Group Theory in Quantum Mechanics

Lecture 18 (3.31.15)

Hexagonal $D_6 \subset D_{6h}$ and octahedral-tetrahedral $O \sim T_d$ symmetry

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

Review: Symmetry reduction and splitting: Subduced irep $D^{\alpha}(D_3)\downarrow C_2 = d^{0_2} \oplus d^{1_2} \oplus$.. correlation
Symmetry induction and clustering: Induced rep $d^{a}(C_2)\uparrow D_3 = D^{\alpha} \oplus D^{\beta} \oplus$.. correlation
Review: Symmetry reduction and splitting: Subduced irep $D^{\alpha}(D_3)\downarrow C_3 = d^{0_3} \oplus d^{1_3} \oplus$.. correlation
Symmetry induction and clustering: Induced rep $d^{c}(C_3)\uparrow D_3 = D^{\alpha} \oplus D^{\beta} \oplus$.. correlation

D_3-C_2 Coset structure of $d^{m_2}(C_2)\uparrow D_3$ induced representation basis
D_3-Projection of $d^{m_2}(C_2)\uparrow D_3$ induced representation basis
Derivation of Frobenius reciprocity

$D_6 \supset D_2 \supset C_2 = D_3 \times C_2$ symmetry and outer product geometry
Irreducible characters
Irreducible representations
Correlations with D_6 characters:
...and $C_2(\mathbf{i}_3)$ characters......and $C_6(\mathbf{1},\mathbf{h}^1,\mathbf{h}^2,...)$ characters
D_6 symmetry and induced representation band structure

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

Review: *Symmetry reduction and splitting: Subduced irep $D^{\alpha}(D_3)\downarrow C_2 = d^{0_2}\oplus d^{1_2}\oplus$.. correlation*

Symmetry induction and clustering: Induced rep $d^{a}(C_2)\uparrow D_3 = D^{\alpha}\oplus D^{\beta}\oplus$.. correlation

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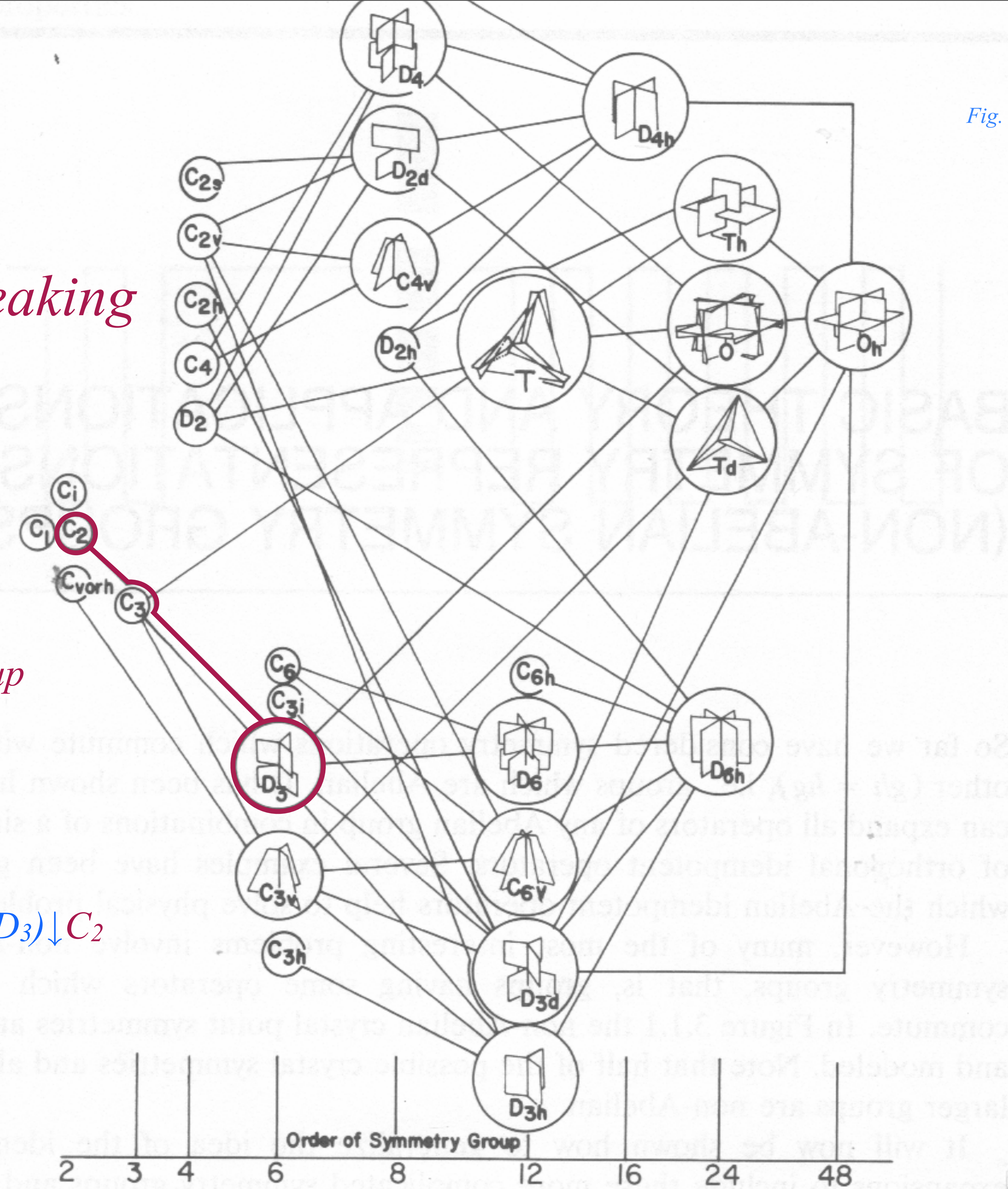
Introduction to octahedral tetrahedral symmetry $O_h\supset O\sim T_d\supset T$

B-Type Symmetry Breaking

Fig. 3.1.1 PSDS



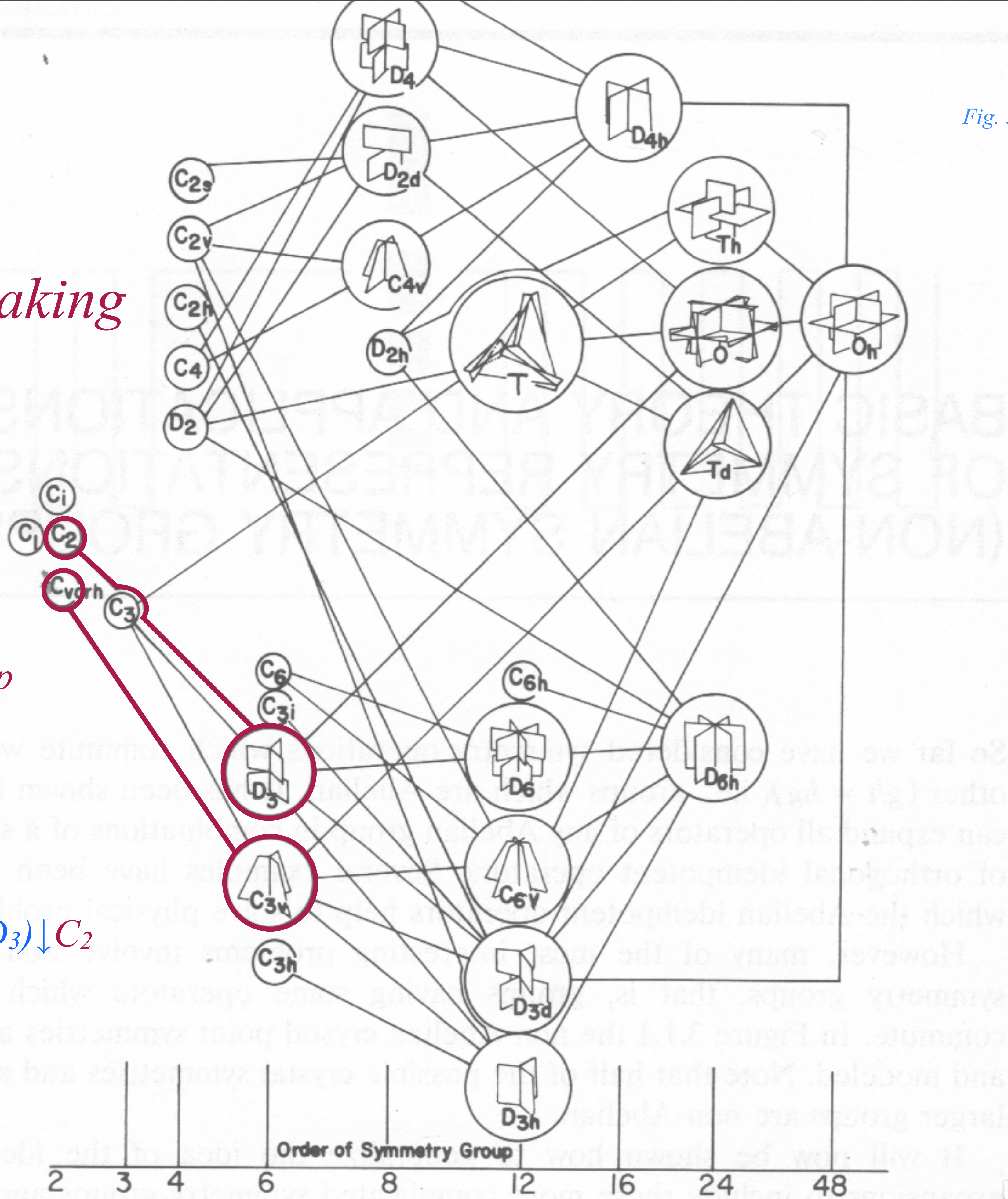
Bilateral subgroup Chain $D_3 \supset C_2$

Subduced irep $D^{\alpha}(D_3){\downarrow}C_2$

Figure 3.1.1 Crystal point symmetry groups. Models are sketched in circles for the

B-Type Symmetry Breaking

Fig. 3.1.1 PSDS



Bilateral subgroup Chain $D_3 \supset C_2$ *(or* $C_{3v} \supset C_v$ *)*

Subduced irep $D^{\alpha}(D_3)\downarrow C_2$

Figure 3.1.1 Crystal point symmetry groups. Models are sketched in circles for the

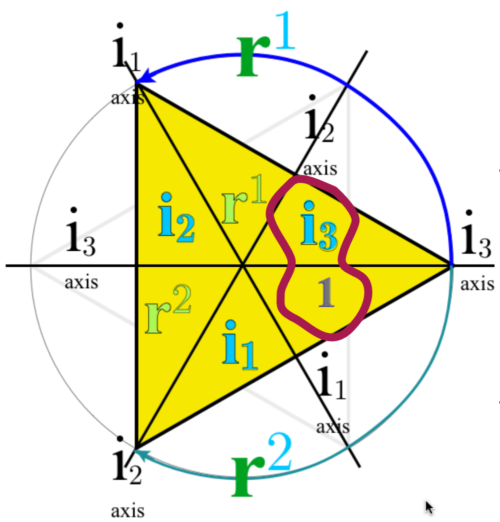
Applied symmetry reduction and splitting: Subduced irep $D^{\alpha}(D_3)\downarrow C_2 = d^{0_2}\oplus d^{1_2}\oplus$.. correlation

$D_3 \supset C_2$	0_2	1_2
A_1	1	·
A_2	·	1
E_1	1	1

$D^{A_1}(D_3)\downarrow C_2 \sim d^{0_2}$

$D^{A_2}(D_3)\downarrow C_2 \sim d^{1_2}$

$D^{E_1}(D_3)\downarrow C_2 \sim d^{0_2}\oplus d^{1_2}$



D_3	$\mathbf{1}$	$\{\mathbf{r}^1,\mathbf{r}^2\}$	$\{\mathbf{i}_1\mathbf{i}_2\mathbf{i}_3\}$
A_1	1	1	1
A_2	1	1	-1
E_1	2	-1	0

$\supset C_2$	$\mathbf{1}$	$\mathbf{i}_3$
$(0)_2$	1	1
$(1)_2$	1	-1

Deriving $D_3 \sim C_{3v}$ products - By group definition $|g\rangle = \mathbf{g}|1\rangle$ of position ket $|g\rangle$

Applied symmetry reduction and splitting: Subduced irep $D^{\alpha}(D_3)\downarrow C_2 = d^{0_2}\oplus d^{1_2}\oplus..$ correlation

$D_3 \supset C_2$	$\mathbf{P}^{\alpha}$ relabel/split	D^{α} relabel/reduce	ω^{α} relabel/split
A_1	$\mathbf{P}^{A_1}=\mathbf{P}^{A_1}\mathbf{P}^{0_2}=\mathbf{P}^{A_1}_{0_2 0_2}$	$\Rightarrow D^{A_1}\downarrow C_2 \sim d^{0_2}$	$\Rightarrow \omega^{A_1} \rightarrow \omega^{0_2}$
A_2	$\mathbf{P}^{A_2}=\mathbf{P}^{A_2}\mathbf{P}^{1_2}=\mathbf{P}^{A_2}_{1_2 1_2}$	$\Rightarrow D^{A_2}\downarrow C_2 \sim d^{1_2}$	$\Rightarrow \omega^{A_2} \rightarrow \omega^{1_2}$
E_1	$\mathbf{P}^{E_1}=\mathbf{P}^{E_1}\mathbf{P}^{0_2}+\mathbf{P}^{E_1}\mathbf{P}^{1_2}$ $=\mathbf{P}^{E_1}_{0_2 0_2}+\mathbf{P}^{E_1}_{1_2 1_2}$	$\Rightarrow D^{E_1}\downarrow C_2 \sim$ $d^{0_2}\oplus d^{1_2}$	$\Rightarrow \omega^{E_1} \rightarrow \omega^{0_2}$ $\searrow \omega^{1_2}$

$D_3 \supset C_2$	0_2	1_2
A_1	1	·
A_2	·	1
E_1	1	1

$D^{A_1}(D_3)\downarrow C_2 \sim d^{0_2}$

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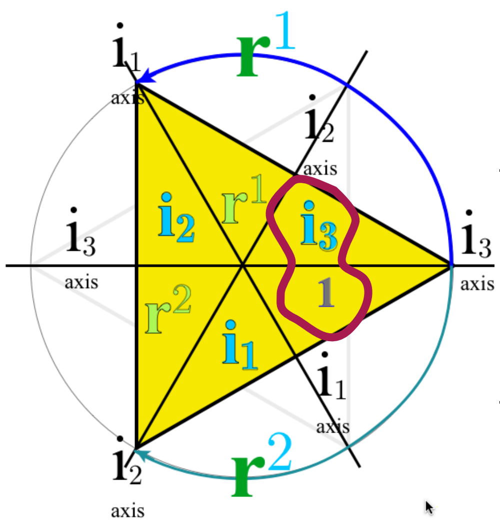

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Irreducible characters

Irreducible representations

Correlations with D_6 characters:

...and C_2($\mathbf{i}_3$) characters......and C_6($\mathbf{1}, \mathbf{h}^1, \mathbf{h}^2$,...) characters

D_6 symmetry and induced representation band structure

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

Applied symmetry reduction and splitting: Subduced irep $D^{\alpha}(D_3)\downarrow C_2 = d^{0_2} \oplus d^{1_2} \oplus$.. correlation

$D_3 \supset C_2$	$\mathbf{P}^{\alpha}$ relabel/split	D^{α} relabel/reduce	ω^{α} relabel/split
A_1	$\mathbf{P}^{A_1} = \mathbf{P}^{A_1}\mathbf{P}^{0_2} = \mathbf{P}^{A_1}_{0_2 0_2}$	$\Rightarrow D^{A_1}\downarrow C_2 \sim d^{0_2}$	$\Rightarrow \omega^{A_1} \rightarrow \omega^{0_2}$
A_2	$\mathbf{P}^{A_2} = \mathbf{P}^{A_2}\mathbf{P}^{1_2} = \mathbf{P}^{A_2}_{1_2 1_2}$	$\Rightarrow D^{A_2}\downarrow C_2 \sim d^{1_2}$	$\Rightarrow \omega^{A_2} \rightarrow \omega^{1_2}$
E_1	$\mathbf{P}^{E_1} = \mathbf{P}^{E_1}\mathbf{P}^{0_2} + \mathbf{P}^{E_1}\mathbf{P}^{1_2}$ $= \mathbf{P}^{E_1}_{0_2 0_2} + \mathbf{P}^{E_1}_{1_2 1_2}$	$\Rightarrow D^{E_1}\downarrow C_2 \sim$ $d^{0_2} \oplus d^{1_2}$	$\Rightarrow \omega^{E_1} \rightarrow \omega^{0_2}$ $\searrow \omega^{1_2}$

$D_3 \supset C_2$	0_2	1_2
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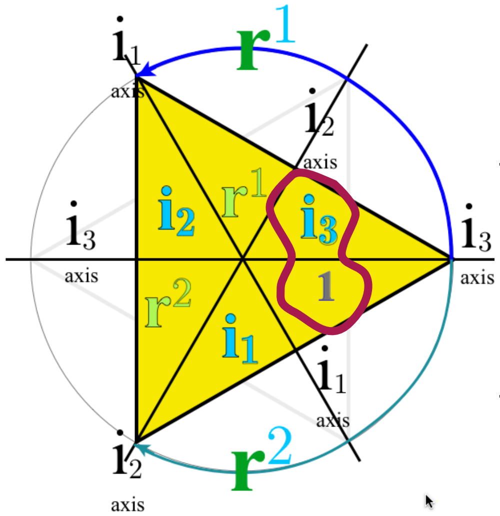
$d^{0_2}(C_2)\uparrow D_3 \sim D^{A_1} \oplus D^{E_1}$ $\quad$ $d^{1_2}(C_2)\uparrow D_3 \sim D^{A_2} \oplus D^{E_1}$

Spontaneous symmetry breaking and clustering: Induced rep $d^{a}(C_2)\uparrow D_3 = D^{\alpha} \oplus D^{\beta} \oplus$.. correlation



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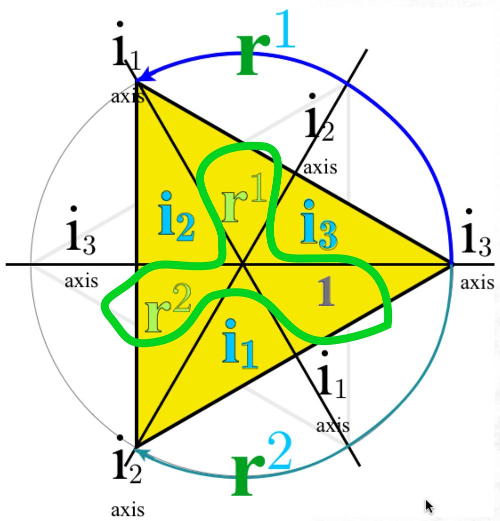
C-Type Symmetry Breaking



Trigonal subgroup Chain $D_3 \supset C_3$
(or $C_{3v} \supset C_3$)

Subduced irep $D^{\alpha}(D_3)\downarrow C_3$

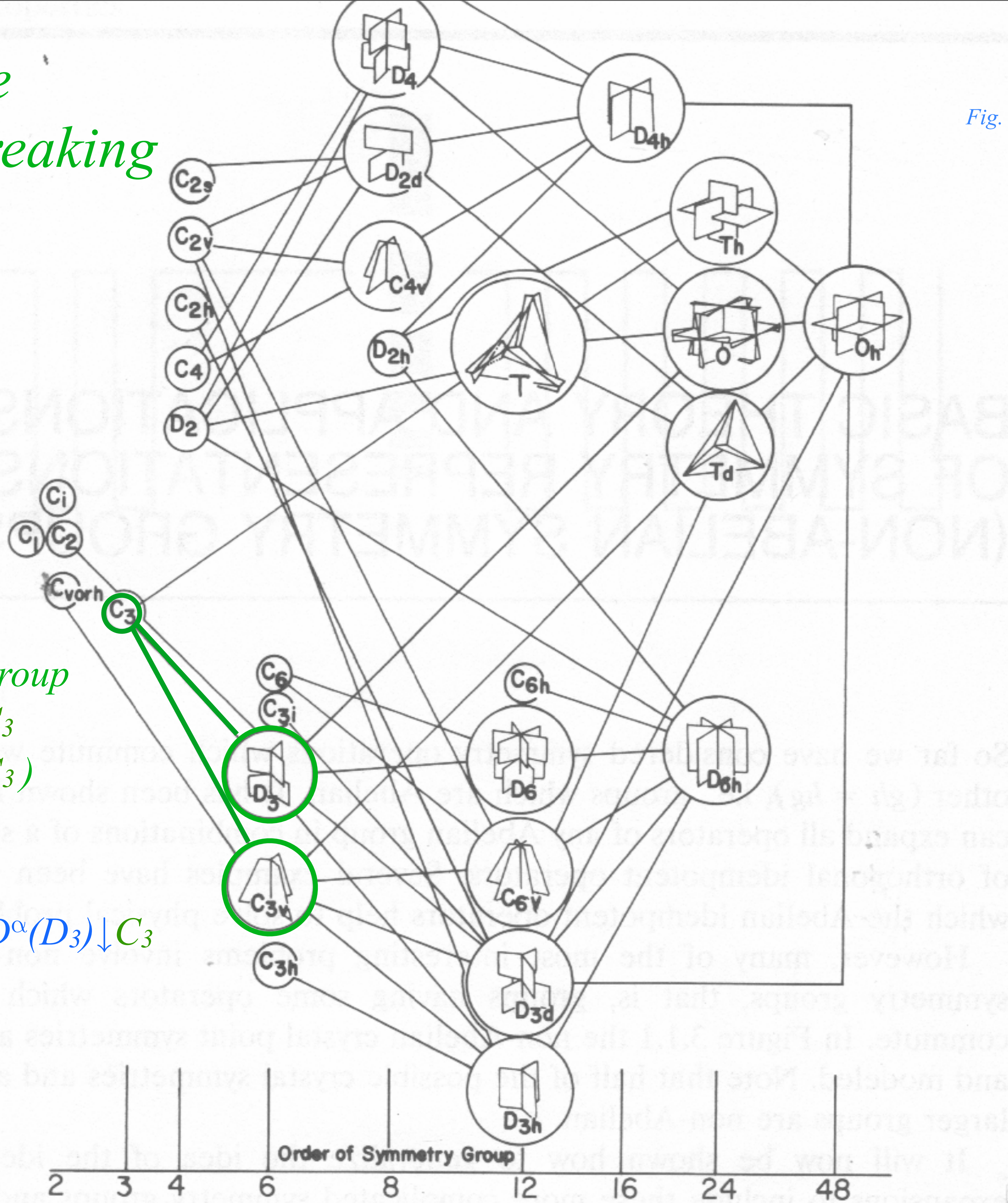


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Fig. 3.1.1 PSDS

Applied symmetry reduction and splitting: Subduced irep $D^\alpha(D_3)\downarrow C_2 = d^{0_2}\oplus d^{1_2}\oplus$.. correlation

$D_3 \supset C_2$	$\mathbf{P}^\alpha$ relabel/split	D^α relabel/reduce	ω^α relabel/split
A_1	$\mathbf{P}^{A_1}=\mathbf{P}^{A_1}\mathbf{P}^{0_2}=\mathbf{P}^{A_1}_{0_2 0_2}$	$\Rightarrow D^{A_1}\downarrow C_2 \sim d^{0_2}$	$\Rightarrow \omega^{A_1} \rightarrow \omega^{0_2}$
A_2	$\mathbf{P}^{A_2}=\mathbf{P}^{A_2}\mathbf{P}^{1_2}=\mathbf{P}^{A_2}_{1_2 1_2}$	$\Rightarrow D^{A_2}\downarrow C_2 \sim d^{1_2}$	$\Rightarrow \omega^{A_2} \rightarrow \omega^{1_2}$
E_1	$\mathbf{P}^{E_1}=\mathbf{P}^{E_1}\mathbf{P}^{0_2}+\mathbf{P}^{E_1}\mathbf{P}^{1_2}$	$\Rightarrow D^{E_1}\downarrow C_2 \sim$	$\Rightarrow \omega^{E_1} \rightarrow \omega^{0_2}$
	$=\mathbf{P}^{E_1}_{0_2 0_2}+\mathbf{P}^{E_1}_{1_2 1_2}$	$d^{0_2}\oplus d^{1_2}$	$\searrow \omega^{1_2}$

$D_3 \supset C_2$	0_2	1_2
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$d^{0_2}(C_2)\uparrow D_3 \sim D^{A_1}\oplus D^{E_1}$

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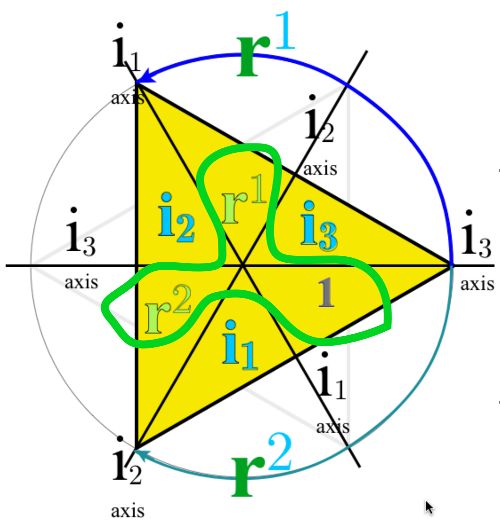

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$(0)_2$	1	1
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$\supset C_3$	$\mathbf{1}=\mathbf{r}^0$	$\mathbf{r}^1$	$\mathbf{r}^2=\mathbf{r}^{-1}$
$(0)_3$	1	1	1
$(+1)_3$	1	ε	ε^*
$(2)_3=(-1)_3$	1	ε^*	ε

Applied symmetry reduction and splitting: Subduced irep $D^{\alpha}(D_3)\downarrow C_2 = d^{0_2}\oplus d^{1_2}\oplus..$ correlation

$D_3\supset C_2$	$\mathbf{P}^{\alpha}$ relabel/split	D^{α} relabel/reduce	ω^{α} relabel/split
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A_2	$\mathbf{P}^{A_2}=\mathbf{P}^{A_2}\mathbf{P}^{1_2}=\mathbf{P}^{A_2}_{1_2 1_2}$	$\Rightarrow D^{A_2}\downarrow C_2 \sim d^{1_2}$	$\Rightarrow \omega^{A_2}\rightarrow\omega^{1_2}$
E_1	$\mathbf{P}^{E_1}=\mathbf{P}^{E_1}\mathbf{P}^{0_2}+\mathbf{P}^{E_1}\mathbf{P}^{1_2}$ $=\mathbf{P}^{E_1}_{0_2 0_2}+\mathbf{P}^{E_1}_{1_2 1_2}$	$\Rightarrow D^{E_1}\downarrow C_2 \sim$ $d^{0_2}\oplus d^{1_2}$	$\Rightarrow \omega^{E_1}\rightarrow\omega^{0_2}$ $\searrow\omega^{1_2}$

$D_3\supset C_2$	0_2	1_2
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A_2	·	1
E_1	1	1

$D^{A_1}(D_3)\downarrow C_2 \sim d^{0_2}$

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$D^{E_1}(D_3)\downarrow C_2 \sim d^{0_2}\oplus d^{1_2}$

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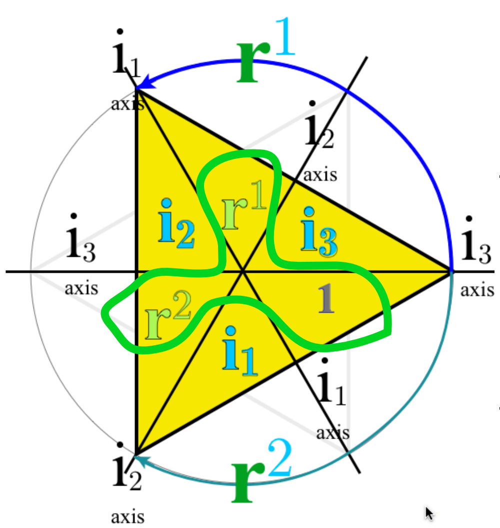

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Applied symmetry reduction and splitting: Subduced irep $D^{\alpha}(D_3)\downarrow C_3 = d^{0_3}\oplus d^{1_3}\oplus..$ correlation

$D_3\supset C_3$	0_3	1_3	2_3
A_1	1	·	·
A_2	1	·	·
E_1	·	1	1

$D^{A_1}(D_3)\downarrow C_3 \sim d^{0_3}$

$D^{A_2}(D_3)\downarrow C_3 \sim d^{0_3}$

$D^{E_1}(D_3)\downarrow C_3 \sim d^{1_3}\oplus d^{2_3}$

Applied symmetry reduction and splitting: Subduced irep $D^{\alpha}(D_3)\downarrow C_2 = d^{0_2}\oplus d^{1_2}\oplus$.. correlation

$D_3 \supset C_2$	$\mathbf{P}^{\alpha}$ relabel/split	D^{α} relabel/reduce	ω^{α} relabel/split
A_1	$\mathbf{P}^{A_1}=\mathbf{P}^{A_1}\mathbf{P}^{0_2}=\mathbf{P}^{A_1}_{0_2 0_2}$	$\Rightarrow D^{A_1}\downarrow C_2 \sim d^{0_2}$	$\Rightarrow \omega^{A_1} \rightarrow \omega^{0_2}$
A_2	$\mathbf{P}^{A_2}=\mathbf{P}^{A_2}\mathbf{P}^{1_2}=\mathbf{P}^{A_2}_{1_2 1_2}$	$\Rightarrow D^{A_2}\downarrow C_2 \sim d^{1_2}$	$\Rightarrow \omega^{A_2} \rightarrow \omega^{1_2}$
E_1	$\mathbf{P}^{E_1}=\mathbf{P}^{E_1}\mathbf{P}^{0_2}+\mathbf{P}^{E_1}\mathbf{P}^{1_2}$	$\Rightarrow D^{E_1}\downarrow C_2 \sim$	$\Rightarrow \omega^{E_1} \rightarrow \omega^{0_2}$
	$=\mathbf{P}^{E_1}_{0_2 0_2}+\mathbf{P}^{E_1}_{1_2 1_2}$	$d^{0_2}\oplus d^{1_2}$	$\searrow \omega^{1_2}$

$D_3 \supset C_2$	0_2	1_2
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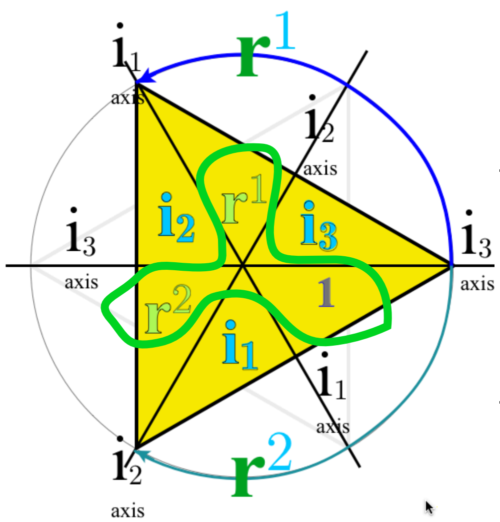

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E_1	$\mathbf{P}^{E_1}=\mathbf{P}^{E_1}\mathbf{P}^{1_3}+\mathbf{P}^{E_1}\mathbf{P}^{2_3}$	$\Rightarrow D^{E_1}\downarrow C_3 \sim$	$\Rightarrow \omega^{E_1} \rightarrow \omega^{1_3}$
	$=\mathbf{P}^{E_1}_{1_3 1_3}+\mathbf{P}^{E_1}_{2_3 2_3}$	$d^{1_3}\oplus d^{2_3}$	$\searrow \omega^{2_3}$

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Symmetry induction and clustering: Induced rep $d^{a}(C_2)\uparrow D_3 = D^{\alpha}\oplus D^{\beta}\oplus$*.. correlation*

Review: *Symmetry reduction and splitting: Subduced irep* $D^{\alpha}(D_3)\downarrow C_3 = d^{0_3}\oplus d^{1_3}\oplus$*.. correlation*

Symmetry induction and clustering: Induced rep $d^{c}(C_3)\uparrow D_3 = D^{\alpha}\oplus D^{\beta}\oplus$*.. correlation*

D_3-C_2 Coset structure of $d^{m_2}(C_2)\uparrow D_3$ induced representation basis

D_3-Projection of $d^{m_2}(C_2)\uparrow D_3$ induced representation basis

Derivation of Frobenius reciprocity

$D_6 \supset D_2 \supset C_2 = D_3 \times C_2$ symmetry and outer product geometry

Irreducible characters

Irreducible representations

Correlations with D_6 characters:

...and $C_2(\mathbf{i}_3)$ characters......and $C_6(\mathbf{1},\mathbf{h}^1,\mathbf{h}^2,...)$ characters

D_6 symmetry and induced representation band structure

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

Applied symmetry reduction and splitting: Subduced irep $D^{\alpha}(D_3)\downarrow C_2 = d^{0_2}\oplus d^{1_2}\oplus$.. correlation

$D_3 \supset C_2$	$\mathbf{P}^{\alpha}$ relabel/split	D^{α} relabel/reduce	ω^{α} relabel/split
A_1	$\mathbf{P}^{A_1}=\mathbf{P}^{A_1}\mathbf{P}^{0_2}=\mathbf{P}^{A_1}_{0_2 0_2}$	$\Rightarrow D^{A_1}\downarrow C_2 \sim d^{0_2}$	$\Rightarrow \omega^{A_1} \rightarrow \omega^{0_2}$
A_2	$\mathbf{P}^{A_2}=\mathbf{P}^{A_2}\mathbf{P}^{1_2}=\mathbf{P}^{A_2}_{1_2 1_2}$	$\Rightarrow D^{A_2}\downarrow C_2 \sim d^{1_2}$	$\Rightarrow \omega^{A_2} \rightarrow \omega^{1_2}$
E_1	$\mathbf{P}^{E_1}=\mathbf{P}^{E_1}\mathbf{P}^{0_2}+\mathbf{P}^{E_1}\mathbf{P}^{1_2}$	$\Rightarrow D^{E_1}\downarrow C_2 \sim$	$\Rightarrow \omega^{E_1} \rightarrow \omega^{0_2}$
	$=\mathbf{P}^{E_1}_{0_2 0_2}+\mathbf{P}^{E_1}_{1_2 1_2}$	$d^{0_2}\oplus d^{1_2}$	$\searrow \omega^{1_2}$

$D_3 \supset C_2$	0_2	1_2
A_1	1	·
A_2	·	1
E_1	1	1

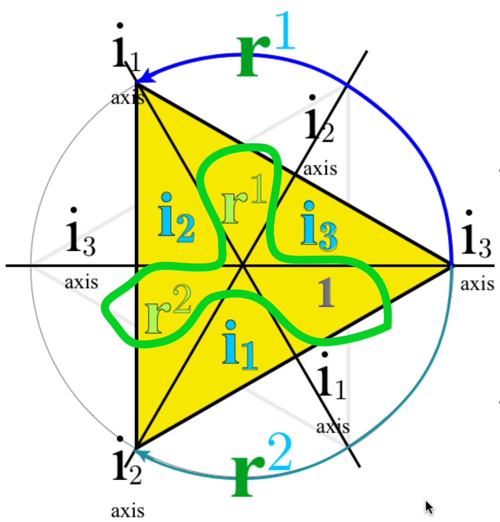
$D^{A_1}(D_3)\downarrow C_2 \sim d^{0_2}$

$D^{A_2}(D_3)\downarrow C_2 \sim d^{1_2}$

$D^{E_1}(D_3)\downarrow C_2 \sim d^{0_2}\oplus d^{1_2}$

$d^{0_2}(C_2)\uparrow D_3 \sim D^{A_1}\oplus D^{E_1}$ $\quad d^{1_2}(C_2)\uparrow D_3 \sim D^{A_2}\oplus D^{E_1}$

Spontaneous symmetry breaking and clustering: Induced rep $d^a(C_2)\uparrow D_3 = D^{\alpha}\oplus D^{\beta}\oplus$.. correlation



D_3	$\mathbf{1}$	$\{\mathbf{r}^1,\mathbf{r}^2\}$	$\{\mathbf{i}_1\mathbf{i}_2\mathbf{i}_3\}$
A_1	1	1	1
A_2	1	1	-1
E_1	2	-1	0

$\supset C_2$	$\mathbf{1}$	$\mathbf{i}_3$
$(0)_2$	1	1
$(1)_2$	1	-1

$\supset C_3$	$\mathbf{1}=\mathbf{r}^0$	$\mathbf{r}^1$	$\mathbf{r}^2=\mathbf{r}^{-1}$
$(0)_3$	1	1	1
$(+1)_3$	1	ε	ε^*
$(2)_3=(-1)_3$	1	ε^*	ε

Applied symmetry reduction and splitting: Subduced irep $D^{\alpha}(D_3)\downarrow C_3 = d^{0_3}\oplus d^{1_3}\oplus$.. correlation

$D_3 \supset C_3$	$\mathbf{P}^{\alpha}$ relabel/split	D^{α} relabel/reduce	ω^{α} relabel/split
A_1	$\mathbf{P}^{A_1}=\mathbf{P}^{A_1}\mathbf{P}^{0_3}=\mathbf{P}^{A_1}_{0_3 0_3}$	$\Rightarrow D^{A_1}\downarrow C_3 \sim d^{0_3}$	$\Rightarrow \omega^{A_1} \rightarrow \omega^{0_3}$
A_2	$\mathbf{P}^{A_2}=\mathbf{P}^{A_2}\mathbf{P}^{0_3}=\mathbf{P}^{A_2}_{0_3 0_3}$	$\Rightarrow D^{A_2}\downarrow C_3 \sim d^{0_3}$	$\Rightarrow \omega^{A_2} \rightarrow \omega^{0_3}$
E_1	$\mathbf{P}^{E_1}=\mathbf{P}^{E_1}\mathbf{P}^{1_3}+\mathbf{P}^{E_1}\mathbf{P}^{2_3}$	$\Rightarrow D^{E_1}\downarrow C_3 \sim$	$\Rightarrow \omega^{E_1} \rightarrow \omega^{1_3}$
	$=\mathbf{P}^{E_1}_{1_3 1_3}+\mathbf{P}^{E_1}_{2_3 2_3}$	$d^{1_3}\oplus d^{2_3}$	$\searrow \omega^{2_3}$

$D_3 \supset C_3$	0_3	1_3	2_3
A_1	1	·	·
A_2	1	·	·
E_1	·	1	1

$D^{A_1}(D_3)\downarrow C_3 \sim d^{0_3}$

$D^{A_2}(D_3)\downarrow C_3 \sim d^{0_3}$

$D^{E_1}(D_3)\downarrow C_3 \sim d^{1_3}\oplus d^{2_3}$

$d^{0_3}(C_3)\uparrow D_3 \sim D^{A_1}\oplus D^{A_2}$ $\quad d^{1_3}(C_3)\uparrow D_3 \sim D^{E_1}$ $\quad d^{2_3}(C_3)\uparrow D_3 \sim D^{E_1}$

Spontaneous symmetry breaking and clustering: Induced rep $d^a(C_3)\uparrow D_3 = D^{\alpha}\oplus D^{\beta}\oplus$.. correlation

Review: Symmetry reduction and splitting: Subduced irep $D^{\alpha}(D_3)\downarrow C_2 = d^{0_2}\oplus d^{1_2}\oplus$.. correlation

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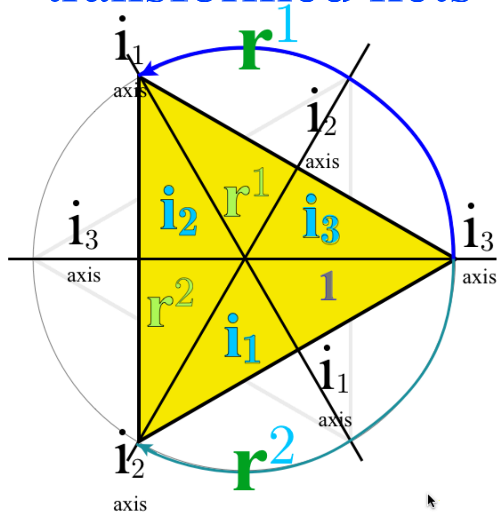
D_3-C_2 Coset structure of $d^{m_2}(C_2)\uparrow D^3$ induced representation basis

Left cosets $[\mathbf{1}C_2 = (\mathbf{1},\mathbf{i}_3), \quad \mathbf{r}^1 C_2 = (\mathbf{r}^1,\mathbf{i}_2), \quad \mathbf{r}^2 C_2 = (\mathbf{r}^2,\mathbf{i}_1)]$ relate to sets of $\mathbf{r}^p$-transformed kets



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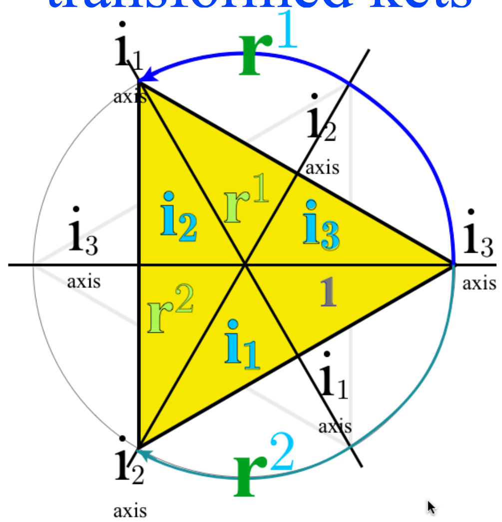
$$[\mathbf{1}(|\mathbf{1}\rangle,|\mathbf{i}_3\rangle) = (|\mathbf{1}\rangle,|\mathbf{i}_3\rangle),\quad \mathbf{r}^1(|\mathbf{1}\rangle,|\mathbf{i}_3\rangle) = (|\mathbf{r}^1\rangle,|\mathbf{i}_2\rangle),\quad \mathbf{r}^2(|\mathbf{1}\rangle,|\mathbf{i}_3\rangle) = (|\mathbf{r}^2\rangle,|\mathbf{i}_1\rangle)]$$



D_3-C_2 Coset structure of $d^{m_2}(C_2)\uparrow D^3$ induced representation basis

Left cosets $[\mathbf{1}C_2=(\mathbf{1},\mathbf{i}_3),\quad \mathbf{r}^1C_2=(\mathbf{r}^1,\mathbf{i}_2),\quad \mathbf{r}^2C_2=(\mathbf{r}^2,\mathbf{i}_1)]$ relate to sets of $\mathbf{r}^p$-transformed kets

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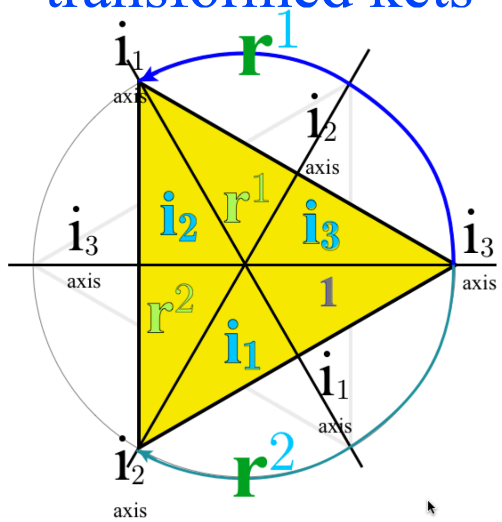
Right cosets $[C_2=(\mathbf{1},\mathbf{i}_3),\ C_2\mathbf{r}^2=(\mathbf{r}^2,\mathbf{i}_2),\ C_2\mathbf{r}=(\mathbf{r},\mathbf{i}_1)]$ relate to sets of bras



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Left cosets $[\mathbf{1}C_2=(\mathbf{1},\mathbf{i}_3),\quad \mathbf{r}^1C_2=(\mathbf{r}^1,\mathbf{i}_2),\quad \mathbf{r}^2C_2=(\mathbf{r}^2,\mathbf{i}_1)]$ relate to sets of $\mathbf{r}^p$-transformed kets

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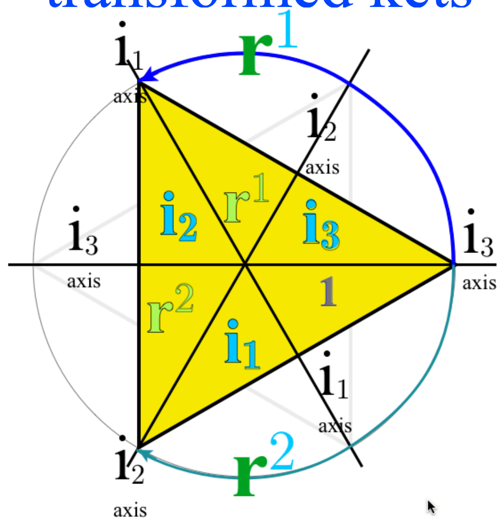
$$[(\langle\mathbf{1}|,\langle\mathbf{i}_3|)\mathbf{1}=(\langle\mathbf{1}|,\langle\mathbf{i}_3|),\quad (\langle\mathbf{1}|,\langle\mathbf{i}_3|)\mathbf{r}^2=(\langle\mathbf{r}^1|,\langle\mathbf{i}_2|),\quad (\langle\mathbf{1}|,\langle\mathbf{i}_3|)\mathbf{r}^1=(\langle\mathbf{r}^2|,\langle\mathbf{i}_1|)]$$



D_3-C_2 Coset structure of $d^{m_2}(C_2)\uparrow D^3$ induced representation basis

Left cosets $[\mathbf{1}C_2=(\mathbf{1},\mathbf{i}_3),\quad \mathbf{r}^1C_2=(\mathbf{r}^1,\mathbf{i}_2),\quad \mathbf{r}^2C_2=(\mathbf{r}^2,\mathbf{i}_1)]$ relate to sets of $\mathbf{r}^p$-transformed kets

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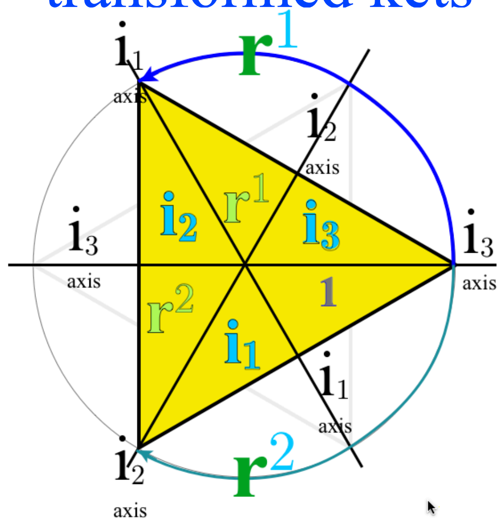

C_2 projectors $\mathbf{P}^{0_2}=\frac{1}{2}(\mathbf{1}+\mathbf{i}_3)=\mathbf{P}^x$ and $\mathbf{P}^{1_2}=\frac{1}{2}(\mathbf{1}-\mathbf{i}_3)=\mathbf{P}^y$ split ket $|\mathbf{r}\rangle=\mathbf{r}|\mathbf{1}\rangle$ or bra $\langle\mathbf{r}|=\langle\mathbf{1}|\mathbf{r}^\dagger$ into ± coset sums

D_3-C_2 Coset structure of $d^{m_2}(C_2)\uparrow D^3$ induced representation basis

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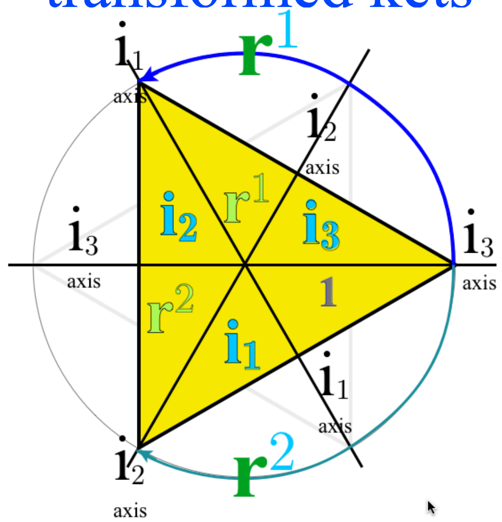

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$$\left[\mathbf{P}^{n_2}|\mathbf{1}\rangle=\tfrac{1}{2}(|\mathbf{1}\rangle\pm|\mathbf{i}_3\rangle),\qquad\qquad\right]=\left[\left|\mathbf{r}^0_n\right\rangle\quad ,\quad\right]$$ basis of $d^{n_2}\uparrow D_3$

D_3-C_2 Coset structure of $d^{m_2}(C_2)\uparrow D^3$ induced representation basis

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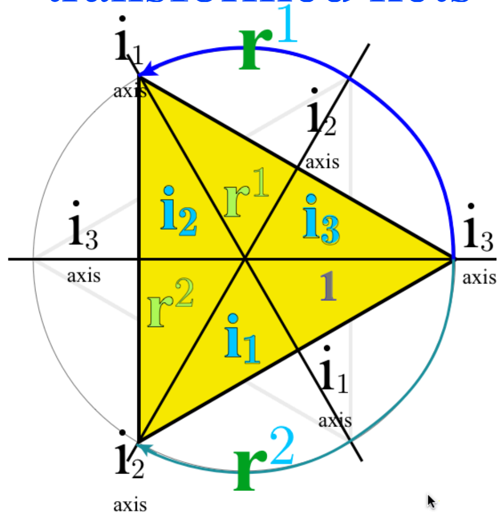

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D_6 *symmetry and induced representation band structure*

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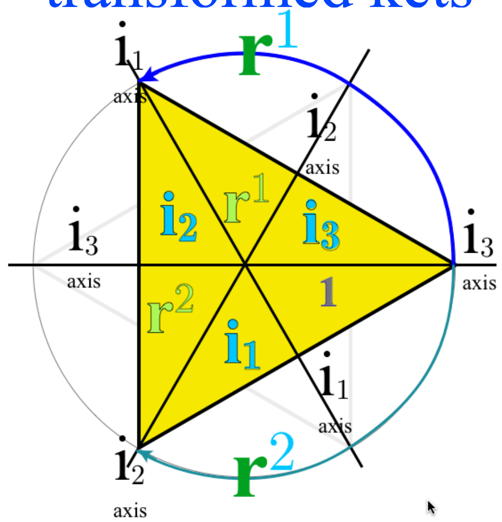

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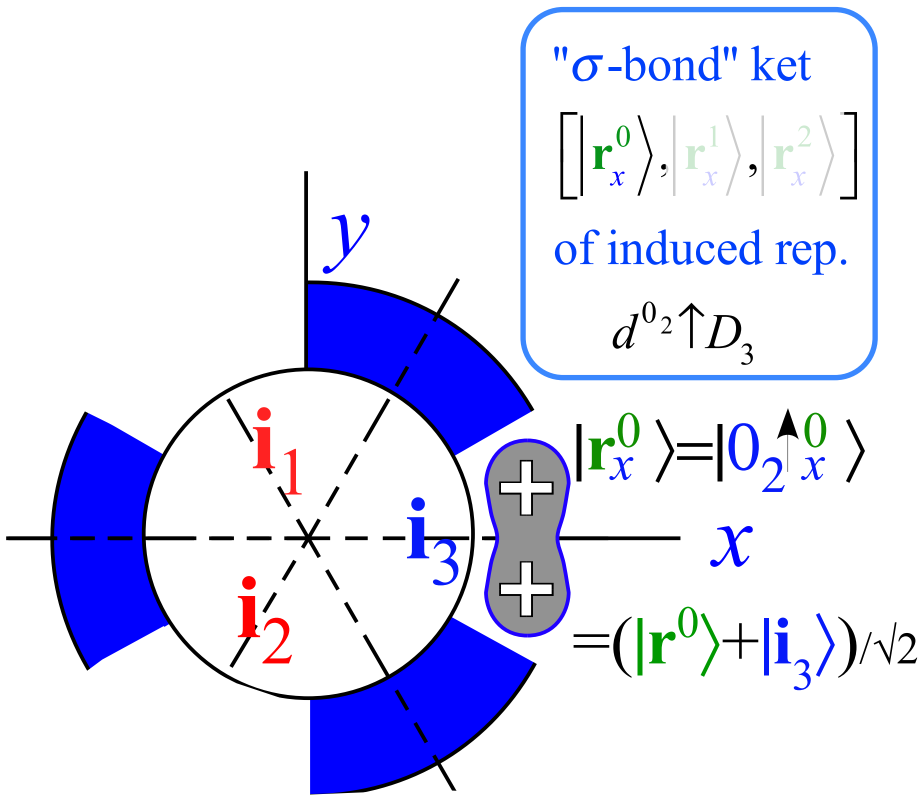

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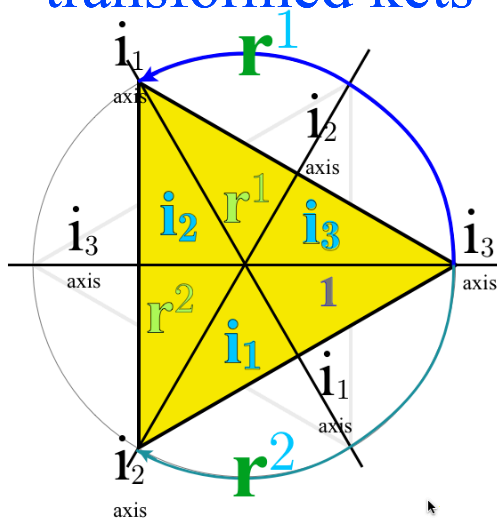

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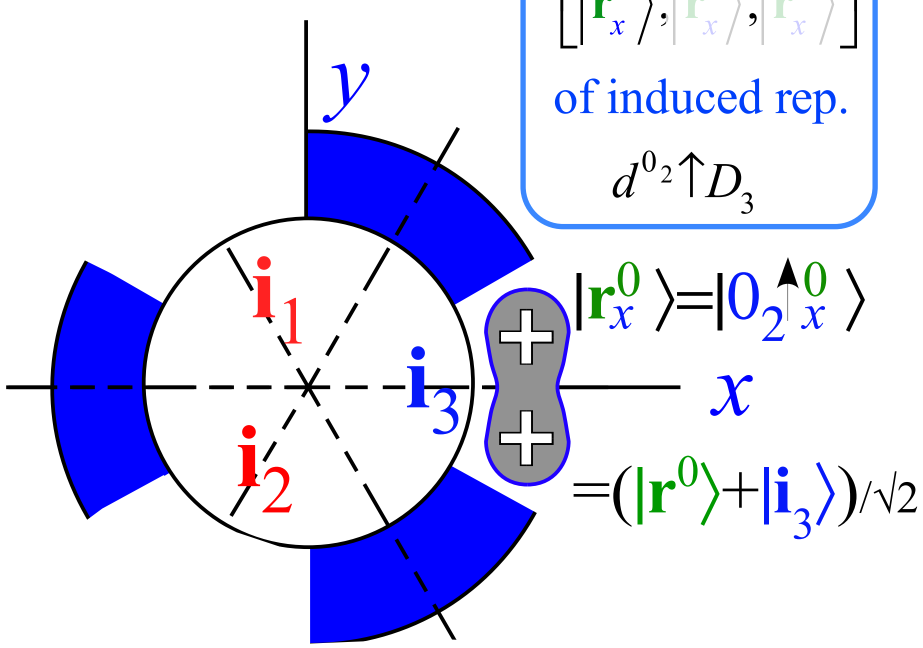
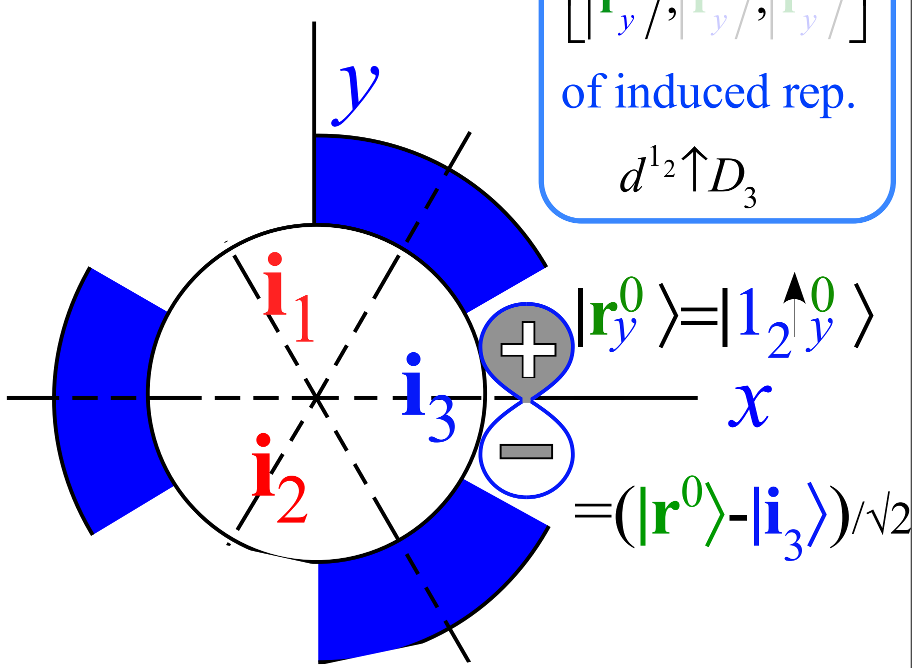
$$\left[\langle\mathbf{1}|\mathbf{P}^{n_2}=\tfrac{1}{2}(\langle\mathbf{1}|\pm\langle\mathbf{i}_3|),\qquad\right]=\left[\langle\mathbf{r}^0_n|\quad,\quad\right]\text{basis of } d^{n_2}\uparrow D_3$$



"σ-bond" ket $[|\mathbf{r}^0_x\rangle,|\mathbf{r}^1_x\rangle,|\mathbf{r}^2_x\rangle]$ of induced rep. $d^{0_2}\uparrow D_3$



"π-bond" ket $[|\mathbf{r}^0_y\rangle,|\mathbf{r}^1_y\rangle,|\mathbf{r}^2_y\rangle]$ of induced rep. $d^{1_2}\uparrow D_3$

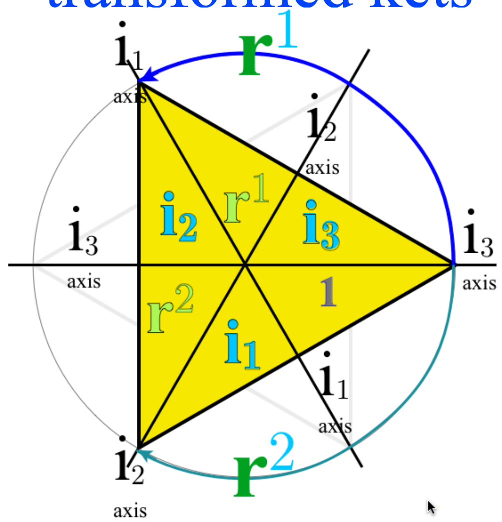
D_3-C_2 Coset structure of $d^{m_2}(C_2)\uparrow D^3$ induced representation basis

Left cosets $[\mathbf{1}C_2 = (\mathbf{1},\mathbf{i}_3),\quad \mathbf{r}^1C_2 = (\mathbf{r}^1,\mathbf{i}_2),\quad \mathbf{r}^2C_2 = (\mathbf{r}^2,\mathbf{i}_1)]$ relate to sets of $\mathbf{r}^p$-transformed kets

$$[\mathbf{1}(|\mathbf{1}\rangle,|\mathbf{i}_3\rangle) = (|\mathbf{1}\rangle,|\mathbf{i}_3\rangle),\quad \mathbf{r}^1(|\mathbf{1}\rangle,|\mathbf{i}_3\rangle) = (|\mathbf{r}^1\rangle,|\mathbf{i}_2\rangle),\quad \mathbf{r}^2(|\mathbf{1}\rangle,|\mathbf{i}_3\rangle) = (|\mathbf{r}^2\rangle,|\mathbf{i}_1\rangle)]$$

Right cosets $[C_2=(\mathbf{1},\mathbf{i}_3),\ C_2\mathbf{r}^2=(\mathbf{r}^2,\mathbf{i}_2),\ C_2\mathbf{r}=(\mathbf{r},\mathbf{i}_1)]$ relate to sets of bras

$$[(\langle\mathbf{1}|,\langle\mathbf{i}_3|)\mathbf{1} = (\langle\mathbf{1}|,\langle\mathbf{i}_3|),\quad (\langle\mathbf{1}|,\langle\mathbf{i}_3|)\mathbf{r}^2 = (\langle\mathbf{r}^1|,\langle\mathbf{i}_2|),\quad (\langle\mathbf{1}|,\langle\mathbf{i}_3|)\mathbf{r}^1 = (\langle\mathbf{r}^2|,\langle\mathbf{i}_1|)]$$

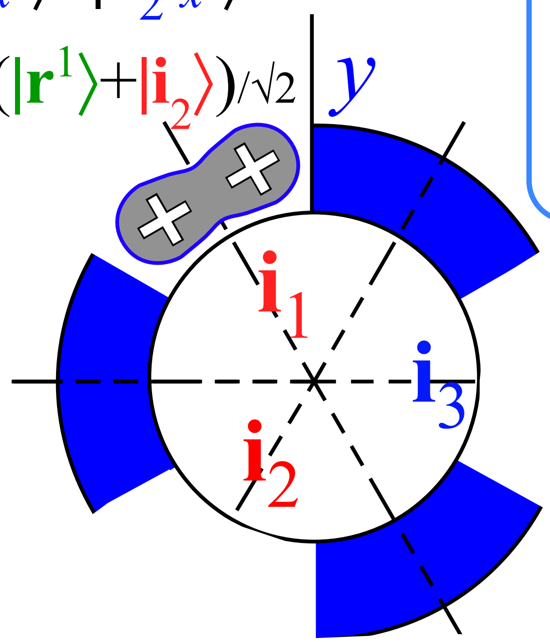


C_2 projectors $\mathbf{P}^{0_2}=\frac{1}{2}(\mathbf{1}+\mathbf{i}_3)=\mathbf{P}^x$ and $\mathbf{P}^{1_2}=\frac{1}{2}(\mathbf{1}-\mathbf{i}_3)=\mathbf{P}^y$ split ket $|\mathbf{r}\rangle=\mathbf{r}|\mathbf{1}\rangle$ or bra $\langle\mathbf{r}|=\langle\mathbf{1}|\mathbf{r}^\dagger$ into $\pm$ coset sums

$$\left[\quad ,\ \mathbf{P}^{n_2}|\mathbf{r}^1\rangle=\tfrac{1}{2}(|\mathbf{r}^1\rangle\pm|\mathbf{i}_2\rangle),\quad\right]=\left[\quad ,|\mathbf{r}^1_n\rangle,\quad\right]$$ basis of $d^{n_2}\uparrow D_3$

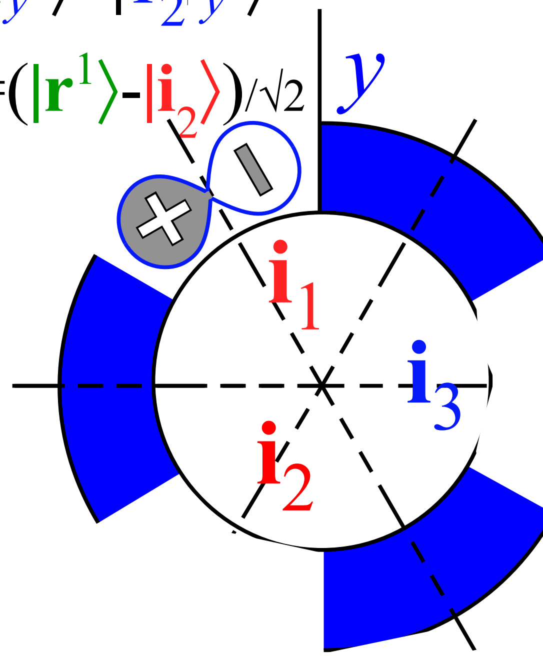
$$\left[\quad ,\ \langle\mathbf{r}^1|\mathbf{P}^{n_2}=\tfrac{1}{2}(\langle\mathbf{r}^1|\pm\langle\mathbf{i}_2|),\quad\right]=\left[\quad ,\langle\mathbf{r}^1_n|,\quad\right]$$ basis of $d^{n_2}\uparrow D_3$

$|\mathbf{r}^1_x\rangle=|0_2{\uparrow}^1_x\rangle$
$=(|\mathbf{r}^1\rangle+|\mathbf{i}_2\rangle)/\sqrt{2}$



"σ-bond" ket
$[|\mathbf{r}^0_x\rangle,|\mathbf{r}^1_x\rangle,|\mathbf{r}^2_x\rangle]$
of induced rep.
$d^{0_2}\uparrow D_3$

$|\mathbf{r}^1_y\rangle=|1_2{\uparrow}^1_y\rangle$
$=(|\mathbf{r}^1\rangle-|\mathbf{i}_2\rangle)/\sqrt{2}$

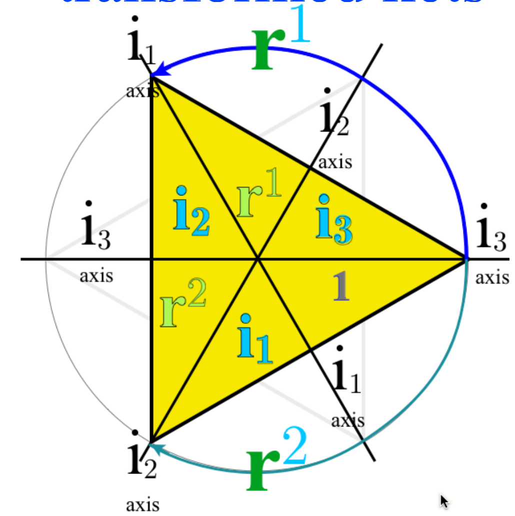


"π-bond" ket
$[|\mathbf{r}^0_y\rangle,|\mathbf{r}^1_y\rangle,|\mathbf{r}^2_y\rangle]$
of induced rep.
$d^{1_2}\uparrow D_3$

D_3-C_2 Coset structure of $d^{m_2}(C_2)\uparrow D^3$ induced representation basis

Left cosets $[\mathbf{1}C_2=(\mathbf{1},\mathbf{i}_3),\quad \mathbf{r}^1C_2=(\mathbf{r}^1,\mathbf{i}_2),\quad \mathbf{r}^2C_2=(\mathbf{r}^2,\mathbf{i}_1)]$ relate to sets of $\mathbf{r}^p$-transformed kets

$$[\mathbf{1}(|\mathbf{1}\rangle,|\mathbf{i}_3\rangle)=(|\mathbf{1}\rangle,|\mathbf{i}_3\rangle),\quad \mathbf{r}^1(|\mathbf{1}\rangle,|\mathbf{i}_3\rangle)=(|\mathbf{r}^1\rangle,|\mathbf{i}_2\rangle),\quad \mathbf{r}^2(|\mathbf{1}\rangle,|\mathbf{i}_3\rangle)=(|\mathbf{r}^2\rangle,|\mathbf{i}_1\rangle)]$$



Right cosets $[C_2=(\mathbf{1},\mathbf{i}_3),\ C_2\mathbf{r}^2=(\mathbf{r}^2,\mathbf{i}_2),\ C_2\mathbf{r}=(\mathbf{r},\mathbf{i}_1)]$ relate to sets of bras

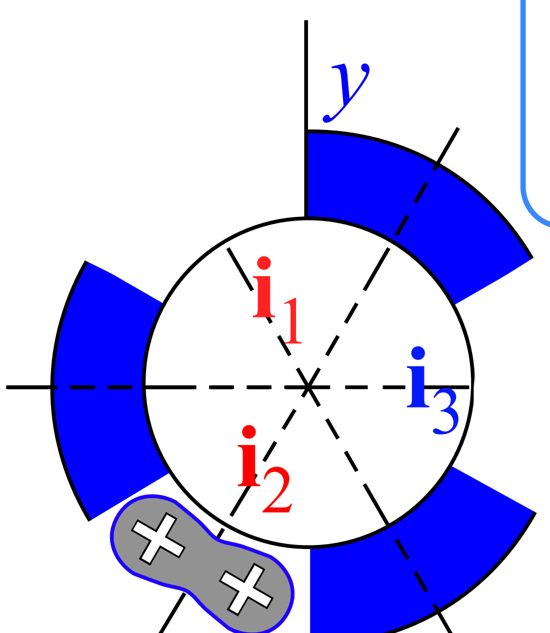
$$[(\langle\mathbf{1}|,\langle\mathbf{i}_3|)\mathbf{1}=(\langle\mathbf{1}|,\langle\mathbf{i}_3|),\quad (\langle\mathbf{1}|,\langle\mathbf{i}_3|)\mathbf{r}^2=(\langle\mathbf{r}^1|,\langle\mathbf{i}_2|),\quad (\langle\mathbf{1}|,\langle\mathbf{i}_3|)\mathbf{r}^1=(\langle\mathbf{r}^2|,\langle\mathbf{i}_1|)]$$

C_2 projectors $\mathbf{P}^{0_2}=\frac{1}{2}(\mathbf{1}+\mathbf{i}_3)=\mathbf{P}^x$ and $\mathbf{P}^{1_2}=\frac{1}{2}(\mathbf{1}-\mathbf{i}_3)=\mathbf{P}^y$ split ket $|\mathbf{r}\rangle=\mathbf{r}|\mathbf{1}\rangle$ or bra $\langle\mathbf{r}|=\langle\mathbf{1}|\mathbf{r}^\dagger$ into $\pm$ coset sums

$$\Big[\qquad\qquad ,\qquad\qquad \mathbf{P}^{n_2}|\mathbf{r}^2\rangle=\tfrac{1}{2}(|\mathbf{r}^2\rangle\pm|\mathbf{i}_1\rangle)\Big]=\Big[\qquad ,|\mathbf{r}_n^2\rangle\Big]$$ basis of $d^{n_2}\uparrow D_3$

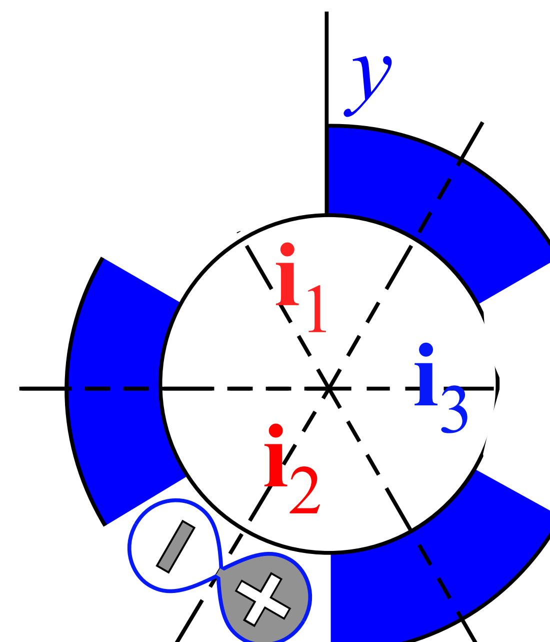
$$\Big[\qquad\qquad ,\qquad\qquad \langle\mathbf{r}^2|\mathbf{P}^{n_2}=\tfrac{1}{2}(\langle\mathbf{r}^2|\pm\langle\mathbf{i}_1|)\Big]=\Big[\qquad ,\langle\mathbf{r}_n^2|\Big]$$ basis of $d^{n_2}\uparrow D_3$

"σ-bond" ket $\left[|\mathbf{r}_x^0\rangle,|\mathbf{r}_x^1\rangle,|\mathbf{r}_x^2\rangle\right]$ of induced rep. $d^{0_2}\uparrow D_3$



$|\mathbf{r}_x^2\rangle=|0_2\uparrow_x^2\rangle=(|\mathbf{r}^2\rangle+|\mathbf{i}_1\rangle)/\sqrt{2}$

"π-bond" ket $\left[|\mathbf{r}_y^0\rangle,|\mathbf{r}_y^1\rangle,|\mathbf{r}_y^2\rangle\right]$ of induced rep. $d^{1_2}\uparrow D_3$



$|\mathbf{r}_y^2\rangle=|1_2\uparrow_y^2\rangle=(|\mathbf{r}^2\rangle-|\mathbf{i}_1\rangle)/\sqrt{2}$

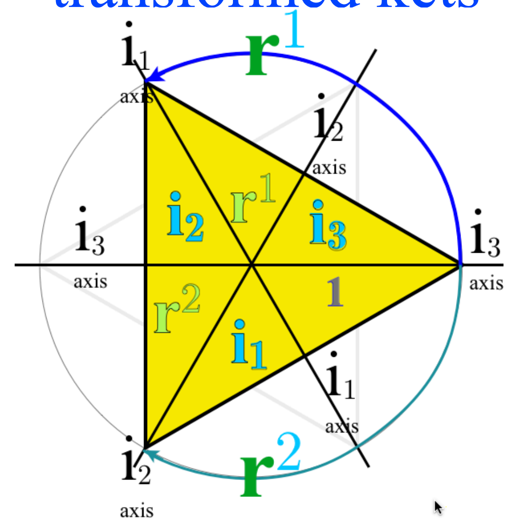
D_3-C_2 Coset structure of $d^{m_2}(C_2)\uparrow D^3$ induced representation basis

Left cosets $[\mathbf{1}C_2=(\mathbf{1},\mathbf{i}_3),\quad \mathbf{r}^1C_2=(\mathbf{r}^1,\mathbf{i}_2),\quad \mathbf{r}^2C_2=(\mathbf{r}^2,\mathbf{i}_1)]$ relate to sets of $\mathbf{r}^p$-transformed kets

$$[\mathbf{1}(|\mathbf{1}\rangle,|\mathbf{i}_3\rangle)=(|\mathbf{1}\rangle,|\mathbf{i}_3\rangle),\quad \mathbf{r}^1(|\mathbf{1}\rangle,|\mathbf{i}_3\rangle)=(|\mathbf{r}^1\rangle,|\mathbf{i}_2\rangle),\quad \mathbf{r}^2(|\mathbf{1}\rangle,|\mathbf{i}_3\rangle)=(|\mathbf{r}^2\rangle,|\mathbf{i}_1\rangle)]$$

Right cosets $[C_2=(\mathbf{1},\mathbf{i}_3),\ C_2\mathbf{r}^2=(\mathbf{r}^2,\mathbf{i}_2),\ C_2\mathbf{r}=(\mathbf{r},\mathbf{i}_1)]$ relate to sets of bras

$$[(\langle\mathbf{1}|,\langle\mathbf{i}_3|)\mathbf{1}=(\langle\mathbf{1}|,\langle\mathbf{i}_3|),\quad (\langle\mathbf{1}|,\langle\mathbf{i}_3|)\mathbf{r}^2=(\langle\mathbf{r}^1|,\langle\mathbf{i}_2|),\quad (\langle\mathbf{1}|,\langle\mathbf{i}_3|)\mathbf{r}^1=(\langle\mathbf{r}^2|,\langle\mathbf{i}_1|)]$$



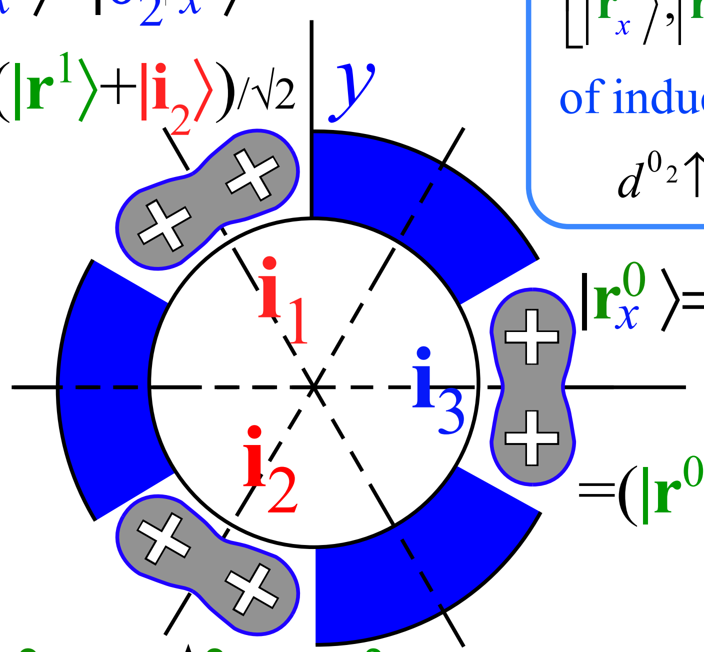
C_2 projectors $\mathbf{P}^{0_2}=\frac{1}{2}(\mathbf{1}+\mathbf{i}_3)=\mathbf{P}^x$ and $\mathbf{P}^{1_2}=\frac{1}{2}(\mathbf{1}-\mathbf{i}_3)=\mathbf{P}^y$ split ket $|\mathbf{r}\rangle=\mathbf{r}|\mathbf{1}\rangle$ or bra $\langle\mathbf{r}|=\langle\mathbf{1}|\mathbf{r}^\dagger$ into $\pm$ coset sums

$$\left[\mathbf{P}^{n_2}|\mathbf{1}\rangle=\tfrac{1}{2}(|\mathbf{1}\rangle\pm|\mathbf{i}_3\rangle),\ \mathbf{P}^{n_2}|\mathbf{r}^1\rangle=\tfrac{1}{2}(|\mathbf{r}^1\rangle\pm|\mathbf{i}_2\rangle),\ \mathbf{P}^{n_2}|\mathbf{r}^2\rangle=\tfrac{1}{2}(|\mathbf{r}^2\rangle\pm|\mathbf{i}_1\rangle)\right]=\left[|\mathbf{r}_n^0\rangle,|\mathbf{r}_n^1\rangle,|\mathbf{r}_n^2\rangle\right] \text{basis of } d^{n_2}\uparrow D_3$$

$$\left[\langle\mathbf{1}|\mathbf{P}^{n_2}=\tfrac{1}{2}(\langle\mathbf{1}|\pm\langle\mathbf{i}_3|),\ \langle\mathbf{r}^1|\mathbf{P}^{n_2}=\tfrac{1}{2}(\langle\mathbf{r}^1|\pm\langle\mathbf{i}_2|),\ \langle\mathbf{r}^2|\mathbf{P}^{n_2}=\tfrac{1}{2}(\langle\mathbf{r}^2|\pm\langle\mathbf{i}_1|)\right]=\left[\langle\mathbf{r}_n^0|,\langle\mathbf{r}_n^1|,\langle\mathbf{r}_n^2|\right] \text{basis of } d^{n_2}\uparrow D_3$$

$|\mathbf{r}_x^1\rangle=|0_2\!\uparrow^1_x\rangle=(|\mathbf{r}^1\rangle+|\mathbf{i}_2\rangle)/\sqrt{2}$

3 "σ-bond" kets $\left[|\mathbf{r}_x^0\rangle,|\mathbf{r}_x^1\rangle,|\mathbf{r}_x^2\rangle\right]$ of induced rep. $d^{0_2}\uparrow D_3$

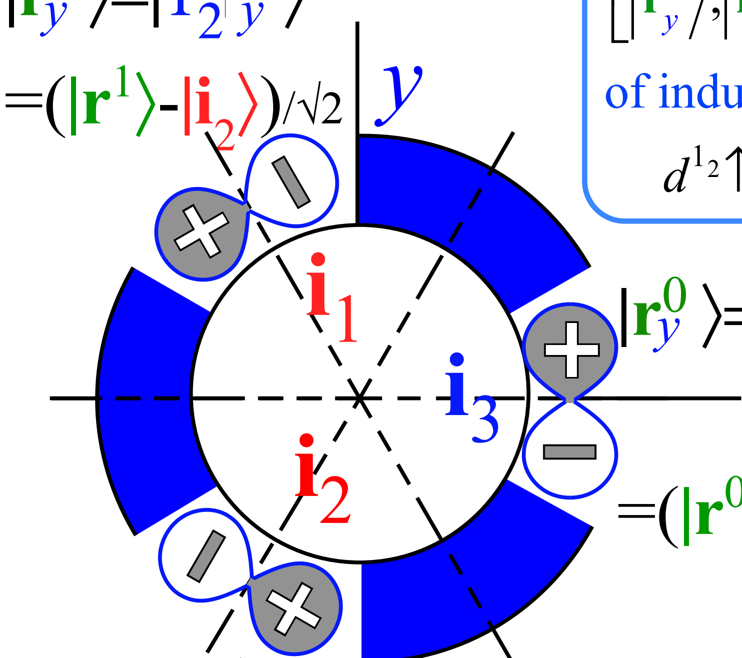


$|\mathbf{r}_x^0\rangle=|0_2\!\uparrow^0_x\rangle=(|\mathbf{r}^0\rangle+|\mathbf{i}_3\rangle)/\sqrt{2}$

$|\mathbf{r}_x^2\rangle=|0_2\!\uparrow^2_x\rangle=(|\mathbf{r}^2\rangle+|\mathbf{i}_1\rangle)/\sqrt{2}$

$|\mathbf{r}_y^1\rangle=|1_2\!\uparrow^1_y\rangle=(|\mathbf{r}^1\rangle-|\mathbf{i}_2\rangle)/\sqrt{2}$

3 "π-bond" kets $\left[|\mathbf{r}_y^0\rangle,|\mathbf{r}_y^1\rangle,|\mathbf{r}_y^2\rangle\right]$ of induced rep. $d^{1_2}\uparrow D_3$



$|\mathbf{r}_y^0\rangle=|1_2\!\uparrow^0_y\rangle=(|\mathbf{r}^0\rangle-|\mathbf{i}_3\rangle)/\sqrt{2}$

$|\mathbf{r}_y^2\rangle=|1_2\!\uparrow^2_y\rangle=(|\mathbf{r}^2\rangle-|\mathbf{i}_1\rangle)/\sqrt{2}$

Review: Symmetry reduction and splitting: Subduced irep $D^{\alpha}(D_3)\downarrow C_2 = d^{0_2} \oplus d^{1_2} \oplus$.. correlation

Symmetry induction and clustering: Induced rep $d^a(C_2)\uparrow D_3 = D^{\alpha} \oplus D^{\beta} \oplus$.. correlation

D_3-C_2 Coset structure of $d^{m_2}(C_2)\uparrow D_3$ induced representation basis

D_3-Projection of $d^{m_2}(C_2)\uparrow D_3$ induced representation basis

Derivation of Frobenius reciprocity

$D_6 \supset D_2 \supset C_2 = D_3 \times C_2$ symmetry and outer product geometry

Irreducible characters

Irreducible representations

Correlations with D_6 characters:

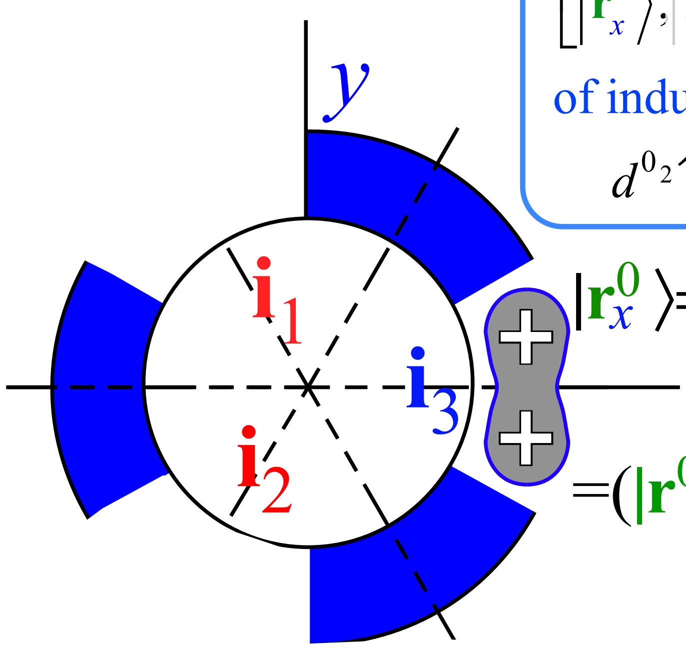
...and $C_2(\mathbf{i}_3)$ characters......and $C_6(\mathbf{1},\mathbf{h}^1,\mathbf{h}^2,...)$ characters

D_6 symmetry and induced representation band structure

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

$D_3 \supset C_2$ projectors $\mathbf{P}^{A_1}_{0_2 0_2}, \mathbf{P}^{A_2}_{1_2 1_2}, \mathbf{P}^{E_1}_{0_2 0_2}, \mathbf{P}^{E_1}_{0_2 1_2}, \mathbf{P}^{E_1}_{1_2 0_2}, \mathbf{P}^{E_1}_{1_2 1_2}$ must reduce induced representation $d^{m_2}(C_2)\uparrow D_3$

"σ-bond" ket $\left[|\mathbf{r}^0_x\rangle, |\mathbf{r}^1_x\rangle, |\mathbf{r}^2_x\rangle\right]$ of induced rep. $d^{0_2}\uparrow D_3$



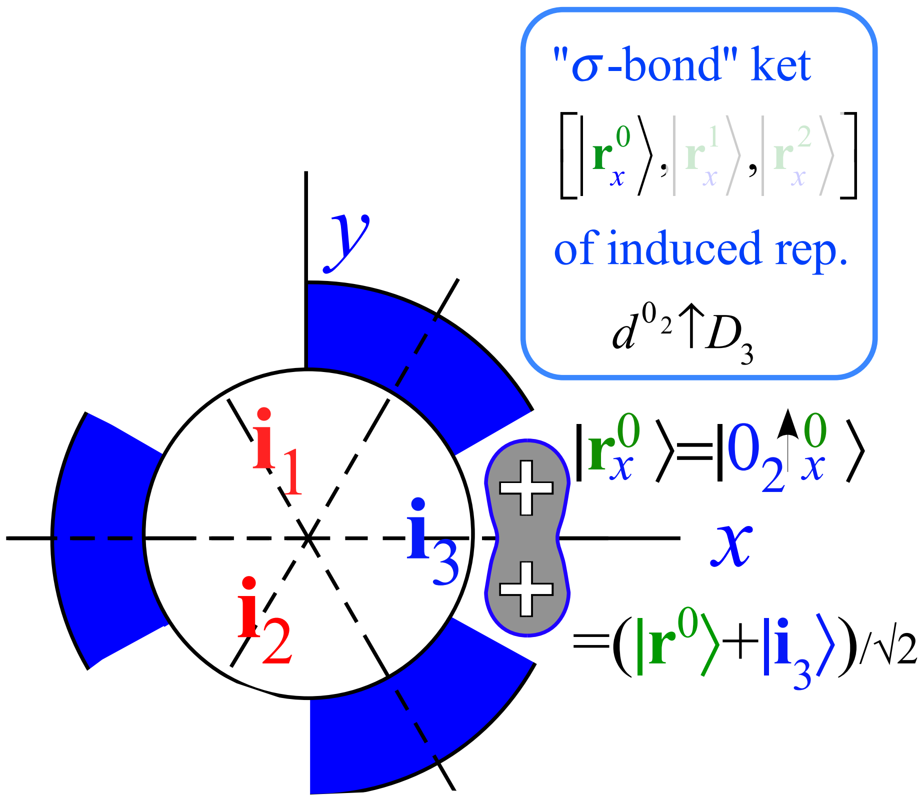
$|\mathbf{r}^0_x\rangle = |0_2 \uparrow^0_x\rangle$

$= (|\mathbf{r}^0\rangle + |\mathbf{i}_3\rangle)/\sqrt{2}$

D_3-C_2 Coset structure of $d^{m_2}(C_2)\uparrow D^3$ induced representation basis

$D_3 \supset C_2$ projectors $\mathbf{P}^{A_1}_{0_2 0_2}, \mathbf{P}^{A_2}_{1_2 1_2}, \mathbf{P}^{E_1}_{0_2 0_2}, \mathbf{P}^{E_1}_{0_2 1_2}, \mathbf{P}^{E_1}_{1_2 0_2}, \mathbf{P}^{E_1}_{1_2 1_2}$ must reduce induced representation $d^{m_2}(C_2)\uparrow D_3$

But, which D_3 projector $\mathbf{P}^{\mu}_{j_2 k_2}$ will work on base $\left|\mathbf{r}^0_{m_2}\right\rangle = \mathbf{p}^{m_2}\left|\mathbf{1}\right\rangle$ of induced representation $d^{m_2}(C_2)\uparrow D_3$

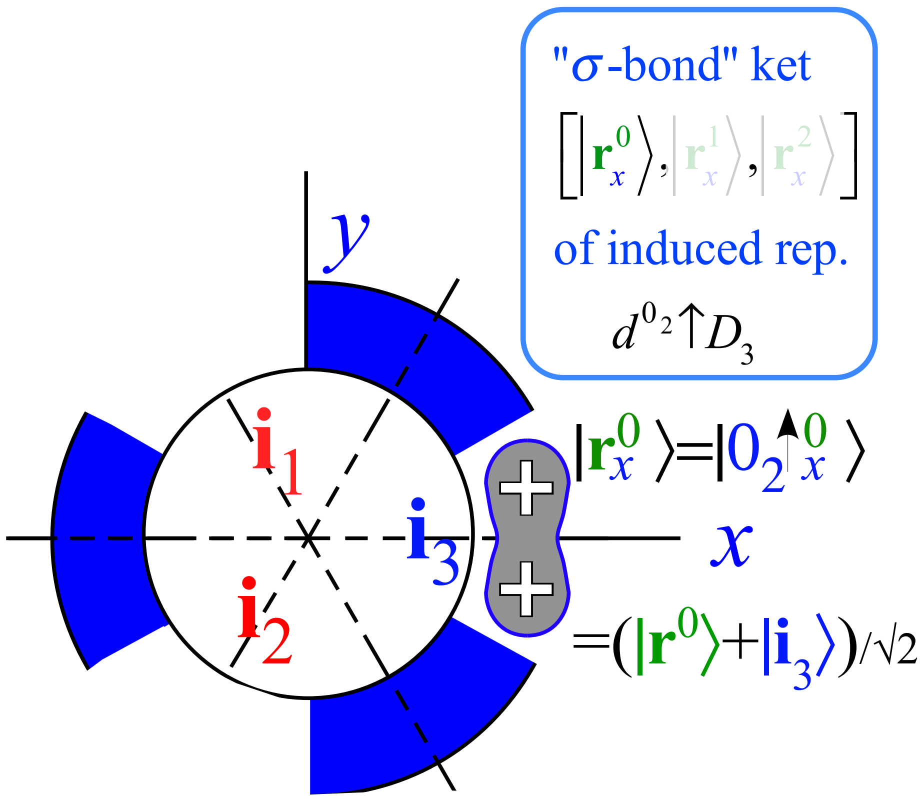


D_3-C_2 Coset structure of $d^{m_2}(C_2)\uparrow D^3$ induced representation basis

$D_3 \supset C_2$ projectors $\mathbf{P}^{A_1}_{0_2 0_2}, \mathbf{P}^{A_2}_{1_2 1_2}, \mathbf{P}^{E_1}_{0_2 0_2}, \mathbf{P}^{E_1}_{0_2 1_2}, \mathbf{P}^{E_1}_{1_2 0_2}, \mathbf{P}^{E_1}_{1_2 1_2}$ must reduce induced representation $d^{m_2}(C_2)\uparrow D_3$

But, which D_3 projector $\mathbf{P}^{\mu}_{j_2 k_2}$ will work on base $\left|\mathbf{r}^0_{m_2}\right\rangle = \mathbf{p}^{m_2}\left|\mathbf{1}\right\rangle$ of induced representation $d^{m_2}(C_2)\uparrow D_3$

$$\mathbf{P}^{\mu}_{j_2 k_2}\left|\mathbf{r}^0_{m_2}\right\rangle = \mathbf{P}^{\mu}_{j_2 k_2}\mathbf{p}^{m_2}\left|\mathbf{1}\right\rangle = ?$$



D_3-C_2 Coset structure of $d^{m_2}(C_2)\uparrow D^3$ induced representation basis

$D_3 \supset C_2$ projectors $\mathbf{P}^{A_1}_{0_2 0_2}, \mathbf{P}^{A_2}_{1_2 1_2}, \mathbf{P}^{E_1}_{0_2 0_2}, \mathbf{P}^{E_1}_{0_2 1_2}, \mathbf{P}^{E_1}_{1_2 0_2}, \mathbf{P}^{E_1}_{1_2 1_2}$ must reduce induced representation $d^{m_2}(C_2)\uparrow D_3$

But, which D_3 projector $\mathbf{P}^{\mu}_{j_2 k_2}$ will work on base $\left|\mathbf{r}^0_{m_2}\right\rangle = \mathbf{p}^{m_2}\left|\mathbf{1}\right\rangle$ of induced representation $d^{m_2}(C_2)\uparrow D_3$

$$\mathbf{P}^{\mu}_{j_2 k_2}\left|\mathbf{r}^0_{m_2}\right\rangle = \mathbf{P}^{\mu}_{j_2 k_2}\mathbf{p}^{m_2}\left|\mathbf{1}\right\rangle = \delta^{m_2}_{k_2}\mathbf{P}^{\mu}_{j_2 m_2}\left|\mathbf{1}\right\rangle$$

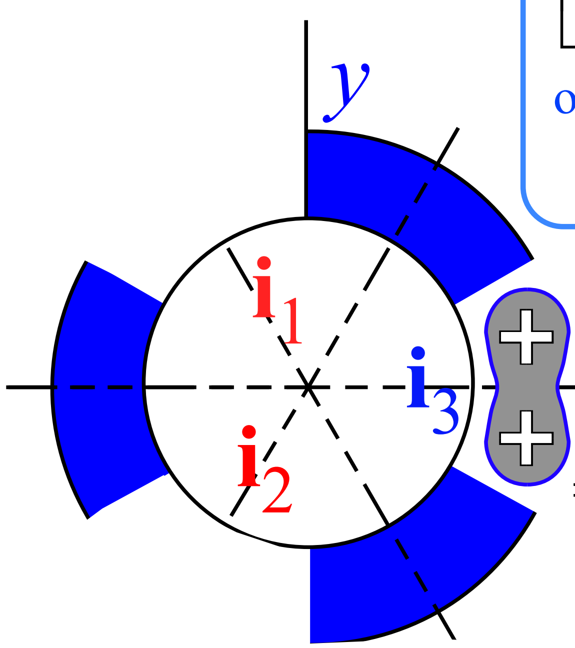
Local symmetry k_2 of $\mathbf{P}^{\mu}_{j_2 k_2}$ must match that of $\left|\mathbf{r}^0_{m_2}\right\rangle$

"σ-bond" ket

$\left[\left|\mathbf{r}^0_x\right\rangle, \left|\mathbf{r}^1_x\right\rangle, \left|\mathbf{r}^2_x\right\rangle\right]$

of induced rep.

$d^{0_2}\uparrow D_3$



$\left|\mathbf{r}^0_x\right\rangle = \left|0_2 \uparrow^0_x\right\rangle$

$= (\left|\mathbf{r}^0\right\rangle + \left|\mathbf{i}_3\right\rangle)/\sqrt{2}$

D_3-C_2 Coset structure of $d^{m_2}(C_2)\uparrow D^3$ induced representation basis

$D_3 \supset C_2$ projectors $\mathbf{P}^{A_1}_{0_2 0_2}, \mathbf{P}^{A_2}_{1_2 1_2}, \mathbf{P}^{E_1}_{0_2 0_2}, \mathbf{P}^{E_1}_{0_2 1_2}, \mathbf{P}^{E_1}_{1_2 0_2}, \mathbf{P}^{E_1}_{1_2 1_2}$ must reduce induced representation $d^{m_2}(C_2)\uparrow D_3$

But, which D_3 projector $\mathbf{P}^{\mu}_{j_2 k_2}$ will work on base $\left|\mathbf{r}^0_{m_2}\right\rangle = \mathbf{p}^{m_2}\left|\mathbf{1}\right\rangle$ of induced representation $d^{m_2}(C_2)\uparrow D_3$

$$\mathbf{P}^{\mu}_{j_2 k_2}\left|\mathbf{r}^0_{m_2}\right\rangle = \mathbf{P}^{\mu}_{j_2 k_2}\mathbf{p}^{m_2}\left|\mathbf{1}\right\rangle = \delta^{m_2}_{k_2}\mathbf{P}^{\mu}_{j_2 m_2}\left|\mathbf{1}\right\rangle$$

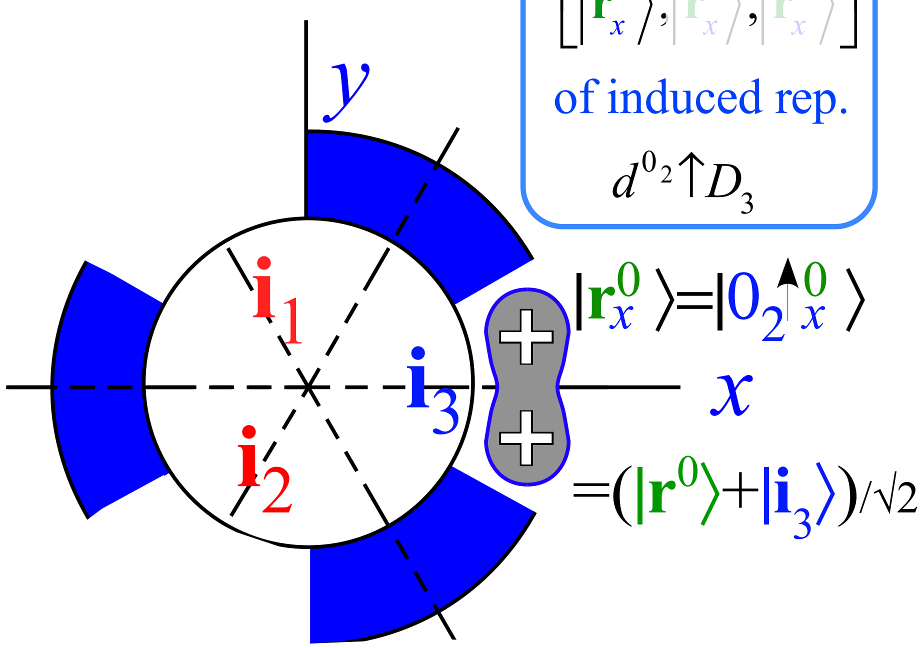
Local symmetry k_2 of $\mathbf{P}^{\mu}_{j_2 k_2}$ must match that m_2 of $\left|\mathbf{r}^0_{m_2}\right\rangle$

For example, base $\left|\mathbf{r}^0_x\right\rangle = \left|\mathbf{r}^0_{0_2}\right\rangle = \mathbf{p}^{0_2}\left|\mathbf{1}\right\rangle$ of $d^{0_2}(C_2)\uparrow D_3$ gives zero for all $\mathbf{P}^{\mu}_{j_2 k_2}$ except $\mathbf{P}^{A_1}_{0_2 0_2}, \mathbf{P}^{E_1}_{0_2 0_2}$, and $\mathbf{P}^{E_1}_{1_2 0_2}$,

D_3 projectors: $\mathbf{P}^{A_1}_{0_2 0_2}$, ~~$\mathbf{P}^{A_2}_{1_2 1_2}$~~, $\mathbf{P}^{E_1}_{0_2 0_2}$, ~~$\mathbf{P}^{E_1}_{0_2 1_2}$~~, $\mathbf{P}^{E_1}_{1_2 0_2}$, ~~$\mathbf{P}^{E_1}_{1_2 1_2}$~~

$C_2\{0_2, 1_2\}$ Notation

"σ-bond" ket $\left[\left|\mathbf{r}^0_x\right\rangle, \left|\mathbf{r}^1_x\right\rangle, \left|\mathbf{r}^2_x\right\rangle\right]$ of induced rep. $d^{0_2}\uparrow D_3$



D_3-C_2 Coset structure of $d^{m_2}(C_2)\uparrow D^3$ induced representation basis

$D_3 \supset C_2$ projectors $\mathbf{P}^{A_1}_{0_2 0_2}, \mathbf{P}^{A_2}_{1_2 1_2}, \mathbf{P}^{E_1}_{0_2 0_2}, \mathbf{P}^{E_1}_{0_2 1_2}, \mathbf{P}^{E_1}_{1_2 0_2}, \mathbf{P}^{E_1}_{1_2 1_2}$ must reduce induced representation $d^{m_2}(C_2)\uparrow D_3$

But, which D_3 projector $\mathbf{P}^{\mu}_{j_2 k_2}$ will work on base $\left|\mathbf{r}^0_{m_2}\right\rangle = \mathbf{p}^{m_2}\left|\mathbf{1}\right\rangle$ of induced representation $d^{m_2}(C_2)\uparrow D_3$

$$\mathbf{P}^{\mu}_{j_2 k_2}\left|\mathbf{r}^0_{m_2}\right\rangle = \mathbf{P}^{\mu}_{j_2 k_2}\mathbf{p}^{m_2}\left|\mathbf{1}\right\rangle = \delta^{m_2}_{k_2}\mathbf{P}^{\mu}_{j_2 m_2}\left|\mathbf{1}\right\rangle$$

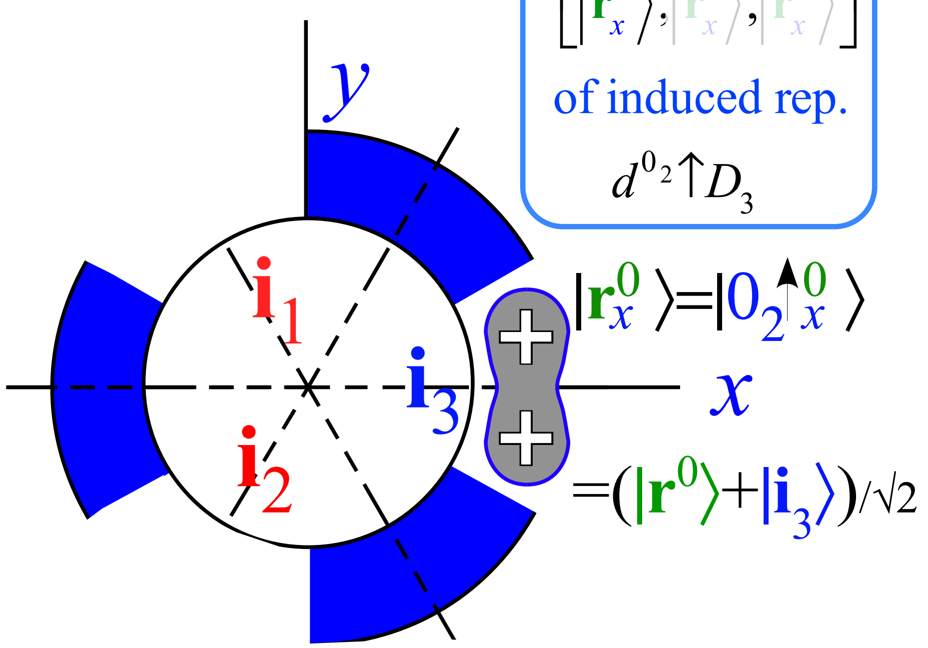
Local symmetry k_2 of $\mathbf{P}^{\mu}_{j_2 k_2}$ must match that m_2 of $\left|\mathbf{r}^0_{m_2}\right\rangle$

For example, base $\left|\mathbf{r}^0_x\right\rangle = \left|\mathbf{r}^0_{0_2}\right\rangle = \mathbf{p}^{0_2}\left|\mathbf{1}\right\rangle$ of $d^{0_2}(C_2)\uparrow D_3$ gives zero for all $\mathbf{P}^{\mu}_{j_2 k_2}$ except $\mathbf{P}^{A_1}_{0_2 0_2}, \mathbf{P}^{E_1}_{0_2 0_2}$, and $\mathbf{P}^{E_1}_{1_2 0_2}$,

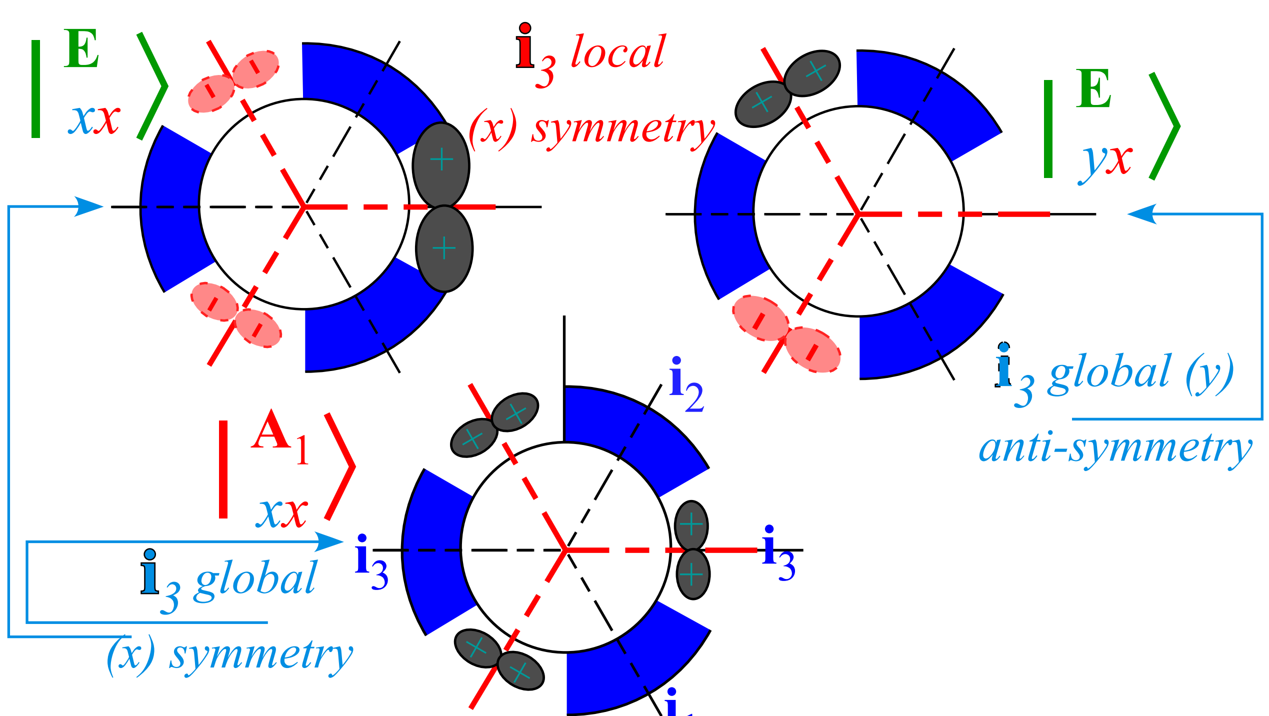
D_3 projectors: $\mathbf{P}^{A_1}_{0_2 0_2}$, ~~$\mathbf{P}^{A_2}_{1_2 1_2}$~~, $\mathbf{P}^{E_1}_{0_2 0_2}$, ~~$\mathbf{P}^{E_1}_{0_2 1_2}$~~, $\mathbf{P}^{E_1}_{1_2 0_2}$, ~~$\mathbf{P}^{E_1}_{1_2 1_2}$~~

C_2 $\{0_2, 1_2\}$ Notation / $\{x, y\}$ Notation: $\mathbf{P}^{A_1}_{xx}$, ~~$\mathbf{P}^{A_2}_{yy}$~~, $\mathbf{P}^{E_1}_{xx}$, ~~$\mathbf{P}^{E_1}_{xy}$~~, $\mathbf{P}^{E_1}_{yx}$, ~~$\mathbf{P}^{E_1}_{yy}$~~

"σ-bond" ket $\left[\left|\mathbf{r}^0_x\right\rangle, \left|\mathbf{r}^1_x\right\rangle, \left|\mathbf{r}^2_x\right\rangle\right]$ of induced rep. $d^{0_2}\uparrow D_3$



These give the "x-band"



D_3-C_2 Coset structure of $d^{m_2}(C_2)\uparrow D^3$ induced representation basis

$D_3 \supset C_2$ projectors $\mathbf{P}^{A_1}_{0_2 0_2}, \mathbf{P}^{A_2}_{1_2 1_2}, \mathbf{P}^{E_1}_{0_2 0_2}, \mathbf{P}^{E_1}_{0_2 1_2}, \mathbf{P}^{E_1}_{1_2 0_2}, \mathbf{P}^{E_1}_{1_2 1_2}$ must reduce induced representation $d^{m_2}(C_2)\uparrow D_3$

But, which D_3 projector $\mathbf{P}^{\mu}_{j_2 k_2}$ will work on base $\left|\mathbf{r}^0_{m_2}\right\rangle = \mathbf{p}^{m_2}\left|\mathbf{1}\right\rangle$ of induced representation $d^{m_2}(C_2)\uparrow D_3$

$$\mathbf{P}^{\mu}_{j_2 k_2}\left|\mathbf{r}^0_{m_2}\right\rangle = \mathbf{P}^{\mu}_{j_2 k_2}\mathbf{p}^{m_2}\left|\mathbf{1}\right\rangle = \delta^{m_2}_{k_2}\mathbf{P}^{\mu}_{j_2 m_2}\left|\mathbf{1}\right\rangle$$

Local symmetry k_2 of $\mathbf{P}^{\mu}_{j_2 k_2}$ must match that m_2 of $\left|\mathbf{r}^0_{m_2}\right\rangle$

For example, base $\left|\mathbf{r}^0_x\right\rangle = \left|\mathbf{r}^0_{0_2}\right\rangle = \mathbf{p}^{0_2}\left|\mathbf{1}\right\rangle$ of $d^{0_2}(C_2)\uparrow D_3$ gives zero for all $\mathbf{P}^{\mu}_{j_2 k_2}$ except $\mathbf{P}^{A_1}_{0_2 0_2}, \mathbf{P}^{E_1}_{0_2 0_2}$, and $\mathbf{P}^{E_1}_{1_2 0_2}$,

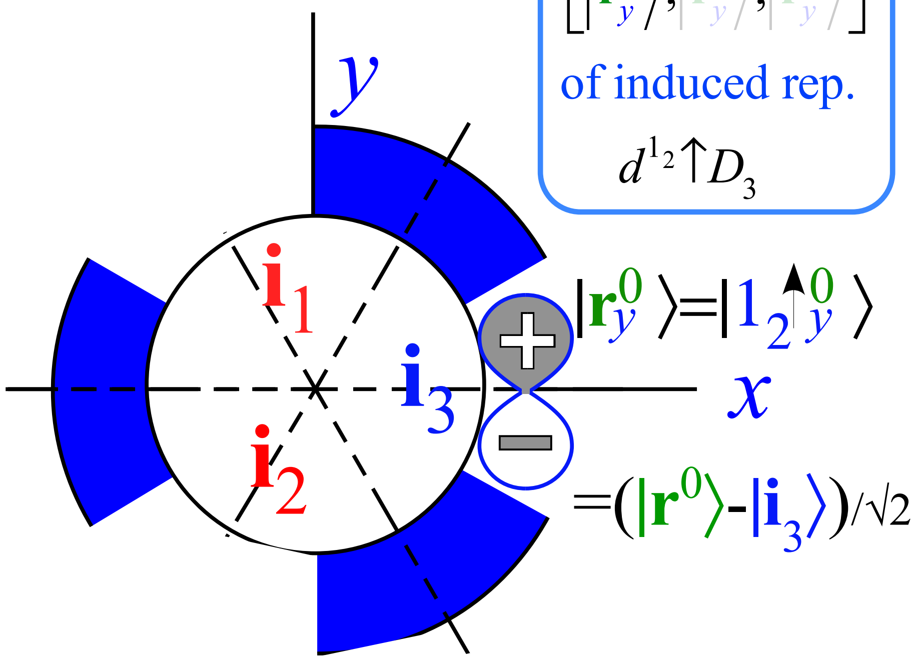
D_3 projectors: ~~$\mathbf{P}^{A_1}_{0_2 0_2}$~~, $\mathbf{P}^{A_2}_{1_2 1_2}$, ~~$\mathbf{P}^{E_1}_{0_2 0_2}$~~, $\mathbf{P}^{E_1}_{0_2 1_2}$, ~~$\mathbf{P}^{E_1}_{1_2 0_2}$~~, $\mathbf{P}^{E_1}_{1_2 1_2}$

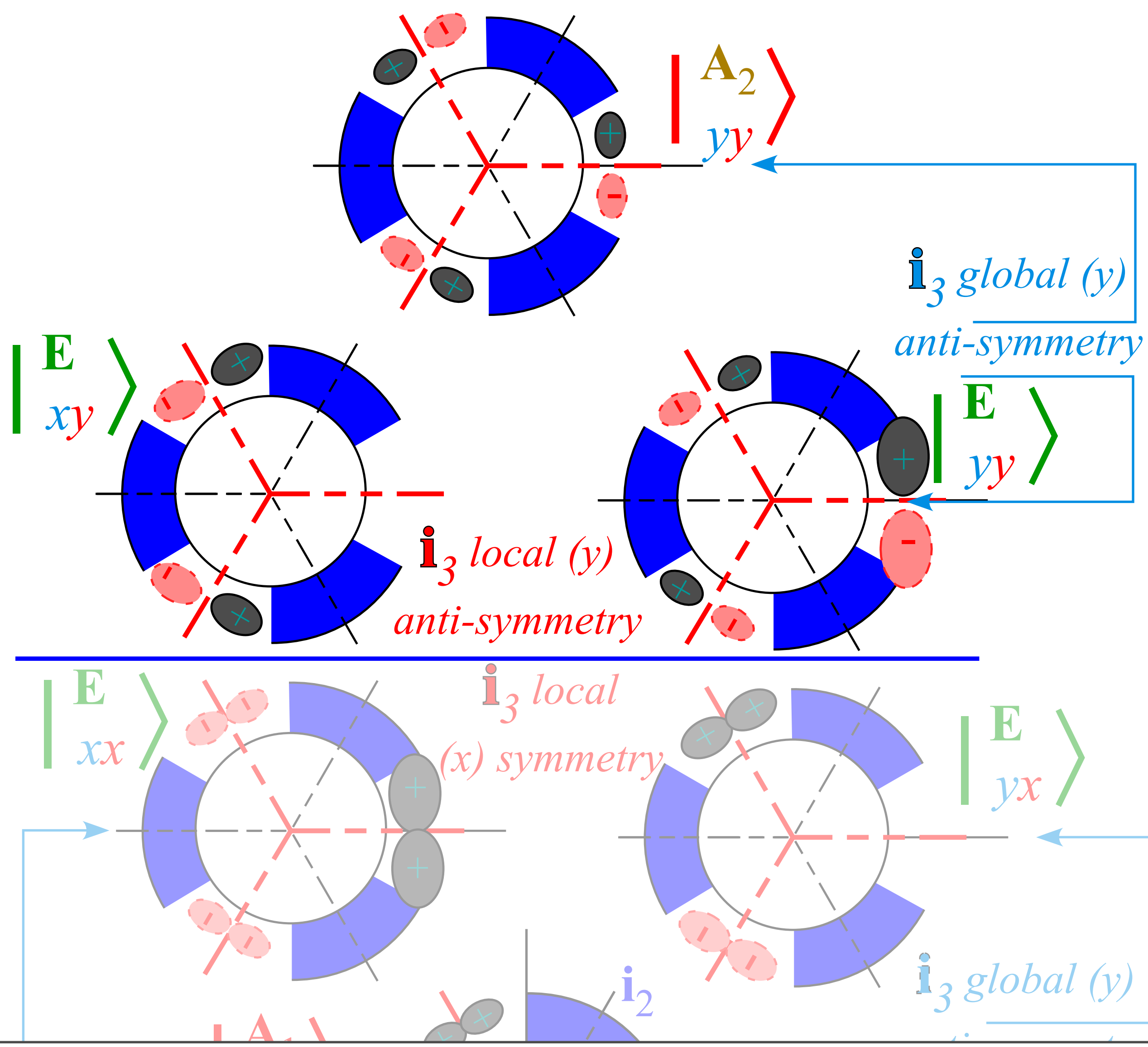
$C_2\{0_2, 1_2\}$Notation

$C_2\{x, y\}$Notation: ~~$\mathbf{P}^{A_1}_{xx}$~~, $\mathbf{P}^{A_2}_{yy}$, ~~$\mathbf{P}^{E_1}_{xx}$~~, $\mathbf{P}^{E_1}_{xy}$, ~~$\mathbf{P}^{E_1}_{yx}$~~, $\mathbf{P}^{E_1}_{yy}$

These give the "y-band"

"π-bond" ket $\left[\left|\mathbf{r}^0_y\right\rangle, \left|\mathbf{r}^1_y\right\rangle, \left|\mathbf{r}^2_y\right\rangle\right]$ of induced rep. $d^{1_2}\uparrow D_3$





Frobenius Reciprocity Theorem for $G \supset K$

$$\text{Number of } D^\alpha \text{ in } d^k(K) \uparrow G = \text{ Number of } d^k \text{ in } D^\alpha(G) \downarrow K$$

Frobenius Reciprocity Theorem for $G \supset K$

$$\text{Number of } D^{\alpha} \text{ in } d^{k}(K) \uparrow G = \text{ Number of } d^{k} \text{ in } D^{\alpha}(G) \downarrow K$$

..applies to regular representation

$D_3 \supset C_1$	$0_1 = 1_1$
A_1	1
A_2	1
E_1	2

Frobenius Reciprocity Theorem for $G \supset K$

$$\text{Number of } D^{\alpha} \text{ in } d^{k}(K) \uparrow G = \text{ Number of } d^{k} \text{ in } D^{\alpha}(G) \downarrow K$$

..applies to regular representation

$D_3 \supset C_1$	$0_1 = 1_1$
A_1	1
A_2	1
E_1	2

..and other induced representations

$D_3 \supset C_2$	0_2	1_2
A_1	1	·
A_2	·	1
E_1	1	1

$D_3 \supset C_3$	0_3	1_3	2_3
A_1	1	·	·
A_2	1	·	·
E_1	·	1	1

Review: Symmetry reduction and splitting: Subduced irep $D^{\alpha}(D_3)\downarrow C_2 = d^{0_2}\oplus d^{1_2}\oplus$.. correlation

Symmetry induction and clustering: Induced rep $d^{a}(C_2)\uparrow D_3 = D^{\alpha}\oplus D^{\beta}\oplus$.. correlation

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$D_6 \supset D_2 \supset C_2 = D_3 \times C_2$ symmetry and outer product geometry

Irreducible characters

Irreducible representations

Correlations with D_6 characters:

...and $C_2(\mathbf{i}_3)$ characters......and $C_6(\mathbf{1},\mathbf{h}^1,\mathbf{h}^2,...)$ characters

D_6 symmetry and induced representation band structure

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

Fig. 3.1.1 PSDS

Bilateral subgroup
Chain $D_6 \supset D_3 \supset C_2$

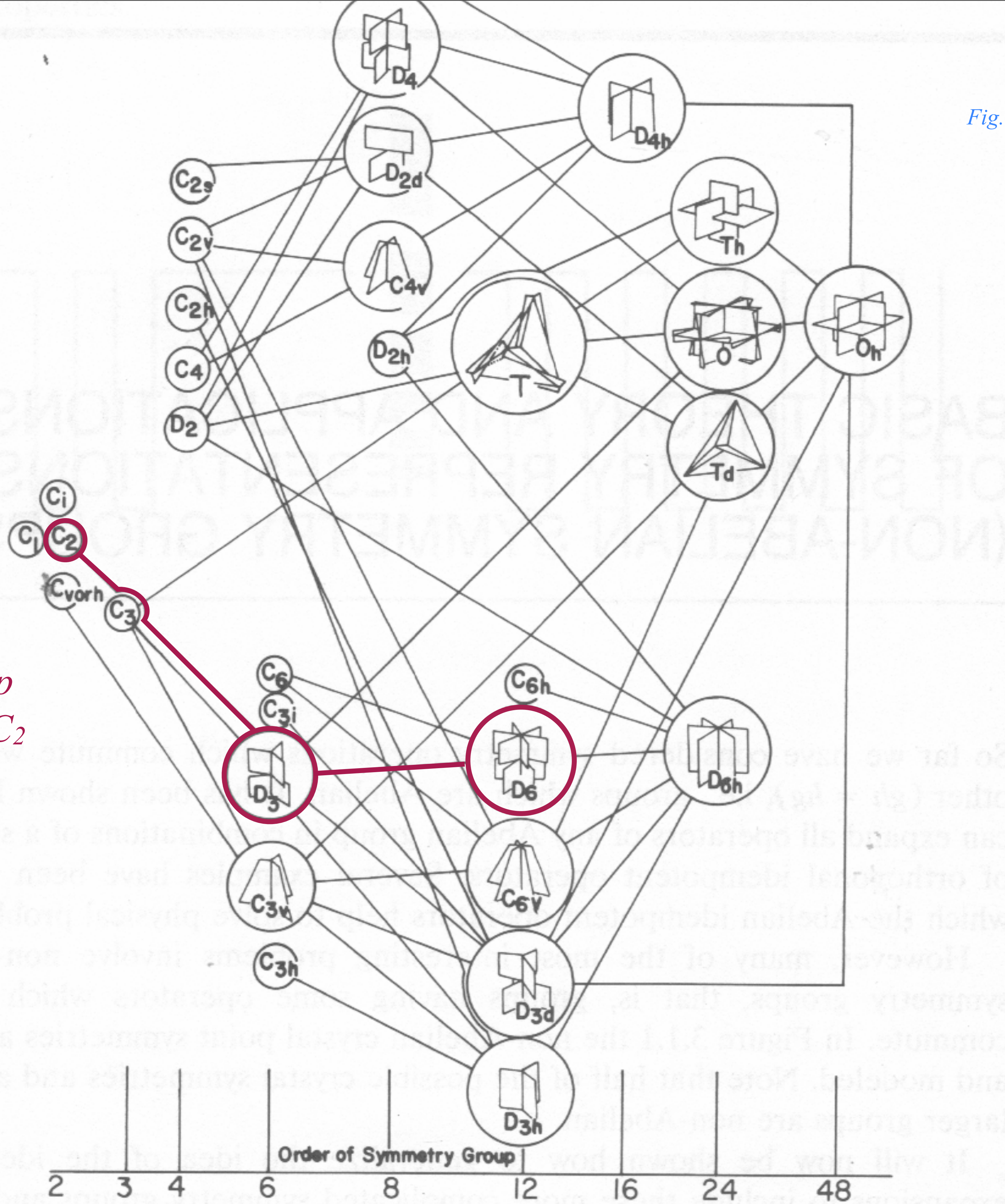
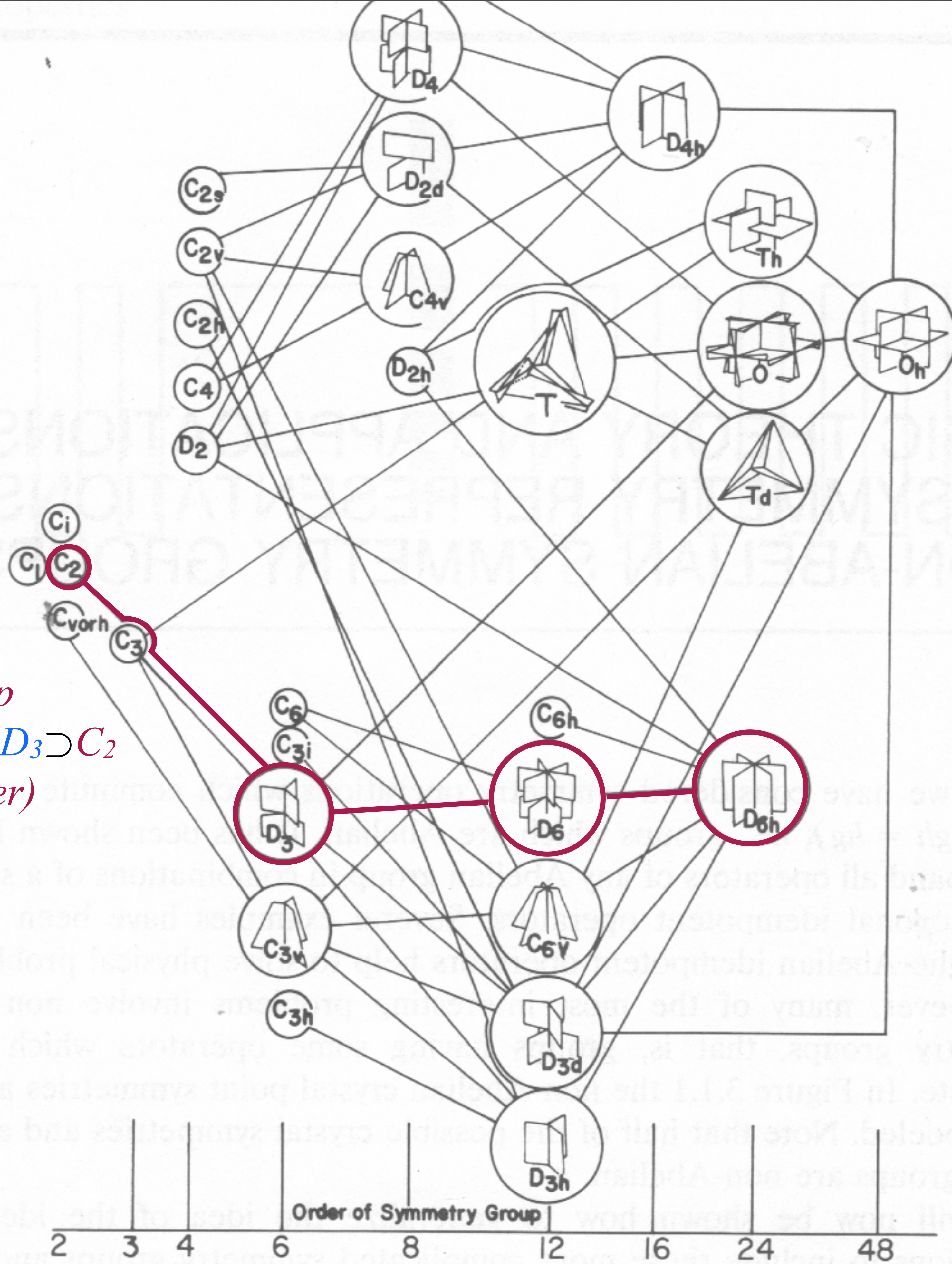


Figure 3.1.1 Crystal point symmetry groups. Models are sketched in circles for the

Fig. 3.1.1 PSDS



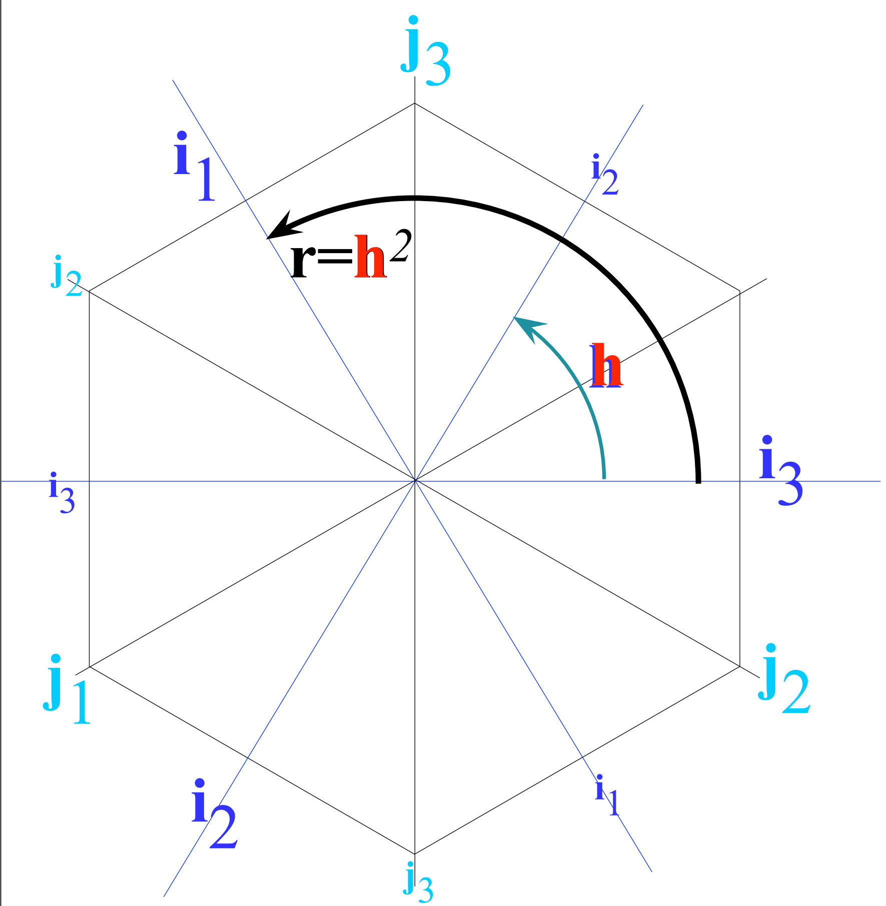
Bilateral subgroup
Chain $D_{6h} \supset D_6 \supset D_3 \supset C_2$
(To be studied later)

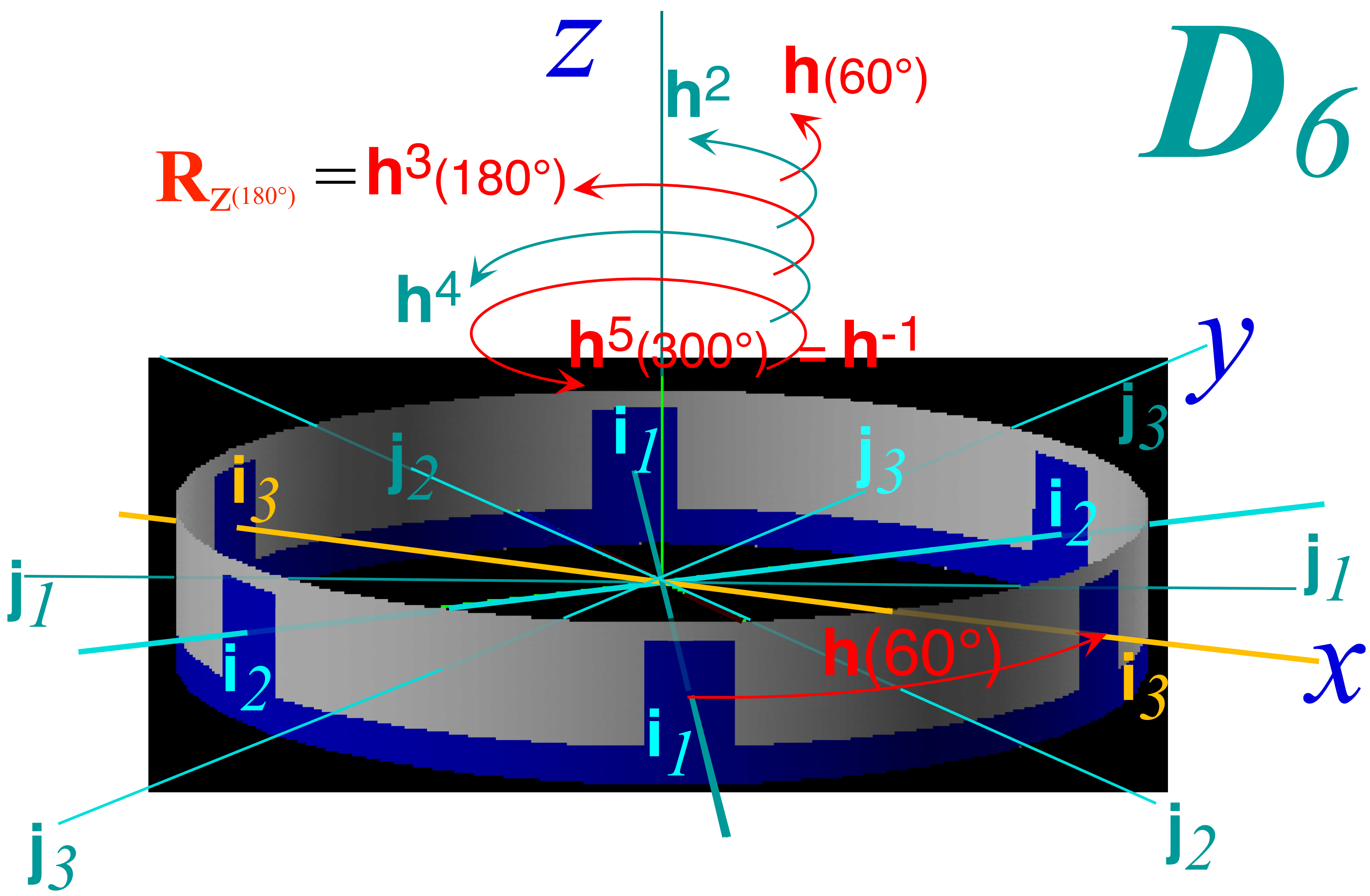
Figure 3.1.1 Crystal point symmetry groups. Models are sketched in circles for the

$D_6 \supset D_2 \supset C_2 = D_3 \times C_2$ *symmetry and outer product geometry*

D_6 is the *outer product* (×) *product* $D_3 \times C_2$ of D_3 and C_2. (Requires C_2 to commute with all of D_3.)

$D_6 = D_3 \times C_2 = \{\mathbf{1}, \mathbf{r}, \mathbf{r}^2, \mathbf{i}_1, \mathbf{i}_2, \mathbf{i}_3\} \times \{\mathbf{1}, \mathbf{R}_z\}$





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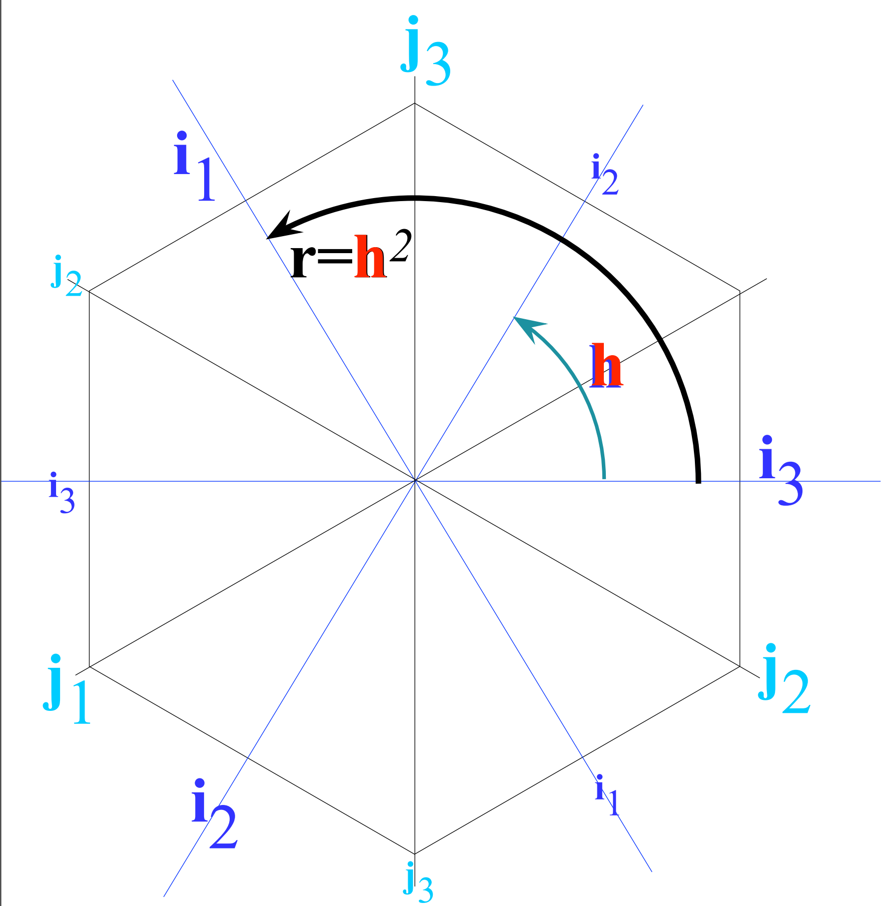
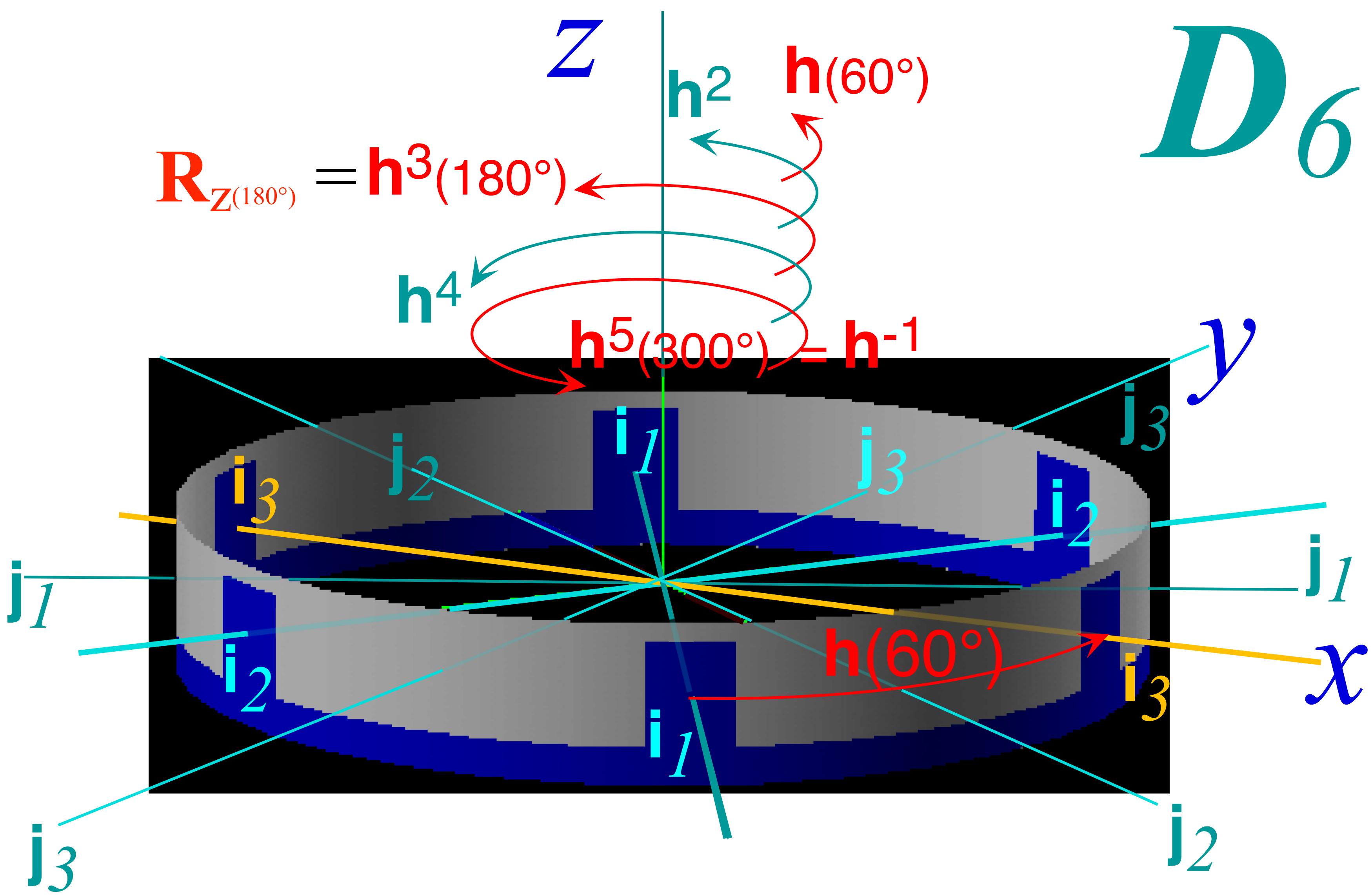
$\times$ product and D_6 operators. Define *hexagonal generator* $\mathbf{h}_{(60°)}$ of subgroup $C_6 = \{\mathbf{1}, \mathbf{h}, \mathbf{h}^2, \mathbf{h}^3, \mathbf{h}^4\ \mathbf{h}^5\}$

$$D_6 = D_3 \times C_2 = \{\mathbf{1}, \mathbf{r}, \mathbf{r}^2, \mathbf{i}_1, \mathbf{i}_2, \mathbf{i}_3, \mathbf{1}\cdot\mathbf{R}_z, \mathbf{r}\cdot\mathbf{R}_z, \mathbf{r}^2\cdot\mathbf{R}_z, \mathbf{i}_1\cdot\mathbf{R}_z, \mathbf{i}_2\cdot\mathbf{R}_z, \mathbf{i}_3\cdot\mathbf{R}_z\}$$

$\mathbf{h}^3{}_{(60°)} = \mathbf{R}_{z(180°)}$





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D_6 is the *outer product* ($\times$) *product* $D_3 \times C_2$ of D_3 and C_2. (Requires C_2 to commute with all of D_3.)

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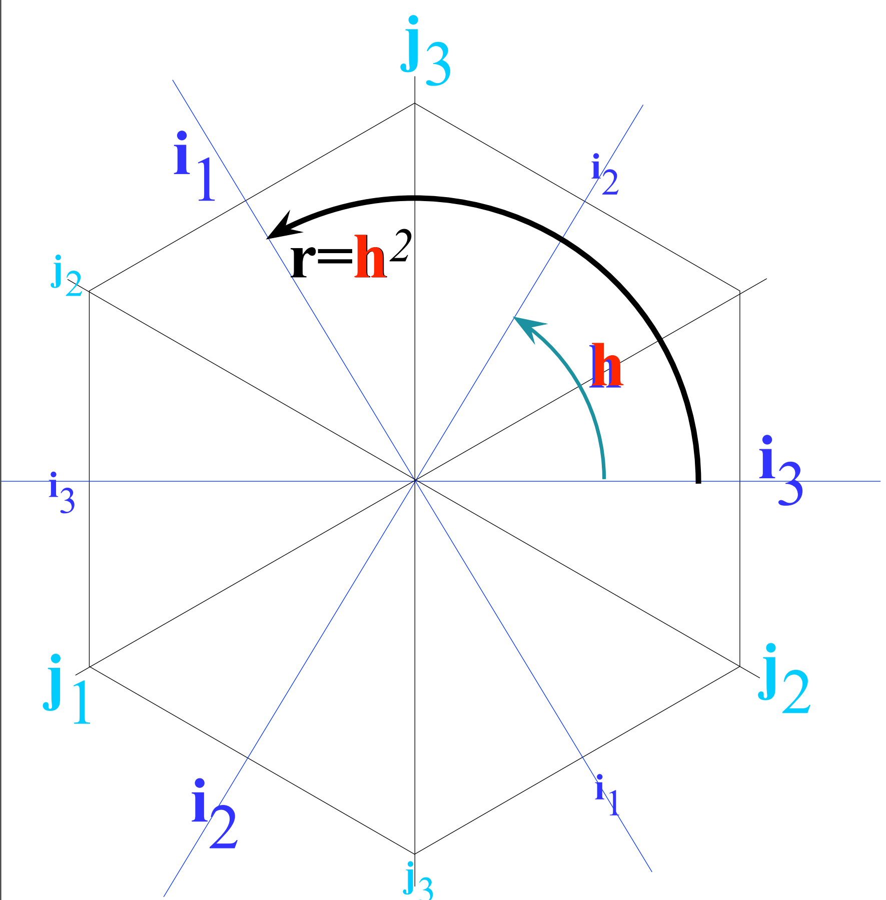

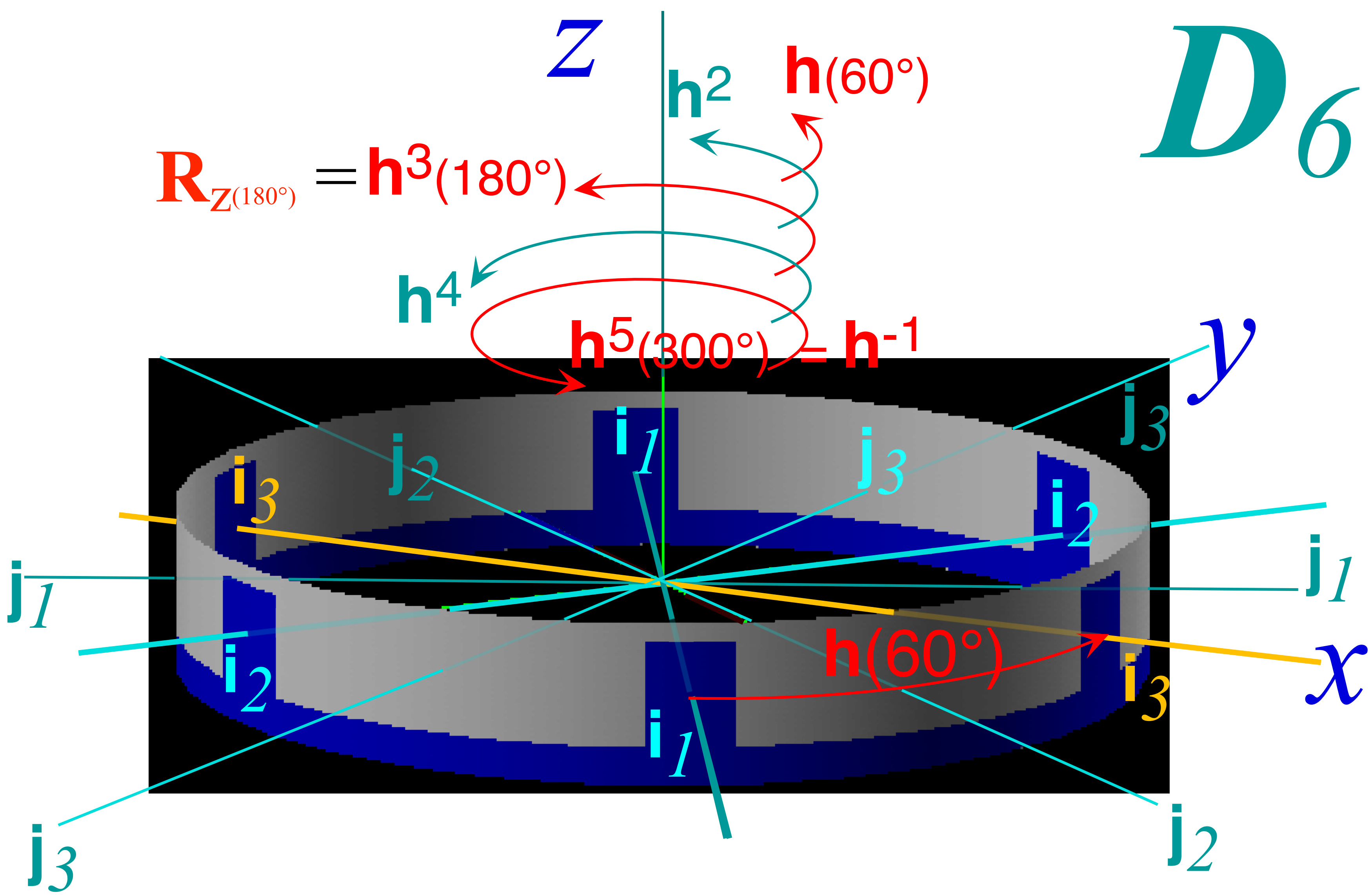

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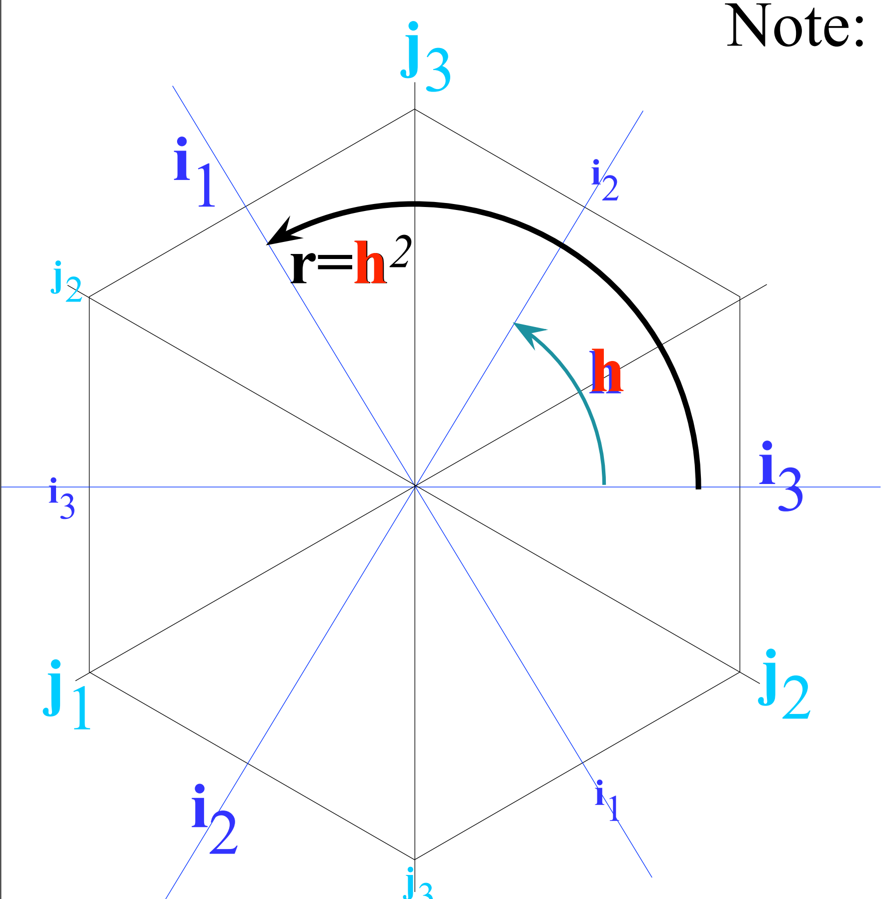
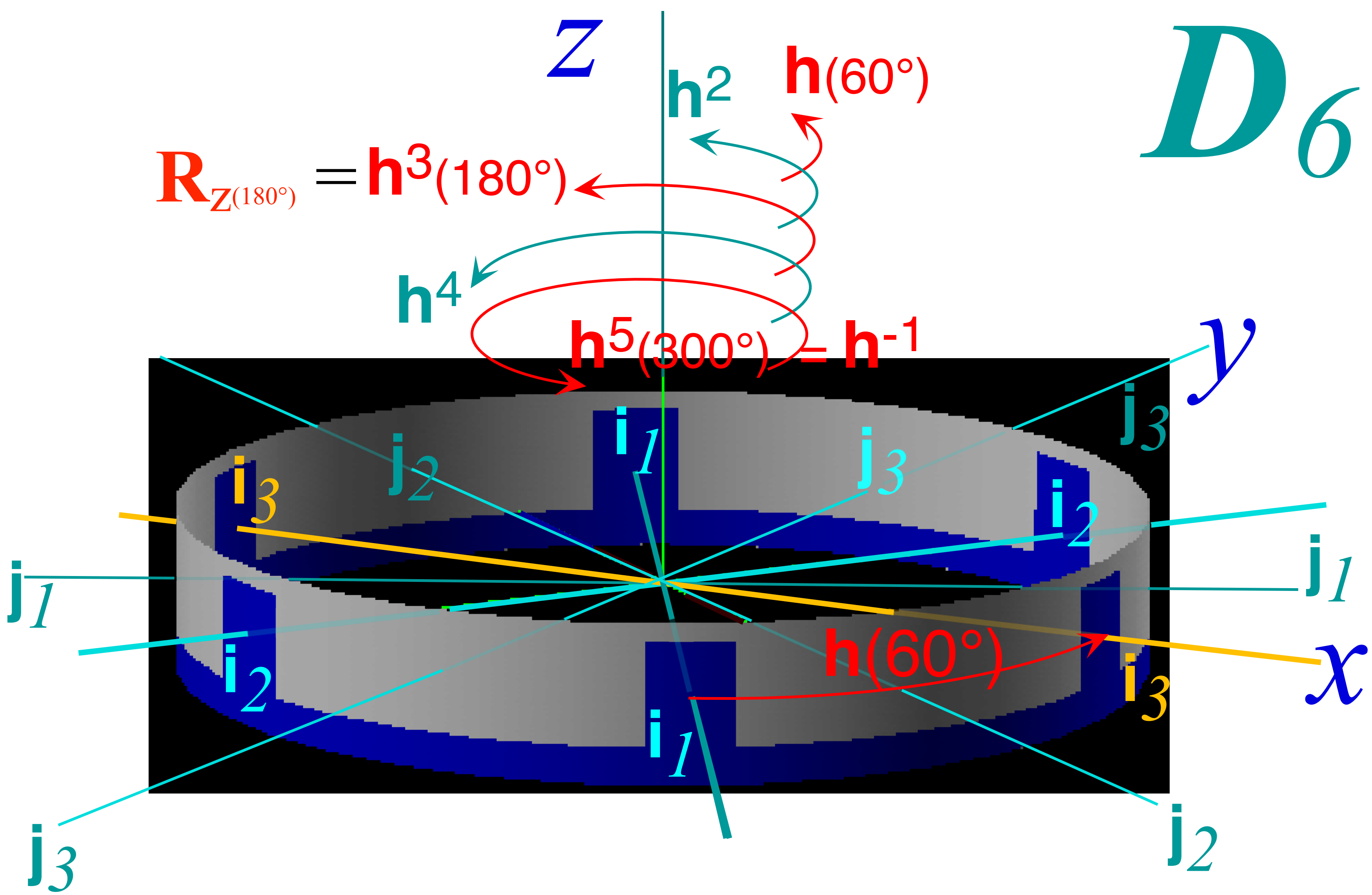
$\mathbf{h}^3_{(60°)} = \mathbf{R}_{z(180°)}$

$D_6 = D_3 \times C_2 = \{\mathbf{1}, \mathbf{h}^2, \mathbf{h}^4, \mathbf{i}_1, \mathbf{i}_2, \mathbf{i}_3, \mathbf{h}^3, \mathbf{h}^5, \mathbf{h}, \mathbf{j}_1, \mathbf{j}_2, \mathbf{j}_3\}$

Note: $\mathbf{h}^2 = \mathbf{r}_{(120°)}$ and $\mathbf{h}^3 = \mathbf{R}_{z(180°)}$ and $\mathbf{h}^4 = \mathbf{r}^2$ and $\mathbf{h}^5 = \mathbf{r}\cdot\mathbf{R}_z$





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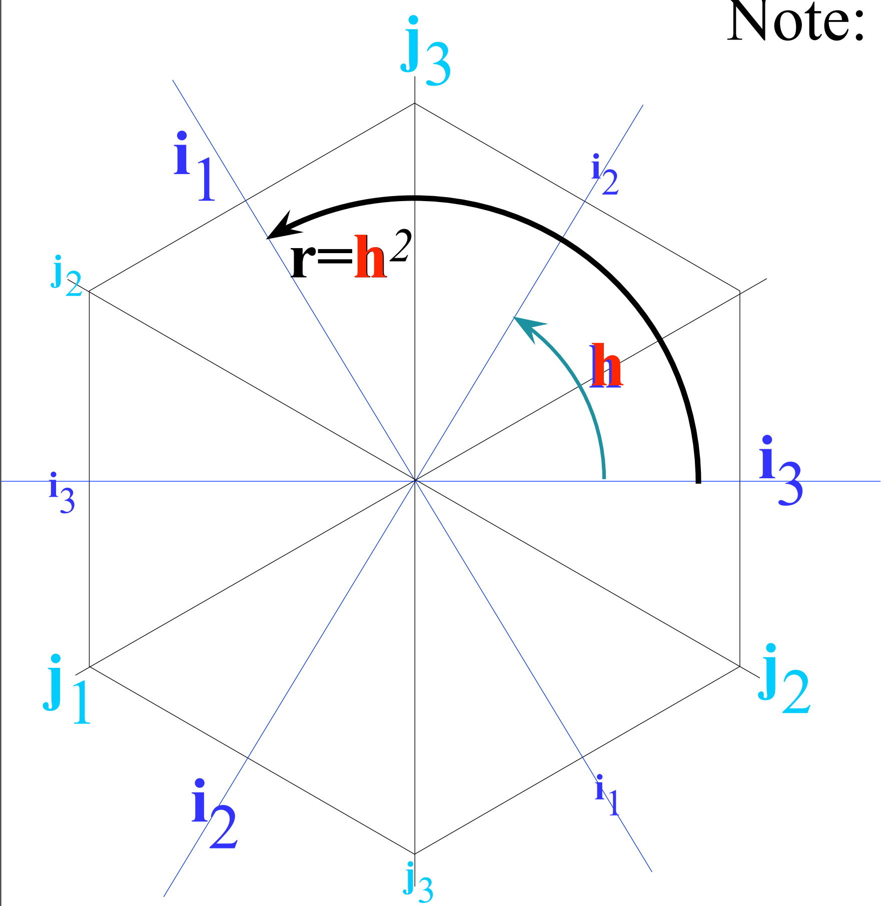
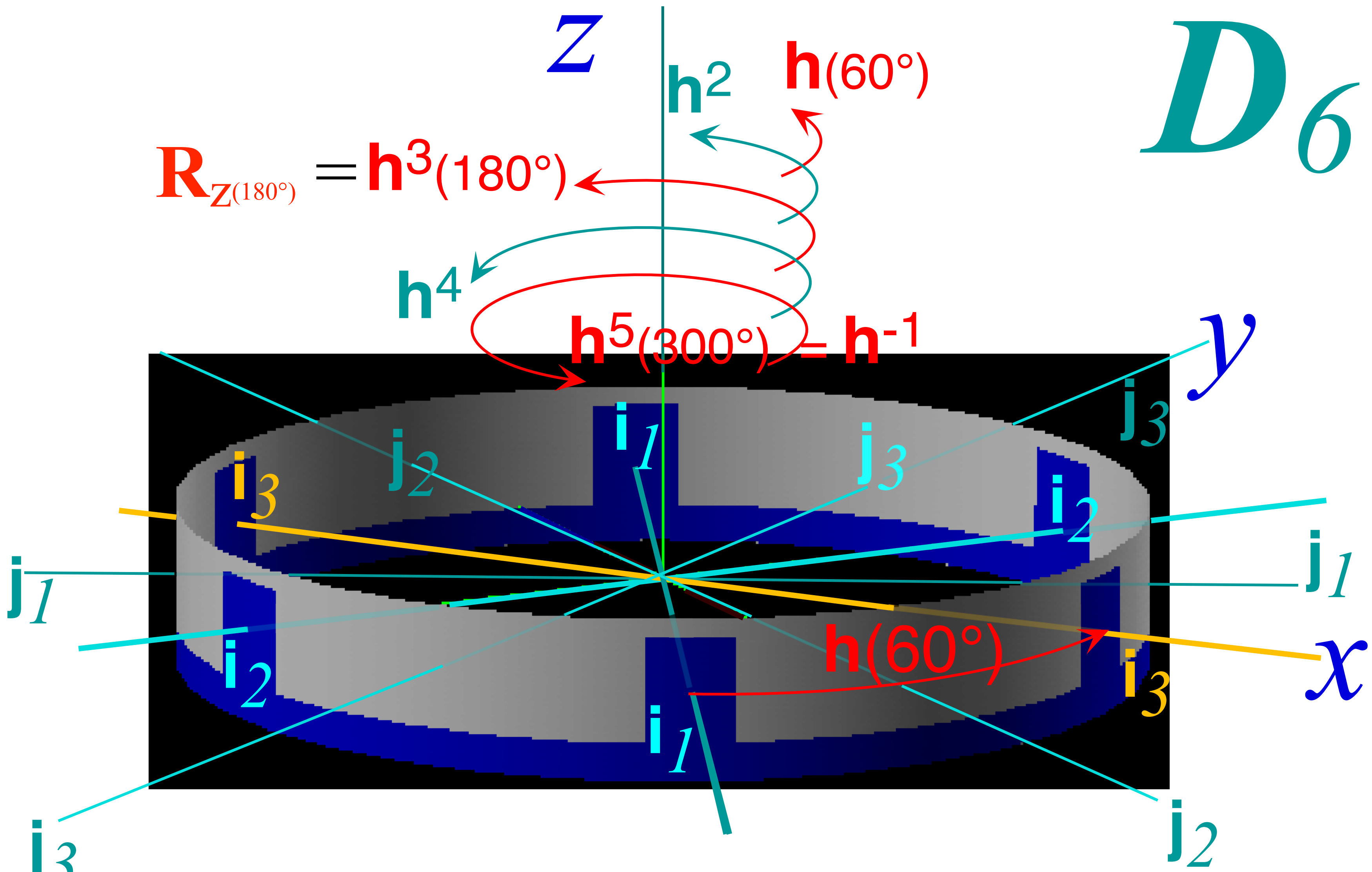
$$D_6 = D_3 \times C_2 = \{\mathbf{1}, \mathbf{h}^2, \mathbf{h}^4, \mathbf{i}_1, \mathbf{i}_2, \mathbf{i}_3, \mathbf{h}^3, \mathbf{h}^5, \mathbf{h}, \mathbf{j}_1, \mathbf{j}_2, \mathbf{j}_3\}$$

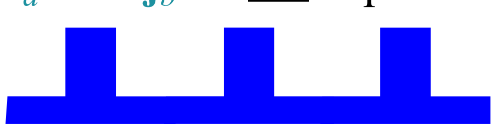
$\mathbf{h}^3{}_{(60°)} = \mathbf{R}_{z(180°)}$

Note: $\mathbf{h}^2 = \mathbf{r}_{(120°)}$ and $\mathbf{h}^3 = \mathbf{R}_{z(180°)}$ and $\mathbf{h}^4 = \mathbf{r}^2$ and $\mathbf{h}^5 = \mathbf{r}\cdot\mathbf{R}_z$





NOTE:
The $\mathbf{i}_a$ and $\mathbf{j}_b$ do not flip over the potential plot.



Electrostatic potential $V(\phi)$ doesn't care which way is "up." Wells remain wells, and barriers remain barriers under all $D6$ operations.

Review: Symmetry reduction and splitting: Subduced irep $D^{\alpha}(D_3)\downarrow C_2 = d^{0_2} \oplus d^{1_2} \oplus$.. correlation

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$D_6 \supset D_2 \supset C_2 = D_3 \times C_2$ symmetry and outer product geometry

Irreducible characters

Irreducible representations

Correlations with D_6 characters:

...and $C_2(\mathbf{i}_3)$ characters......and $C_6(\mathbf{1},\mathbf{h}^1,\mathbf{h}^2,...)$ characters

D_6 symmetry and induced representation band structure

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

$D_6 \supset D_2 \supset C_2 = D_3 \times C_2$ Irreducible characters

D_3	$\mathbf{1}$	$\{\mathbf{r},\mathbf{r}^2\}$	$\{\mathbf{i}_1,\mathbf{i}_2,\mathbf{i}_3\}$
$\chi^{A_1}(\mathbf{g})$	1	1	1
$\chi^{A_2}(\mathbf{g})$	1	1	−1
$\chi^{E_1}(\mathbf{g})$	2	−1	0

×

C_2^Z	$\mathbf{1}$	$\mathbf{R}_z$
(A)	1	1
(B)	1	−1

=

$D_3 \times C_2^Z$	$\mathbf{1}$	$\{\mathbf{r},\mathbf{r}^2\}$	$\{\mathbf{i}_1,\mathbf{i}_2,\mathbf{i}_3\}$	$\mathbf{1}\cdot\mathbf{R}_z$	$\{\mathbf{r},\mathbf{r}^2\}\cdot\mathbf{R}_z$	$\{\mathbf{i}_1,\mathbf{i}_2,\mathbf{i}_3\}\cdot\mathbf{R}_z$
$A_1\cdot(A)$	$1\cdot1$	$1\cdot1$	$1\cdot1$	$1\cdot1$	$1\cdot1$	$1\cdot1$
$A_2\cdot(A)$	$1\cdot1$	$1\cdot1$	$-1\cdot1$	$1\cdot1$	$1\cdot1$	$-1\cdot1$
$E_1\cdot(A)$	$2\cdot1$	$-1\cdot1$	$0\cdot1$	$2\cdot1$	$-1\cdot1$	$0\cdot1$
$A_1\cdot(B)$	$1\cdot1$	$1\cdot1$	$1\cdot1$	$1\cdot(-1)$	$1\cdot(-1)$	$1\cdot(-1)$
$A_2\cdot(B)$	$1\cdot1$	$1\cdot1$	$-1\cdot1$	$1\cdot(-1)$	$1\cdot(-1)$	$-1\cdot(-1)$
$E_1\cdot(B)$	$2\cdot1$	$-1\cdot1$	$0\cdot1$	$2\cdot(-1)$	$-1\cdot(-1)$	$0\cdot(-1)$

$D_6 \supset D_2 \supset C_2 = D_3 \times C_2$ Irreducible characters

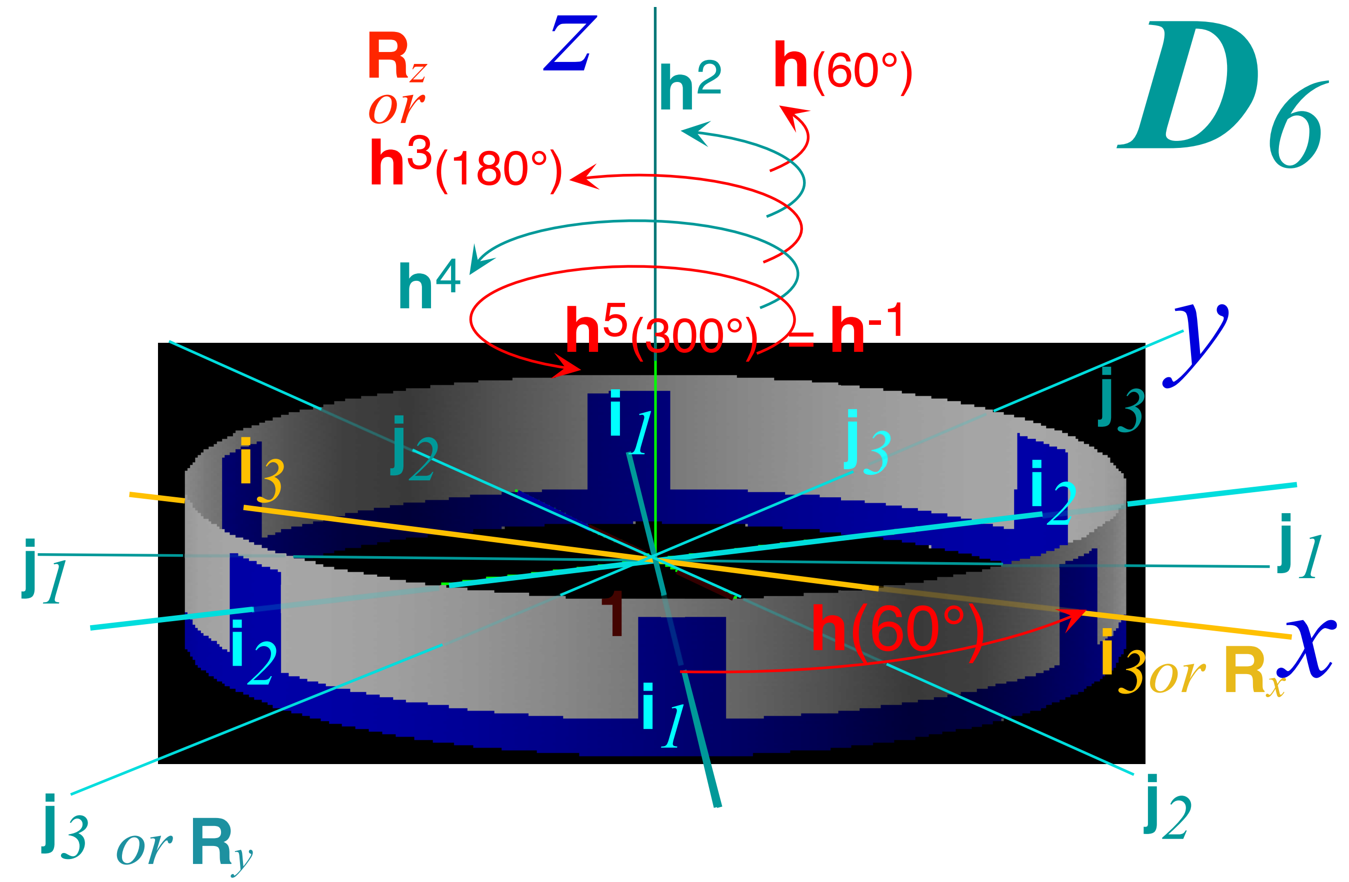
D_3	$\mathbf{1}$	$\{\mathbf{r},\mathbf{r}^2\}$	$\{\mathbf{i}_1,\mathbf{i}_2,\mathbf{i}_3\}$
$\chi^{A_1}(\mathbf{g})$	1	1	1
$\chi^{A_2}(\mathbf{g})$	1	1	-1
$\chi^{E_1}(\mathbf{g})$	2	-1	0

$\times$

C_2^Z	$\mathbf{1}$	$\mathbf{R}_z$
(A)	1	1
(B)	1	-1

$=$

$D_3 \times C_2^Z$	$\mathbf{1}$	$\{\mathbf{r},\mathbf{r}^2\}$	$\{\mathbf{i}_1,\mathbf{i}_2,\mathbf{i}_3\}$	$\mathbf{1}\cdot\mathbf{R}_z$	$\{\mathbf{r},\mathbf{r}^2\}\cdot\mathbf{R}_z$	$\{\mathbf{i}_1,\mathbf{i}_2,\mathbf{i}_3\}\cdot\mathbf{R}_z$
$A_1\cdot(A)$	$1\cdot1$	$1\cdot1$	$1\cdot1$	$1\cdot1$	$1\cdot1$	$1\cdot1$
$A_2\cdot(A)$	$1\cdot1$	$1\cdot1$	$-1\cdot1$	$1\cdot1$	$1\cdot1$	$-1\cdot1$
$E_1\cdot(A)$	$2\cdot1$	$-1\cdot1$	$0\cdot1$	$2\cdot1$	$-1\cdot1$	$0\cdot1$
$A_1\cdot(B)$	$1\cdot1$	$1\cdot1$	$1\cdot1$	$1\cdot(-1)$	$1\cdot(-1)$	$1\cdot(-1)$
$A_2\cdot(B)$	$1\cdot1$	$1\cdot1$	$-1\cdot1$	$1\cdot(-1)$	$1\cdot(-1)$	$-1\cdot(-1)$
$E_1\cdot(B)$	$2\cdot1$	$-1\cdot1$	$0\cdot1$	$2\cdot(-1)$	$-1\cdot(-1)$	$0\cdot(-1)$



$D_6 \supset D_2 \supset C_2 = D_3 \times C_2$ Irreducible characters

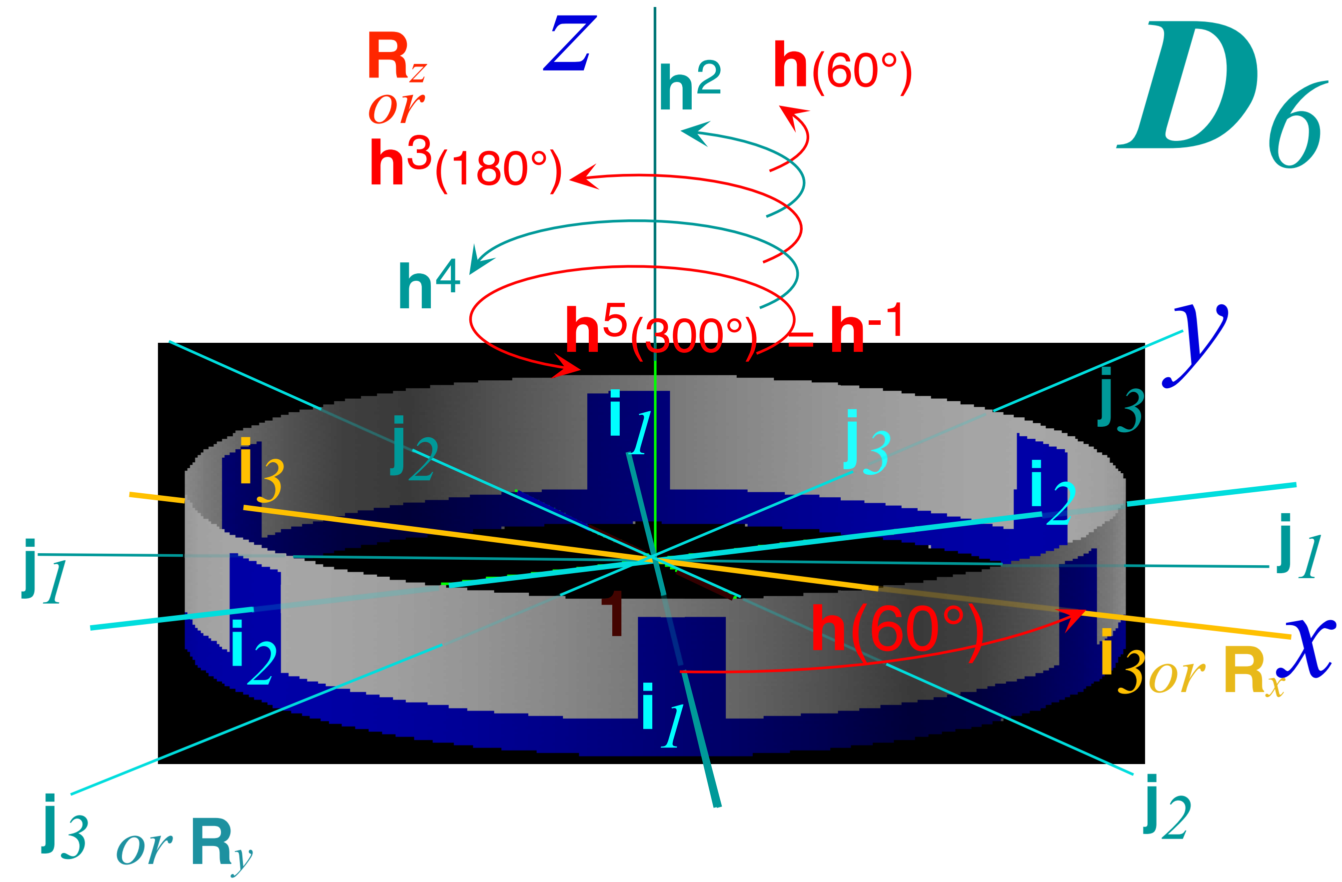
D_3	$\mathbf{1}$	$\{\mathbf{r},\mathbf{r}^2\}$	$\{\mathbf{i}_1,\mathbf{i}_2,\mathbf{i}_3\}$
$\chi^{A_1}(\mathbf{g})$	1	1	1
$\chi^{A_2}(\mathbf{g})$	1	1	-1
$\chi^{E_1}(\mathbf{g})$	2	-1	0

×

C_2^Z	$\mathbf{1}$	$\mathbf{R}_z$
(A)	1	1
(B)	1	-1

=

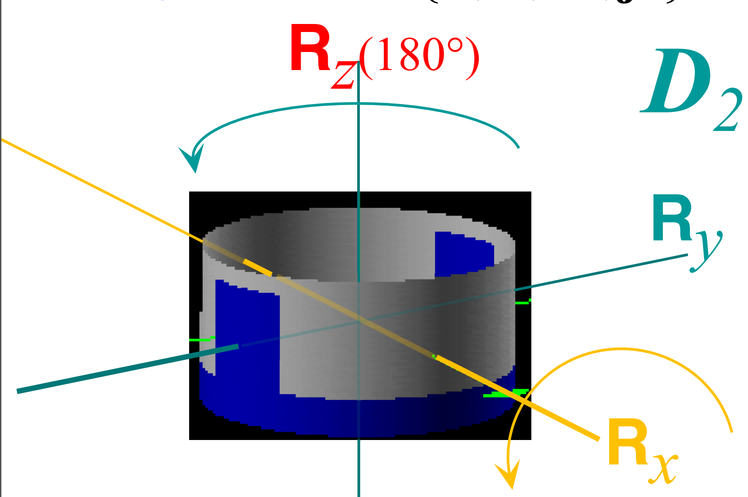
$D_3 \times C_2^Z$	$\mathbf{1}$	$\{\mathbf{r},\mathbf{r}^2\}$	$\{\mathbf{i}_1,\mathbf{i}_2,\mathbf{i}_3\}$	$\mathbf{1}\cdot\mathbf{R}_z$	$\{\mathbf{r},\mathbf{r}^2\}\cdot\mathbf{R}_z$	$\{\mathbf{i}_1,\mathbf{i}_2,\mathbf{i}_3\}\cdot\mathbf{R}_z$
$A_1\cdot(A)$	$1\cdot1$	$1\cdot1$	$1\cdot1$	$1\cdot1$	$1\cdot1$	$1\cdot1$
$A_2\cdot(A)$	$1\cdot1$	$1\cdot1$	$-1\cdot1$	$1\cdot1$	$1\cdot1$	$-1\cdot1$
$E_1\cdot(A)$	$2\cdot1$	$-1\cdot1$	$0\cdot1$	$2\cdot1$	$-1\cdot1$	$0\cdot1$
$A_1\cdot(B)$	$1\cdot1$	$1\cdot1$	$1\cdot1$	$1\cdot(-1)$	$1\cdot(-1)$	$1\cdot(-1)$
$A_2\cdot(B)$	$1\cdot1$	$1\cdot1$	$-1\cdot1$	$1\cdot(-1)$	$1\cdot(-1)$	$-1\cdot(-1)$
$E_1\cdot(B)$	$2\cdot1$	$-1\cdot1$	$0\cdot1$	$2\cdot(-1)$	$-1\cdot(-1)$	$0\cdot(-1)$



Recall $C_2 \times C_2 = D_2 = \{\mathbf{1}, \mathbf{R}_x, \mathbf{R}_z, \mathbf{R}_y\}$ characters

(*Lect.12 p.50-60*)

D_6 has $D_2 = \{\mathbf{1}, \mathbf{i}_3, \mathbf{h}^3, \mathbf{j}_3\}$ subgroup



D_2

$\mathbf{1}$	$\mathbf{R}_x$	$\mathbf{R}_z$	$\mathbf{R}_y$
$\mathbf{R}_x$	$\mathbf{1}$	$\mathbf{R}_y$	$\mathbf{R}_z$
$\mathbf{R}_z$	$\mathbf{R}_y$	$\mathbf{1}$	$\mathbf{R}_x$
$\mathbf{R}_y$	$\mathbf{R}_z$	$\mathbf{R}_x$	$\mathbf{1}$

C_2^X	$\mathbf{1}$	$\mathbf{R}_X$
$+=1$	1	1
$-=2$	1	-1

×

C_2^Z	$\mathbf{1}$	$\mathbf{R}_Z$
$+=A$	1	1
$-=B$	1	-1

=

$C_2^X \times C_2^Z$	$\mathbf{1}\cdot\mathbf{1}$	$\mathbf{R}_X\cdot\mathbf{1}$	$\mathbf{1}\cdot\mathbf{R}_Z$	$\mathbf{R}_X\cdot\mathbf{R}_Z$
$+\cdot+=A_1$	$1\cdot1$	$1\cdot1$	$1\cdot1$	$1\cdot1$
$-\cdot+=A_2$	$1\cdot1$	$-1\cdot1$	$1\cdot1$	$-1\cdot1$
$+\cdot-=B_1$	$1\cdot1$	$1\cdot1$	$1\cdot(-1)$	$1\cdot(-1)$
$-\cdot-=B_2$	$1\cdot1$	$-1\cdot1$	$1\cdot(-1)$	$-1\cdot(-1)$

$D_6 \supset D_2 \supset C_2 = D_3 \times C_2$ Irreducible characters

D_3	$\mathbf{1}$	$\{\mathbf{r},\mathbf{r}^2\}$	$\{\mathbf{i}_1,\mathbf{i}_2,\mathbf{i}_3\}$
$\chi^{A_1}(\mathbf{g})$	1	1	1
$\chi^{A_2}(\mathbf{g})$	1	1	-1
$\chi^{E_1}(\mathbf{g})$	2	-1	0

$\times$

C_2^Z	$\mathbf{1}$	$\mathbf{R}_z$
(A)	1	1
(B)	1	-1

$=$

$D_3 \times C_2^Z$	$\mathbf{1}$	$\{\mathbf{r},\mathbf{r}^2\}$	$\{\mathbf{i}_1,\mathbf{i}_2,\mathbf{i}_3\}$	$\mathbf{1}\cdot\mathbf{R}_z$	$\{\mathbf{r},\mathbf{r}^2\}\cdot\mathbf{R}_z$	$\{\mathbf{i}_1,\mathbf{i}_2,\mathbf{i}_3\}\cdot\mathbf{R}_z$
$A_1\cdot(A)$	$1\cdot1$	$1\cdot1$	$1\cdot1$	$1\cdot1$	$1\cdot1$	$1\cdot1$
$A_2\cdot(A)$	$1\cdot1$	$1\cdot1$	$-1\cdot1$	$1\cdot1$	$1\cdot1$	$-1\cdot1$
$E_1\cdot(A)$	$2\cdot1$	$-1\cdot1$	$0\cdot1$	$2\cdot1$	$-1\cdot1$	$0\cdot1$
$A_1\cdot(B)$	$1\cdot1$	$1\cdot1$	$1\cdot1$	$1\cdot(-1)$	$1\cdot(-1)$	$1\cdot(-1)$
$A_2\cdot(B)$	$1\cdot1$	$1\cdot1$	$-1\cdot1$	$1\cdot(-1)$	$1\cdot(-1)$	$-1\cdot(-1)$
$E_1\cdot(B)$	$2\cdot1$	$-1\cdot1$	$0\cdot1$	$2\cdot(-1)$	$-1\cdot(-1)$	$0\cdot(-1)$

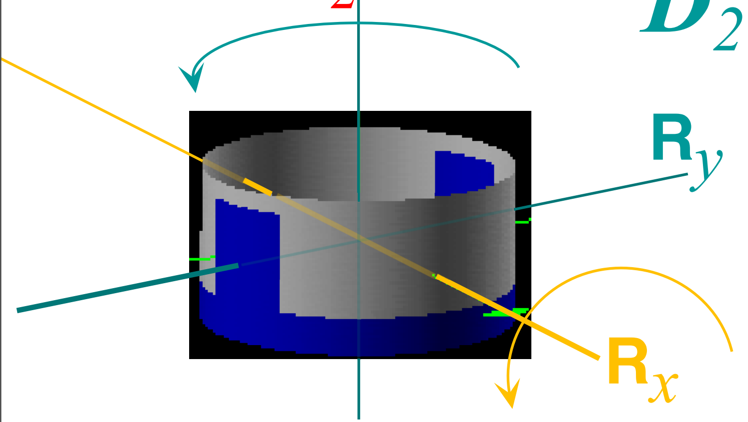
$\chi_g^\mu(D_6) =$

$D_3 \times C_2^z$	$\mathbf{1}$	$\{\mathbf{h}^2,\mathbf{h}^4\}$	$\{\mathbf{i}_1,\mathbf{i}_2,\mathbf{i}_3\}$	$\mathbf{h}^3$	$\{\mathbf{h},\mathbf{h}^5\}$	$\{\mathbf{j}_1,\mathbf{j}_2,\mathbf{j}_3\}$
A_1	1	1	1	1	1	1
A_2	1	1	-1	1	1	-1
E_2	2	-1	0	2	-1	0
B_1	1	1	1	-1	-1	-1
B_2	1	1	-1	-1	-1	1
E_1	2	-1	0	-2	1	0

Recall $C_2 \times C_2 = D_2 = \{\mathbf{1}, \mathbf{R}_x, \mathbf{R}_z, \mathbf{R}_y\}$ characters

($Lect.12\ p.50$-60)

D_6 has $D_2 = \{\mathbf{1}, \mathbf{i}_3, \mathbf{h}^3, \mathbf{j}_3\}$ subgroup



D_2

$\mathbf{1}$	$\mathbf{R}_x$	$\mathbf{R}_z$	$\mathbf{R}_y$
$\mathbf{R}_x$	$\mathbf{1}$	$\mathbf{R}_y$	$\mathbf{R}_z$
$\mathbf{R}_z$	$\mathbf{R}_y$	$\mathbf{1}$	$\mathbf{R}_x$
$\mathbf{R}_y$	$\mathbf{R}_z$	$\mathbf{R}_x$	$\mathbf{1}$

C_2^X	$\mathbf{1}$	$\mathbf{R}_X$
$+=1$	1	1
$-=2$	1	-1

$\times$

C_2^Z	$\mathbf{1}$	$\mathbf{R}_Z$
$+=A$	1	1
$-=B$	1	-1

$=$

$C_2^X \times C_2^Z$	$\mathbf{1}\cdot\mathbf{1}$	$\mathbf{R}_X\cdot\mathbf{1}$	$\mathbf{1}\cdot\mathbf{R}_Z$	$\mathbf{R}_X\cdot\mathbf{R}_Z$
$+\cdot+=A_1$	$1\cdot1$	$1\cdot1$	$1\cdot1$	$1\cdot1$
$-\cdot+=A_2$	$1\cdot1$	$-1\cdot1$	$1\cdot1$	$-1\cdot1$
$+\cdot-=B_1$	$1\cdot1$	$1\cdot1$	$1\cdot(-1)$	$1\cdot(-1)$
$-\cdot-=B_2$	$1\cdot1$	$-1\cdot1$	$1\cdot(-1)$	$-1\cdot(-1)$

$D_6 \supset D_2 \supset C_2 = D_3 \times C_2$ Irreducible characters

D_3	$\mathbf{1}$	$\{\mathbf{r},\mathbf{r}^2\}$	$\{\mathbf{i}_1,\mathbf{i}_2,\mathbf{i}_3\}$
$\chi^{A_1}(\mathbf{g})$	1	1	1
$\chi^{A_2}(\mathbf{g})$	1	1	−1
$\chi^{E_1}(\mathbf{g})$	2	−1	0

×

C_2^Z	$\mathbf{1}$	$\mathbf{R}_z$
(A)	1	1
(B)	1	−1

=

$D_3 \times C_2^Z$	$\mathbf{1}$	$\{\mathbf{r},\mathbf{r}^2\}$	$\{\mathbf{i}_1,\mathbf{i}_2,\mathbf{i}_3\}$	$\mathbf{1}\cdot\mathbf{R}_z$	$\{\mathbf{r},\mathbf{r}^2\}\cdot\mathbf{R}_z$	$\{\mathbf{i}_1,\mathbf{i}_2,\mathbf{i}_3\}\cdot\mathbf{R}_z$
$A_1\cdot(A)$	$1\cdot1$	$1\cdot1$	$1\cdot1$	$1\cdot1$	$1\cdot1$	$1\cdot1$
$A_2\cdot(A)$	$1\cdot1$	$1\cdot1$	$-1\cdot1$	$1\cdot1$	$1\cdot1$	$-1\cdot1$
$E_1\cdot(A)$	$2\cdot1$	$-1\cdot1$	$0\cdot1$	$2\cdot1$	$-1\cdot1$	$0\cdot1$
$A_1\cdot(B)$	$1\cdot1$	$1\cdot1$	$1\cdot1$	$1\cdot(-1)$	$1\cdot(-1)$	$1\cdot(-1)$
$A_2\cdot(B)$	$1\cdot1$	$1\cdot1$	$-1\cdot1$	$1\cdot(-1)$	$1\cdot(-1)$	$-1\cdot(-1)$
$E_1\cdot(B)$	$2\cdot1$	$-1\cdot1$	$0\cdot1$	$2\cdot(-1)$	$-1\cdot(-1)$	$0\cdot(-1)$

Recall $C_2 \times C_2 = D_2 = \{\mathbf{1}, \mathbf{R}_x, \mathbf{R}_z, \mathbf{R}_y\}$
characters
(*Lect.12 p.50-60*)

D_6 has $D_2 = \{\mathbf{1}, \mathbf{i}_3, \mathbf{h}^3, \mathbf{j}_3\}$ subgroup

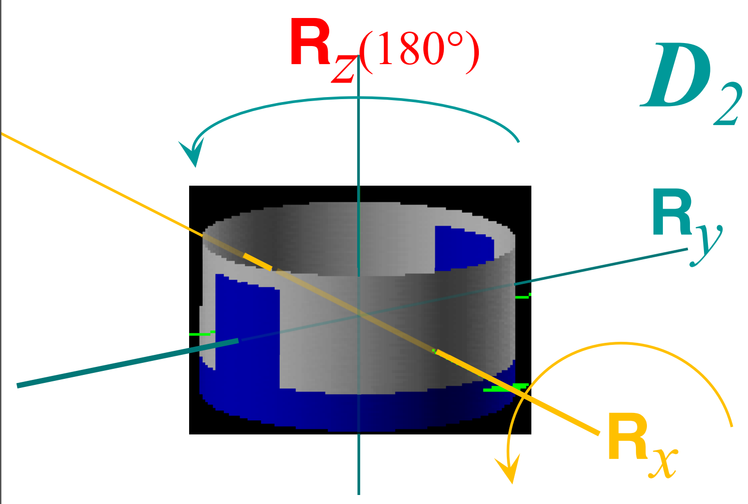
$\chi_g^\mu(D_6) =$

$D_3 \times C_2^z$	$\mathbf{1}$	$\{\mathbf{h}^2,\mathbf{h}^4\}$	$\{\mathbf{i}_1,\mathbf{i}_2,\mathbf{i}_3\}$	$\mathbf{h}^3$	$\{\mathbf{h},\mathbf{h}^5\}$	$\{\mathbf{j}_1,\mathbf{j}_2,\mathbf{j}_3\}$
A_1	1	1	1	1	1	1
A_2	1	1	-1	1	1	-1
E_2	2	-1	0	2	-1	0
B_1	1	1	1	-1	-1	-1
B_2	1	1	-1	-1	-1	1
E_1	2	-1	0	−2	1	0

Let X-rotation or 180° *X-flip* $\mathbf{i}_3$ *determine* A_1 or B_1 *vs* A_2 or B_2 (+1) *vs* (-1)

Let unit translation or 60° *hex-Z rotation* $\mathbf{h}$ *determine* A_p *vs* B_p (+1) *vs* (-1)

So also does: 180° $\mathbf{h}^3$



D_2

$\mathbf{1}$	$\mathbf{R}_x$	$\mathbf{R}_z$	$\mathbf{R}_y$
$\mathbf{R}_x$	$\mathbf{1}$	$\mathbf{R}_y$	$\mathbf{R}_z$
$\mathbf{R}_z$	$\mathbf{R}_y$	$\mathbf{1}$	$\mathbf{R}_x$
$\mathbf{R}_y$	$\mathbf{R}_z$	$\mathbf{R}_x$	$\mathbf{1}$

C_2^X	$\mathbf{1}$	$\mathbf{R}_X$
$+=1$	1	1
$-=2$	1	−1

×

C_2^Z	$\mathbf{1}$	$\mathbf{R}_Z$
$+=A$	1	1
$-=B$	1	−1

=

$C_2^X \times C_2^Z$	$\mathbf{1}\mathbf{1}$	$\mathbf{R}_X\mathbf{1}$	$\mathbf{1}\mathbf{R}_Z$	$\mathbf{R}_X\mathbf{R}_Z$
$+\cdot+=A_1$	$1\cdot1$	$1\cdot1$	$1\cdot1$	$1\cdot1$
$-\cdot+=A_2$	$1\cdot1$	$-1\cdot1$	$1\cdot1$	$-1\cdot1$
$+\cdot-=B_1$	$1\cdot1$	$1\cdot1$	$1\cdot(-1)$	$1\cdot(-1)$
$-\cdot-=B_2$	$1\cdot1$	$-1\cdot1$	$1\cdot(-1)$	$-1\cdot(-1)$

Review: *Symmetry reduction and splitting: Subduced irep* $D^{\alpha}(D_3)\downarrow C_2 = d^{0_2}\oplus d^{1_2}\oplus$*.. correlation*

Symmetry induction and clustering: Induced rep $d^{a}(C_2)\uparrow D_3 = D^{\alpha}\oplus D^{\beta}\oplus$*.. correlation*

D_3*-*C_2 *Coset structure of* $d^{m_2}(C_2)\uparrow D_3$ *induced representation basis*

D_3*-Projection of* $d^{m_2}(C_2)\uparrow D_3$ *induced representation basis*

Derivation of Frobenius reciprocity

$D_6\supset D_2\supset C_2 = D_3\times C_2$ *symmetry and outer product geometry*

Irreducible characters

→ *Irreducible representations* ←

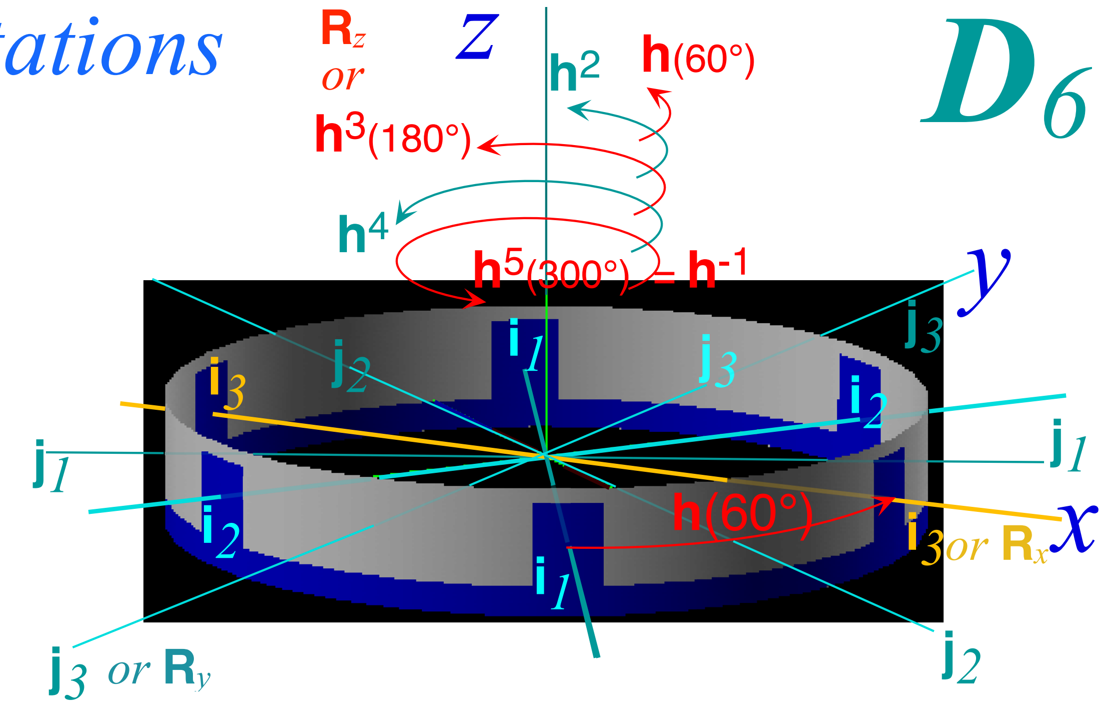
Correlations with D_6 *characters:*

...and $C_2(\mathbf{i}_3)$ *characters......and* $C_6(\mathbf{1},\mathbf{h}^1,\mathbf{h}^2,...)$ *characters*

D_6 *symmetry and induced representation band structure*

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

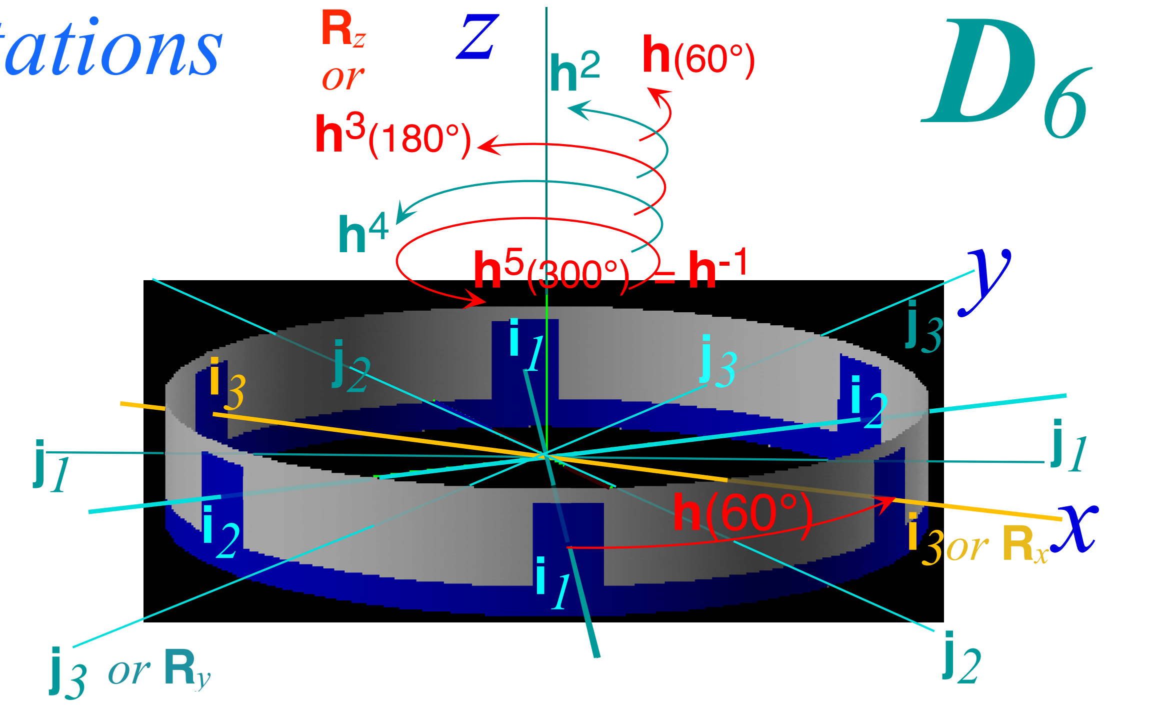
$D_6 \supset D_2 \supset C_2 = D_3 \times C_2$ Irreducible representations



g =	1	$r=h^2$	$r^2=h^4$	i_1	i_2	i_3
$D^{A_1}(g)=$	1	1	1	1	1	1
$D^{A_2}(g)=$	1	1	1	-1	-1	-1
$D^{E_2}(g)=$	$\begin{pmatrix}1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{-\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{-\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}1&0\\0&-1\end{pmatrix}$
$D^{B_1}(g)=$	1	1	1	1	1	1
$D^{B_2}(g)=$	1	1	1	-1	-1	-1
$D^{E_1}(g)=$	$\begin{pmatrix}1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{-\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{-\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}1&0\\0&-1\end{pmatrix}$

g =	h^3	$h^3r=h^5$	$h^3r^2=h^1$	$h^3i_1=j_1$	$h^3i_2=j_2$	$h^3i_3=j_3$
$D^{A_1}(g)=$	1	1	1	1	1	1
$D^{A_2}(g)=$	1	1	1	-1	-1	-1
$D^{E_2}(g)=$	$\begin{pmatrix}1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{-\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{-\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}1&0\\0&-1\end{pmatrix}$
$D^{B_1}(g)=$	-1	-1	-1	- 1	-1	-1
$D^{B_2}(g)=$	-1	-1	-1	1	1	1
$D^{E_1}(g)=$	$\begin{pmatrix}-1&0\\0&-1\end{pmatrix}$	$\begin{pmatrix}\frac{1}{2}&\frac{\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{1}{2}&\frac{-\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{1}{2}&\frac{\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{1}{2}&\frac{-\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}-1&0\\0&1\end{pmatrix}$

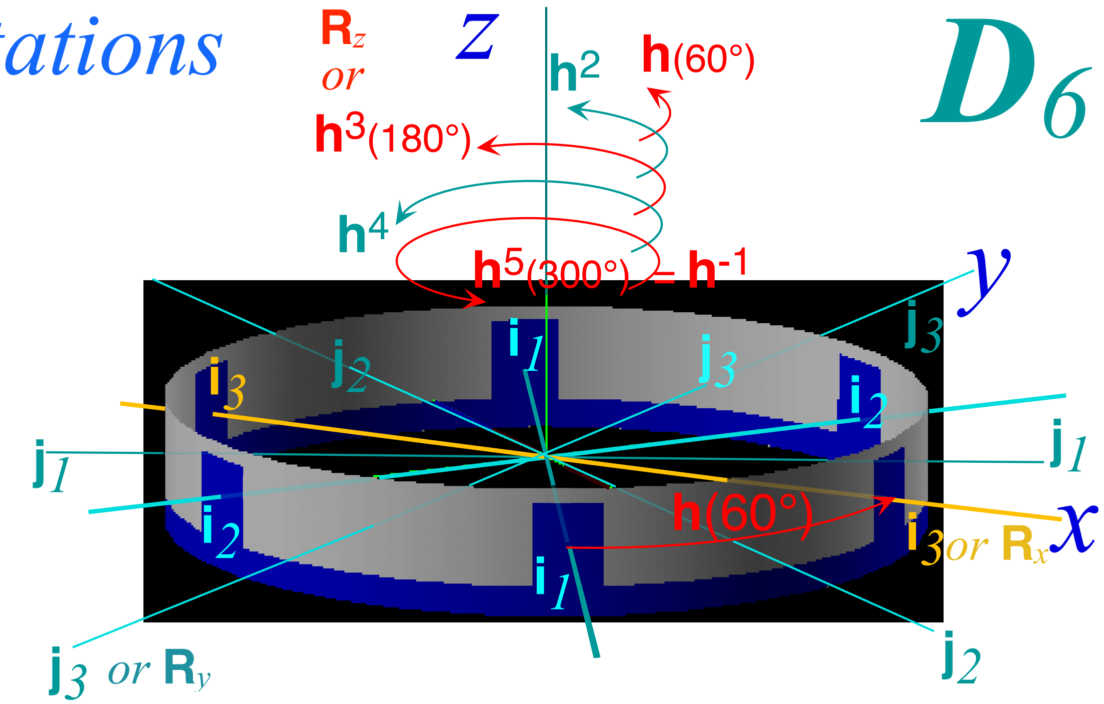
$D_6 \supset D_2 \supset C_2 = D_3 \times C_2$ Irreducible representations



$g =$	$\mathbf{1}$	$\mathbf{r}=\mathbf{h}^2$	$\mathbf{r}^2=\mathbf{h}^4$	$\mathbf{i}_1$	$\mathbf{i}_2$	$\mathbf{i}_3$	$\mathbf{h}^3$	$\mathbf{h}^3\mathbf{r}=\mathbf{h}^5$	$\mathbf{h}^3\mathbf{r}^2=\mathbf{h}^1$	$\mathbf{h}^3\mathbf{i}_1=\mathbf{j}_1$	$\mathbf{h}^3\mathbf{i}_2=\mathbf{j}_2$	$\mathbf{h}^3\mathbf{i}_3=\mathbf{j}_3$
$D^{A_1}(g)=$	1	1	1	1	1	1	1	1	1	1	1	1
$D^{A_2}(g)=$	1	1	1	-1	-1	-1	1	1	1	-1	-1	-1
$D^{E_2}(g)=$	$\begin{pmatrix}1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{-\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{-\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}1&0\\0&-1\end{pmatrix}$	$\begin{pmatrix}1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{-\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{-\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}1&0\\0&-1\end{pmatrix}$
$D^{B_1}(g)=$	1	1	1	1	1	1	-1	-1	-1	- 1	-1	-1
$D^{B_2}(g)=$	1	1	1	-1	-1	-1	-1	-1	-1	1	1	1
$D^{E_1}(g)=$	$\begin{pmatrix}1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{-\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{-\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}1&0\\0&-1\end{pmatrix}$	$\begin{pmatrix}-1&0\\0&-1\end{pmatrix}$	$\begin{pmatrix}\frac{1}{2}&\frac{\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{1}{2}&\frac{-\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{1}{2}&\frac{\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{1}{2}&\frac{-\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}-1&0\\0&1\end{pmatrix}$

Let X-rotation
or
180° *X-flip* $\mathbf{i}_3$
determines
A_1 or B_1 *vs* A_2 or B_2
(+1) *vs* (-1)

$D_6 \supset D_2 \supset C_2 = D_3 \times C_2$ Irreducible representations

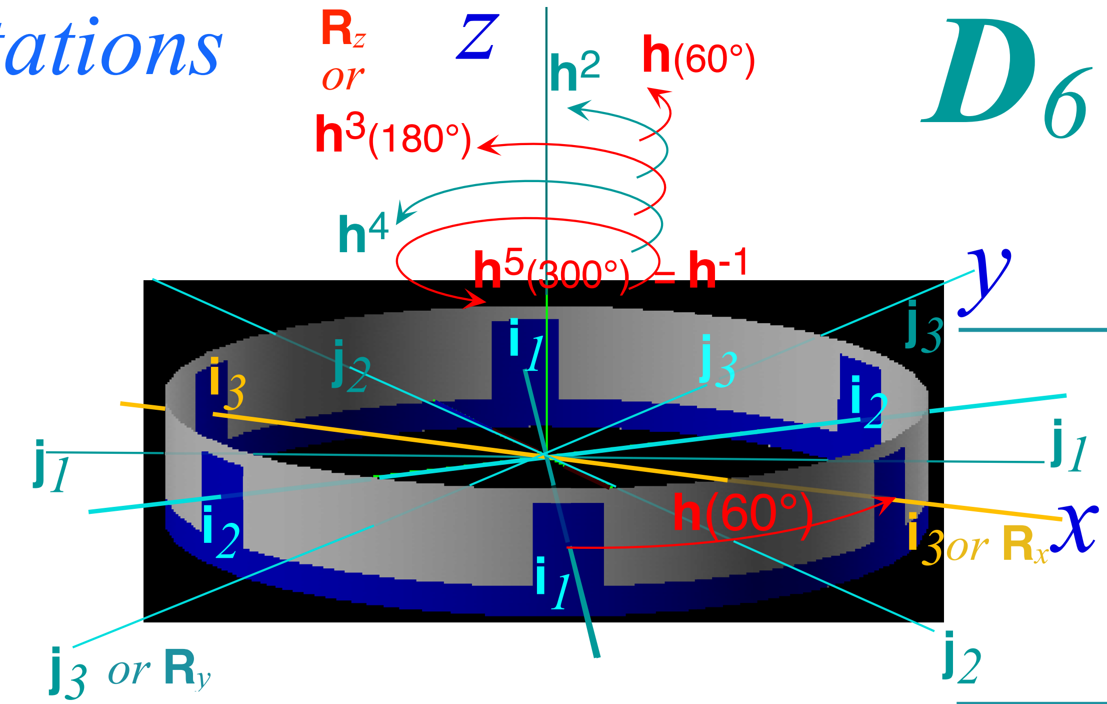


g =	1	$r=h^2$	$r^2=h^4$	i_1	i_2	i_3	h^3	$h^3r=h^5$	$h^3r^2=h^1$	$h^3i_1=j_1$	$h^3i_2=j_2$	$h^3i_3=j_3$
$D^{A_1}(g)=$	1	1	1	1	1	1	1	1	1	1	1	1
$D^{A_2}(g)=$	1	1	1	-1	-1	-1	1	1	1	-1	-1	-1
$D^{E_2}(g)=$	$\begin{pmatrix}1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{-\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{-\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}1&0\\0&-1\end{pmatrix}$	$\begin{pmatrix}1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{-\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{-\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}1&0\\0&-1\end{pmatrix}$
$D^{B_1}(g)=$	1	1	1	1	1	1	-1	-1	-1	-1	-1	-1
$D^{B_2}(g)=$	1	1	1	-1	-1	-1	-1	-1	-1	1	1	1
$D^{E_1}(g)=$	$\begin{pmatrix}1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{-\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{-\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}1&0\\0&-1\end{pmatrix}$	$\begin{pmatrix}-1&0\\0&-1\end{pmatrix}$	$\begin{pmatrix}\frac{1}{2}&\frac{\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{1}{2}&\frac{-\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{1}{2}&\frac{\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{1}{2}&\frac{-\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}-1&0\\0&1\end{pmatrix}$

Let X-rotation
or
180° *X-flip* $\mathbf{i}_3$
determines
A_1 or B_1 *vs* A_2 or B_2
(+1) *vs* (-1)

Let unit translation
or
60° *hex-Z rotation* **h**
determine
A_p *vs* B_p
(+1) *vs* (-1)
So also does:
180° $\mathbf{h}^3$

$D_6 \supset D_2 \supset C_2 = D_3 \times C_2$ Irreducible representations



$g =$	1	$r=h^2$	$r^2=h^4$	i_1	i_2	i_3	h^3	$h^3r=h^5$	$h^3r^2=h^1$	$h^3i_1=j_1$	$h^3i_2=j_2$	$h^3i_3=j_3$
$D^{A_1}(g)=$	1	1	1	1	1	1	1	1	1	1	1	1
$D^{A_2}(g)=$	1	1	1	-1	-1	-1	1	1	1	-1	-1	-1
$D^{E_2}(g)=$	$\begin{pmatrix}1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{-\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{-\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}1&0\\0&-1\end{pmatrix}$	$\begin{pmatrix}1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{-\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{-\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}1&0\\0&-1\end{pmatrix}$
$D^{B_1}(g)=$	1	1	1	1	1	1	-1	-1	-1	- 1	-1	-1
$D^{B_2}(g)=$	1	1	1	-1	-1	-1	-1	-1	-1	1	1	1
$D^{E_1}(g)=$	$\begin{pmatrix}1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{-\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{-\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}1&0\\0&-1\end{pmatrix}$	$\begin{pmatrix}-1&0\\0&-1\end{pmatrix}$	$\begin{pmatrix}\frac{1}{2}&\frac{\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{1}{2}&\frac{-\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{1}{2}&\frac{\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{1}{2}&\frac{-\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}-1&0\\0&1\end{pmatrix}$

Let X-rotation
or
180° *X-flip* $\mathbf{i}_3$
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Let unit translation
or
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determine
A_p *vs* B_p
(+1) *vs* (-1)
So also does:
180° $\mathbf{h}^3$

Y-rotation
or
180° *flip* $\mathbf{j}_3$
is product
$\mathbf{i}_3\mathbf{h}^3 = \mathbf{h}^3\mathbf{i}_3$

Review: Symmetry reduction and splitting: Subduced irep $D^\alpha(D_3)\downarrow C_2 = d^{0_2}\oplus d^{1_2}\oplus$*.. correlation*

Symmetry induction and clustering: Induced rep $d^a(C_2)\uparrow D_3 = D^\alpha\oplus D^\beta\oplus$*.. correlation*

D_3-C_2 *Coset structure of* $d^{m_2}(C_2)\uparrow D_3$ *induced representation basis*

D_3-*Projection of* $d^{m_2}(C_2)\uparrow D_3$ *induced representation basis*

Derivation of Frobenius reciprocity

$D_6 \supset D_2 \supset C_2 = D_3 \times C_2$ *symmetry and outer product geometry*

Irreducible characters

Irreducible representations

Correlations with D_6 *characters:*

➡ *...and* $C_2(\mathbf{i}_3)$ *characters......and* $C_6(\mathbf{1},\mathbf{h}^1,\mathbf{h}^2,...)$ *characters* ⬅

D_6 *symmetry and induced representation band structure*

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

Correlations by D_6 characters: $\chi_g^\mu(D_6)=$

$D_3 \times C_2^z$	$\mathbf{1}$	$\{\mathbf{h}^2,\mathbf{h}^4\}$	$\{\mathbf{i}_1,\mathbf{i}_2,\mathbf{i}_3\}$	$\mathbf{h}^3$	$\{\mathbf{h},\mathbf{h}^5\}$	$\{\mathbf{j}_1,\mathbf{j}_2,\mathbf{j}_3\}$
A_1	1	1	1	1	1	1
A_2	1	1	-1	1	1	-1
E_2	2	-1	0	2	-1	0
B_1	1	1	1	-1	-1	-1
B_2	1	1	-1	-1	-1	1
E_1	2	-1	0	−2	1	0

...and $C_2(\mathbf{i}_3)$ characters:

C_2^X	$\mathbf{1}$	$\mathbf{i}_3$
0_2	1	1
1_2	1	−1

Let X-rotation or 180° *X-flip* $\mathbf{i}_3$ *determine*
A_1 or B_1 *vs* A_2 or B_2
(+1) *vs* (-1)

$D_6 \supset C_2^X(\mathbf{i}_3)$	0_2	1_2
A_1	1	·
A_2	·	1
E_2	1	1
B_1	1	·
B_2	·	1
E_1	1	1

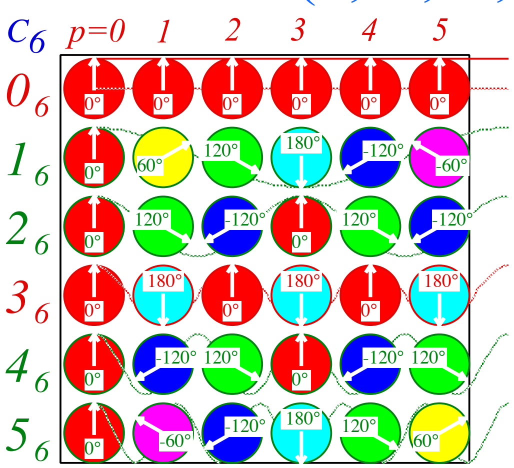
Correlations by D_6 characters: $\chi_g^{\mu}(D_6) =$

$D_3 \times C_2^z$	$\mathbf{1}$	$\{\mathbf{h}^2,\mathbf{h}^4\}$	$\{\mathbf{i}_1,\mathbf{i}_2,\mathbf{i}_3\}$	$\mathbf{h}^3$	$\{\mathbf{h},\mathbf{h}^5\}$	$\{\mathbf{j}_1,\mathbf{j}_2,\mathbf{j}_3\}$
A_1	1	1	1	1	1	1
A_2	1	1	-1	1	1	-1
E_2	2	-1	0	2	-1	0
B_1	1	1	1	-1	-1	-1
B_2	1	1	-1	-1	-1	1
E_1	2	-1	0	−2	1	0

...and $C_2(\mathbf{i}_3)$ characters:

C_2^X	$\mathbf{1}$	$\mathbf{i}_3$
0_2	1	1
1_2	1	−1

...and $C_6(\mathbf{1},\mathbf{h}^1,\mathbf{h}^2,...)$ characters:



C_6	1	$\mathbf{h}^1$	$\mathbf{h}^2$	$\mathbf{h}^3$	$\mathbf{h}^{-2}$	$\mathbf{h}^{-1}$
0_6	1	1	1	1	1	1
1_6	1	ε^1	ε^2	−1	ε^{-2}	ε^{-1}
2_6	1	ε^2	ε^4	1	ε^{-4}	ε^{-2}
3_6	1	−1	1	−1	1	−1
-2_6	1	ε^{-2}	ε^{-4}	−1	ε^4	ε^2
-1_6	1	ε^{-1}	ε^{-2}	ε^{-3}	ε^{-4}	ε^{-5}

$(\varepsilon = e^{\pi i/3})$

Let X-rotation or 180° *X-flip* $\mathbf{i}_3$ *determine* A_1 or B_1 *vs* A_2 or B_2 (+1) *vs* (-1)

Let unit translation or 60° *hex-Z rotation* $\mathbf{h}$ *determine* A_p *vs* B_p (+1) *vs* (-1)

So also does: 180° $\mathbf{h}^3$

Y-rotation or 180° *flip* $\mathbf{j}_3$ *is product* $\mathbf{i}_3\mathbf{h}^3 = \mathbf{h}^3\mathbf{i}_3$

Correlations by D_6 characters: $\chi^{\mu}_{g}(D_6)=$

$D_3 \times C_2^z$	$\mathbf{1}$	$\{\mathbf{h}^2,\mathbf{h}^4\}$	$\{\mathbf{i}_1,\mathbf{i}_2,\mathbf{i}_3\}$	$\mathbf{h}^3$	$\{\mathbf{h},\mathbf{h}^5\}$	$\{\mathbf{j}_1,\mathbf{j}_2,\mathbf{j}_3\}$
A_1	1	1	1	1	1	1
A_2	1	1	-1	1	1	-1
E_2	2	-1	0	2	-1	0
B_1	1	1	1	-1	-1	-1
B_2	1	1	-1	-1	-1	1
E_1	2	-1	0	-2	1	0

...and $C_2(\mathbf{i}_3)$ characters:

C_2^X	$\mathbf{1}$	$\mathbf{i}_3$
0_2	1	1
1_2	1	−1

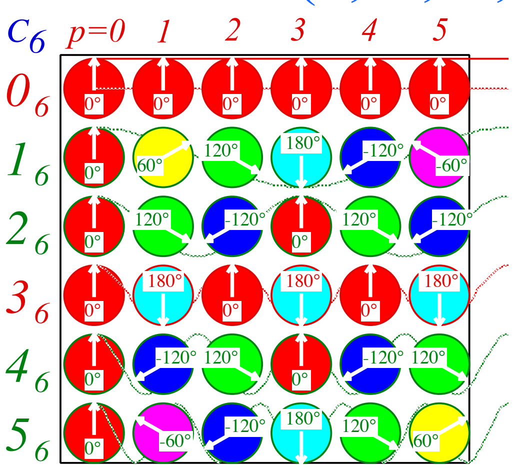
Let X-rotation or 180° X-flip $\mathbf{i}_3$ determine A_1 or B_1 vs A_2 or B_2 (+1) vs (-1)

Let unit translation or 60° hex-Z rotation $\mathbf{h}$ determine A_p vs B_p (+1) vs (-1)

So also does: 180° $\mathbf{h}^3$

Y-rotation or 180° flip $\mathbf{j}_3$ is product $\mathbf{i}_3\mathbf{h}^3=\mathbf{h}^3\mathbf{i}_3$

...and $C_6(\mathbf{1},\mathbf{h}^1,\mathbf{h}^2,...)$ characters:



C_6	1	$\mathbf{h}^1$	$\mathbf{h}^2$	$\mathbf{h}^3$	$\mathbf{h}^{-2}$	$\mathbf{h}^{-1}$
0_6	1	1	1	1	1	1
1_6	1	ε^1	ε^2	−1	ε^{-2}	ε^{-1}
2_6	1	ε^2	ε^4	1	ε^{-4}	ε^{-2}
3_6	1	−1	1	−1	1	−1
-2_6	1	ε^{-2}	ε^{-4}	−1	ε^4	ε^2
-1_6	1	ε^{-1}	ε^{-2}	ε^{-3}	ε^{-4}	ε^{-5}

$(\varepsilon=e^{\pi i/3})$

$D_6 \supset C_2^X(\mathbf{i}_3)$	0_2	1_2
A_1	1	·
A_2	·	1
E_2	1	1
B_1	1	·
B_2	·	1
E_1	1	1

$D_6 \supset C_6(\mathbf{h})$	0_6	1_6	2_6	3_6	4_6	5_6
A_1	1	·	·	·	·	·
A_2	1	·	·	·	·	·
E_2	·	·	1	·	1	·
B_2	·	·	·	1	·	·
B_1	·	·	·	1	·	·
E_1	·	1	·	·	·	1

Review: Symmetry reduction and splitting: Subduced irep $D^{\alpha}(D_3)\downarrow C_2 = d^{0_2}\oplus d^{1_2}\oplus$.. correlation

Symmetry induction and clustering: Induced rep $d^{a}(C_2)\uparrow D_3 = D^{\alpha}\oplus D^{\beta}\oplus$.. correlation

D_3-C_2 Coset structure of $d^{m_2}(C_2)\uparrow D_3$ induced representation basis

D_3-Projection of $d^{m_2}(C_2)\uparrow D_3$ induced representation basis

Derivation of Frobenius reciprocity

$D_6 \supset D_2 \supset C_2 = D_3 \times C_2$ symmetry and outer product geometry

Irreducible characters

Irreducible representations

Correlations with D_6 characters:

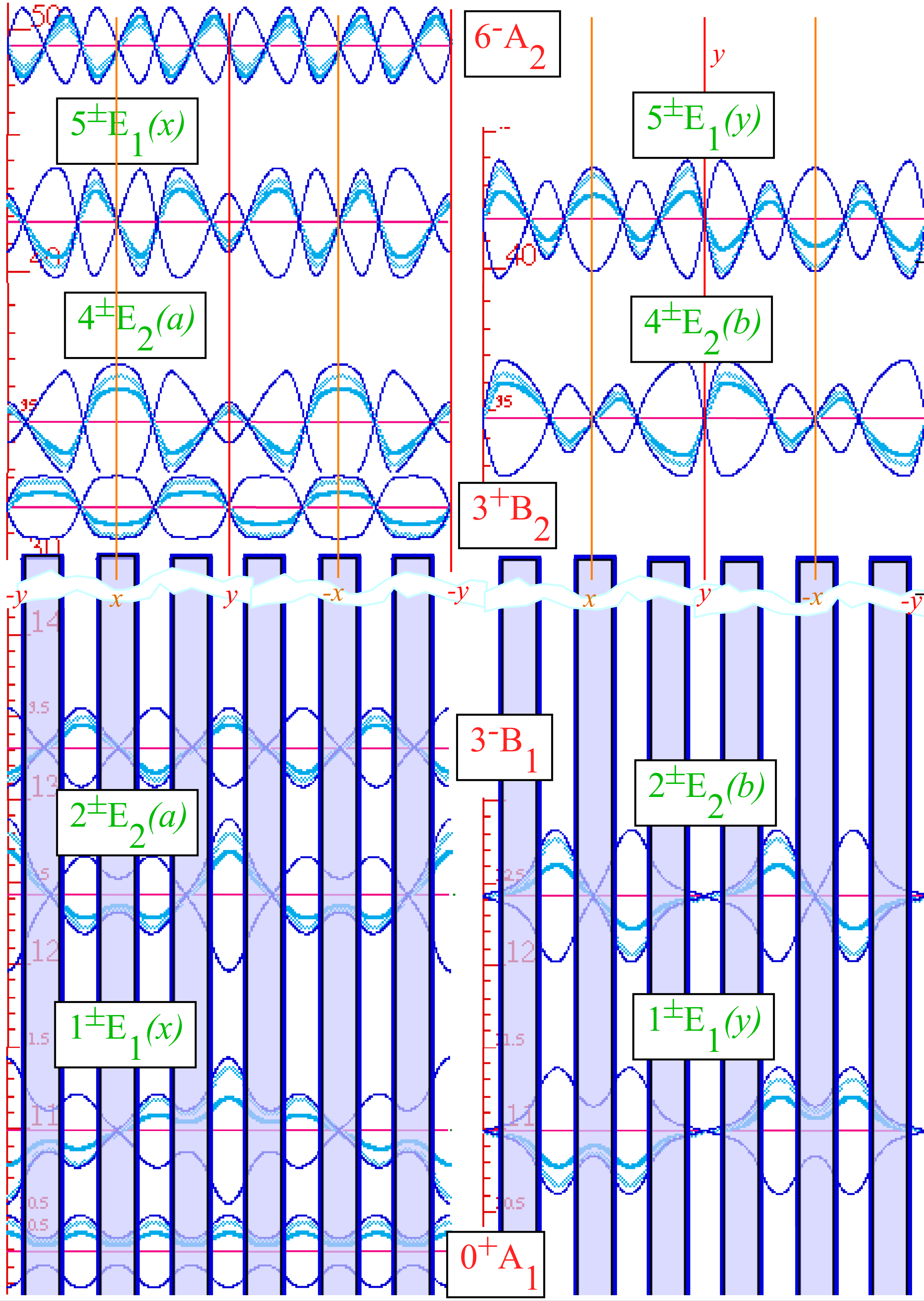
...and $C_2(\mathbf{i}_3)$ characters......and $C_6(\mathbf{1},\mathbf{h}^1,\mathbf{h}^2,...)$ characters

➡ *D_6 symmetry and induced representation band structure* ⬅

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

D_6 symmetry and induced representation band structure

D_6 Band structure and related induced representations



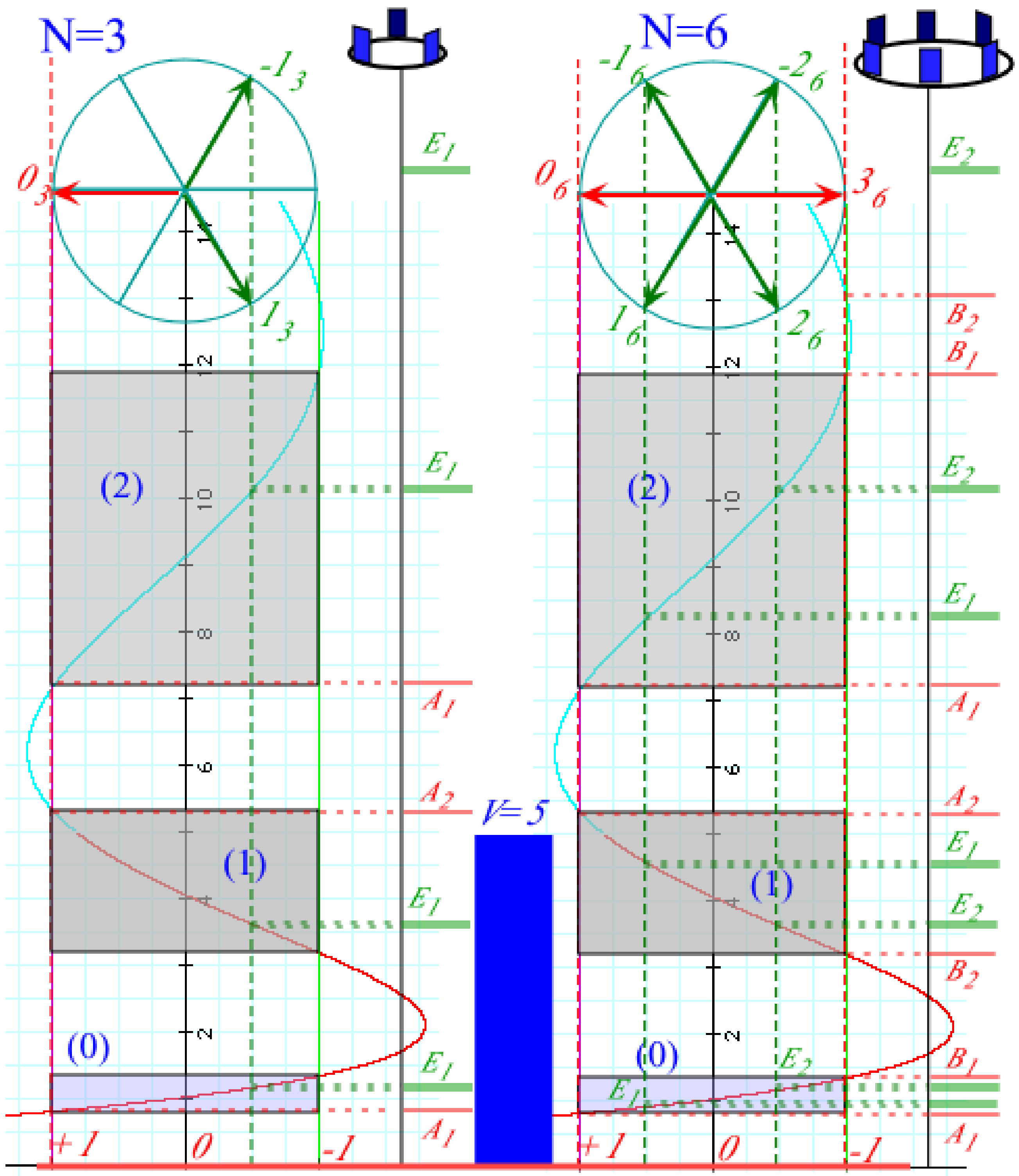
For high energy above potential barriers local C_2 symmetry is replaced by global C_6 angular momentum doublets such as $E_{\pm m}$, A_1A_2, and B_1B_2

$D_6 \supset C_3(h)$	0_6	1_6	2_6	3_6	4_6	5_6
A_1	1	·	·	·	·	·
A_2	1	·	·	·	·	·
E_2	·	·	1	·	1	·
B_2	·	·	·	1	·	·
B_1	·	·	·	1	·	·
E_1	·	1	·	·	·	1

For low energy deep in potential local C_2 symmetry dominates and the bands $A_1E_1E_2B_1$ and $B_2E_2E_1A_2$ that become tight clusters

$D_3 \supset C_2(j_3)$	0_2	1_2
A_1	1	·
A_2	·	1
E_2	1	1
B_2	·	1
B_1	1	·
E_1	1	1

D_6 symmetry and induced representation band structure



For high energy above potential barriers local C_2 symmetry is replaced by global C_6 angular momentum doublets such as $E_{\pm m}$, A_1A_2, and B_1B_2

$D_6 \supset C_3(h)$	0_6	1_6	2_6	3_6	4_6	5_6
A_1	1	.	.	.	.	.
A_2	1	.	.	.	.	.
E_2	.	.	1	.	1	.
B_2	.	.	.	1	.	.
B_1	.	.	.	1	.	.
E_1	.	1	.	.	.	1

For low energy deep in potential local C_2 symmetry dominates and the bands $A_1E_1E_2B_1$ and $B_2E_2E_1A_2$ then become tight clusters

$D_6 \supset C_2(j_3)$	0_2	1_2
A_1	1	.
A_2	.	1
E_2	1	1
B_2	.	1
B_1	1	.
E_1	1	1

Review: *Symmetry reduction and splitting: Subduced irep $D^{\alpha}(D_3)\downarrow C_2 = d^{0_2} \oplus d^{1_2} \oplus$.. correlation*

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Derivation of Frobenius reciprocity

$D_6 \supset D_2 \supset C_2 = D_3 \times C_2$ symmetry and outer product geometry

Irreducible characters

Irreducible representations

Correlations with D_6 characters:

...and $C_2(\mathbf{i}_3)$ characters......and $C_6(\mathbf{1},\mathbf{h}^1,\mathbf{h}^2,...)$ characters

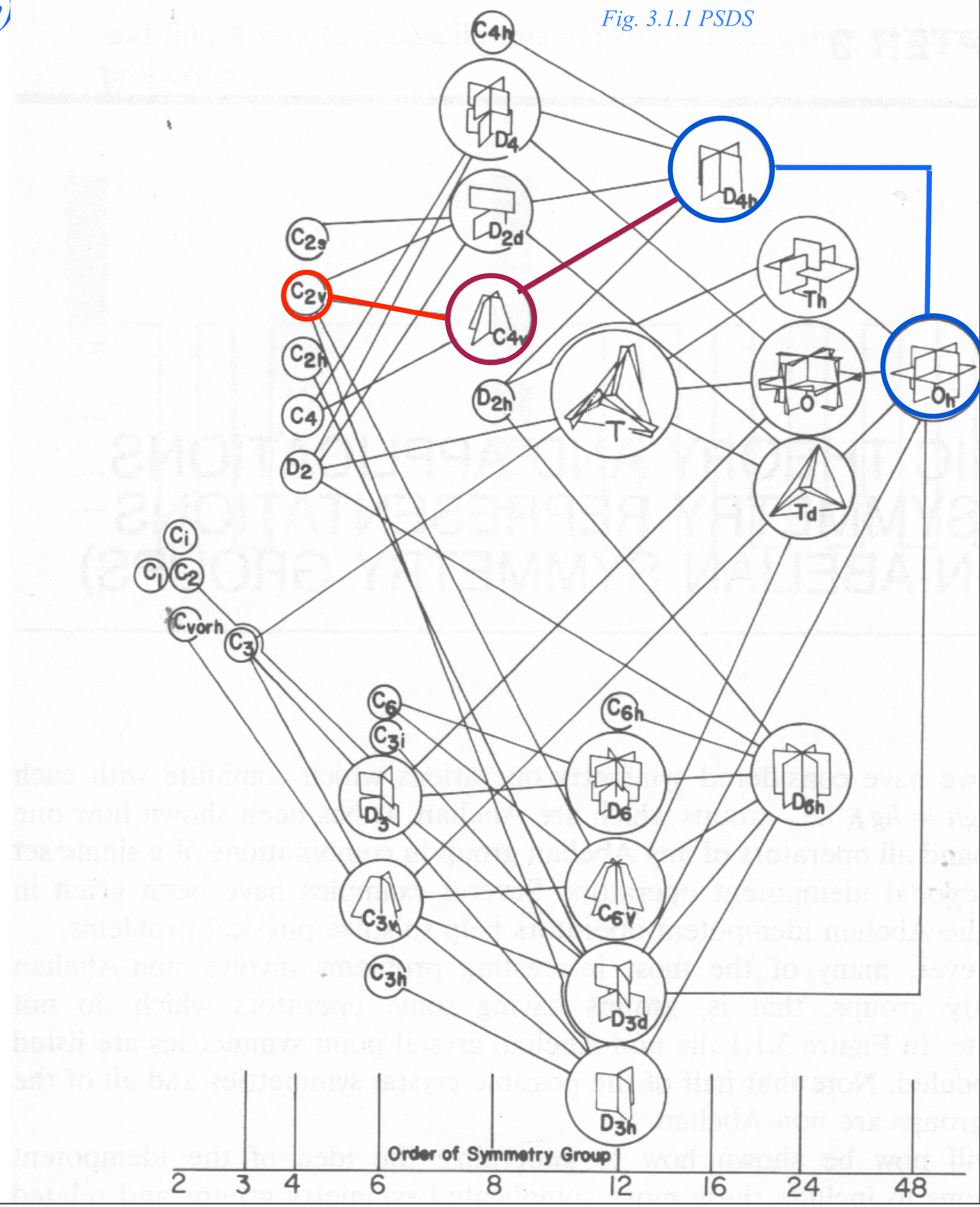
D_6 symmetry and induced representation band structure

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

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

...(one of very many)

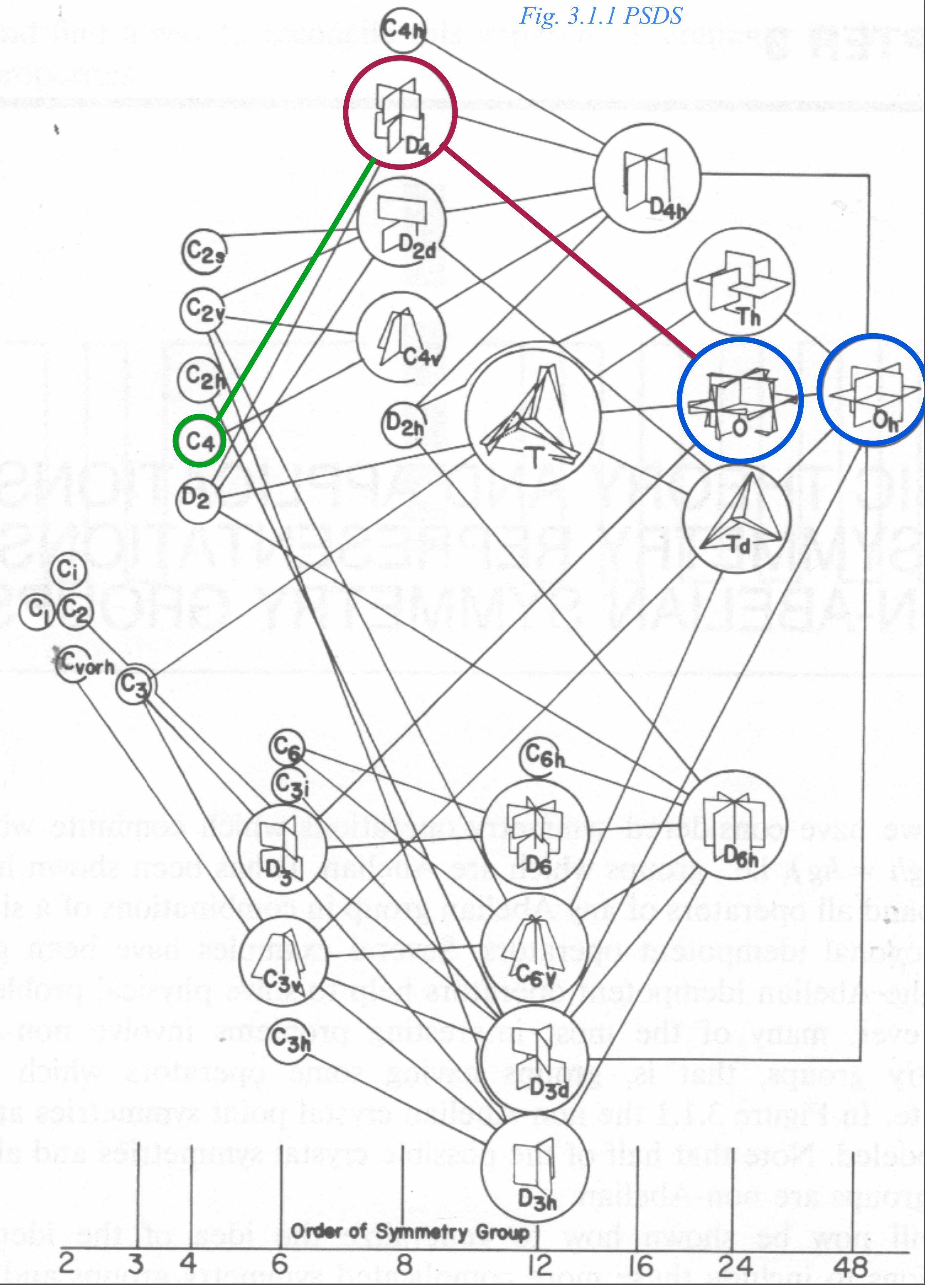
Fig. 3.1.1 PSDS



$O_h \supset O \supset D_4 \supset C_4$ *subgroup chain*

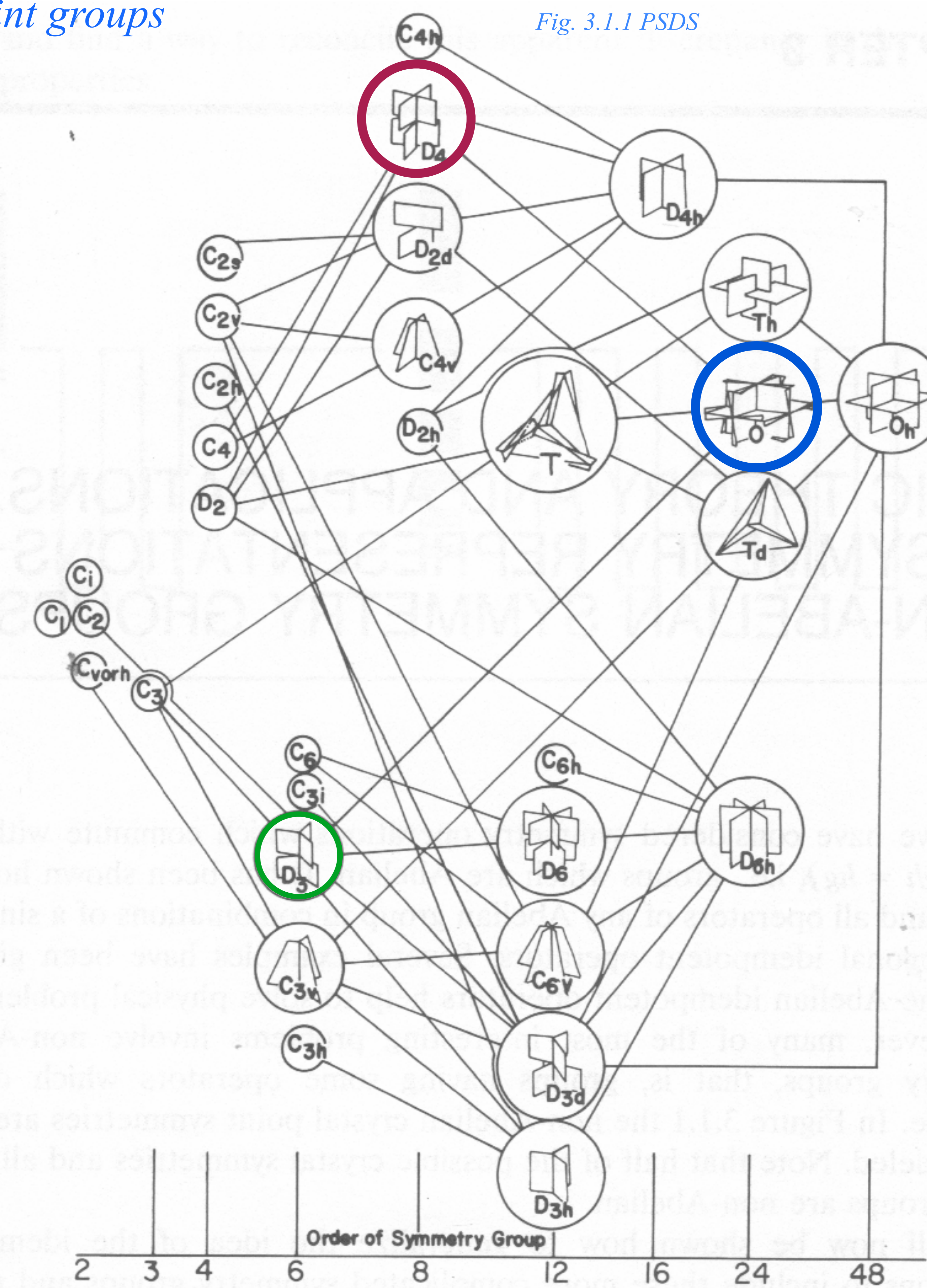
...(one of my favorites)

Fig. 3.1.1 PSDS



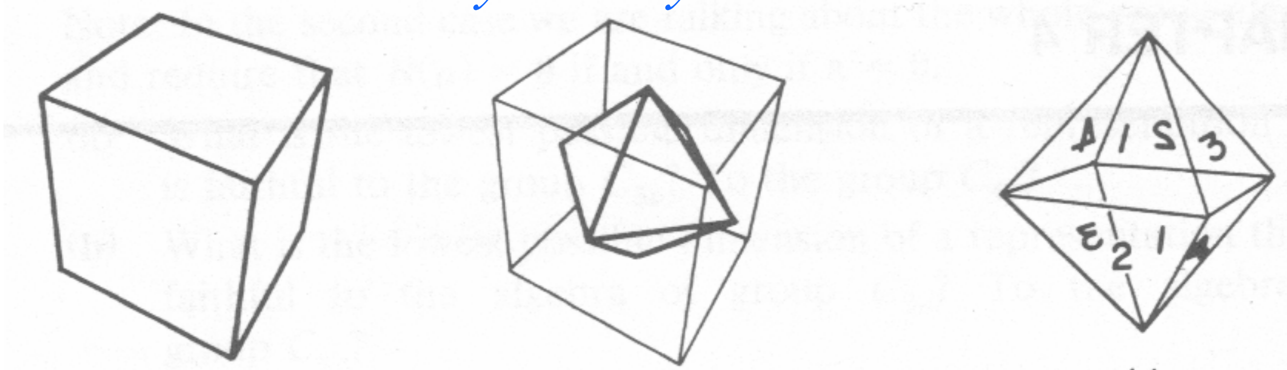
Three groups: O, D_4, and D_3 let you "do"
all the other 32 crystal point groups

Fig. 3.1.1 PSDS



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

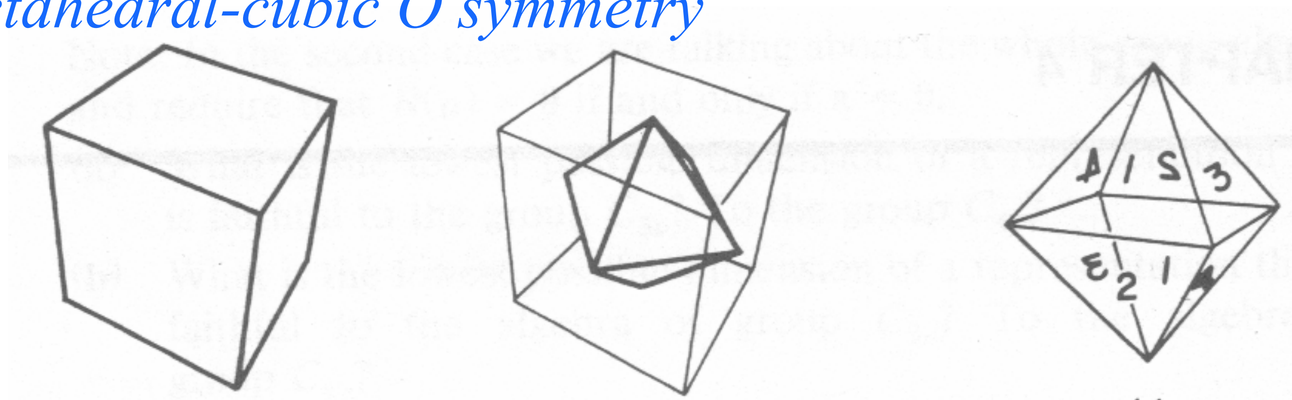
Octahedral-cubic O symmetry



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

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

Octahedral-cubic O symmetry



Order °O=6 hexahedron squares · 4 pts =24

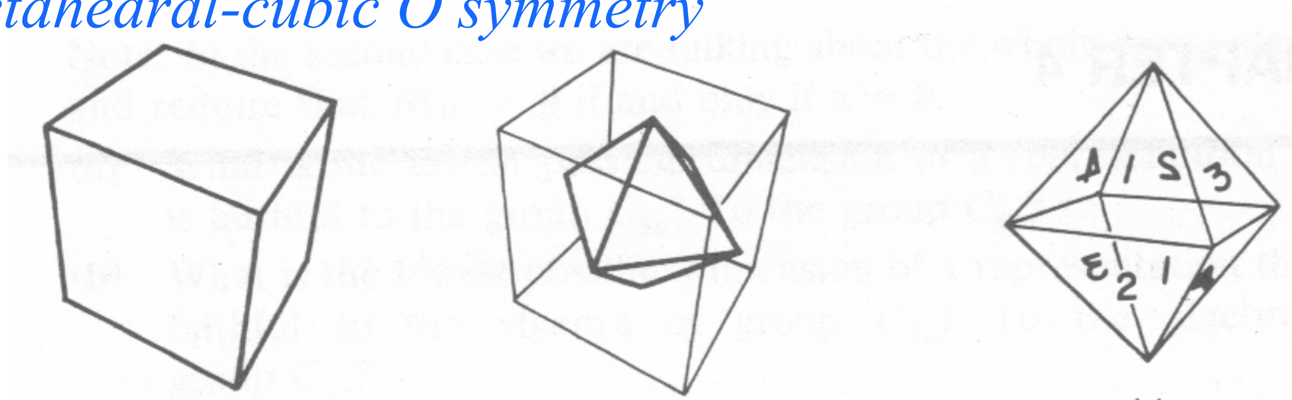
=8 octahedron triangles · 3 pts =24

=12 lines · 2 pts =24 positions

Octahedral group O operations

Class of 1: **1**

Octahedral-cubic O symmetry



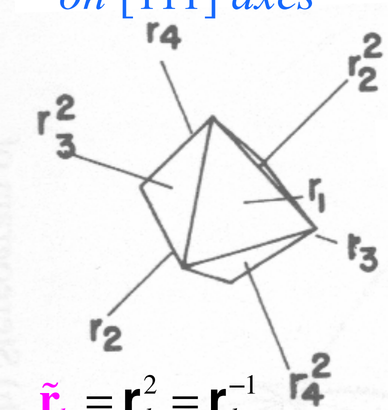
Order °O=6 hexahedron squares · 4 pts =24
=8 octahedron triangles · 3 pts =24
=12 lines · 2 pts =24 positions

Octahedral group O operations

Class of 1: **1**

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

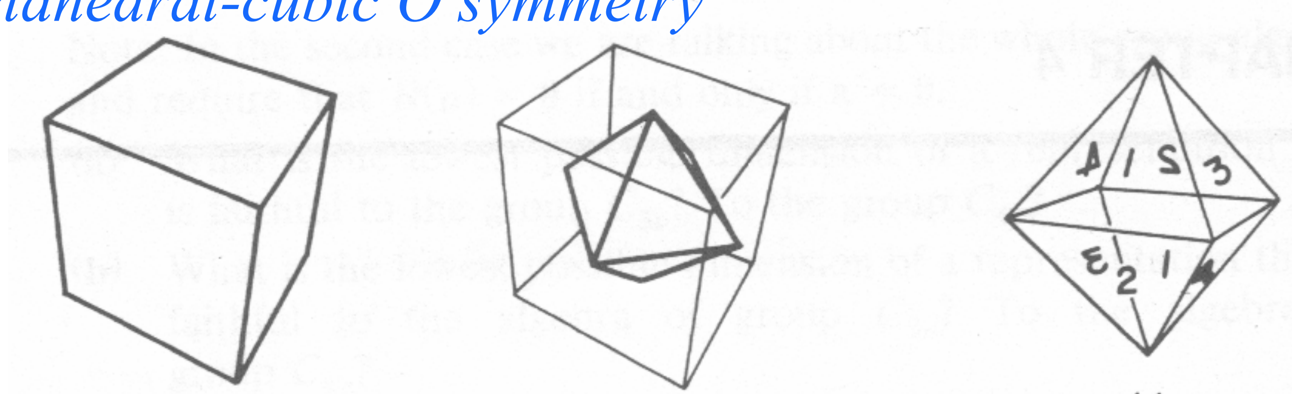
Class of 8:
120° rotations
on [111] *axes*



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

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

Octahedral-cubic O symmetry



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Octahedral group O operations

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Class of 8:
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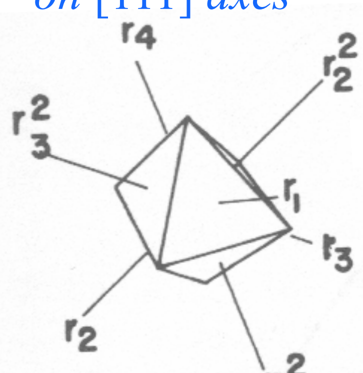
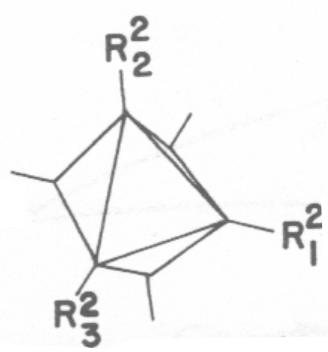


$\tilde{\mathbf{r}}_k = \mathbf{r}_k^2 = \mathbf{r}_k^{-1}$

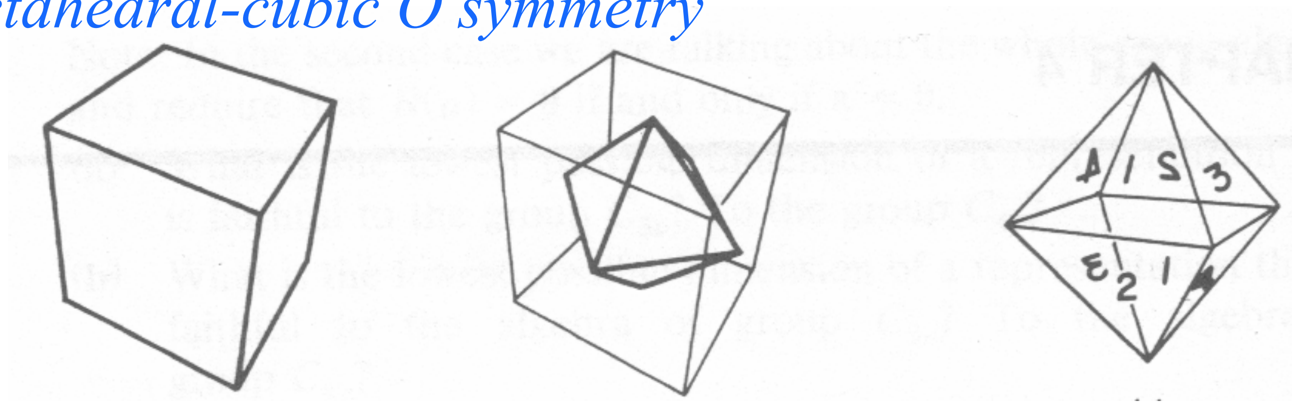


Class of 3
180° rotations
on [100] axes

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

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

Octahedral-cubic O symmetry



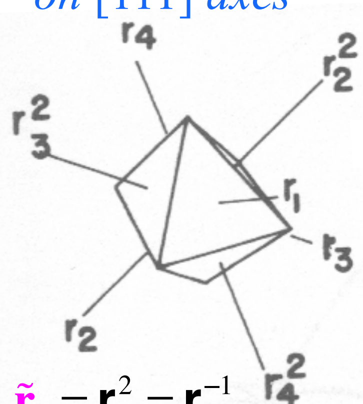
Order °O=6 hexahedron squares · 4 pts =24
=8 octahedron triangles · 3 pts =24
=12 lines · 2 pts =24 positions

Octahedral group O operations

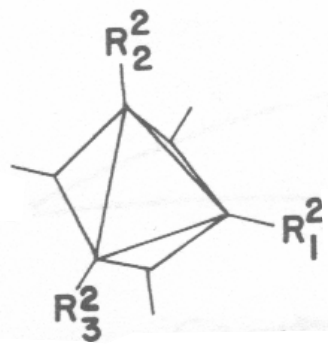
Class of 1: **1**

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

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



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

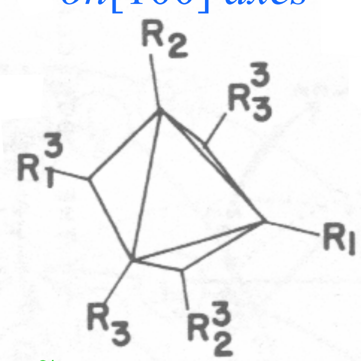


Class of 3
180° rotations
on [100] axes

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

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

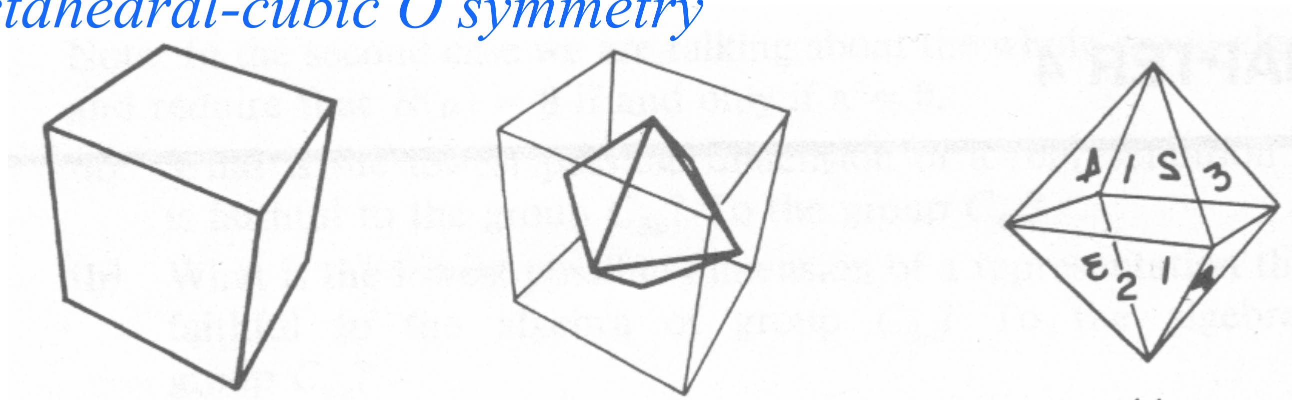
Class of 6
±90° rotations
on[100] axes



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

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

Octahedral-cubic O symmetry

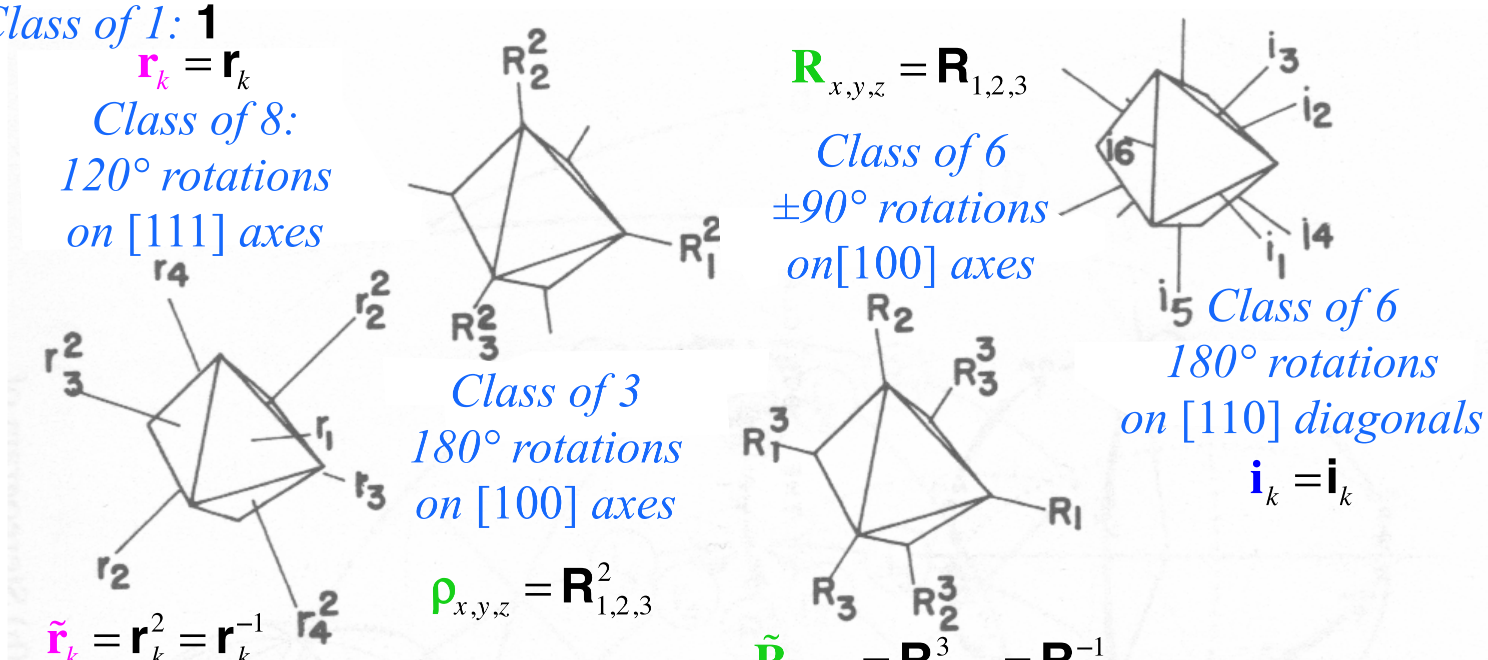


Order °O=6 hexahedron squares · 4 pts =24

=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

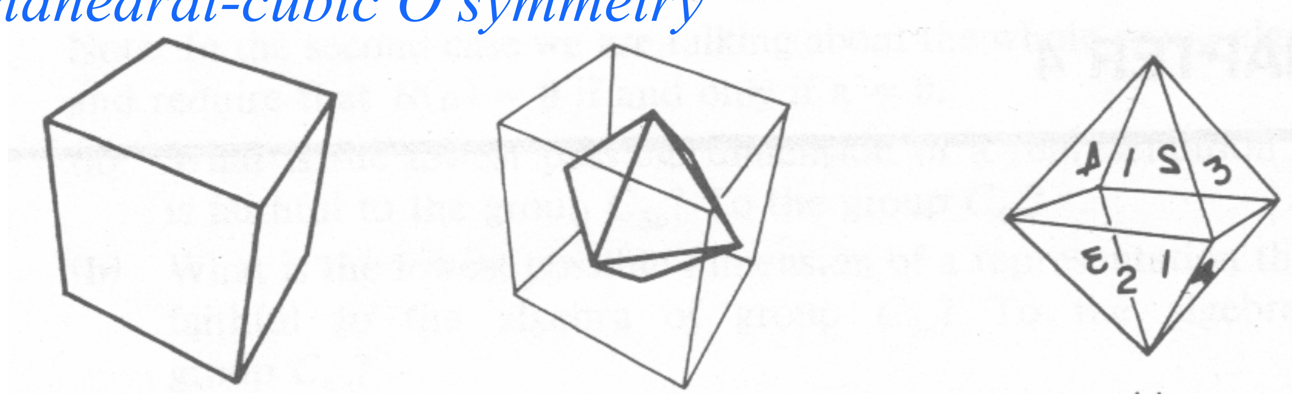
$\tilde{\mathbf{R}}_{x,y,z} = \mathbf{R}_{1,2,3}^3 = \mathbf{R}_{1,2,3}^{-1}$

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



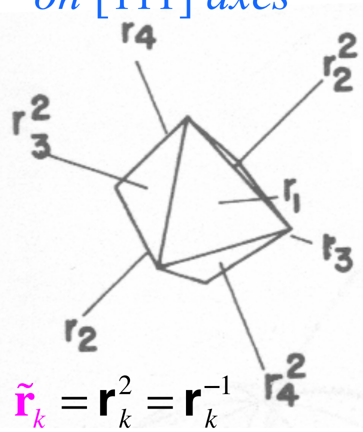
Order °O=6 hexahedron squares · 4 pts =24
=8 octahedron triangles · 3 pts =24
=12 lines · 2 pts =24 positions

Octahedral group O operations

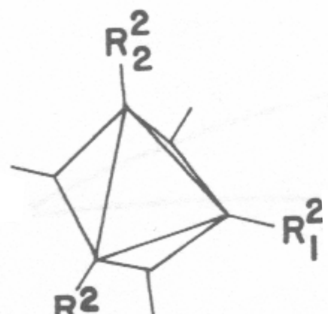
Class of 1: **1**

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

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



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

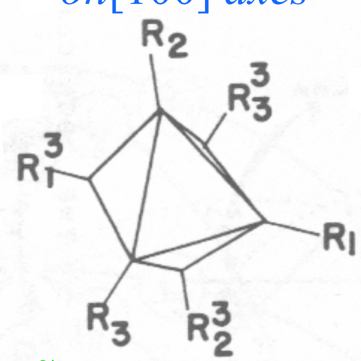


Class of 3:
180° rotations
on [100] axes

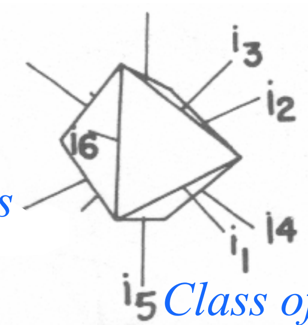
$\rho_{x,y,z} = \mathbf{R}^2_{1,2,3}$

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

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

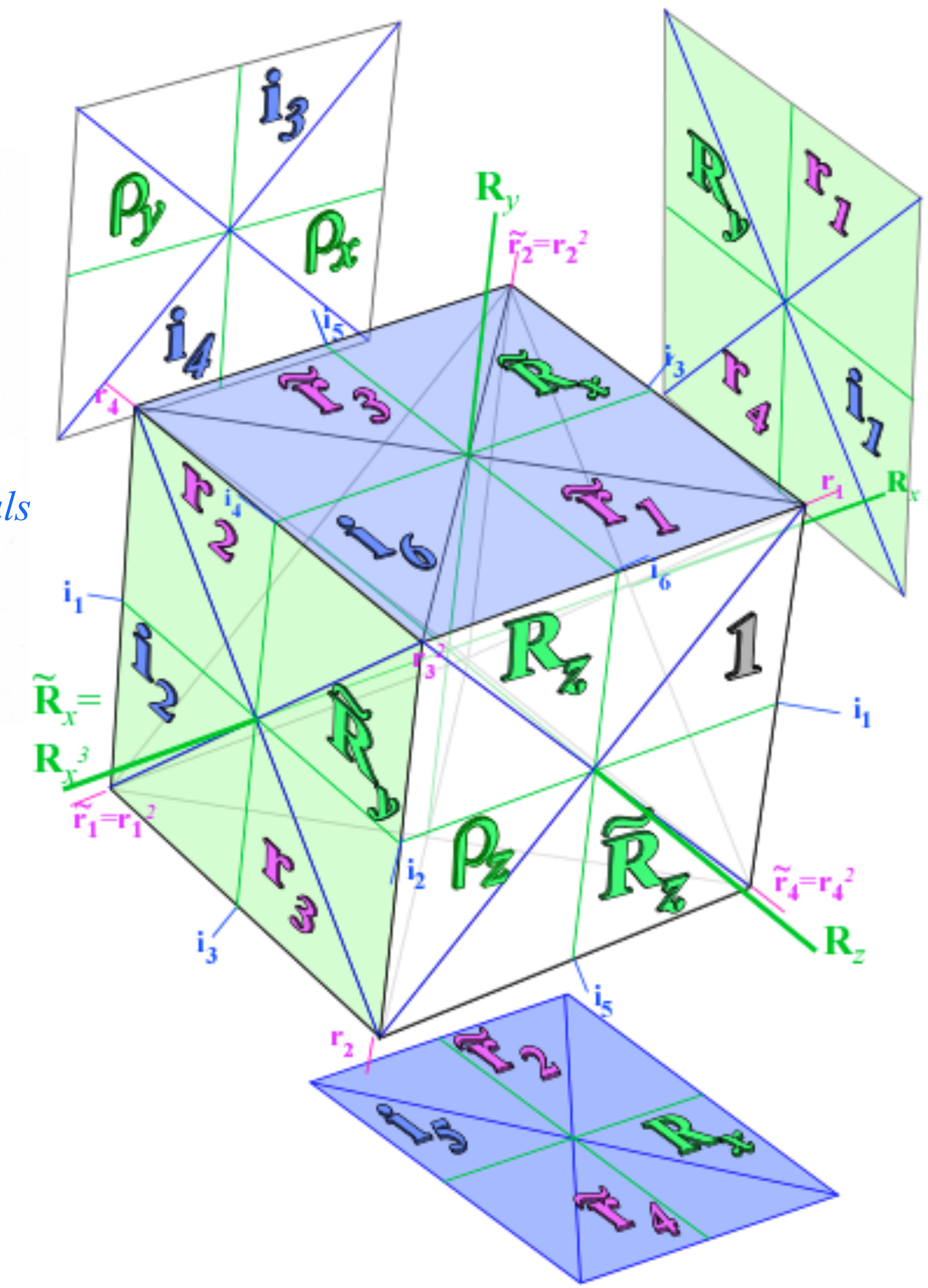


$\tilde{\mathbf{R}}_{x,y,z} = \mathbf{R}^3_{1,2,3} = \mathbf{R}^{-1}_{1,2,3}$



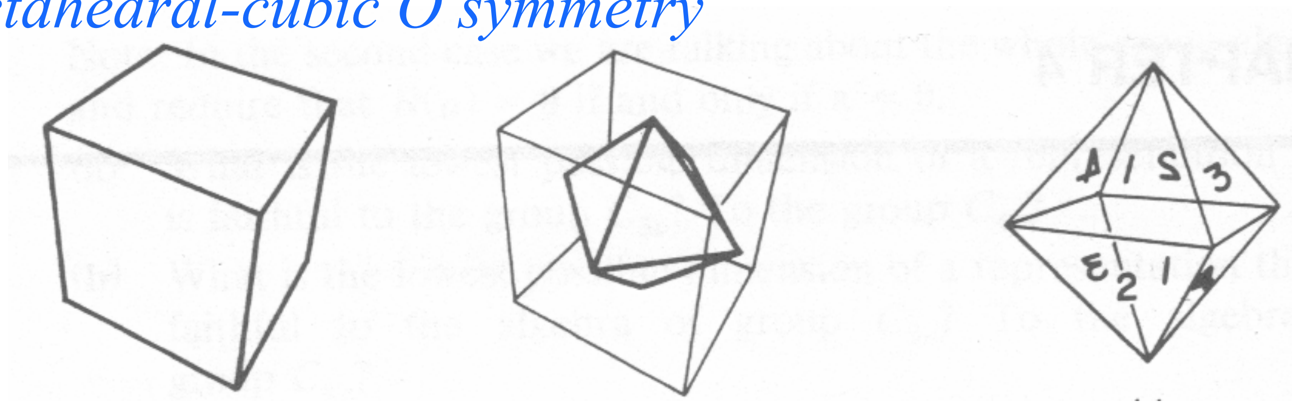
Class of 6:
180° rotations
on [110] diagonals

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



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

Octahedral-cubic O symmetry



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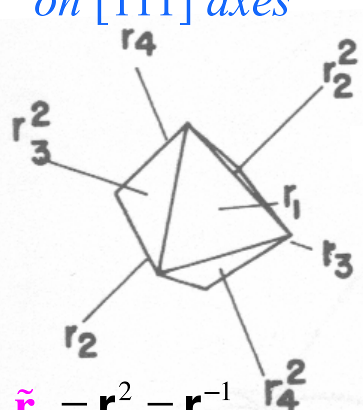
=8 octahedron triangles · 3 pts =24
=12 lines · 2 pts =24 positions

Octahedral group O operations

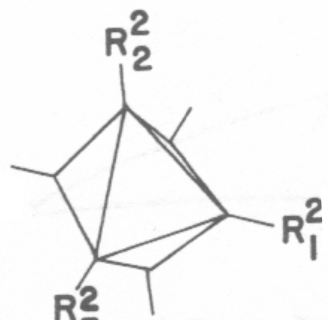
Class of 1: **1**

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

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



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

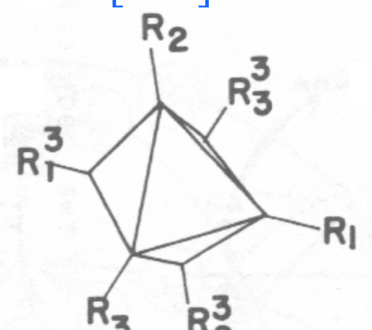


Class of 3: 180° rotations on [100] axes

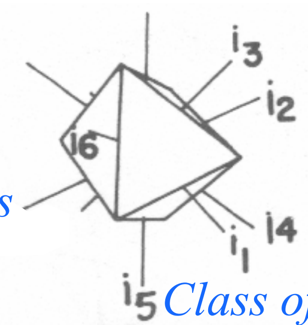
$\rho_{x,y,z} = \mathbf{R}^2_{1,2,3}$

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

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

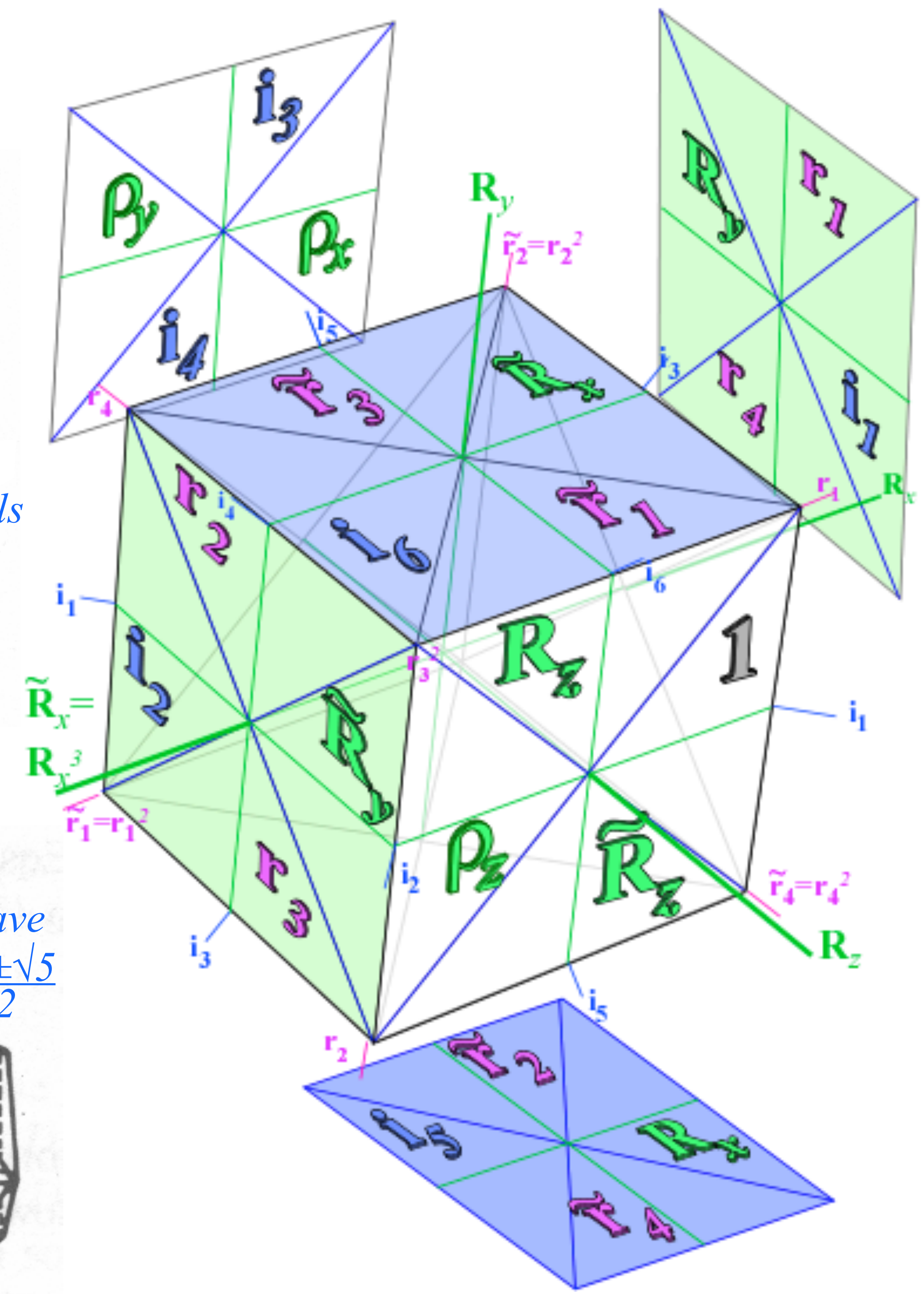


$\tilde{\mathbf{R}}_{x,y,z} = \mathbf{R}^3_{1,2,3} = \mathbf{R}^{-1}_{1,2,3}$

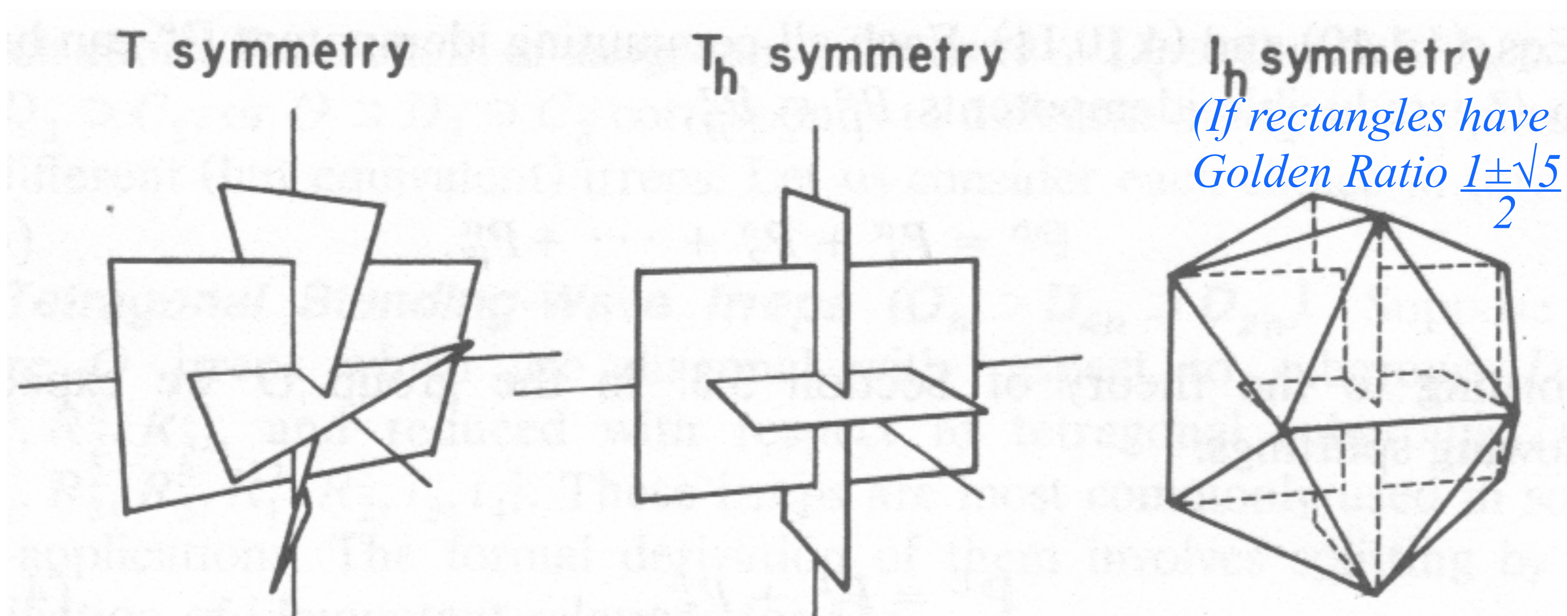


Class of 6: 180° rotations on [110] diagonals

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



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 $O_h \supset O \sim T_d \supset T$

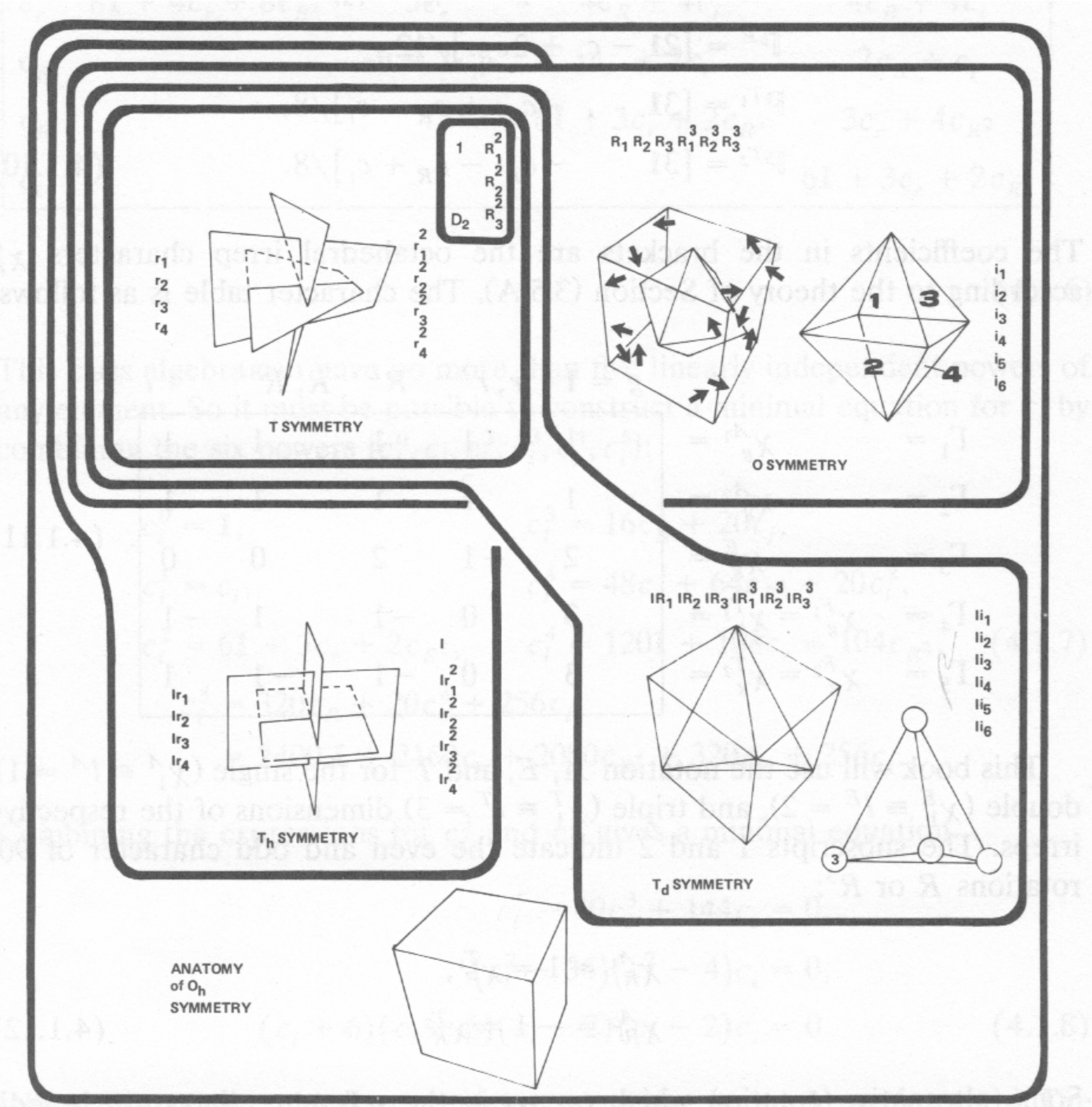
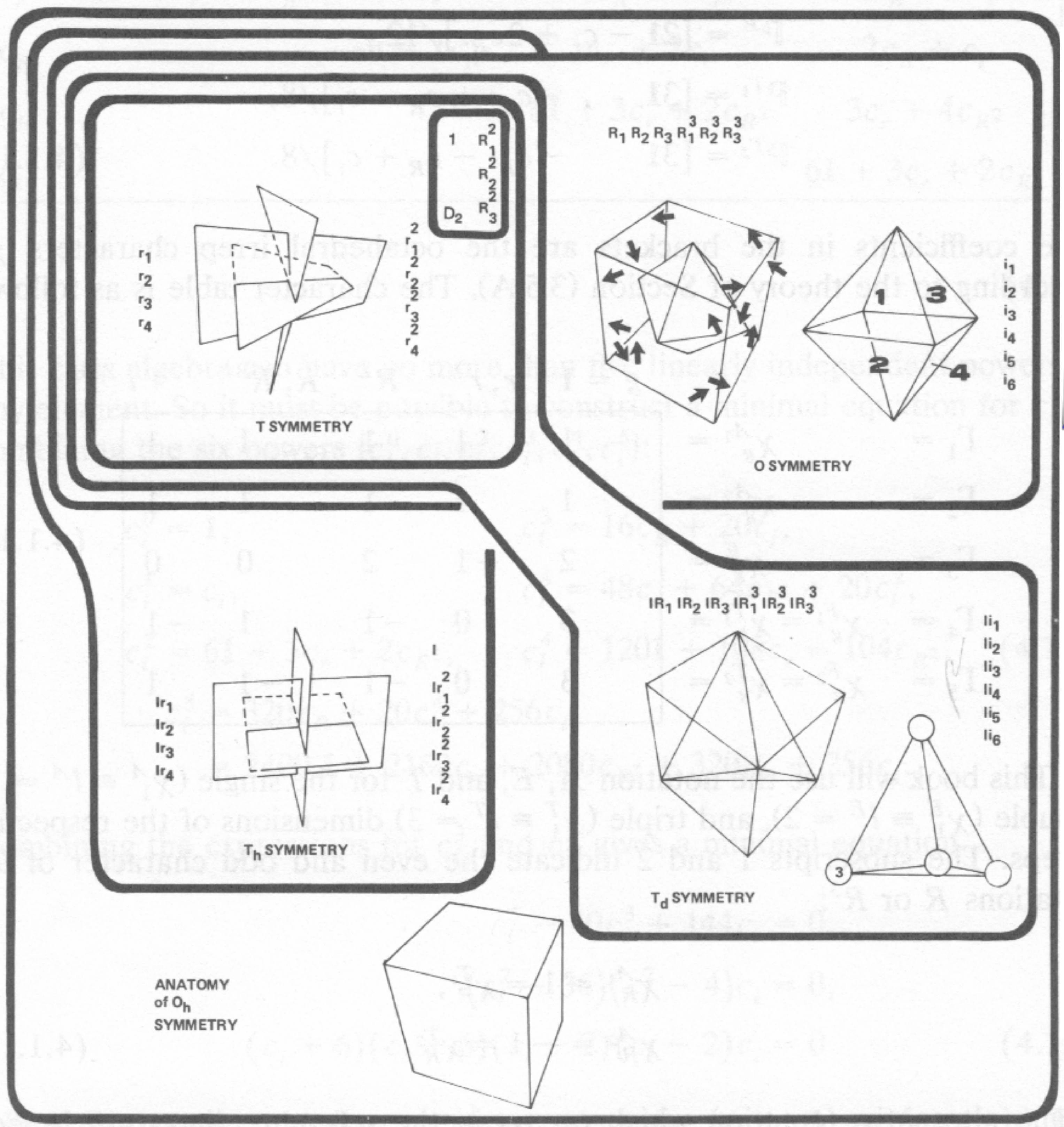


Figure 4.1.5 The full octahedral group (O_h) and four non-Abelian subgroups T, T_h, T_d, and O. The Abelian D_2 subgroup of T is indicated also.

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

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



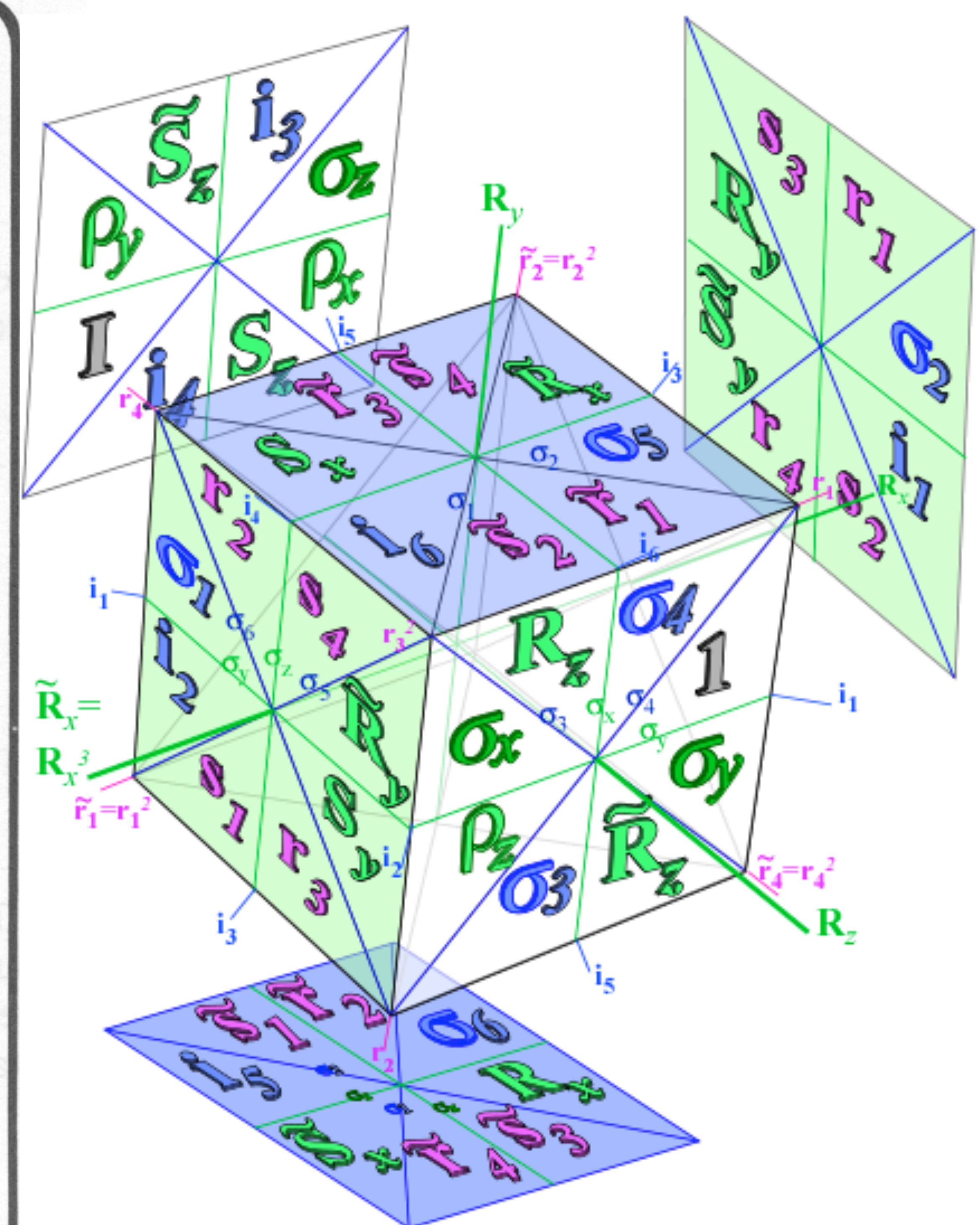


Figure 4.1.5 The full octahedral group (O_h) and four non-Abelian subgroups T, T_h, T_d, and O. The Abelian D_2 subgroup of T is indicated also.

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

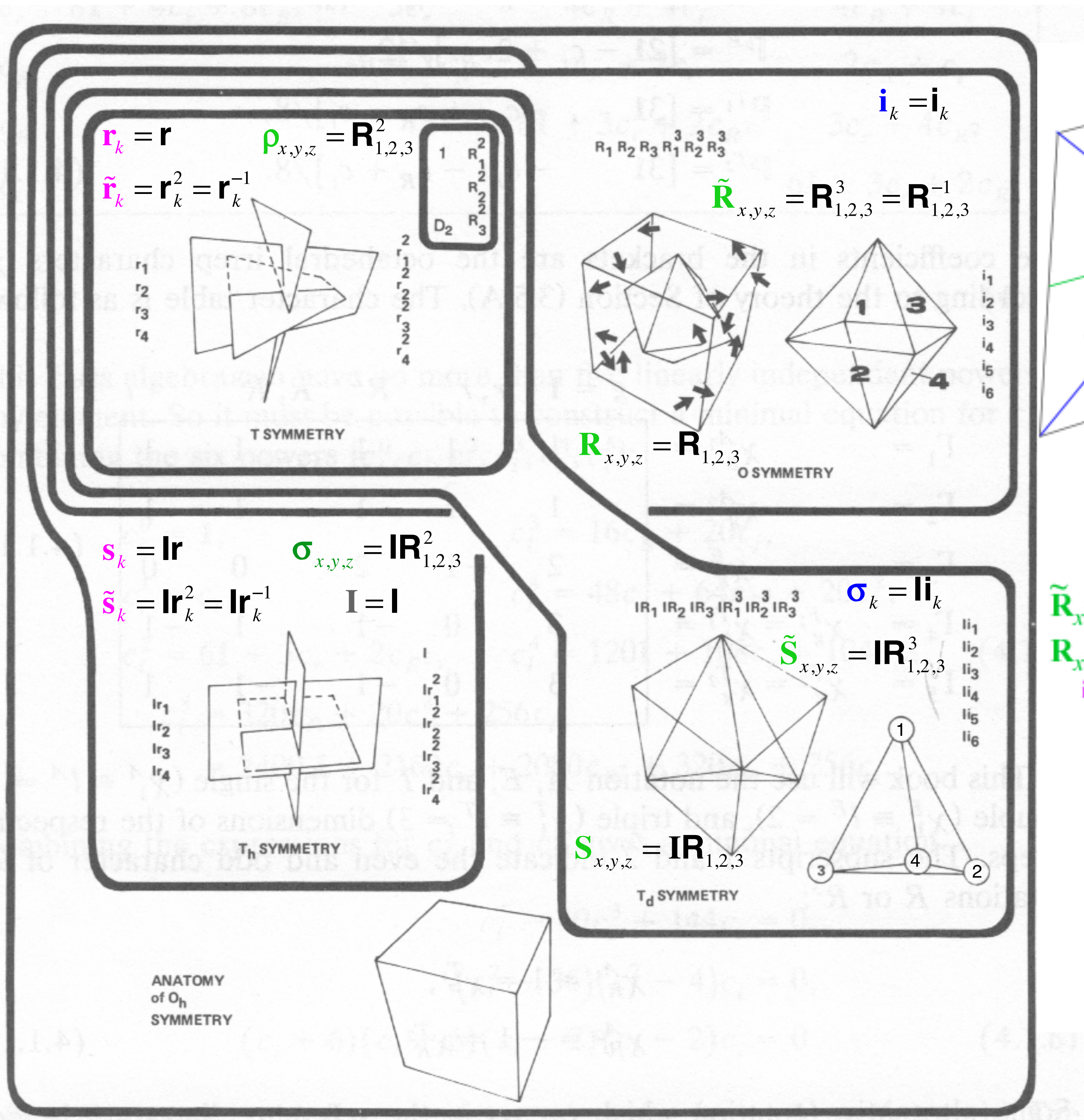
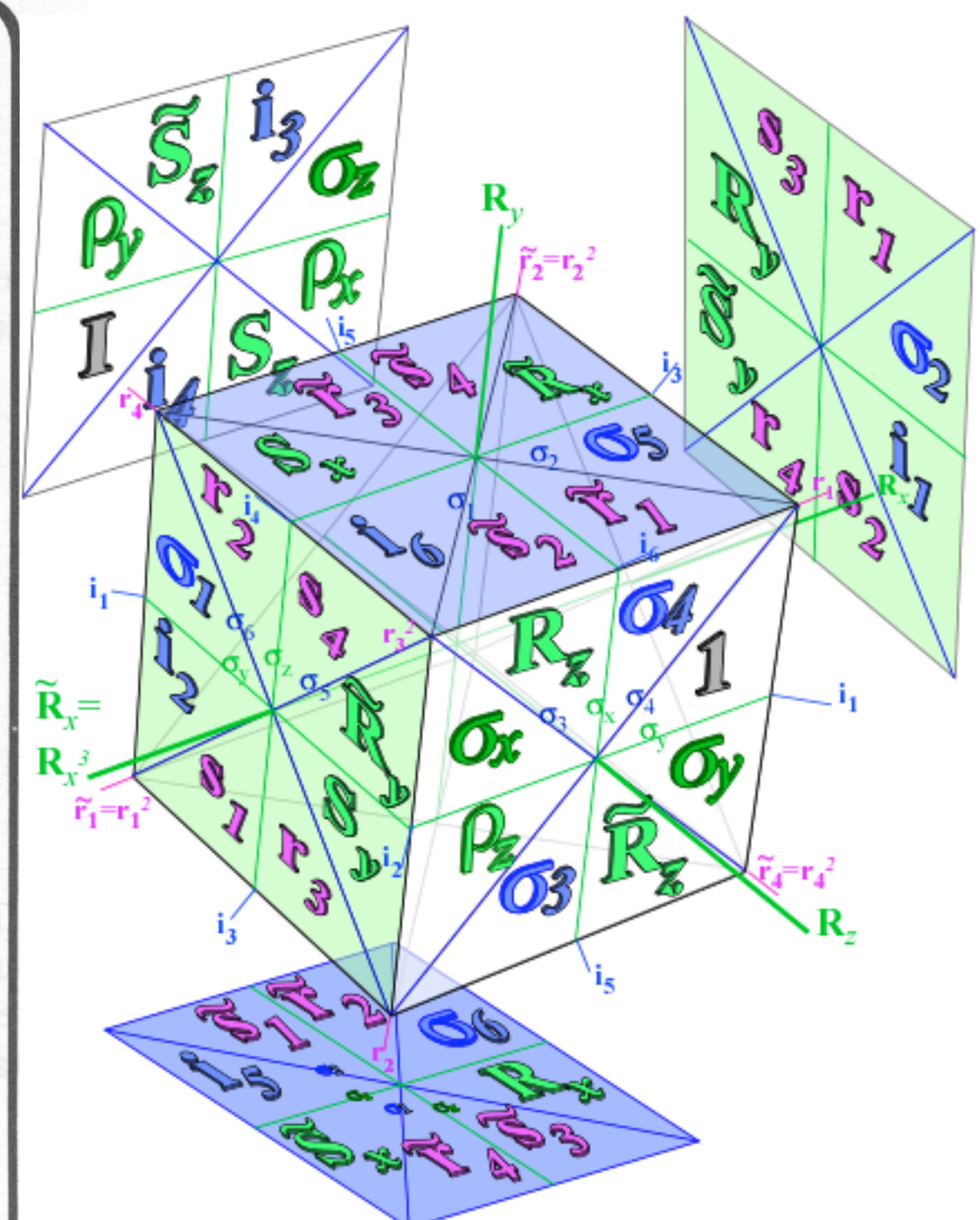
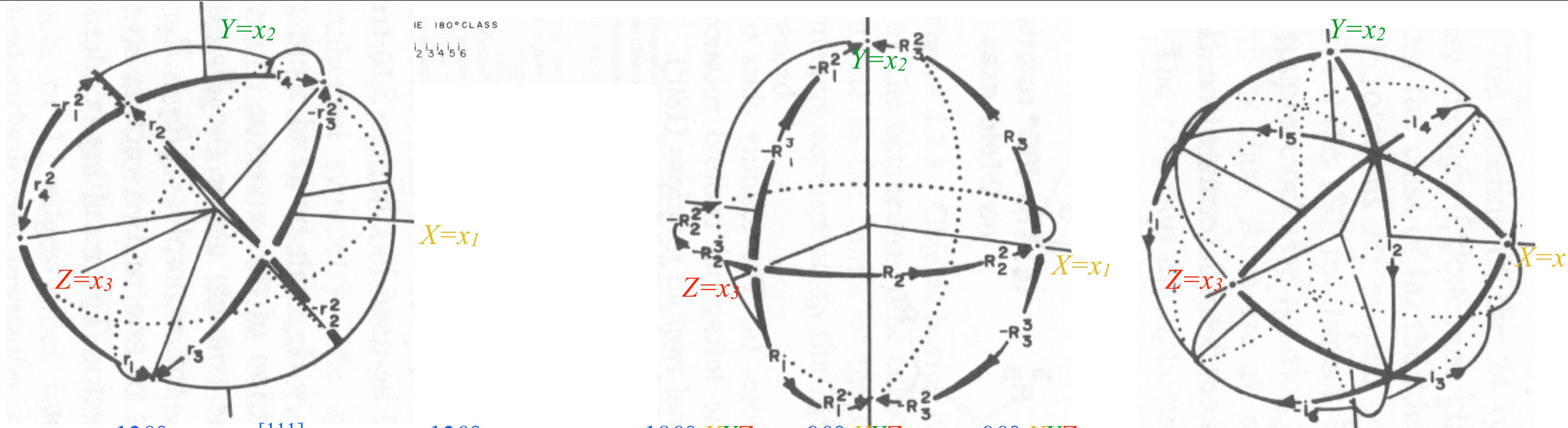


Figure 4.1.5 The full octahedral group (O_h) and four non-Abelian subgroups T, T_h, T_d, and O. The Abelian D_2 subgroup of T is indicated also.

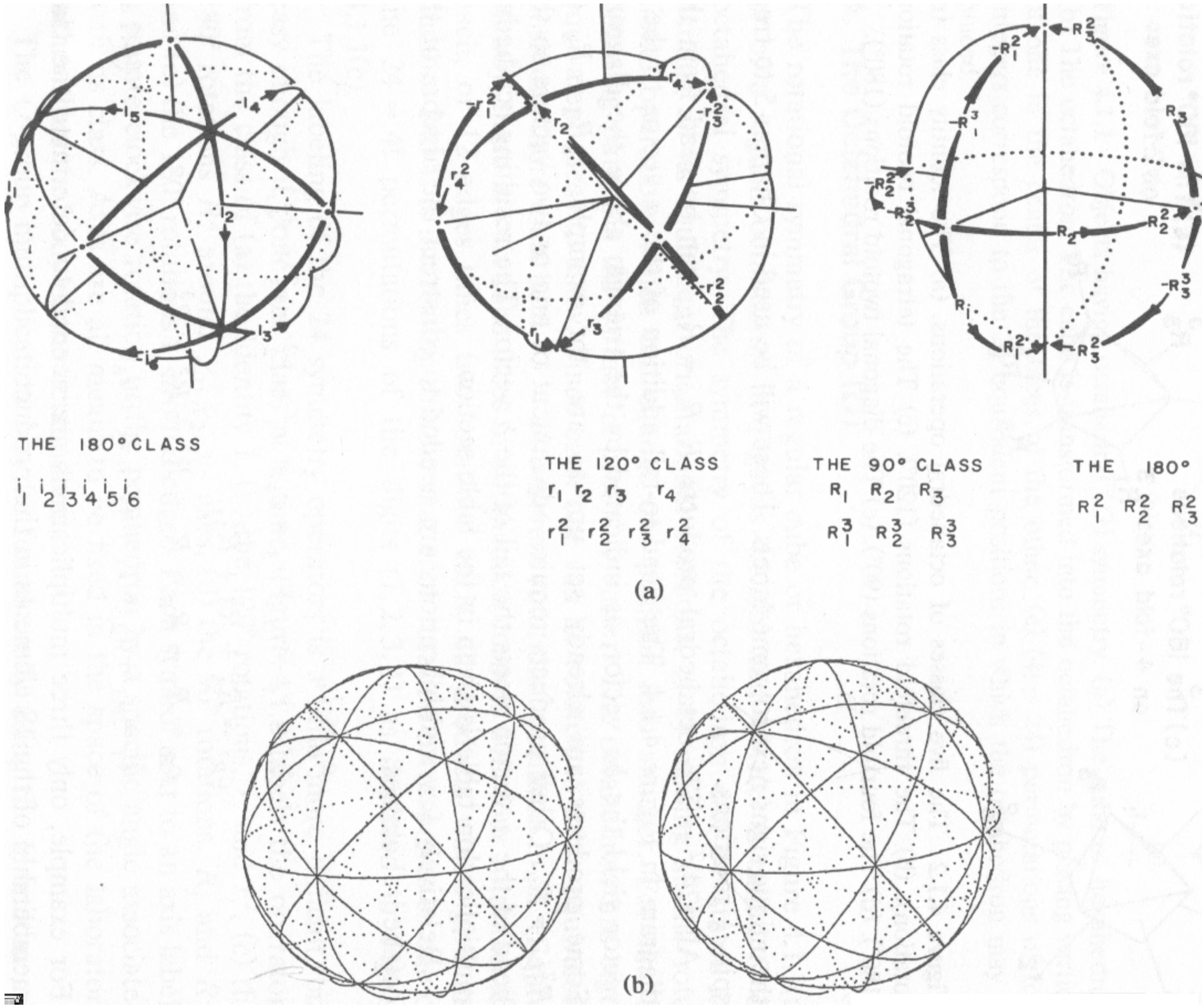
Fig. 4.1.5 from Principles of Symmetry, Dynamics and Spectroscopy





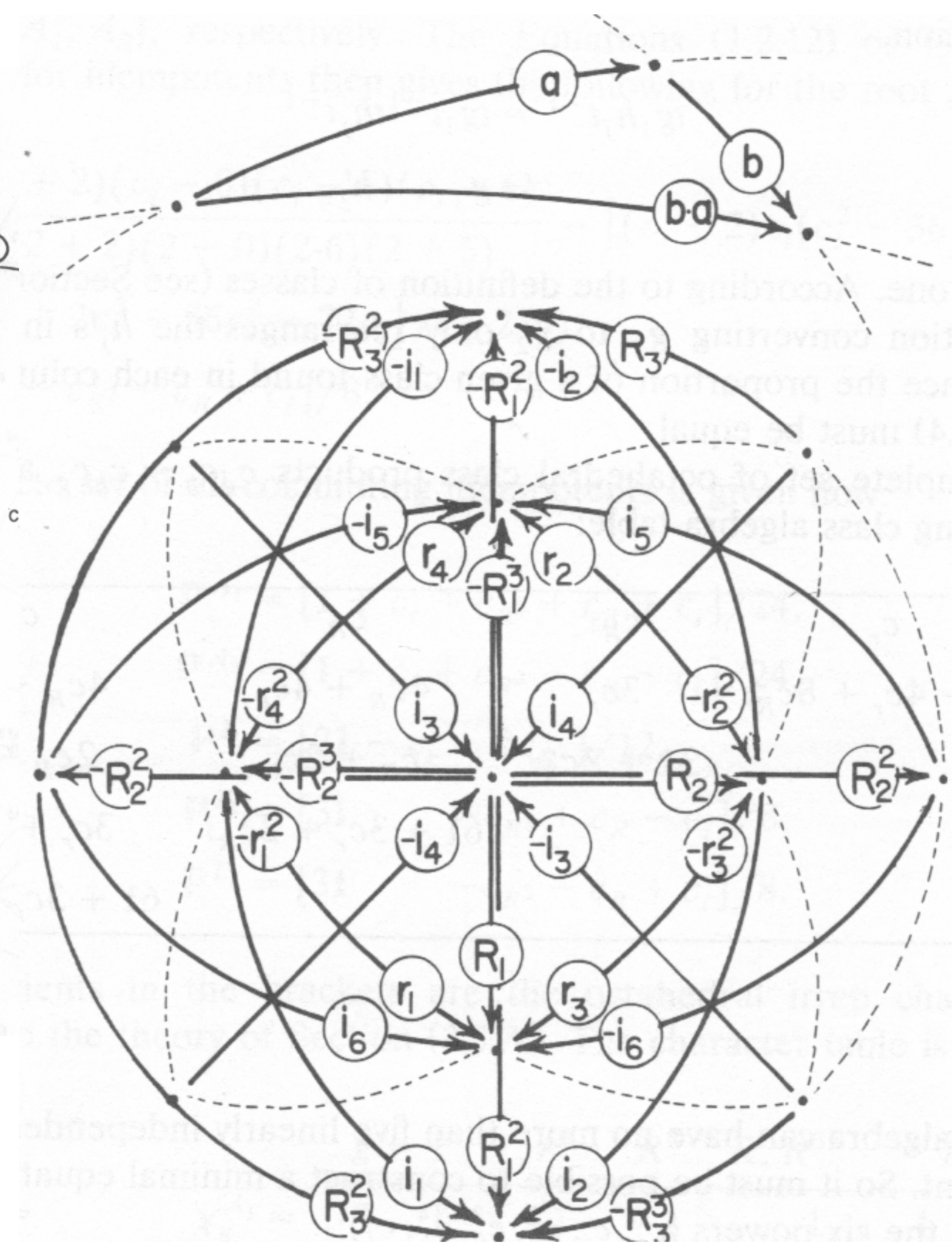
1	[1 1 1] r_1	[1 1 $\bar{1}$] r_2	[1 $\bar{1}$ $\bar{1}$] r_3	[$\bar{1}$ $\bar{1}$ $\bar{1}$] r_4	[1 1 1] r_1^2	[1 1 $\bar{1}$] r_2^2	[1 $\bar{1}$ $\bar{1}$] r_3^2	[$\bar{1}$ $\bar{1}$ $\bar{1}$] r_4^2	[1 0 0] R_1^2	[0 1 0] R_2^2	[0 0 1] R_3^2	[1 0 0] R_1	[0 1 0] R_2	[0 0 1] R_3	[1 0 0] R_1^3	[0 1 0] R_2^3	[0 0 1] 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 rotation product Table F.2.1 from Principles of Symmetry, Dynamics and Spectroscopy


THE 180° CLASS
i1 i2 i3 i4 i5 i6
THE 120° CLASS
r1 r2 r3 r4
r1² r2² r3² r4²
THE 90° CLASS
R1 R2 R3
R1³ R2³ R3³
THE 180° C
R1² R2² R3²

(a)

(b)


a
b
b·a
-R3²
-i1
-R1²
-i2
R3
-i5
r4
-R1³
r2
i5
-r4²
i3
i4
-r2²
-R2²
-R2³
R2
R2²
-r1²
-i4
-i3
-r3²
R1
r1
r3
i6
-i6
R1²
i1
i2
R3²
-R3³

$\ell^{A_1} = 1$

$\ell^{A_2} = 1$

$\ell^{E} = 2$

$\ell^{T_1} = 3$

$\ell^{T_2} = 3$

Example: $G = O$

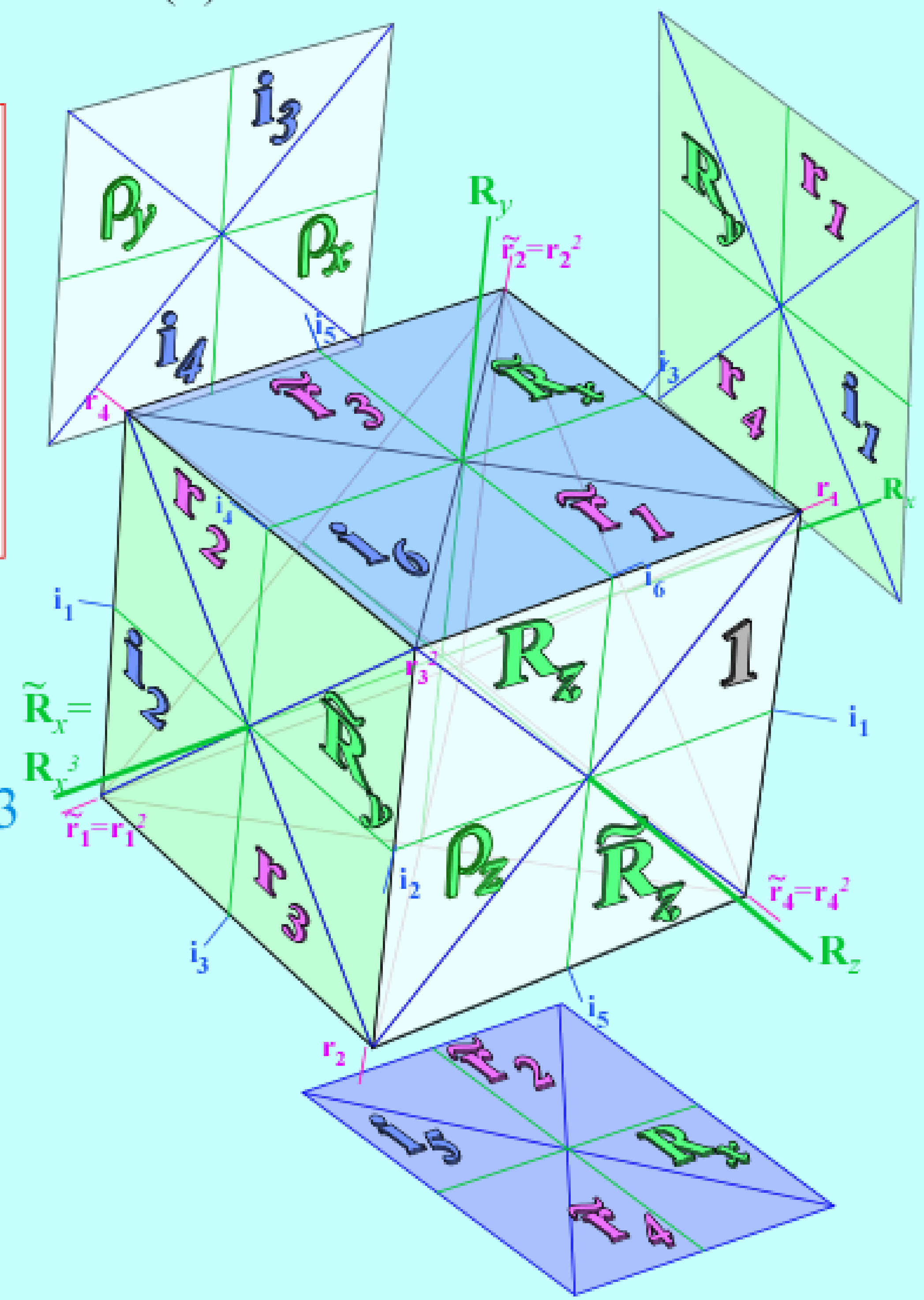
Cubic-Octahedral Group O

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

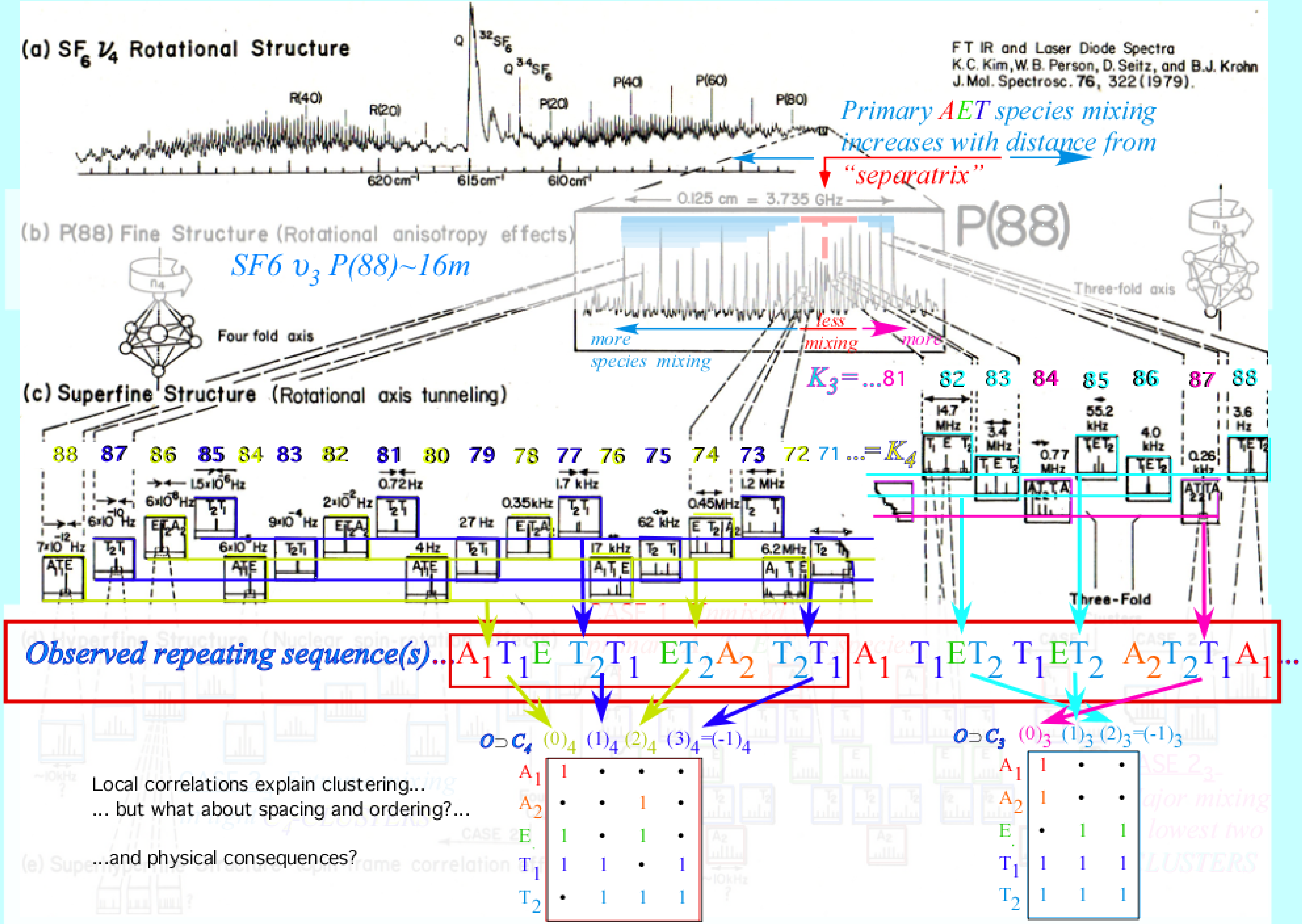


$O \supset C_4$

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



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

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

Deriving $D_3 \sim C_{3v}$ products - By group definition $|g\rangle = \mathbf{g}|1\rangle$ of position ket $|g\rangle$