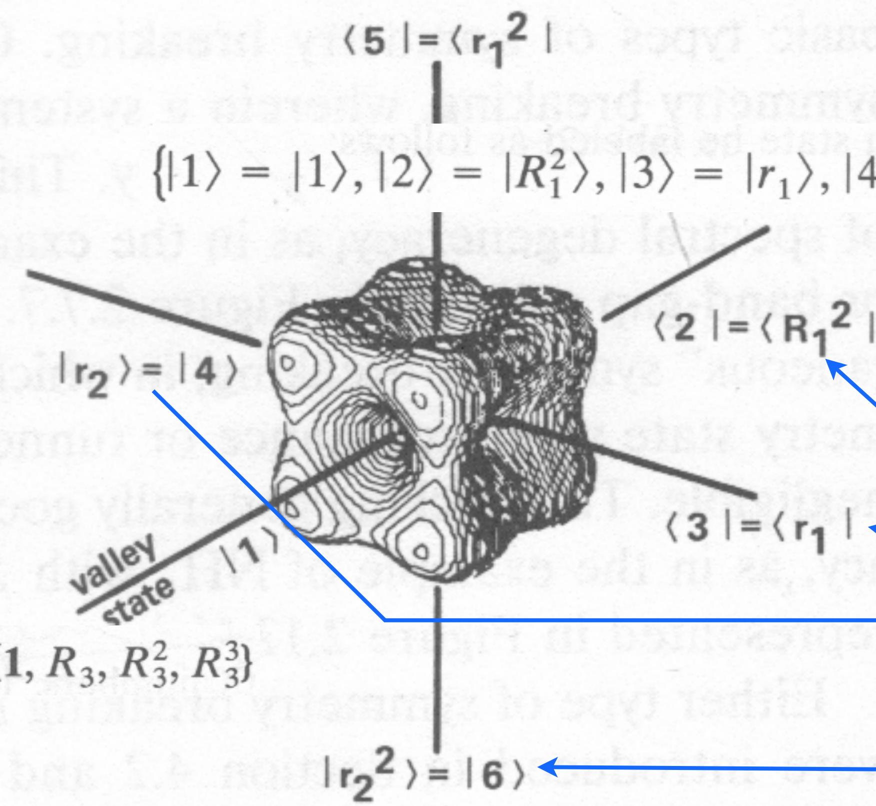
$\mathbf{1}$	$\mathbf{r}_1$	$\mathbf{r}_2$	$\mathbf{r}_3$	$\mathbf{r}_4$	$\mathbf{r}_1^2$	$\mathbf{r}_2^2$	$\mathbf{r}_3^2$	$\mathbf{r}_4^2$	$\mathbf{R}_1^2$	$\mathbf{R}_2^2$	$\mathbf{R}_3^2$	$\mathbf{R}_1$	$\mathbf{R}_2$	$\mathbf{R}_3$	$\mathbf{R}_1^3$	$\mathbf{R}_2^3$	$\mathbf{R}_3^3$	$\mathbf{i}_1$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

Simplest $O_h \supset O \supset D_4 \supset C_4$ spectral analysis problems



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

Fig. 4.3.1 PSDS



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

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

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

$$R_1^2(\mathbf{1}, R_3, R_3^2, R_3^3) = (R_1^2, i_4, R_2^2, i_3),$$

$$r_1(\mathbf{1}, R_3, R_3^2, R_3^3) = (r_1, i_1, r_4, R_2),$$

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

$$r_1^2(\mathbf{1}, R_3, R_3^2, R_3^3) = (r_1^2, R_1^3, r_3^2, i_6),$$

$$r_2^2(\mathbf{1}, R_3, R_3^2, R_3^3) = (r_2^2, R_1, r_4^2, i_5),$$

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* $\quad P^A \equiv P^{0_4} = (\mathbf{1} + R_3 + R_3^2 + R_3^3)/4$

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

These apply to all six $|\mathbf{g}\rangle = \mathbf{g}|\mathbf{1}\rangle$-base states. $\quad |g\rangle = |gR_3\rangle = |gR_3^2\rangle = |gR_3^3\rangle$

$$|g\rangle = g|1\rangle = gR_3|1\rangle = gR_3^2|1\rangle = gR_3^3|1\rangle$$

O operators (Two notations)

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

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

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

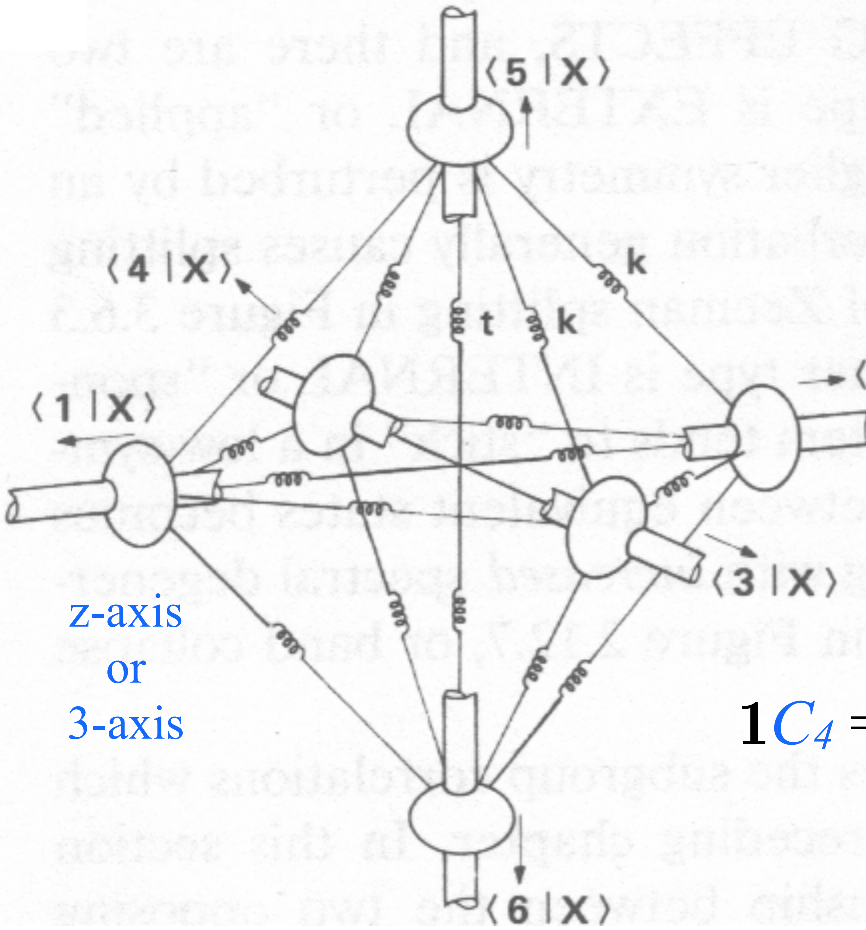
Comparison of $O \supset D_4 \supset C_4$ *and* $O \supset D_4 \supset D_2$ *correlations and level/projector splitting*

- $O \supset D_4 \supset C_4$ *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*

Simplest $O_h \supset O \supset D_4 \supset C_4$ *spectral analysis problems*

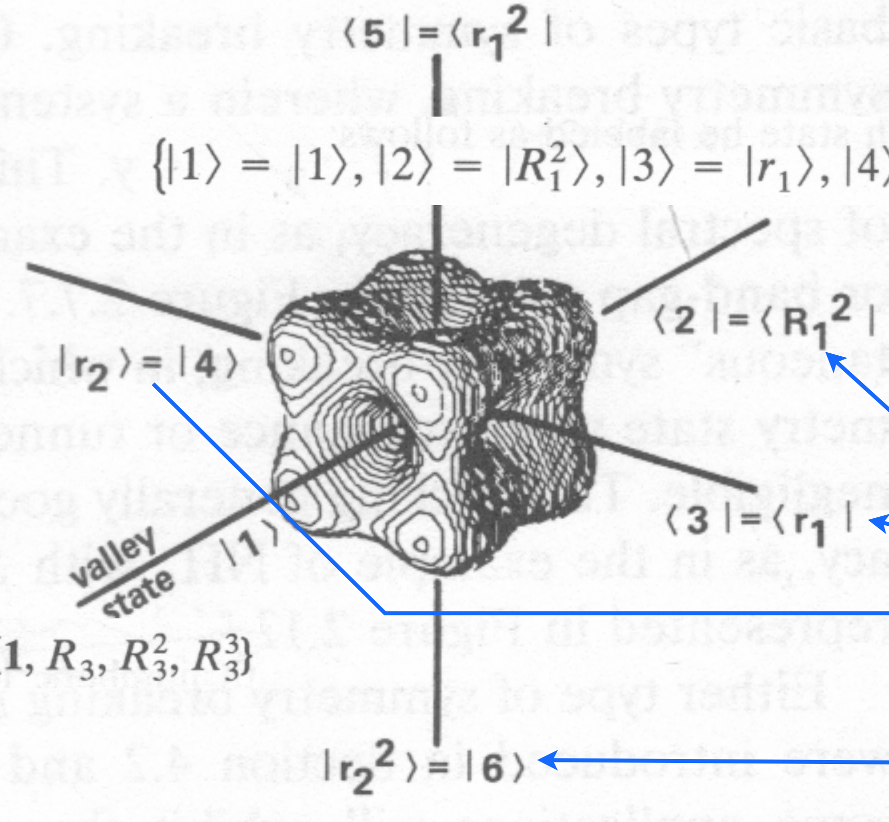
- *Elementary induced representation* $0_4(C_4)\uparrow O$
- *Projection reduction of induced representation* $0_4(C_4)\uparrow O$
- *Introduction to ortho-complete eigenvalue expression*

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



z-axis
or
3-axis

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

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

$R_1^2(\mathbf{1}, R_3, R_3^2, R_3^3) = (R_1^2, i_4, R_2^2, i_3),$

$r_1(\mathbf{1}, R_3, R_3^2, R_3^3) = (r_1, i_1, r_4, R_2),$

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

$r_1^2(\mathbf{1}, R_3, R_3^2, R_3^3) = (r_1^2, R_1^3, r_3^2, i_6),$

$r_2^2(\mathbf{1}, R_3, R_3^2, R_3^3) = (r_2^2, R_1, r_4^2, i_5),$

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

$i_4\vert 1\rangle = i_4\vert 1\rangle,$	$i_4\vert 2\rangle = i_4 R_1^2\vert 1\rangle,$	$i_4\vert 3\rangle = i_4 r_1\vert 1\rangle,$	$i_4\vert 4\rangle = i_4 r_2\vert 1\rangle,$	$i_4\vert 5\rangle = i_4 r_1^2\vert 1\rangle,$	$i_4\vert 6\rangle = i_4 r_2^2\vert 1\rangle,$
$= R_1^2\vert 1\rangle,$	$= R_3^3\vert 1\rangle,$	$= i_5\vert 1\rangle,$	$= i_6\vert 1\rangle,$	$= i_2\vert 1\rangle,$	$= i_1\vert 1\rangle,$
$= \vert 2\rangle,$	$= \vert 1\rangle,$	$= \vert 6\rangle,$	$= \vert 5\rangle,$	$= \vert 4\rangle,$	$= \vert 3\rangle,$

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

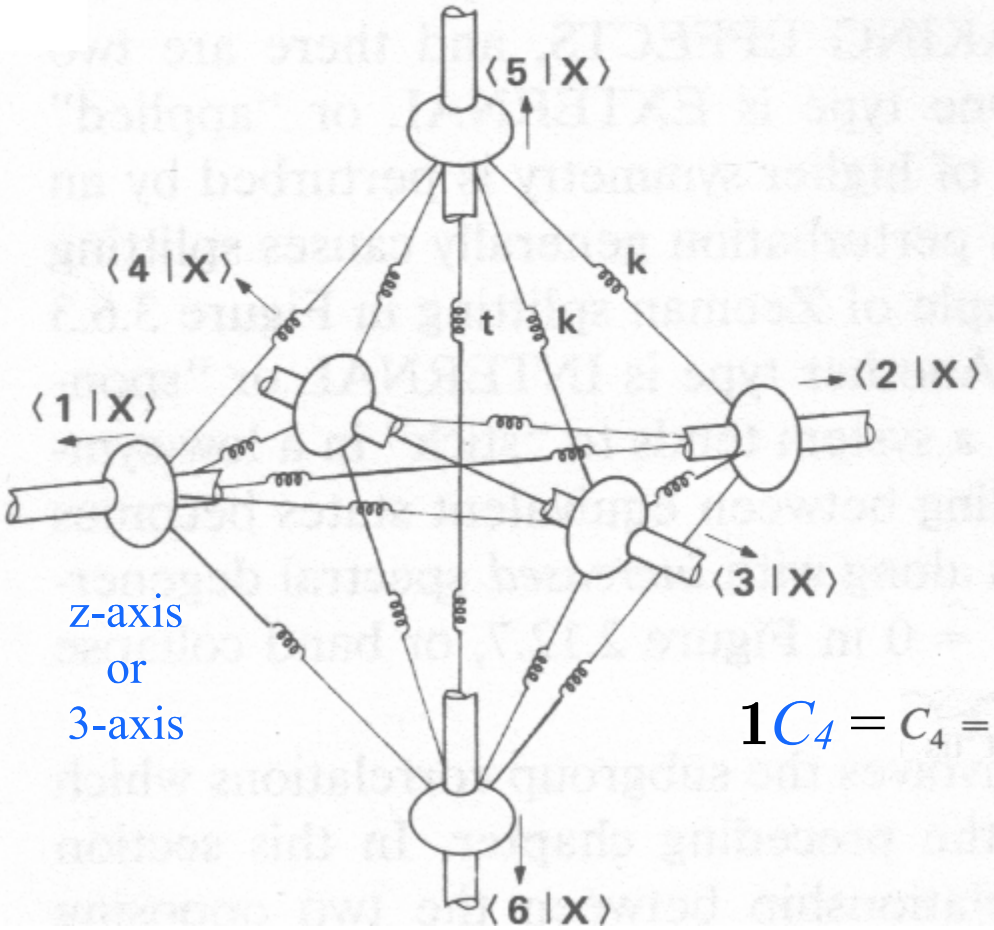
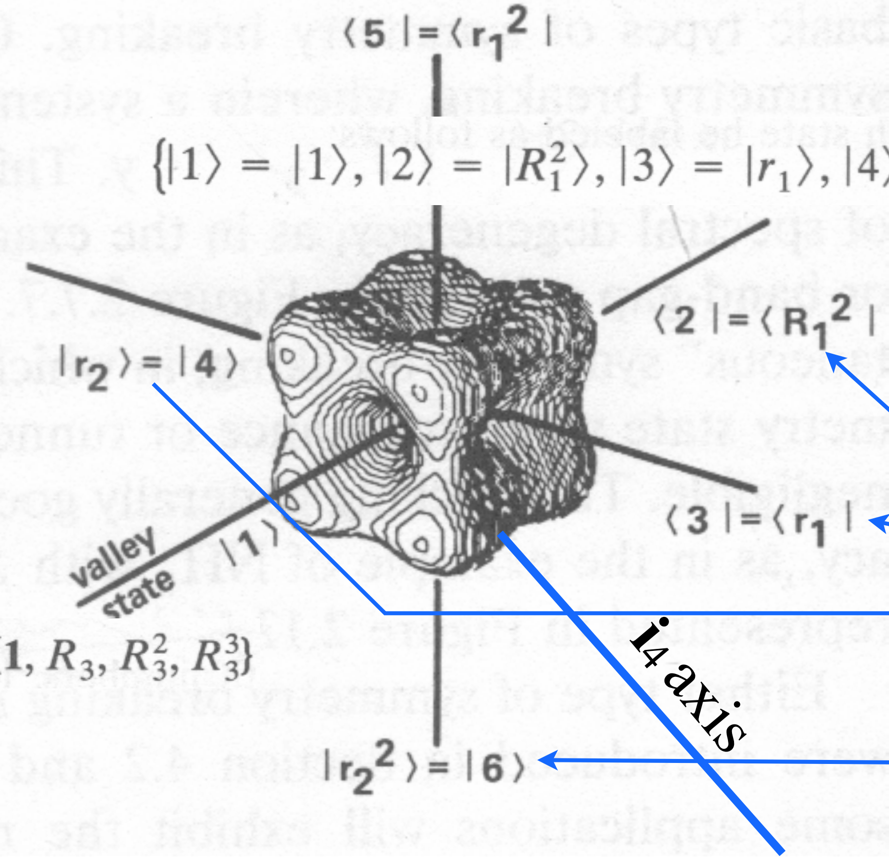


Fig. 4.3.1 PSDS



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

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

$$\mathbf{1}C_4 = C_4 = \{1, R_3, R_3^2, R_3^3\}$$
$$R_1^2(1, R_3, R_3^2, R_3^3) = (R_1^2, i_4, R_2^2, i_3),$$
$$r_1(1, R_3, R_3^2, R_3^3) = (r_1, i_1, r_4, R_2),$$
$$r_2(1, R_3, R_3^2, R_3^3) = (r_2, i_2, r_3, R_2^3),$$
$$r_1^2(1, R_3, R_3^2, R_3^3) = (r_1^2, R_1^3, r_3^2, i_6),$$
$$r_2^2(1, R_3, R_3^2, R_3^3) = (r_2^2, R_1, r_4^2, i_5),$$

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

$$\begin{array}{llllll}
i_4|1\rangle = i_4|1\rangle, & i_4|2\rangle = i_4R_1^2|1\rangle, & i_4|3\rangle = i_4r_1|1\rangle, & i_4|4\rangle = i_4r_2|1\rangle, & i_4|5\rangle = i_4r_1^2|1\rangle, & i_4|6\rangle = i_4r_2^2|\rangle, \\
= R_1^2|1\rangle, & = R_3^3|1\rangle, & = i_5|1\rangle, & = i_6|1\rangle, & = i_2|1\rangle, & = i_1|1\rangle, \\
= |2\rangle, & = |1\rangle, & = |6\rangle, & = |5\rangle, & = |4\rangle, & = |3\rangle,
\end{array}$$

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

$$\mathcal{I}^{0_4\uparrow 0}(i_4) = \begin{pmatrix} \langle 1|i_4|1\rangle & \langle 1|i_4|2\rangle & \cdots & \langle 1|i_4|6\rangle \\ \langle 2|i_4|1\rangle & \langle 2|i_4|2\rangle & & \cdot \\ \cdot & & & \cdot \\ \cdot & & & \cdot \\ \cdot & & & \cdot \\ \langle 6|i_4|1\rangle & \langle 6|i_4|2\rangle & \cdots & \langle 6|i_4|6\rangle \end{pmatrix} = \begin{pmatrix} \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \end{pmatrix}$$

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*

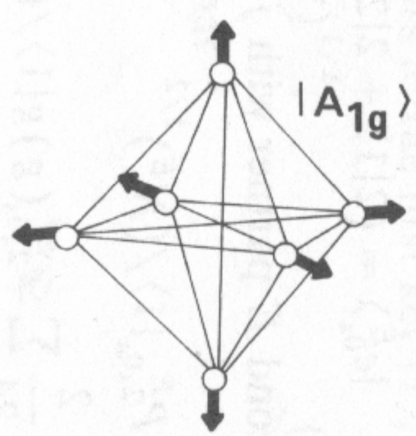
Simplest $O_h \supset O \supset D_4 \supset C_4$ *spectral analysis problems*

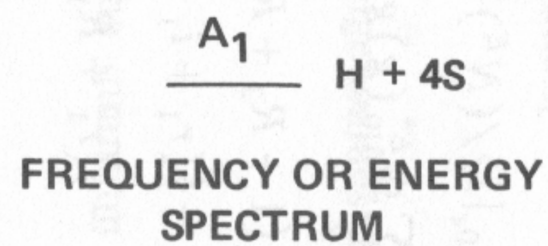
- *Elementary induced representation* $0_4(C_4)\uparrow O$
- *Projection reduction of induced representation* $0_4(C_4)\uparrow O$
- *Introduction to ortho-complete eigenvalue expression*

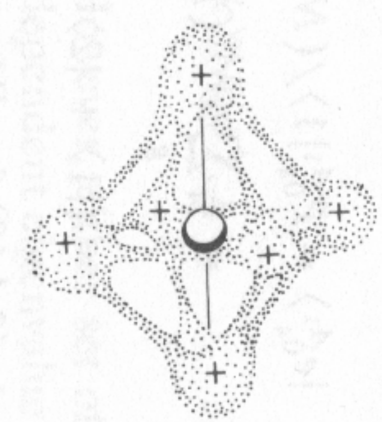
Projection reduction of induced representation $0_4(C_4)\uparrow O$

Scalar A_1 eigenket

$$
\begin{aligned}
|e^{A_1}_{0_4}\rangle &= P^{A_1}_{0_4}|1\rangle/(N^{A_1})^{1/2} \\
&= \tfrac{1}{24}\sum_g \mathscr{D}^{A_1^*}(g)\, g|1\rangle/(N^{A_1})^{1/2} \\
&= (|1\rangle + |2\rangle + |3\rangle + |4\rangle + |5\rangle + |6\rangle)/(6)^{1/2}.
\end{aligned}
$$







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

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

Scalar A_1 eigenket 0_40_4

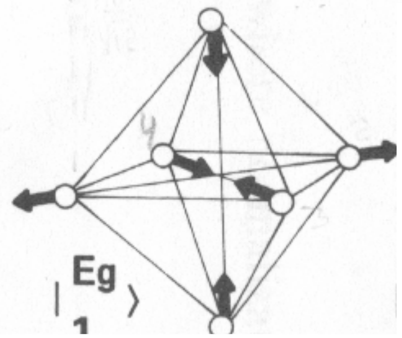
$$|e^{A_1}_{0_4}\rangle = P^{A_1}_{0_4}|1\rangle/(N^{A_1})^{1/2}$$
$$= \frac{1}{24}\sum_g \mathscr{D}^{A_1^*}(g)\,g|1\rangle/(N^{A_1})^{1/2}$$
$$= (|1\rangle + |2\rangle + |3\rangle + |4\rangle + |5\rangle + |6\rangle)/(6)^{1/2}.$$

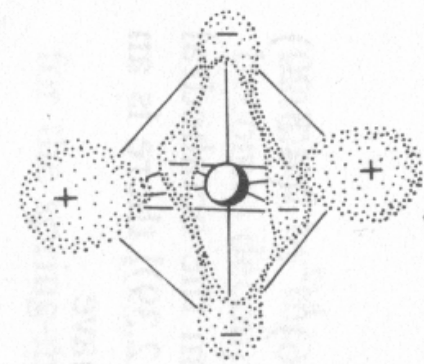
Tensor E-eigenket 0_40_4

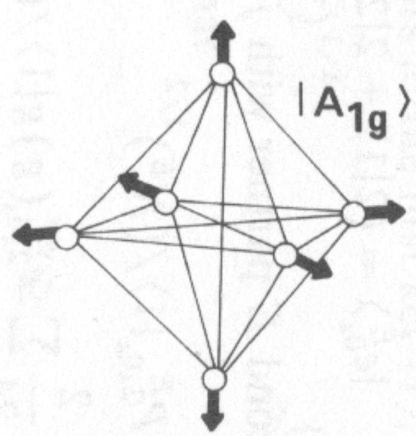
$$|e^{E}_{0_4}\rangle = P^{E}_{0_40_4}|1\rangle/(N^{E})^{1/2}$$
$$= \frac{2}{24}\sum_g \mathscr{D}^{E^*}_{0_40_4}(g)\,g|1\rangle/(N^{E})^{1/2}$$
$$= \frac{2}{24}\Big[(1 + R_3 + R_3^2 + R_3^3) + (R_1^2 + i_4 + R_2^2 + i_3) - \tfrac{1}{2}(r_1 + i_1 + r_4 + R_2) - \tfrac{1}{2}(r_2 + i_2 + r_3 + R_2^3) - \tfrac{1}{2}(r_1^2 + R_1^3 + r_3^2 + i_6) - \tfrac{1}{2}(r_2^2 + R_1 + r_4^2 + i_5)\Big]|1\rangle/(N^E)^{1/2},$$

$$|e^{E}_{0_4}\rangle = (2|1\rangle + 2|2\rangle - |3\rangle - |4\rangle - |5\rangle - |6\rangle)/(2\sqrt{3}).$$

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

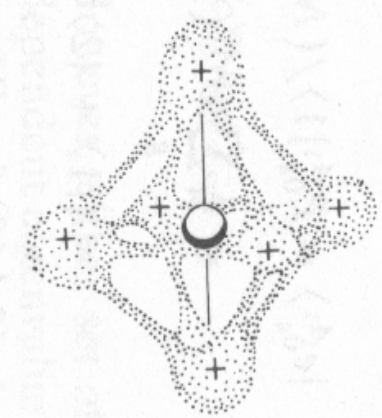






A_1 H + 4S

FREQUENCY OR ENERGY SPECTRUM



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

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

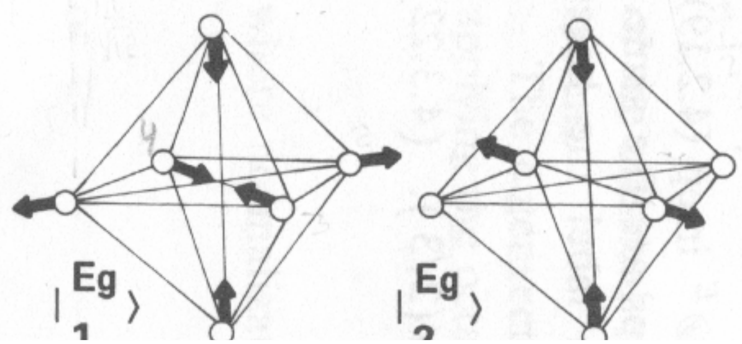
Scalar A_1 eigenket 0_40_4

$$|e^{A_1}_{0_4}\rangle = P^{A_1}_{0_4}|1\rangle/(N^{A_1})^{1/2}$$
$$= \tfrac{1}{24}\sum_g \mathscr{D}^{A_1^*}(g)\,g|1\rangle/(N^{A_1})^{1/2}$$
$$= (|1\rangle + |2\rangle + |3\rangle + |4\rangle + |5\rangle + |6\rangle)/(6)^{1/2}.$$

Tensor E-eigenket 2_40_4

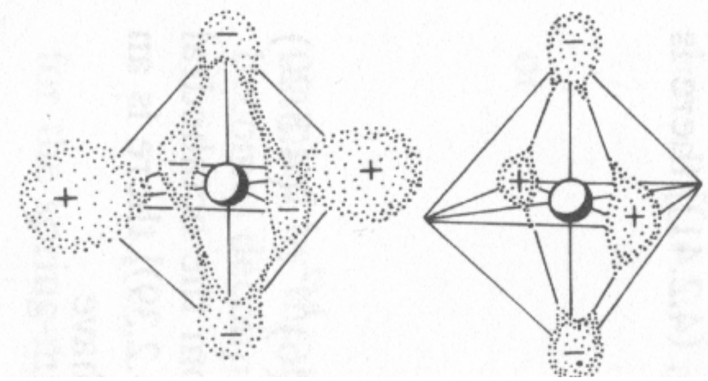
$$|e^{E}_{2_4}\rangle = P^{E}_{2_40_4}|1\rangle/(N^{E})^{1/2}$$
$$= \frac{2}{24}\sum_g \mathscr{D}^{E*}_{2_40_4}(g)\,g|1\rangle/(N^{E})^{1/2}$$
$$= \frac{2}{24}\left[\frac{\sqrt{3}}{2}(r_1+i_1+r_4+R_2) + \frac{\sqrt{3}}{2}(r_2+i_2+r_3+R_2^3) - \frac{\sqrt{3}}{2}(r_1^2+R_1^3+r_3^2+i_6) - \frac{\sqrt{3}}{2}(r_2^2+R_1+r_4^2+i_5)\right]|1\rangle/(N^{E})^{1/2},$$
$$|e^{E}_{2_4}\rangle = (|3\rangle + |4\rangle - |5\rangle - |6\rangle)/2.$$

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

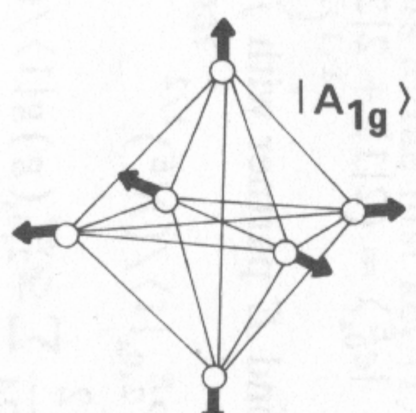


E

H − 2S



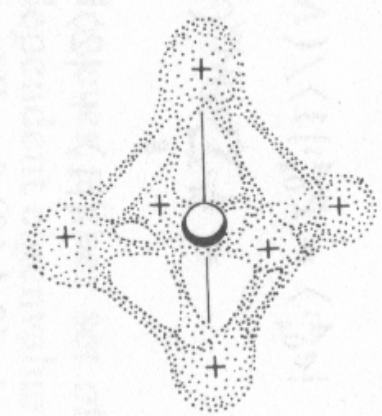
$$\left|{}^{E}_{2_40_4}\right\rangle = \begin{pmatrix}0\\0\\1\\1\\-1\\-1\end{pmatrix}\frac{1}{2}$$



A_1

H + 4S

FREQUENCY OR ENERGY SPECTRUM



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

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

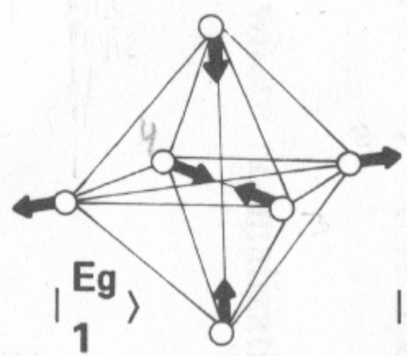
Scalar A_1 eigenket 0_40_4

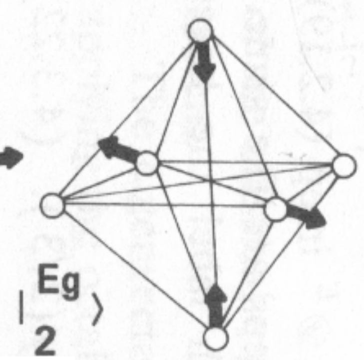
$$|e^{A_1}_{0_4}\rangle = P^{A_1}_{0_4}|1\rangle/(N^{A_1})^{1/2}$$
$$= \tfrac{1}{24}\sum_g \mathscr{D}^{A_1^*}(g)\,g|1\rangle/(N^{A_1})^{1/2}$$
$$= (|1\rangle + |2\rangle + |3\rangle + |4\rangle + |5\rangle + |6\rangle)/(6)^{1/2}.$$

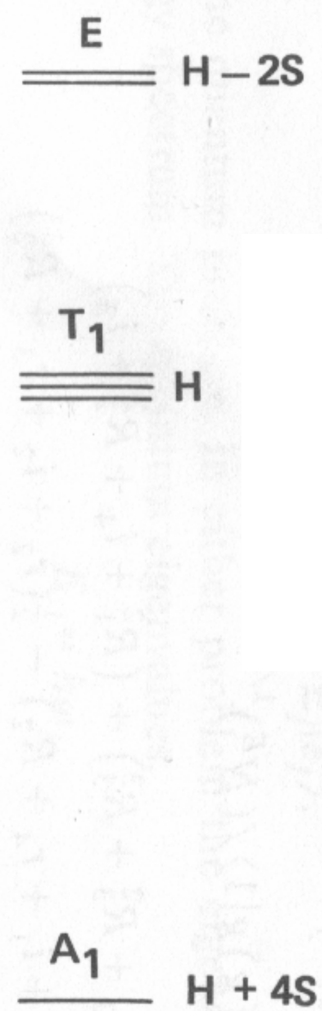
Vector T_1-eigenket 3_40_4=-1_40_4 and 0_40_4

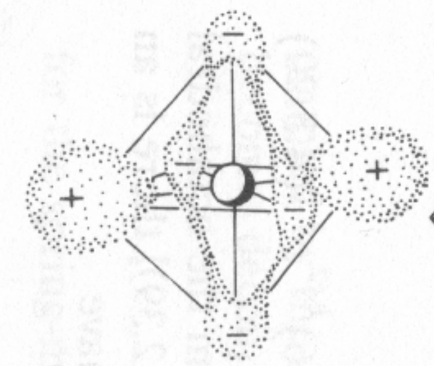
$$|e^{T_1}_{3_4}\rangle = (|3\rangle - |4\rangle - i|5\rangle + i|6\rangle)/2,$$
$$|e^{T_1}_{0_4}\rangle = (|1\rangle - |2\rangle)/\sqrt{2}\,.$$

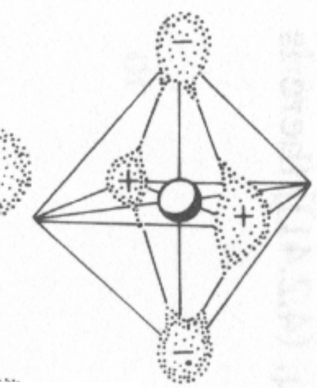
$$\left|{}^{E}_{0_40_4}\right\rangle = \begin{pmatrix}2\\2\\-1\\-1\\-1\\-1\end{pmatrix}\frac{1}{2\sqrt{3}}$$



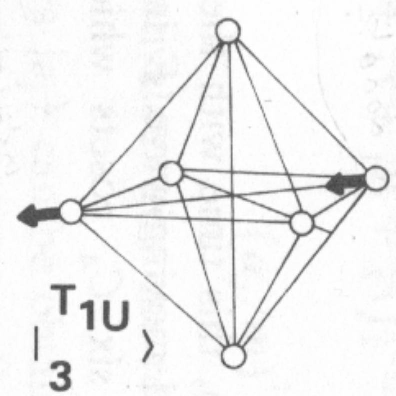


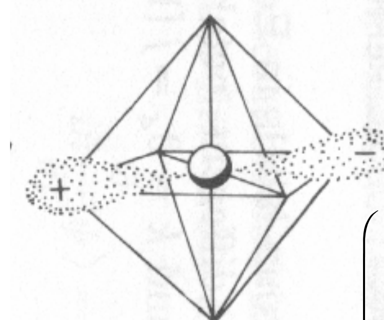




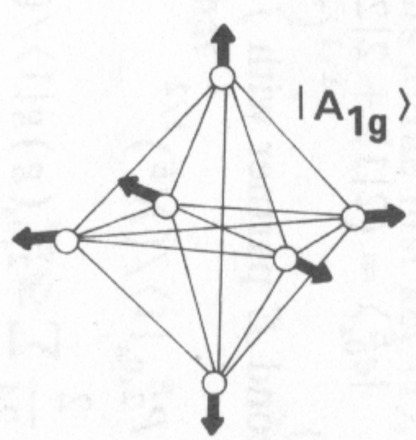


$$\left|{}^{E}_{2_40_4}\right\rangle = \begin{pmatrix}0\\0\\1\\1\\-1\\-1\end{pmatrix}\frac{1}{2}$$

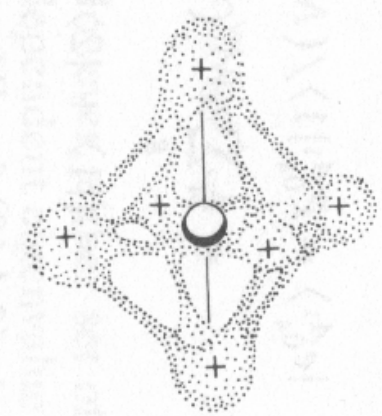




$$\left|{}^{T_1}_{0_40_4}\right\rangle = \begin{pmatrix}1\\-1\\0\\0\\0\\0\end{pmatrix}\frac{1}{\sqrt{2}}$$



FREQUENCY OR ENERGY SPECTRUM



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

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

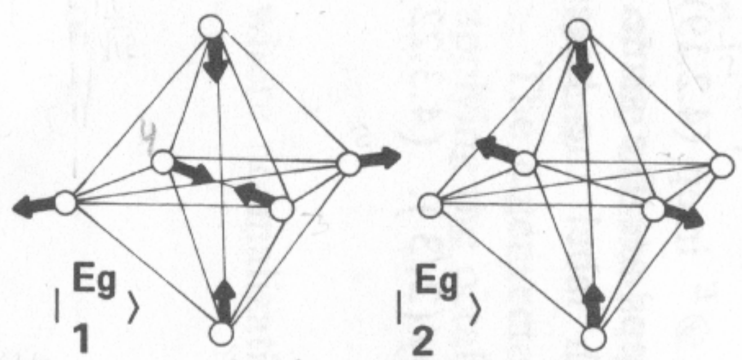
Scalar A_1 eigenket $0_4 0_4$

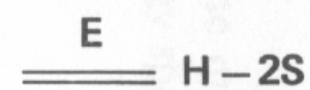
$$|e^{A_1}_{0_4}\rangle = P^{A_1}_{0_4}|1\rangle/(N^{A_1})^{1/2}$$
$$= \frac{1}{24}\sum_g \mathscr{D}^{A_1^*}(g)\,g|1\rangle/(N^{A_1})^{1/2}$$
$$= (|1\rangle + |2\rangle + |3\rangle + |4\rangle + |5\rangle + |6\rangle)/(6)^{1/2}.$$

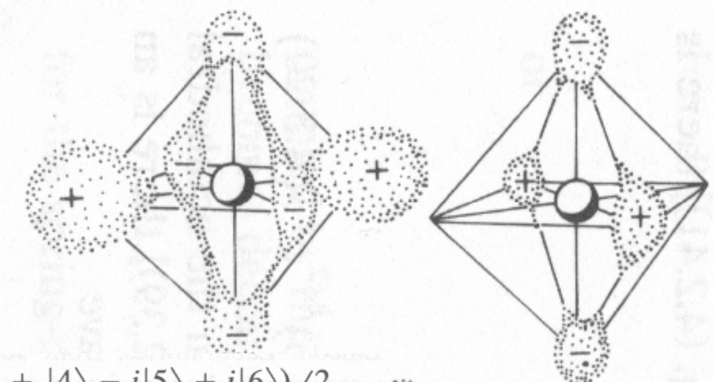
Vector T_1-eigenket $\pm 1_4 0_4$ and $0_4 0_4$

$$|e^{T_1}_{1_4}\rangle = P^{T_1}_{1_4 0_4}|1\rangle/(N^{T_1})^{1/2}$$
$$= \frac{3}{24}\sum_g \mathscr{D}^{T_1^*}_{1_4 0_4}(g)\,g|1\rangle/(N^{T_1})^{1/2}$$
$$= \frac{3}{24}\Big[-\frac{1}{\sqrt{2}}(r_1 + i_1 + r_4 + R_2) + \frac{1}{\sqrt{2}}(r_2 + i_2 + r_3 + R_2^3)$$
$$-\frac{i}{\sqrt{2}}(r_1^2 + R_1^3 + r_3^2 + i_6) + \frac{i}{\sqrt{2}}(r_2^2 + R_1 + r_4^2 + i_5)\Big]|1\rangle/(N^{T_1})^{1/2}$$

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

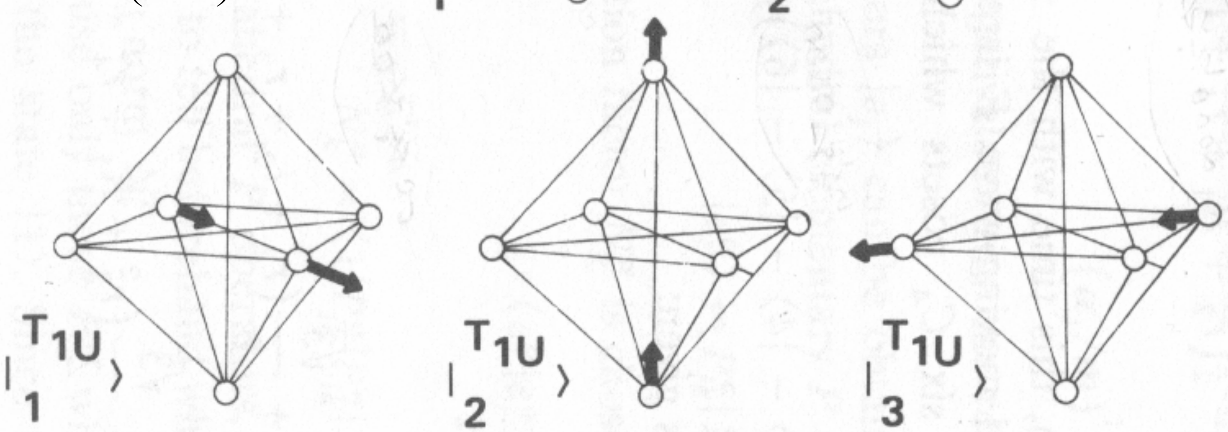


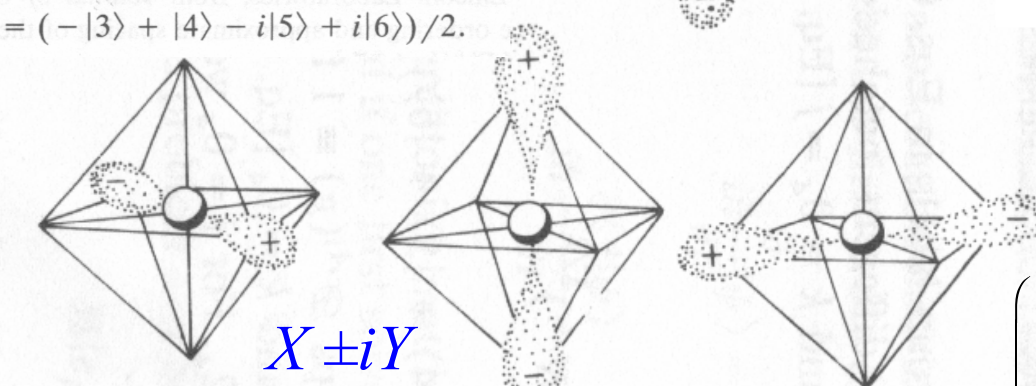




$$\left|{}^{E}_{2_4 0_4}\right\rangle = \begin{pmatrix}0\\0\\1\\1\\-1\\-1\end{pmatrix}\frac{1}{2}$$

$$|e^{T_1}_{1_4}\rangle = (-|3\rangle + |4\rangle - i|5\rangle + i|6\rangle)/2.$$



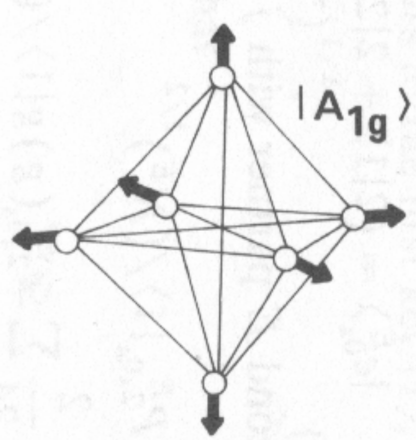


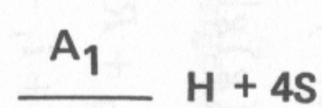
$$\left|{}^{T_1}_{1_4 0_4}\right\rangle = \begin{pmatrix}0\\0\\-1\\1\\-i\\i\end{pmatrix}\frac{1}{2}$$

$X \pm iY$

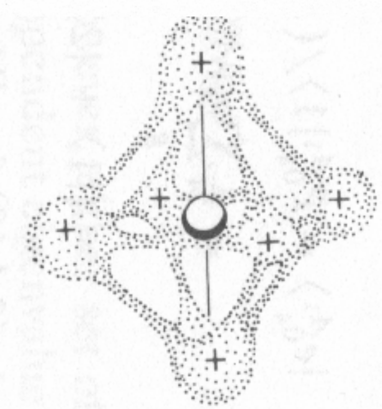
$$|e^{T_1}_x\rangle = \left(-|e^{T_1}_{1_4}\rangle + |e^{T_1}_{3_4}\rangle\right)/\sqrt{2} = (|3\rangle - |4\rangle)/\sqrt{2}$$
$$|e^{T_1}_y\rangle = i\left(|e^{T_1}_{1_4}\rangle + |e^{T_1}_{3_4}\rangle\right)/\sqrt{2} = (|5\rangle - |6\rangle)/\sqrt{2}$$
$$|e^{T_1}_z\rangle = |e^{T_1}_{0_4}\rangle = (|1\rangle - |2\rangle)/\sqrt{2}$$

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





FREQUENCY OR ENERGY SPECTRUM



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

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

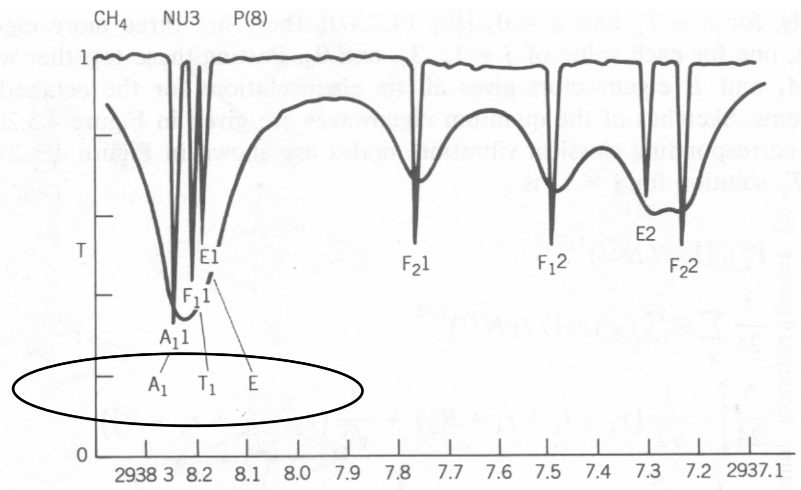
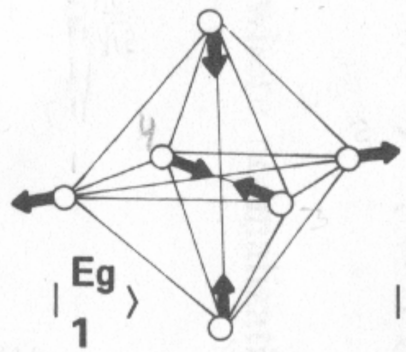
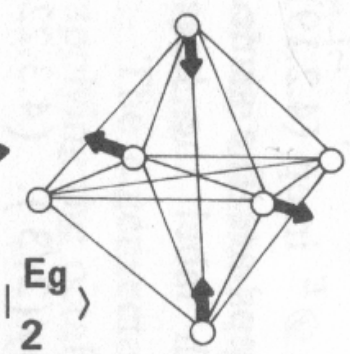


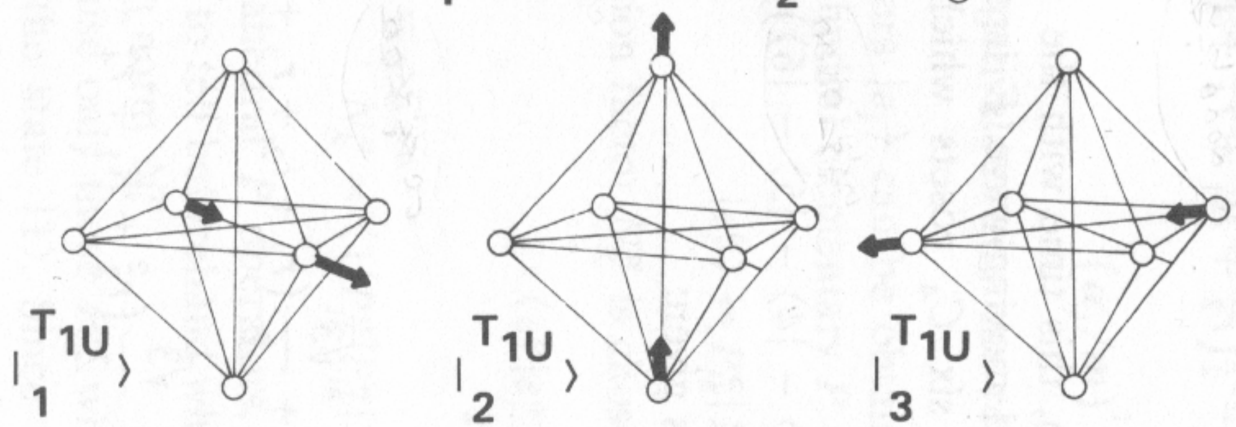
Figure 4.3.3 Evidence of an (A_1T_1E) spectral cluster in methane laser spectra. (Courtesy of Dr. Allan Pine, MIT Lincoln Laboratories, from *Journal of Optical Society of America* **66**, 97 (1976)). The ordering and approximate spacing of the A_1T_1 and E lines is consistent with that of Figure 4.3.2.

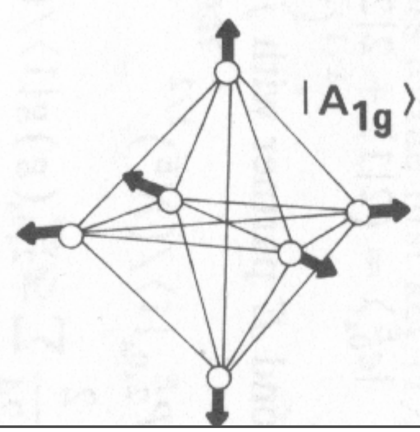
$$\begin{pmatrix} \langle 1|\mathbf{H}|1\rangle & \langle 1|\mathbf{H}|2\rangle & \cdots & \langle 1|\mathbf{H}|6\rangle \\ \langle 2|\mathbf{H}|1\rangle & \langle 2|\mathbf{H}|2\rangle & \cdots & \langle 2|\mathbf{H}|6\rangle \\ \cdot & & & \cdot \\ \cdot & & & \cdot \\ \cdot & & & \cdot \\ \langle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

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









E

H – 2S

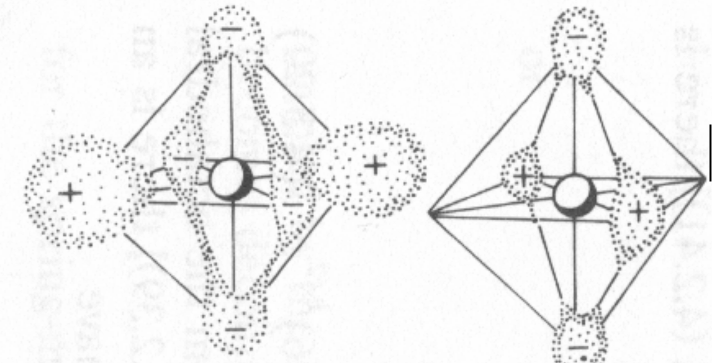
T1

H

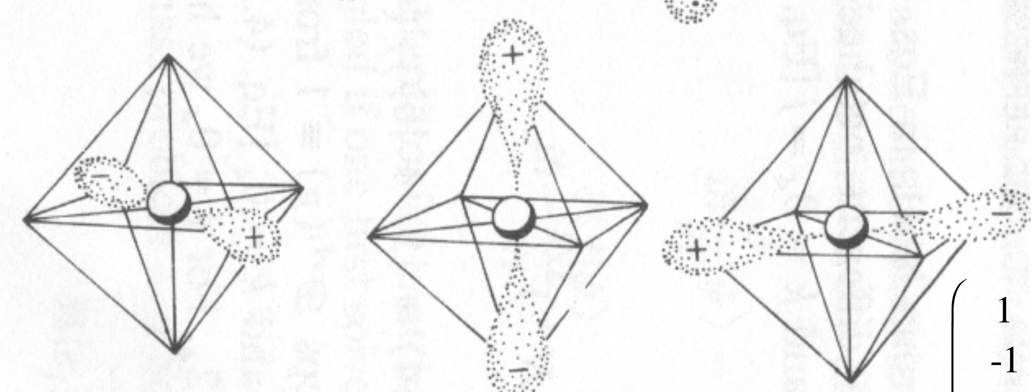
A1

H + 4S

FREQUENCY OR ENERGY SPECTRUM

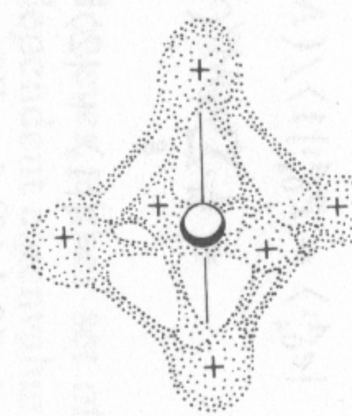


$$\left|\begin{smallmatrix}E\\2_40_4\end{smallmatrix}\right\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 1 \\ -1 \\ -1 \end{pmatrix} \frac{1}{2}$$



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

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



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

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*

Simplest $O_h \supset O \supset D_4 \supset C_4$ *spectral analysis problems*

- *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 expression*

Introduction to ortho-complete eigenvalue calculations
Right and Left cosets of C_4 extracted from group table

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

TABLE F.2.1 ***O*-Group Table**

1	r_1	r_2	r_3	r_4	$\tilde r_1$ r_1^2	$\tilde r_2$ r_2^2	$\tilde r_3$ r_3^2	$\tilde r_4$ r_4^2	ρ_x R_1^2	ρ_y R_2^2	ρ_z R_3^2	R_1	R_2	R_3	$\tilde R_x$ R_1^3	$\tilde R_y$ R_2^3	$\tilde R_z$ R_3^3	i_1	i_2	i_3	i_4	i_5	i_6
r_1	r_1^2	$-r_4^2$	$-r_2^2$	$-r_3^2$	-1	$-R_2^2$	$-R_3^2$	$-R_1^2$	$-r_2$	$-r_3$	$-r_4$	i_3	i_6	i_1	$-R_3$	$-R_1$	$-R_2$	R_1^3	i_5	R_2^3	i_2	$-i_4$	R_3^3
r_2	$-r_3^2$	r_2^2	$-r_4^2$	$-r_1^2$	R_2^2	-1	R_1^2	$-R_3^2$	r_1	r_4	$-r_3$	R_3	$-R_1^3$	i_2	i_3	$-i_5$	R_2^3	i_6	$-R_1$	R_2	$-i_1$	R_3^3	i_4
r_3	$-r_4^2$	$-r_1^2$	r_3^2	$-r_2^2$	R_3^2	$-R_1^2$	-1	R_2^2	$-r_4$	r_1	r_2	$-i_4$	R_1	$-R_2^3$	R_3^3	i_6	i_2	i_5	$-R_1^3$	i_1	R_2	$-i_3$	R_3
r_4	$-r_2^2$	$-r_3^2$	$-r_1^2$	r_4^2	R_1^2	R_3^2	$-R_2^2$	-1	r_3	$-r_2$	r_1	$-R_3^3$	$-i_5$	R_2	$-i_4$	R_1^3	i_1	R_1	i_6	$-i_2$	R_2^3	R_3	i_3
r_1^2	-1	R_1^2	R_2^2	R_3^2	$-r_1$	r_3	r_4	r_2	r_4^2	r_2^2	r_3^2	R_2^3	R_3^3	R_1^3	$-i_1$	$-i_3$	$-i_6$	$-R_3$	$-i_4$	$-R_1$	i_5	$-i_2$	$-R_2$
r_2^2	$-R_1^2$	-1	R_3^2	$-R_2^2$	r_4	$-r_2$	r_1	r_3	$-r_3^2$	$-r_1^2$	r_4^2	i_2	$-i_3$	$-R_1$	R_2	$-R_3^3$	$-i_5$	i_4	$-R_3$	$-R_1^3$	$-i_6$	R_2^3	$-i_1$
r_3^2	$-R_2^2$	$-R_3^2$	-1	R_1^2	r_2	r_4	$-r_3$	r_1	r_2^2	$-r_4^2$	$-r_1^2$	$-R_2$	$-i_4$	$-i_6$	i_2	R_3	$-R_1^3$	$-i_3$	$-R_3^3$	i_5	R_1	$-i_1$	$-R_2^3$
r_4^2	$-R_3^2$	R_2^2	$-R_1^2$	-1	r_3	r_1	r_2	$-r_4$	$-r_1^2$	r_3^2	$-r_2^2$	$-i_1$	$-R_3$	$-i_5$	$-R_2^3$	$-i_4$	R_1	$-R_3^3$	i_3	$-i_6$	R_1^3	R_2	$-i_2$
R_1^2	$-r_4$	r_3	$-r_2$	r_1	r_2^2	$-r_1^2$	r_4^2	$-r_3^2$	-1	R_3^2	$-R_2^2$	R_1^3	i_1	$-i_4$	$-R_1$	i_2	$-i_3$	$-R_2$	$-R_2^3$	R_3^3	R_3	$-i_6$	i_5
R_2^2	$-r_2$	r_1	r_4	$-r_3$	r_3^2	$-r_4^2$	$-r_1^2$	r_2^2	$-R_3^2$	-1	R_1^2	$-i_5$	R_2^3	i_3	$-i_6$	$-R_2$	$-i_4$	$-i_2$	i_1	$-R_3$	R_3^3	R_1	R_1^3
R_3^2	$-r_3$	$-r_4$	r_1	r_2	r_4^2	r_3^2	$-r_2^2$	$-r_1^2$	R_2^2	$-R_1^2$	-1	i_6	i_2	R_3^3	$-i_5$	$-i_1$	$-R_3$	R_2^3	$-R_2$	i_4	$-i_3$	R_1^3	$-R_1$
R_1	i_1	$-R_2^3$	$-i_2$	R_2	R_3^3	$-i_3$	$-R_3$	i_4	R_1^3	i_6	i_5	R_1^2	r_1	$-r_4^2$	-1	$-r_3$	r_2^2	$-r_4$	r_2	r_1^2	$-r_3^2$	$-R_2^2$	R_3^2
R_2	i_3	R_3	$-R_3^3$	i_4	R_1^3	i_5	$-i_6$	$-R_1$	$-i_2$	R_2^3	i_1	$-r_2^2$	R_2^2	r_1	r_3^2	-1	$-r_4$	R_1^2	R_3^2	$-r_2$	$-r_3$	$-r_4^2$	r_1^2
R_3	i_6	i_5	R_1	$-R_1^3$	R_2^3	$-R_2$	$-i_2$	$-i_1$	i_3	i_4	R_3^3	r_1	$-r_3^2$	R_3^2	$-r_2$	r_4^2	-1	r_1^2	r_2^2	R_2^2	$-R_1^2$	$-r_4$	$-r_3$
R_1^3	$-R_2$	$-i_2$	R_2^3	i_1	$-i_3$	$-R_3^3$	i_4	R_3	$-R_1$	i_5	$-i_6$	-1	$-r_4$	r_3^2	$-R_1^2$	r_2	$-r_1^2$	$-r_1$	r_3	r_2^2	$-r_4^2$	$-R_3^2$	$-R_2^2$
R_2^3	$-R_3$	i_3	i_4	R_3^3	$-i_6$	R_1	$-R_1^3$	i_5	$-i_1$	$-R_2$	$-i_2$	r_4^2	-1	$-r_2$	$-r_1^2$	$-R_2^2$	r_3	$-R_3^2$	R_1^2	$-r_1$	$-r_4$	$-r_2^2$	r_3^2
R_3^3	$-R_1$	R_1^3	i_6	i_5	$-i_1$	$-i_2$	R_2	$-R_2^3$	i_4	$-i_3$	$-R_3$	$-r_3$	r_2^2	-1	r_4	$-r_1^2$	$-R_3^2$	r_4^2	r_3^2	$-R_1^2$	$-R_2^2$	$-r_2$	$-r_1$
i_1	R_3^3	$-i_4$	i_3	R_3	$-R_1$	$-i_6$	$-i_5$	$-R_1^3$	R_2^3	i_2	$-R_2$	r_1^2	R_3^2	$-r_4$	r_4^2	$-R_1^2$	$-r_1$	-1	$-R_2^2$	$-r_3$	r_2	r_3^2	r_2^2
i_2	i_4	R_3^3	R_3	$-i_3$	$-i_5$	R_1^3	R_1	$-i_6$	R_2	$-i_1$	R_2^3	$-r_3^2$	$-R_1^2$	$-r_3$	$-r_2^2$	$-R_3^2$	$-r_2$	R_2^2	-1	r_4	$-r_1$	r_1^2	r_4^2
i_3	R_1^3	R_1	$-i_5$	i_6	$-R_2$	$-R_2^3$	$-i_1$	i_2	$-R_3$	R_3^3	$-i_4$	$-r_2$	r_1^2	R_1^2	$-r_1$	r_2^2	$-R_2^2$	r_3^2	$-r_4^2$	-1	R_3^2	r_3	$-r_4$
i_4	$-i_5$	i_6	$-R_1^3$	$-R_1$	$-i_2$	i_1	$-R_2^3$	$-R_2$	$-R_3^3$	$-R_3$	i_3	r_4	r_4^2	R_2^2	r_3	r_3^2	R_1^2	$-r_2^2$	r_1^2	$-R_3^3$	-1	r_1	$-r_2$
i_5	i_2	$-R_2$	i_1	$-R_2^3$	i_4	$-R_3$	i_3	$-R_3^3$	i_6	$-R_1^3$	$-R_1$	R_3^2	r_2	r_2^2	R_2^2	r_4	r_4^2	$-r_3$	$-r_1$	$-r_3^2$	$-r_1^2$	-1	$-R_1^2$
i_6	R_2^3	i_1	R_2	i_2	$-R_3$	$-i_4$	$-R_3^3$	$-i_3$	$-i_5$	$-R_1$	R_1^3	R_2^2	$-r_3$	r_1^2	$-R_3^2$	$-r_1$	r_3^2	$-r_2$	$-r_4$	r_4^2	r_2^2	R_1^2	-1

Examples of multiple Left cosets of C_4 from group table

Will be used later to derive eigensolutions and simplified formulae.

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

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

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

C_4 subgroup correlation to O

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

C_4 Projectors to split octahedral P^α

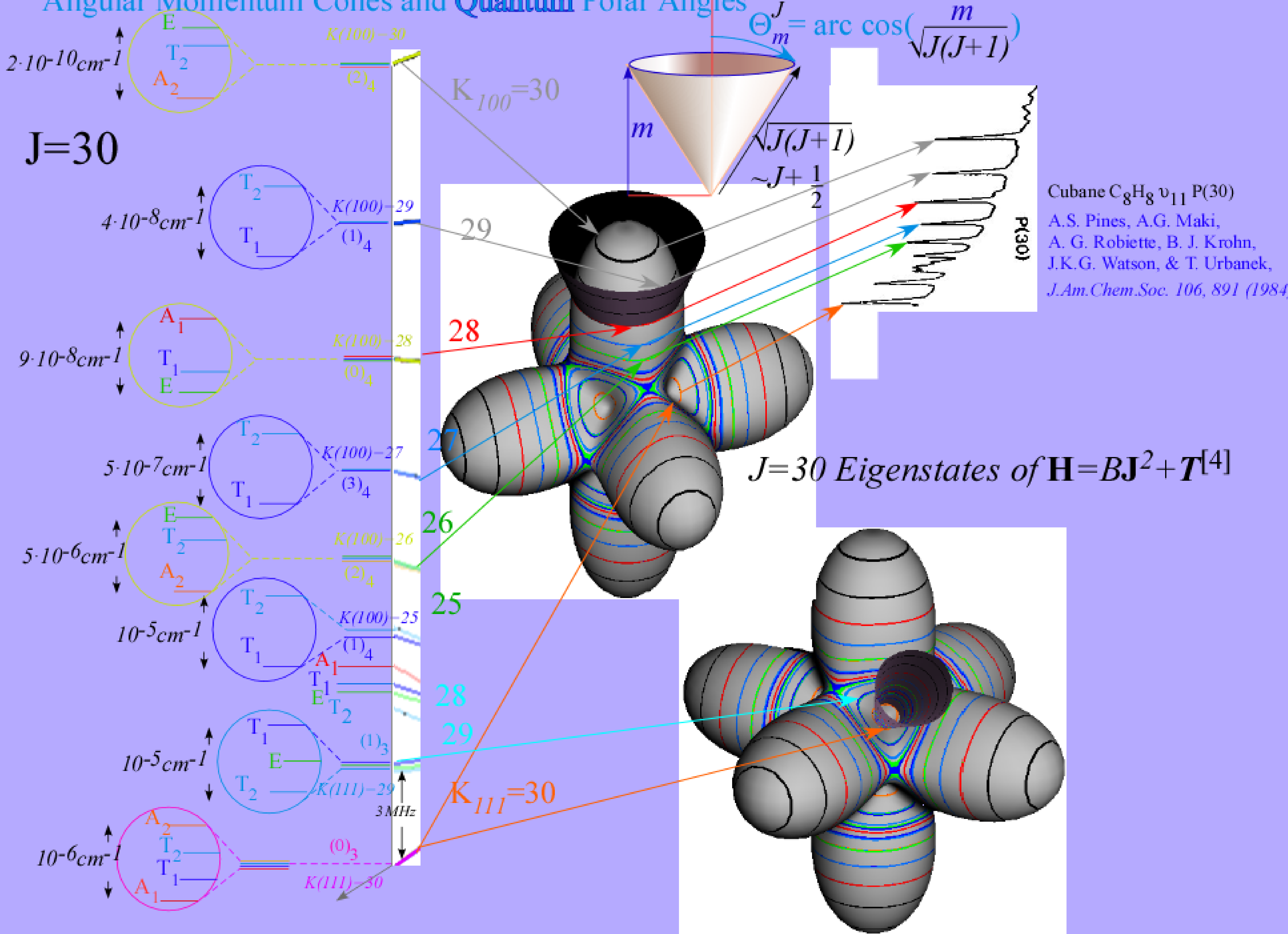
$$\mathbf{p}_{m_4} = \sum_{p=0}^{3} \frac{e^{2\pi i m\cdot p/4}}{4}\mathbf{R}_z^p = \begin{cases} \mathbf{p}_{0_4} = (\mathbf{1} + \mathbf{R}_z + \rho_z + \tilde{\mathbf{R}}_z)/4 \\ \mathbf{p}_{1_4} = (\mathbf{1} + i\mathbf{R}_z - \rho_z - i\tilde{\mathbf{R}}_z)/4 \\ \mathbf{p}_{2_4} = (\mathbf{1} -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

$\mathbf{1}\cdot\mathbf{P}^\alpha =$	$(\mathbf{p}_{0_4}$	$+\mathbf{p}_{1_4}$	$+\mathbf{p}_{2_4}$	$+\mathbf{p}_{3_4})\cdot\mathbf{P}^\alpha$
$\mathbf{1}\cdot\mathbf{P}^{A_1} =$	$\mathbf{P}^{A_1}_{0_40_4}$	$+0$	$+0$	$+0$
$\mathbf{1}\cdot\mathbf{P}^{A_2} =$	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	$+\mathbf{P}^{T_2}_{1_41_4}$	$+\mathbf{P}^{T_2}_{2_42_4}$	$+\mathbf{P}^{T_2}_{3_43_4}$

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

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

Angular Momentum Cones and Quantum Polar Angles



$\ell^{A_1}=1$

$\ell^{A_2}=1$

$\ell^{E}=2$

$\ell^{T_1}=3$

$\ell^{T_2}=3$

Example: $G=O$

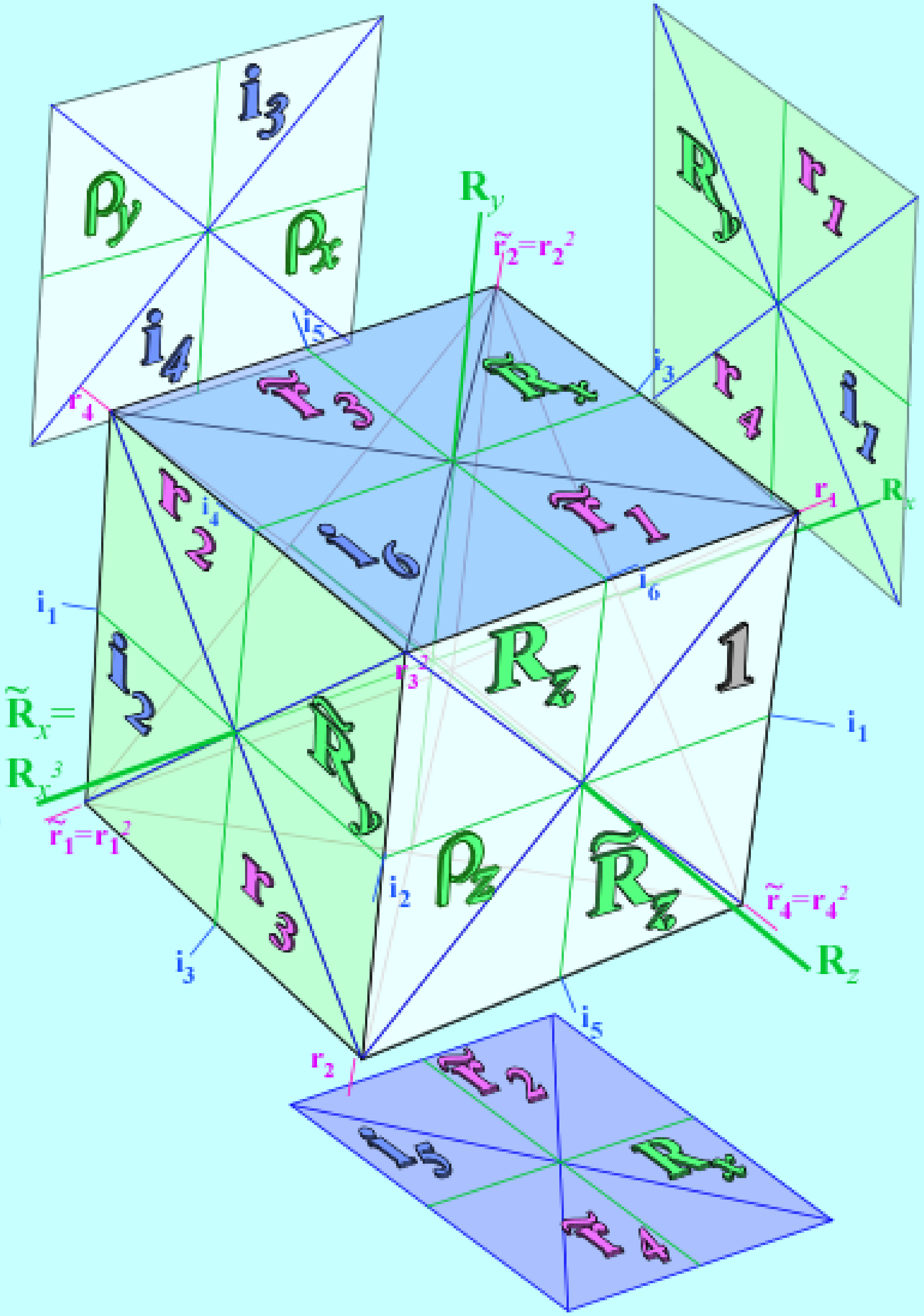
Cubic-Octahedral Group O

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
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

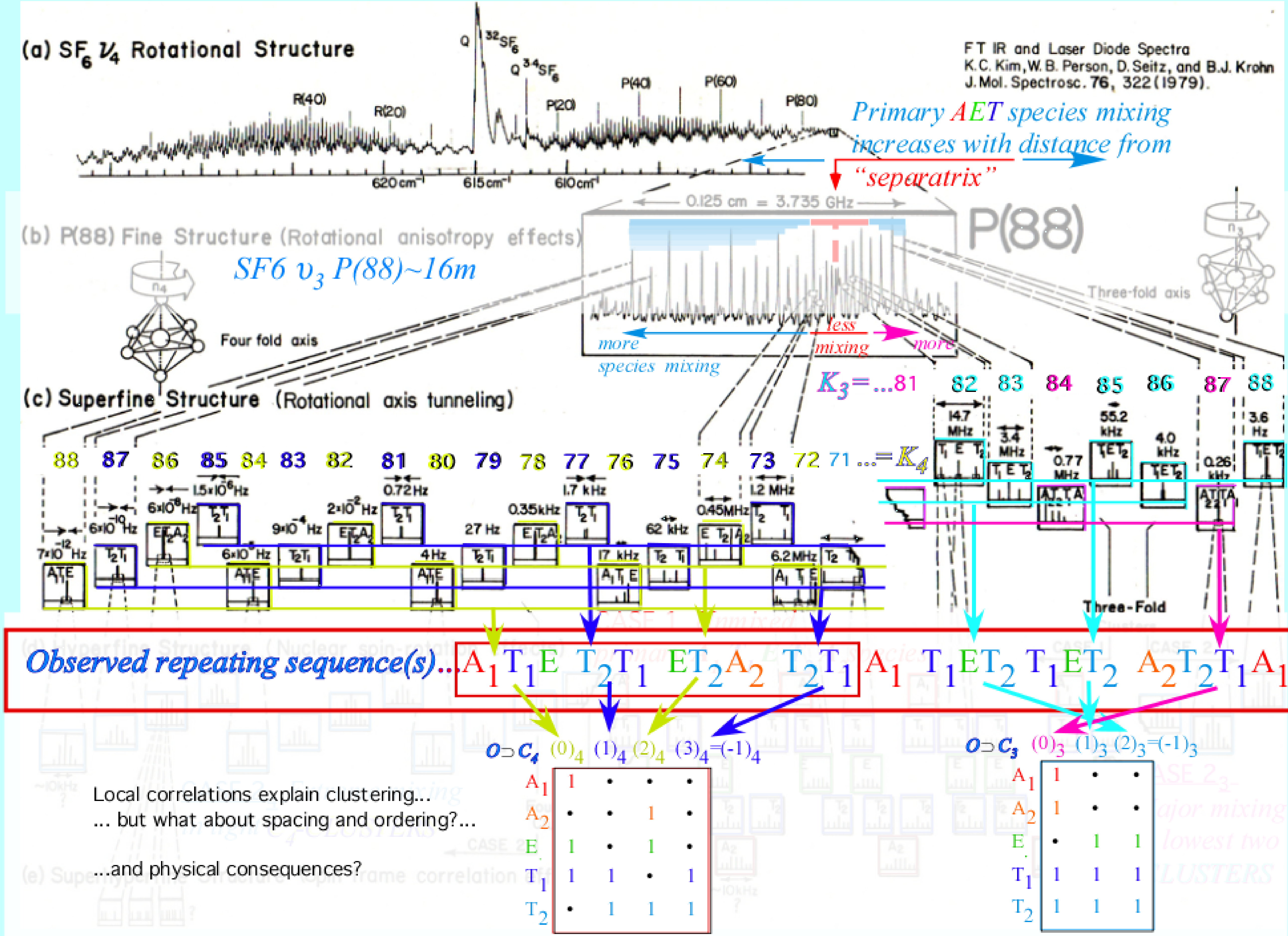


$O\supset C_4$

	$(0)_4$	$(1)_4$	$(2)_4$	$(3)_4=(-1)_4$
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



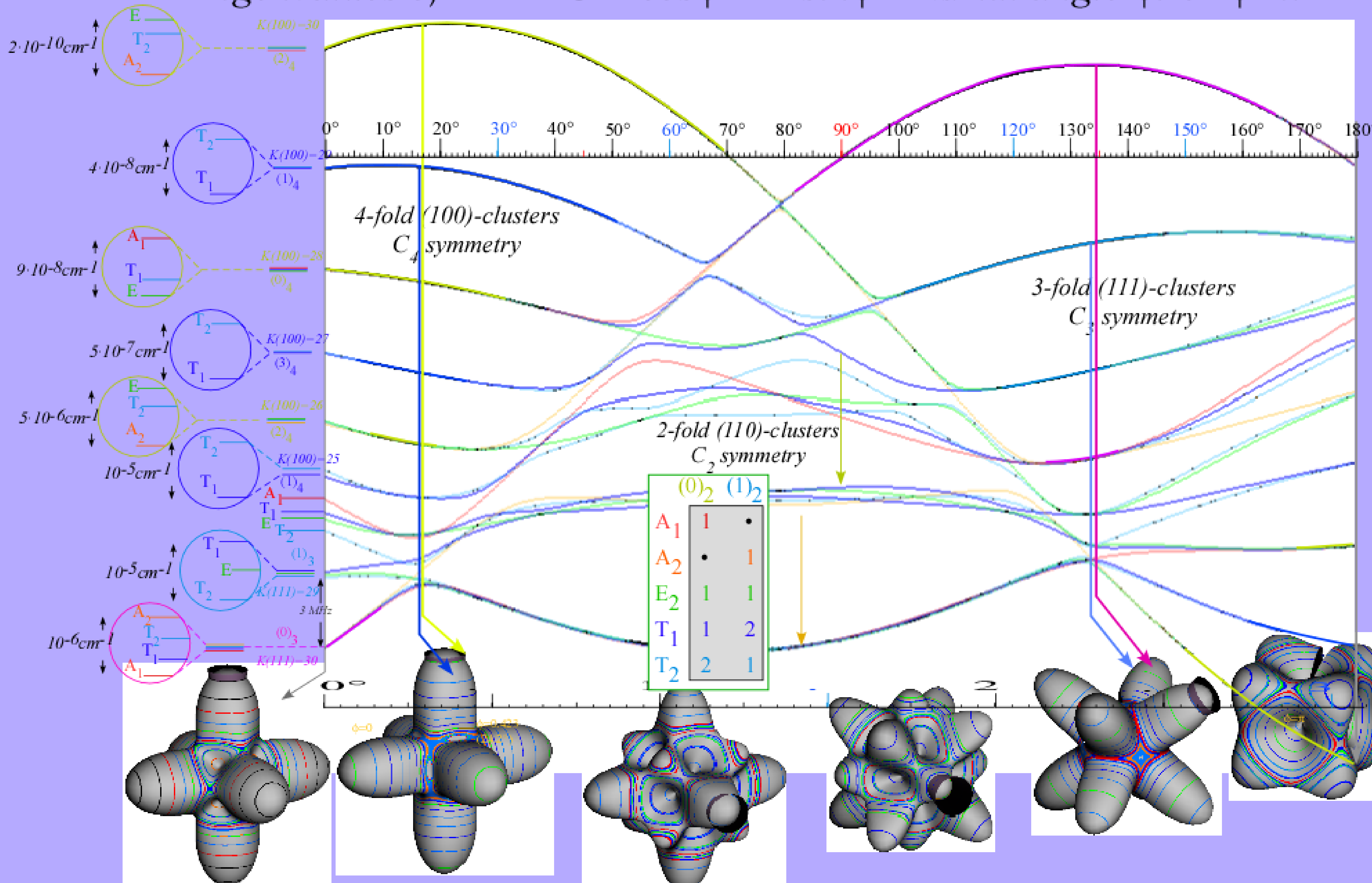
	$(0)_4$	$(1)_4$	$(2)_4$	$(3)_4=(-1)_4$
A_1	1	•	•	•
A_2	•	•	1	•
E	1	•	1	•
T_1	1	1	•	1
T_2	•	1	1	1

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

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

...and physical consequences?

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



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

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

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

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

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