AMOP
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3.05.18 class 15.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Discrete symmetry subgroups of O(3)$\supset$(Octahedral $O_h \supset O \sim T_d$, Cubic-Tetrahedral $T_h \supset T$): Characters and subgroup-chain defined ireps, and applications to SF_6 and CF_4 spectra

Review: *General all-commuting class-character-projector formula derivations.* *f^{μ} derivation 2015 Lect15 p.40-45.*

$\mathbb{P}^{\mu}$ in χ^{μ}-terms of $\boldsymbol{\kappa}_{\mathbf{g}}$ *$\boldsymbol{\kappa}_{\mathbf{g}}$ in $\chi^{\mu *}$-terms of $\mathbb{P}^{\mu}$* *Irep frequency f^{μ} in $\chi^{\mu *}$-terms of Trace$R(\mathbf{g})$*

Introducing octahedral/ tetrahedral symmetry $O_h \supset O \sim T_d \supset T$: relating $D_4 \supset C_4$ and $D_3 \supset C_3$

- *Octahedral-cubic O symmetry and group operations,* *O slide-rule*
- *Tetrahedral symmetry leads to Icosahedral*
- *Octahedral groups $O_h \supset O \sim T_d \supset T$ and its large subgroups.* *O_h slide-rule*
  - *Octahedral O and spin-$O \subset U(2)$ nomograms*

Tetrahedral T class algebra *minimal equations* *centrum projectors and characters*
Octahedral O class algebra *minimal equations* *centrum projectors and characters*

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- *Octahedral $O_h \supset O \supset C_{\mathbf{I}}$ subgroup correlations*

Octahedral subgroup correlation *$O_h \supset O \supset D_4$* *$O_h \supset O \supset D_4 \supset C_4$* *and level-splitting*

- *Comparing $O \supset C_4$ and $O \supset C_3$ and $O \supset C_2$*

$R(3) \subset O(3) \supset O_h \supset O$ character analysis: Crystal field splitting *p, d, f,…orbitals*

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Global vs Local *External LAB splitting vs Internal BODY clustering*

- *Detailed superfine structure for A_1T_1E cluster* *preview of next lecture*

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

Web Resources - front page
UAF Physics UTube channel

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

2014 AMOP
2017 Group Theory for QM
2018 AMOP

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

Theory of hyperfine and superfine levels in symmetric polyatomic molecules.

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

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

Rotation–vibration spectra of icosahedral molecules.

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

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

RESONANCE AND REVIVALS

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

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

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

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$\mathbb{P}^{\mu}$ *in terms of* $\boldsymbol{\kappa}_{\mathbf{g}}$ (class sum: $\mathbf{g+g'+g''+\ldots}$)

$\boldsymbol{\kappa}_{\mathbf{g}}$ *in terms of* $\mathbb{P}^{\mu}$ (all-commuting **P**rojectors)

$\mathbb{P}^{\mu}$ *in terms of* $\boldsymbol{\kappa}_{\mathbf{g}}$ (class sum: **g+g′+g″+…**)

$(\mu)^{th}$ *irep characters* $\chi^{(\mu)}(\mathbf{g})$ given by trace definition: $\chi^{\mu}(\mathbf{g}) \equiv Trace\ D^{\mu}(\mathbf{g}) = \sum_{m=1}^{\ell^{\mu}} D^{\mu}_{mm}(\mathbf{g})$

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irep projectors vs. **g**

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

for unitary D^{μ}_{nm}

$$D^{\mu^{*}}_{mn}(g) = D^{\mu}_{nm}\left(g^{-1}\right)$$

Weyl expansion p40
used here.
(Lect.13 p40 to p78.)

$\kappa_{\mathbf{g}}$ *in terms of* $\mathbb{P}^{\mu}$ (all-commuting **P**rojectors)

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$\boldsymbol{\kappa}_{\mathbf{g}}$ *in terms of* $\mathbb{P}^{\mu}$ (all-commuting **P**rojectors)

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$$\boxed{\mathbb{P}^{\mu} = \sum_{classes\,\boldsymbol{\kappa}_{\mathbf{g}}} \frac{\ell^{\mu}}{{}^{\circ}G}\chi^{\mu^{*}}_{g}\boldsymbol{\kappa}_{\mathbf{g}}}\ , \quad \text{where: } \chi^{\mu}_{g} = \chi^{\mu}(\mathbf{g}) = \chi^{\mu}(\mathbf{hgh}^{-1})$$

(by χ^{μ} trace invariance)

$\boldsymbol{\kappa}_{\mathbf{g}}$ *in terms of* $\mathbb{P}^{\mu}$ (all-commuting **P**rojectors)

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$$\mathbb{P}^{\mu} = \sum_{m=1}^{\ell^{\mu}} \mathbf{P}^{\mu}_{mm} = \frac{\ell^{\mu}}{{}^{\circ}G} \sum_{\mathbf{g}}^{{}^{\circ}G} \sum_{m=1}^{\ell^{\mu}} D^{\mu *}_{mm}(g)\, \mathbf{g} = \frac{\ell^{\mu}}{{}^{\circ}G} \sum_{\mathbf{g}}^{{}^{\circ}G} \chi^{\mu *}(g)\, \mathbf{g}$$

$$\boxed{\mathbb{P}^{\mu} = \sum_{classes\, \kappa_{\mathbf{g}}} \frac{\ell^{\mu}}{{}^{\circ}G} \chi^{\mu^{*}}_{g} \kappa_{\mathbf{g}}}$$

, where: $\chi^{\mu}_{g} = \chi^{\mu}(\mathbf{g}) = \chi^{\mu}\left(\mathbf{h}\mathbf{g}\mathbf{h}^{-1}\right)$ (by χ^{μ} trace invariance)

$\kappa_{\mathbf{g}}$ *in terms of* $\mathbb{P}^{\mu}$ (all-commuting **P**rojectors)

Find *all-commuting class* $\kappa_{\mathbf{g}}$ in terms of $\mathbb{P}^{\mu}$ given $\mathbf{g}$ vs. *irep projectors* $\mathbf{P}^{\mu}_{mn}$:

$$\boxed{\mathbf{g} = \sum_{\mu} \sum_{m}^{\ell^{\mu}} \sum_{n}^{\ell^{\mu}} D^{\mu}_{mn}(g)\, \mathbf{P}^{\mu}_{mn}}$$

$\mathbb{P}^{\mu}$ *in terms of* $\boldsymbol{\kappa}_{\mathbf{g}}$ (class sum: **g+g′+g″+…**)

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Find *all-commuting class* $\boldsymbol{\kappa}_{\mathbf{g}}$ in terms of $\mathbb{P}^{\mu}$ given **g** vs. *irep projectors* $\mathbf{P}^{\mu}_{mn}$:

$$\boxed{\mathbf{g}=\sum_{\mu}\sum_{m}^{\ell^{\mu}}\sum_{n}^{\ell^{\mu}}D^{\mu}_{mn}(g)\,\mathbf{P}^{\mu}_{mn}}$$

$D^{\mu}_{mn}\left(\boldsymbol{\kappa}_{\mathbf{g}}\right)$ commutes with $D^{\mu}_{mn}\left(\mathbf{P}^{\mu}_{pr}\right)=\delta_{mp}\delta_{nr}$ for *all p and r* :

$\mathbb{P}^{\mu}$ *in terms of* $\boldsymbol{\kappa}_{\mathbf{g}}$ (class sum: **g+g′+g″+…**)

$(\mu)^{\text{th}}$ *irep characters* $\chi^{(\mu)}(\mathbf{g})$ given by trace definition: $\chi^{\mu}(\mathbf{g}) \equiv Trace\, D^{\mu}(\mathbf{g}) = \sum_{m=1}^{\ell^{\mu}} D^{\mu}_{mm}(\mathbf{g})$

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$\boldsymbol{\kappa}_{\mathbf{g}}$ *in terms of* $\mathbb{P}^{\mu}$ (all-commuting **P**rojectors)

Find *all-commuting class* $\boldsymbol{\kappa}_{\mathbf{g}}$ in terms of $\mathbb{P}^{\mu}$ given **g** vs. *irep projectors* $\mathbf{P}^{\mu}_{mn}$:

$$\boxed{\mathbf{g} = \sum_{\mu} \sum_{m}^{\ell^{\mu}} \sum_{n}^{\ell^{\mu}} D^{\mu}_{mn}(g)\, \mathbf{P}^{\mu}_{mn}}$$

$D^{\mu}_{mn}(\boldsymbol{\kappa}_{\mathbf{g}})$ commutes with $D^{\mu}_{mn}(\mathbf{P}^{\mu}_{pr}) = \delta_{mp}\delta_{nr}$ for *all p and r* :

$$\sum_{b=1}^{\ell^{\mu}} D^{\mu}_{ab}(\boldsymbol{\kappa}_{\mathbf{g}}) D^{\mu}_{bc}(\mathbf{P}^{\mu}_{pr}) = \sum_{d=1}^{\ell^{\mu}} D^{\mu}_{ad}(\mathbf{P}^{\mu}_{pr}) D^{\mu}_{dc}(\boldsymbol{\kappa}_{\mathbf{g}})$$

$\mathbb{P}^{\mu}$ *in terms of* $\boldsymbol{\kappa}_{\mathbf{g}}$ (class sum: **g+g′+g″+…**)

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$$\sum_{b=1}^{\ell^{\mu}} D^{\mu}_{ab}(\boldsymbol{\kappa}_{\mathbf{g}})\; \delta_{bp}\delta_{cr} = \sum_{d=1}^{\ell^{\mu}} \delta_{ap}\delta_{dr}\; D^{\mu}_{dc}(\boldsymbol{\kappa}_{\mathbf{g}})$$

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$$D^{\mu}_{ap}(\kappa_{\mathbf{g}})\; \delta_{cr} = \delta_{ap}\; D^{\mu}_{rc}(\kappa_{\mathbf{g}})$$

$$D^{\mu}_{aa}(\kappa_{\mathbf{g}})\; \delta_{cc} = \delta_{aa}\; D^{\mu}_{cc}(\kappa_{\mathbf{g}})$$

$\mathbb{P}^{\mu}$ *in terms of* $\kappa_{\mathbf{g}}$ (class sum: $\mathbf{g}+\mathbf{g}'+\mathbf{g}''+\ldots$)

$(\mu)^{\text{th}}$ *irep characters* $\chi^{(\mu)}(\mathbf{g})$ given by trace definition: $\chi^{\mu}(\mathbf{g}) \equiv \mathit{Trace}\; D^{\mu}(\mathbf{g}) = \sum_{m=1}^{\ell^{\mu}} D^{\mu}_{mm}(\mathbf{g})$

$(\mu)^{\text{th}}$ *all-commuting class projector* given by sum $\mathbb{P}^{\mu} = \mathbf{P}^{\mu}_{11} + \mathbf{P}^{\mu}_{22} + \ldots + \mathbf{P}^{\mu}_{\ell^{\mu}\ell^{\mu}}$ of

irep projectors vs. $\mathbf{g}$

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

(for unitary D^{μ}_{nm}

$$D^{\mu^{*}}_{mn}(g) = D^{\mu}_{nm}(g^{-1})$$
)

$$\mathbb{P}^{\mu} = \sum_{m=1}^{\ell^{\mu}} \mathbf{P}^{\mu}_{mm} = \frac{\ell^{\mu}}{{}^{\circ}G} \sum_{\mathbf{g}}^{{}^{\circ}G} \sum_{m=1}^{\ell^{\mu}} D^{\mu^{*}}_{mm}(g)\,\mathbf{g} = \frac{\ell^{\mu}}{{}^{\circ}G} \sum_{\mathbf{g}}^{{}^{\circ}G} \chi^{\mu^{*}}(g)\,\mathbf{g}$$

$$\boxed{\mathbb{P}^{\mu} = \sum_{classes\,\kappa_{\mathbf{g}}} \frac{\ell^{\mu}}{{}^{\circ}G} \chi^{\mu^{*}}_{g} \kappa_{\mathbf{g}}}$$

, where: $\chi^{\mu}_{g} = \chi^{\mu}(\mathbf{g}) = \chi^{\mu}(\mathbf{hgh}^{-1})$ (by χ^{μ} trace invariance)

$\kappa_{\mathbf{g}}$ *in terms of* $\mathbb{P}^{\mu}$ (all-commuting **P**rojectors)

Find *all-commuting class* $\kappa_{\mathbf{g}}$ in terms of $\mathbb{P}^{\mu}$ given $\mathbf{g}$ vs. *irep projectors* $\mathbf{P}^{\mu}_{mn}$:

$$\boxed{\mathbf{g} = \sum_{\mu} \sum_{m}^{\ell^{\mu}} \sum_{n}^{\ell^{\mu}} D^{\mu}_{mn}(g)\,\mathbf{P}^{\mu}_{mn}}$$

$D^{\mu}_{mn}(\kappa_{\mathbf{g}})$ commutes with $D^{\mu}_{mn}(\mathbf{P}^{\mu}_{pr}) = \delta_{mp}\delta_{nr}$ for *all p and r* :

$$\sum_{b=1}^{\ell^{\mu}} D^{\mu}_{ab}(\kappa_{\mathbf{g}}) D^{\mu}_{bc}(\mathbf{P}^{\mu}_{pr}) = \sum_{d=1}^{\ell^{\mu}} D^{\mu}_{ad}(\mathbf{P}^{\mu}_{pr}) D^{\mu}_{dc}(\kappa_{\mathbf{g}})$$

$$\sum_{b=1}^{\ell^{\mu}} D^{\mu}_{ab}(\kappa_{\mathbf{g}})\; \delta_{bp}\delta_{cr} = \sum_{d=1}^{\ell^{\mu}} \delta_{ap}\delta_{dr}\; D^{\mu}_{dc}(\kappa_{\mathbf{g}})$$

$$D^{\mu}_{ap}(\kappa_{\mathbf{g}})\quad \delta_{cr} = \delta_{ap}\quad D^{\mu}_{rc}(\kappa_{\mathbf{g}})$$

$$D^{\mu}_{aa}(\kappa_{\mathbf{g}}) = D^{\mu}_{cc}(\kappa_{\mathbf{g}})$$

Key result called: *Schur's Lemma*

So: $D^{\mu}_{mn}(\kappa_{\mathbf{g}})$ is multiple of ℓ^{μ}-by-ℓ^{μ} unit matrix:

$$D^{\mu}_{mn}(\kappa_{\mathbf{g}}) = \delta_{mn} \frac{\chi^{\mu}(\kappa_{\mathbf{g}})}{\ell^{\mu}} = \delta_{mn} \frac{{}^{\circ}\kappa_{g}\chi^{\mu}_{g}}{\ell^{\mu}}$$

$\mathbb{P}^\mu$ *in terms of* $\boldsymbol{\kappa}_\mathbf{g}$ (class sum: **g+g′+g″+…**)

(μ)th *irep characters* $\chi^{(\mu)}(\mathbf{g})$ given by trace definition: $\chi^\mu(\mathbf{g}) \equiv Trace\, D^\mu(\mathbf{g}) = \sum_{m=1}^{\ell^\mu} D^\mu_{mm}(\mathbf{g})$

(μ)th *all-commuting class projector* given by sum $\mathbb{P}^\mu = \mathbf{P}^\mu_{11} + \mathbf{P}^\mu_{22} + \ldots + \mathbf{P}^\mu_{\ell^\mu \ell^\mu}$ of

irep projectors vs. **g**

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

for unitary D^μ_{nm}

$$D^{\mu^*}_{mn}(g) = D^\mu_{nm}(g^{-1})$$

$$\mathbb{P}^\mu = \sum_{m=1}^{\ell^\mu} \mathbf{P}^\mu_{mm} = \frac{\ell^\mu}{{}^\circ G} \sum_{\mathbf{g}}^{{}^\circ G} \sum_{m=1}^{\ell^\mu} D^{\mu *}_{mm}(g)\,\mathbf{g} = \frac{\ell^\mu}{{}^\circ G} \sum_{\mathbf{g}}^{{}^\circ G} \chi^{\mu *}(g)\,\mathbf{g}$$

$$\boxed{\mathbb{P}^\mu = \sum_{classes\, \boldsymbol{\kappa}_\mathbf{g}} \frac{\ell^\mu}{{}^\circ G} \chi^{\mu *}_g \boldsymbol{\kappa}_\mathbf{g}}$$

where: $\chi^\mu_g = \chi^\mu(\mathbf{g}) = \chi^\mu(\mathbf{h}\mathbf{g}\mathbf{h}^{-1})$ (by χ^μ trace invariance)

$\boldsymbol{\kappa}_\mathbf{g}$ *in terms of* $\mathbb{P}^\mu$ (all-commuting **P**rojectors)

Find *all-commuting class* $\boldsymbol{\kappa}_\mathbf{g}$ in terms of $\mathbb{P}^\mu$ given **g** vs. *irep projectors* $\mathbf{P}^\mu_{mn}$:

$$\boxed{\mathbf{g} = \sum_\mu \sum_m^{\ell^\mu} \sum_n^{\ell^\mu} D^\mu_{mn}(g)\,\mathbf{P}^\mu_{mn}}$$

$D^\mu_{mn}(\boldsymbol{\kappa}_\mathbf{g})$ commutes with $D^\mu_{mn}(\mathbf{P}^\mu_{pr}) = \delta_{mp}\delta_{nr}$ for *all p and r* :

$$\sum_{b=1}^{\ell^\mu} D^\mu_{ab}(\boldsymbol{\kappa}_\mathbf{g}) D^\mu_{bc}(\mathbf{P}^\mu_{pr}) = \sum_{d=1}^{\ell^\mu} D^\mu_{ad}(\mathbf{P}^\mu_{pr}) D^\mu_{dc}(\boldsymbol{\kappa}_\mathbf{g})$$

$$\sum_{b=1}^{\ell^\mu} D^\mu_{ab}(\boldsymbol{\kappa}_\mathbf{g})\, \delta_{bp}\delta_{cr} = \sum_{d=1}^{\ell^\mu} \delta_{ap}\delta_{dr}\, D^\mu_{dc}(\boldsymbol{\kappa}_\mathbf{g})$$

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Key result called: *Schur's Lemma*

So: $D^\mu_{mn}(\boldsymbol{\kappa}_\mathbf{g})$ is multiple of ℓ^μ-by-ℓ^μ unit matrix:

$$D^\mu_{mn}(\boldsymbol{\kappa}_\mathbf{g}) = \delta_{mn} \frac{\chi^\mu(\boldsymbol{\kappa}_\mathbf{g})}{\ell^\mu} = \delta_{mn} \frac{{}^\circ\kappa_g \chi^\mu_g}{\ell^\mu}$$

$$\boxed{\boldsymbol{\kappa}_\mathbf{g} = \sum_\mu \frac{{}^\circ\kappa_g \chi^\mu_g}{\ell^\mu} \mathbb{P}^\mu}$$

AMOP reference links on page 2

3.05.18 class 15.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Discrete symmetry subgroups of $O(3)\supset$(Octahedral $O_h\supset O\sim T_d$, Cubic-Tetrahedral $T_h\supset T$): Characters and subgroup-chain defined ireps, and applications to SF_6 and CF_4 spectra

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Octahedral groups $O_h\supset O\sim T_d\supset T$ and its large subgroups. *O_h slide-rule*

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Octahedral O class algebra *minimal equations* *centrum projectors and characters*

Characters of full Octahedral symmetry $O_h=O\times C_\mathbf{I}=O\times\{\mathbf{1},\mathbf{I}\}$

Octahedral $O_h\supset O\supset C_\mathbf{I}$ subgroup correlations

Octahedral subgroup correlation *$O_h\supset O\supset D_4$* *$O_h\supset O\supset D_4\supset C_4$* *and level-splitting*

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$R(3)\subset O(3)\supset O_h\supset O$ character analysis: Crystal field splitting *p, d, f,…orbitals*

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Detailed superfine structure for A_1T_1E cluster *preview of next lecture*

Introducing octahedral / tetrahedral symmetry $O_h \supset O \sim T_d \supset T$:
relating $D_4 \supset C_4$ and $D_3 \supset C_3$

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

The others are isomorphic to
O, D_4, or D_3
or outer products of these with
C_2 or C_3 or C_4.

Examples: $D_2 = C_2 \times C_2$
$D_6 = D_3 \times C_2$
$D_{6h} = D_3 \times C_2 \times C_2$

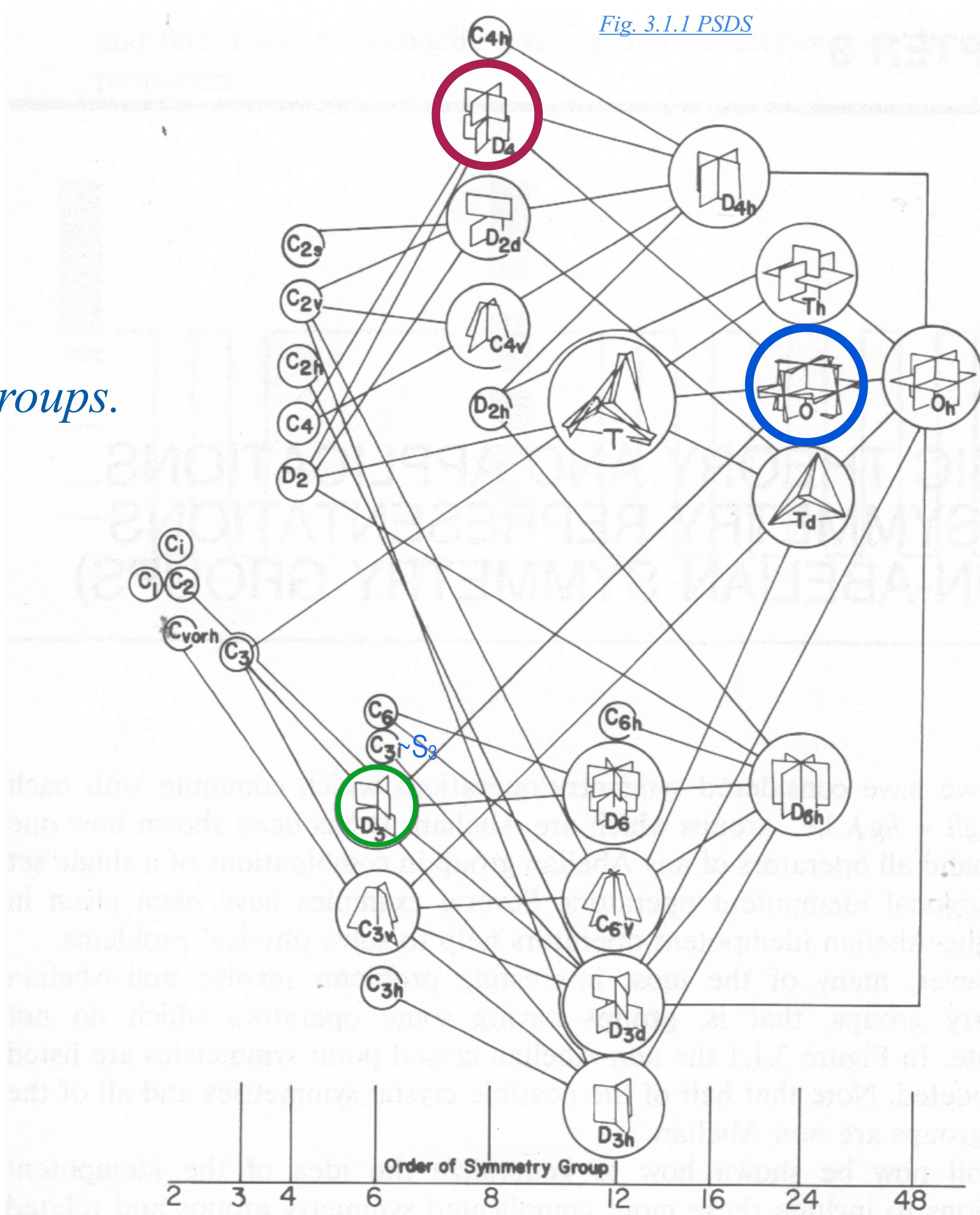
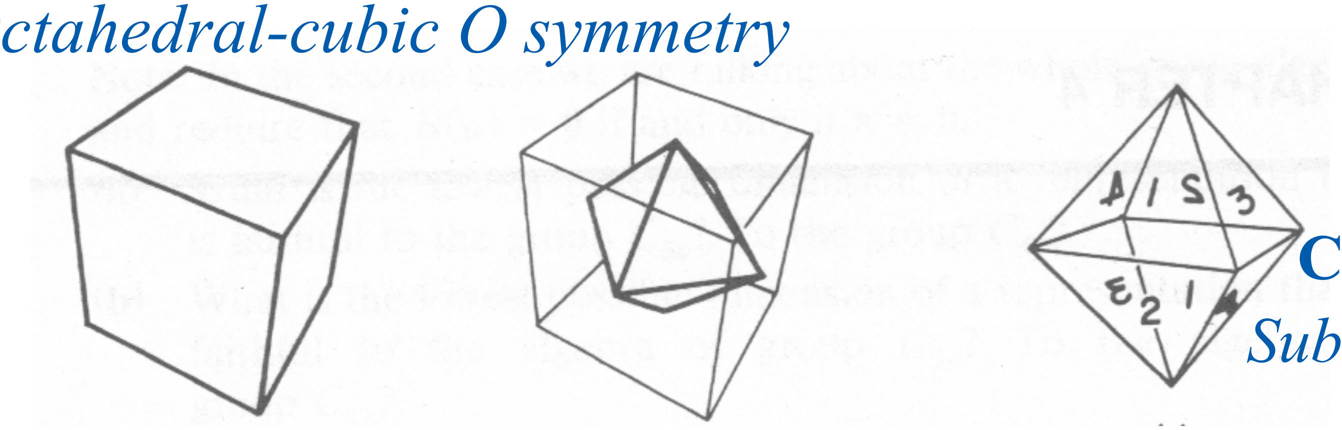


Fig. 3.1.1 PSDS

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

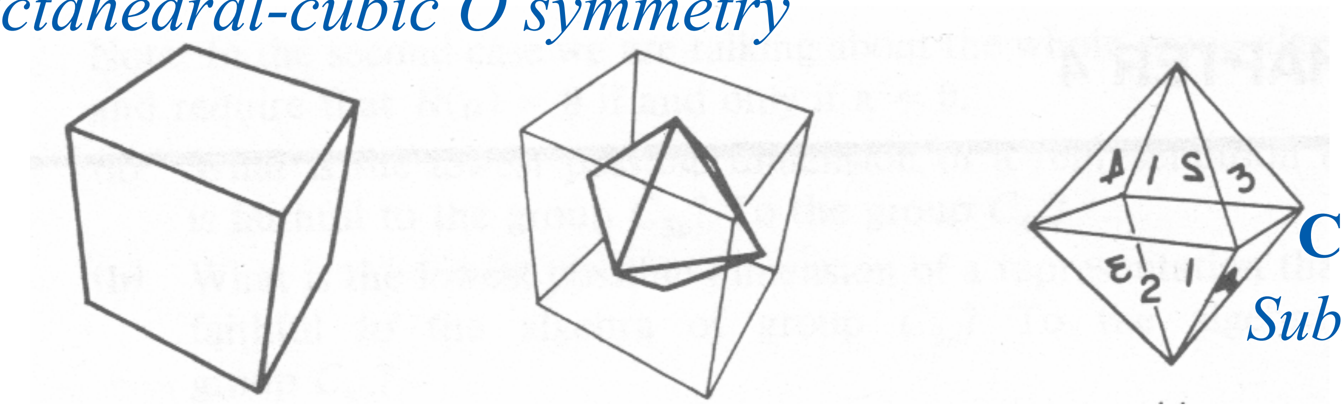
=12 lines · 2 pts =24

Counting an octahedron's symmetry positions

Substitution or *Permutation group-S_4* $°S_4=4!=24$

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

Octahedral-cubic O symmetry



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Counting an octahedron's symmetry positions

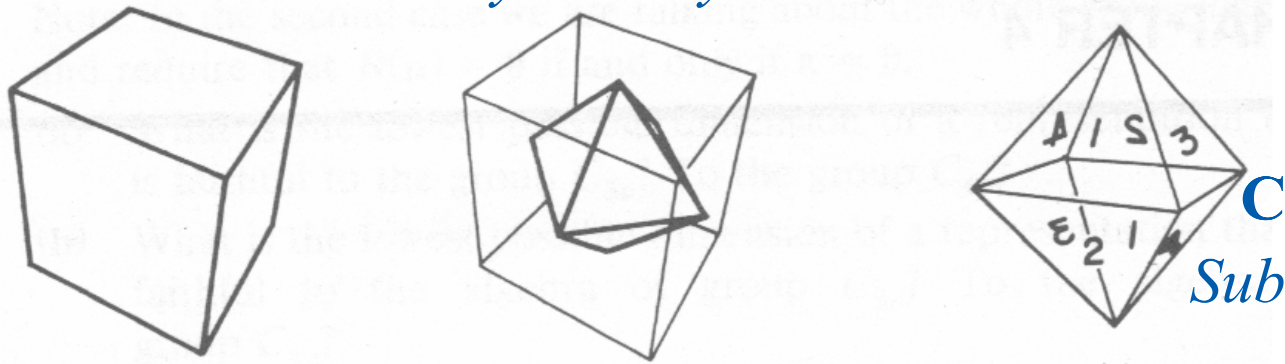
Substitution or *Permutation group-S_4* $°S_4=4!=24$

Octahedral group O ***operations***

Class of 1: **1**

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

Octahedral-cubic *O* symmetry



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Counting an octahedron's symmetry positions

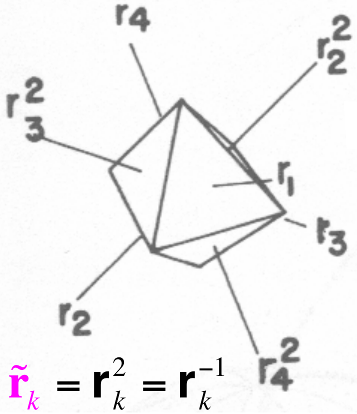
Substitution or *Permutation group-S_4* $°S_4=4!=24$

Octahedral group *O* **operations**

Class of 1: **1**

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

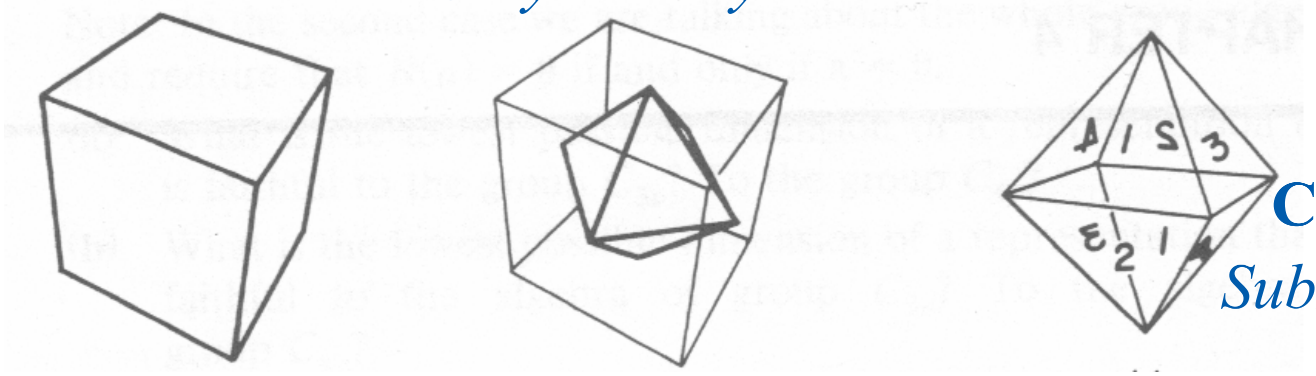
Class of 8:
120° rotations
on [111] *axes*



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

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

Octahedral-cubic O symmetry



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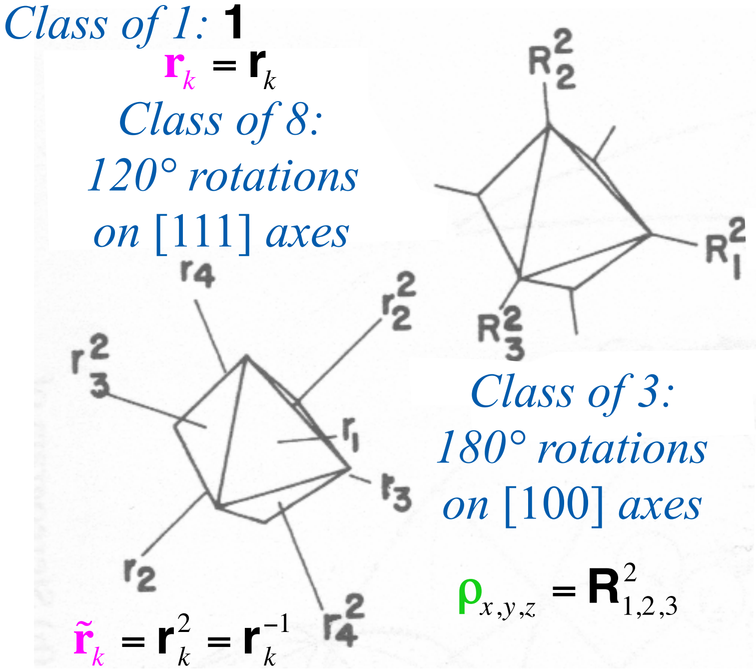
Counting an octahedron's symmetry positions

Substitution or *Permutation group-S_4* $°S_4=4!=24$

Octahedral group O ***operations***



Class of 1: **1**

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

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

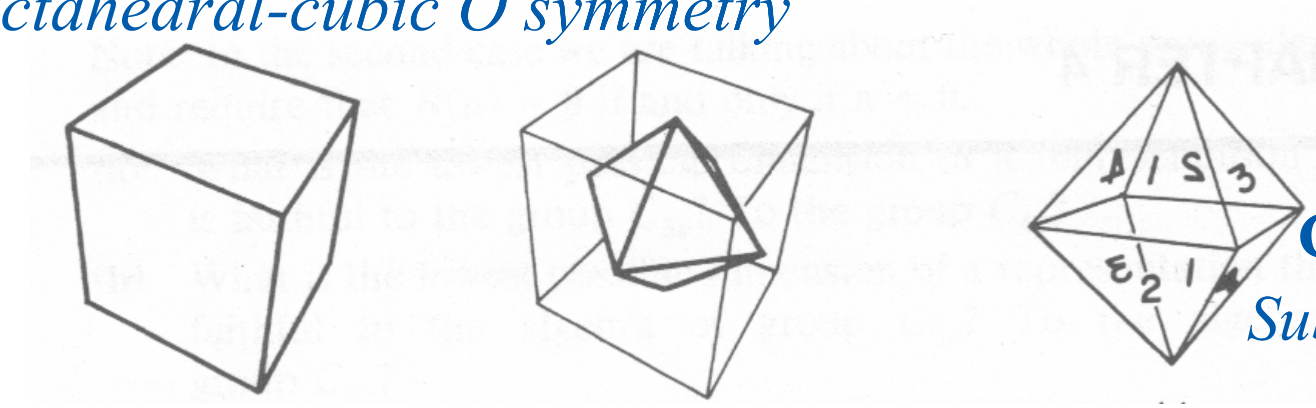
Class of 3:
180° rotations
on [100] *axes*

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

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

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

Octahedral-cubic O symmetry



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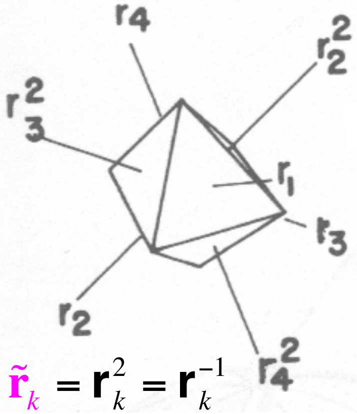
Octahedral group O **operations**

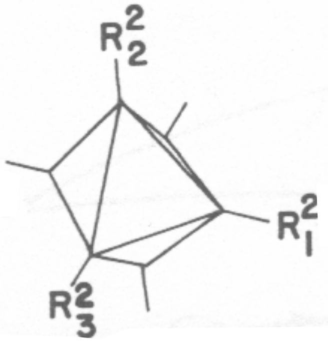
Class of 1: **1**

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

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



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

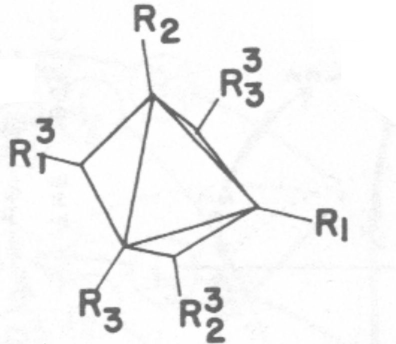


Class of 3: 180° rotations on [100] axes

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

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

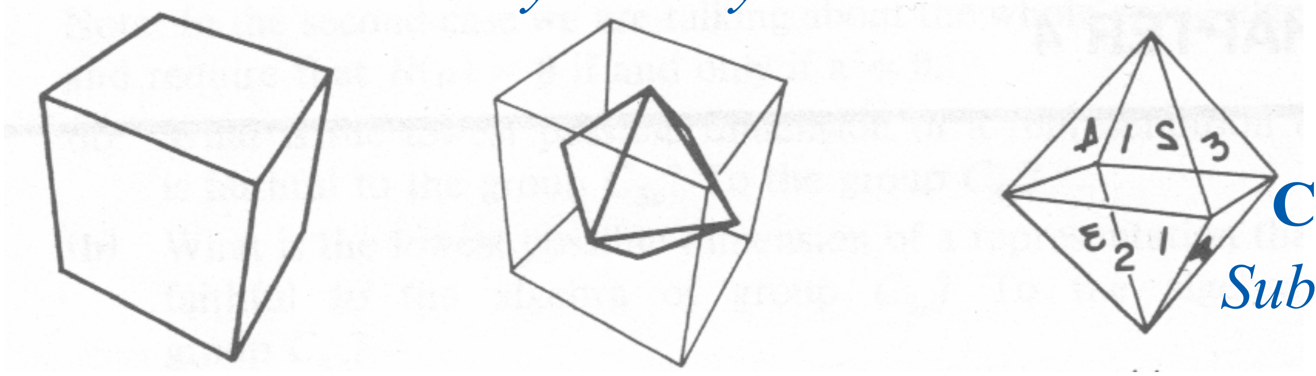
Class of 6: ±90° rotations on[100] axes



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

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

Octahedral-cubic O symmetry



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Counting an octahedron's symmetry positions

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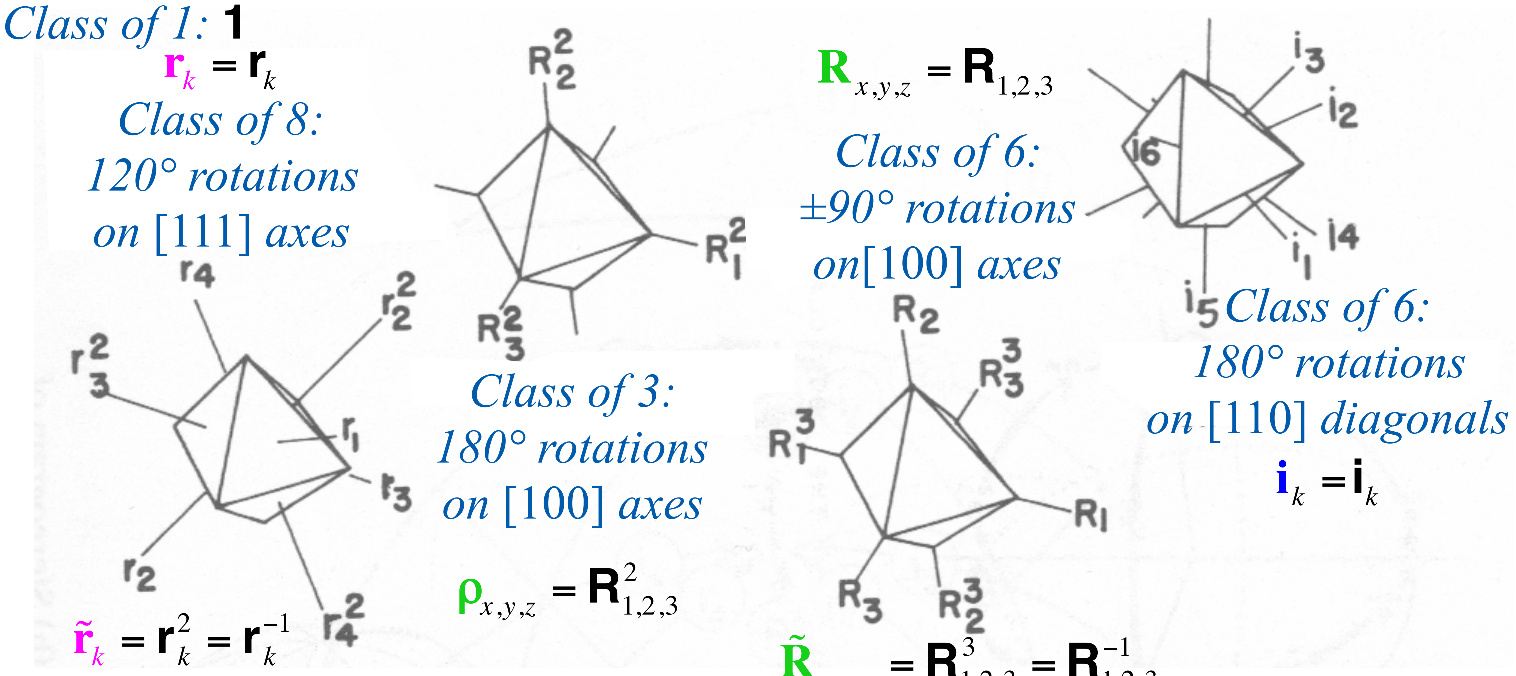
Octahedral group O **operations**



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

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

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

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

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

PSDS Fig. 4.1.2.

AMOP reference links on page 2

3.05.18 class 15.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Discrete symmetry subgroups of O(3)⊃(Octahedral $O_h \supset O \sim T_d$, Cubic-Tetrahedral $T_h \supset T$): Characters and subgroup-chain defined ireps, and applications to SF_6 and CF_4 spectra

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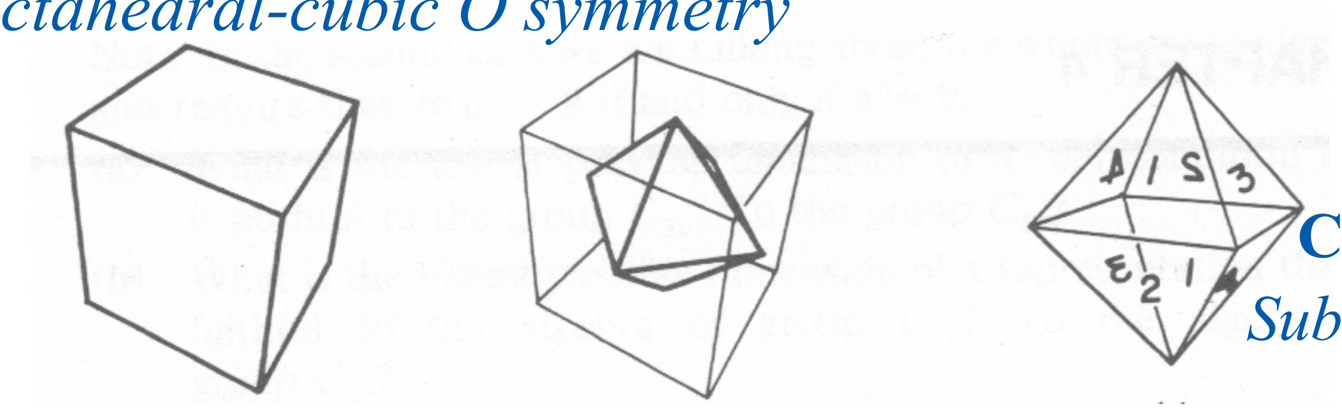

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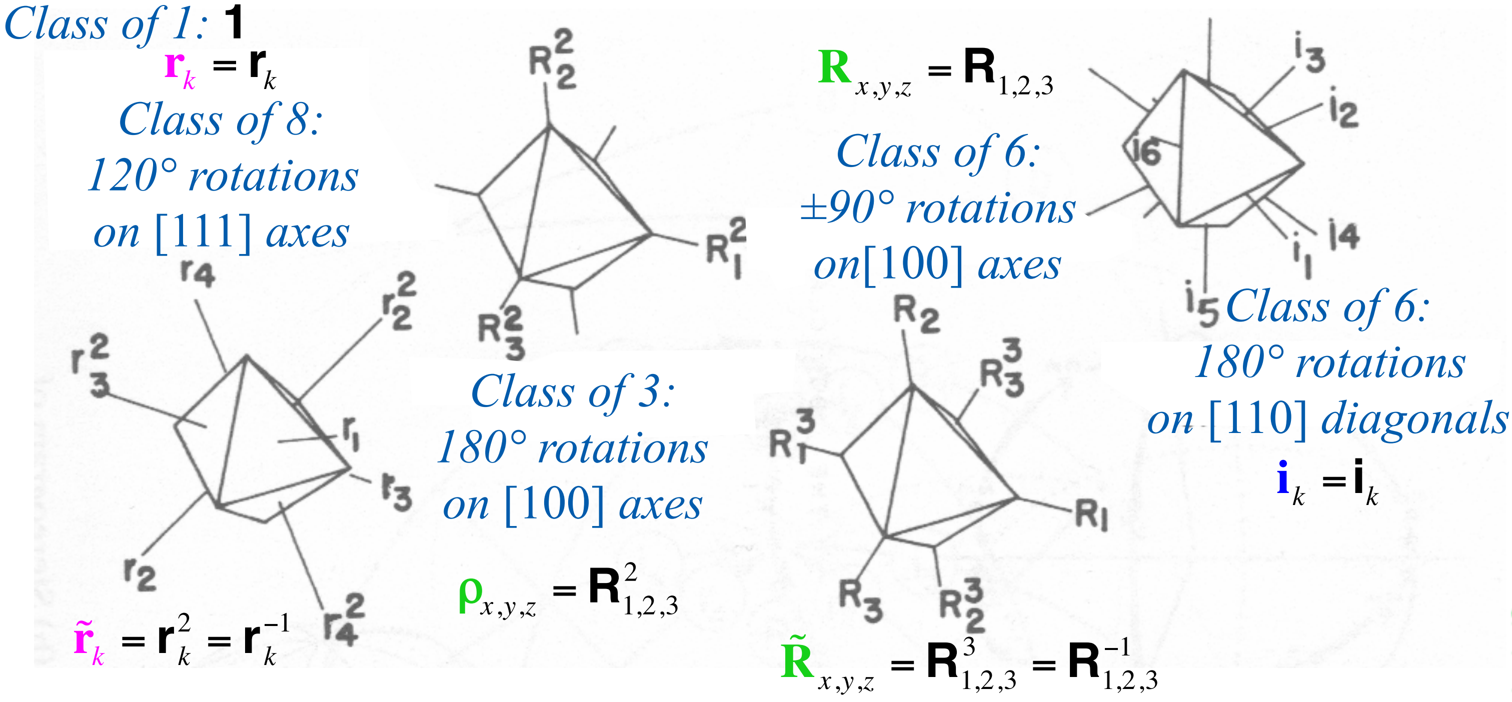
Octahedral group O *operations*



Class of 1: **1**

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180° rotations
on [100] *axes*

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Class of 6:
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on [110] *diagonals*

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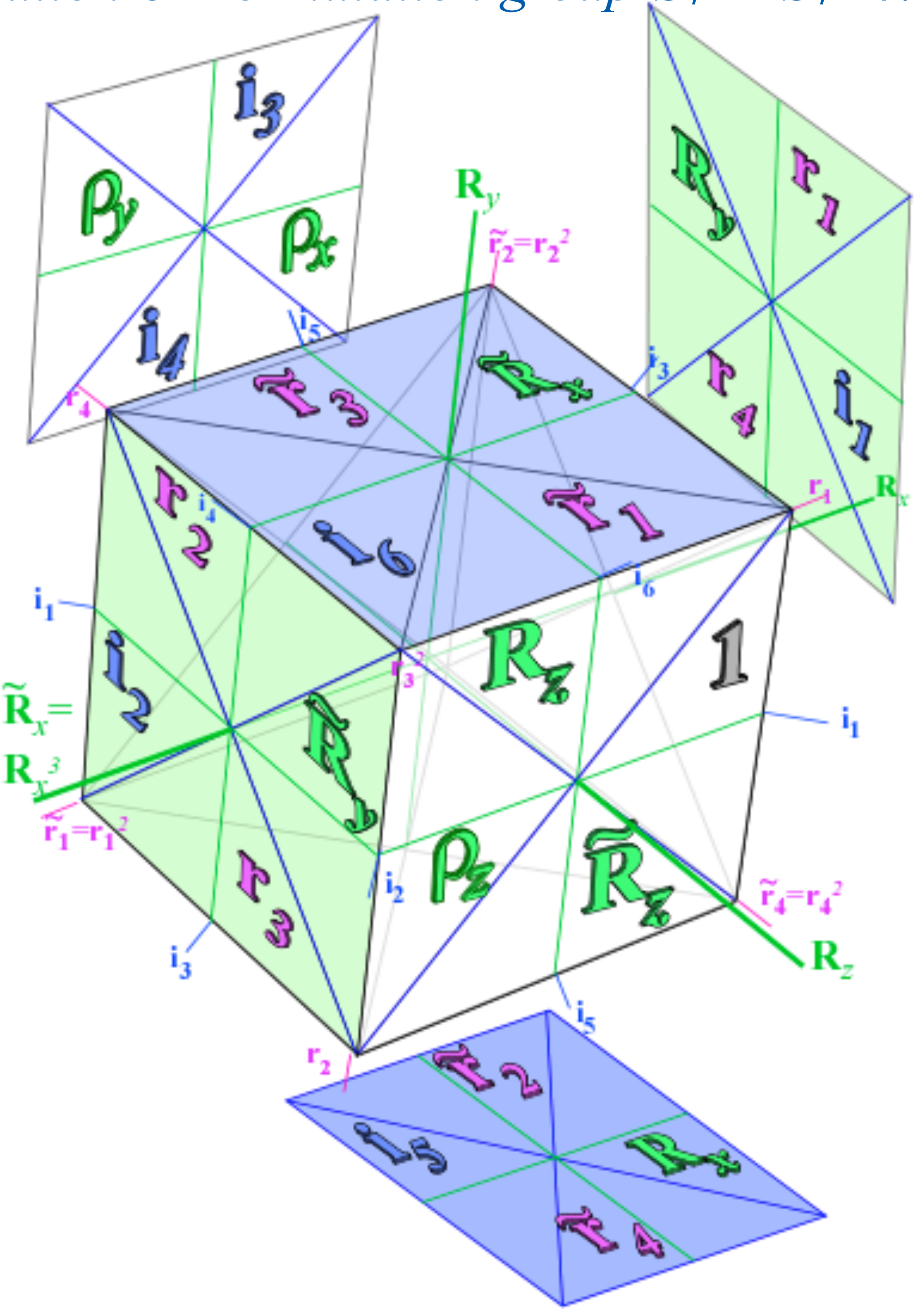

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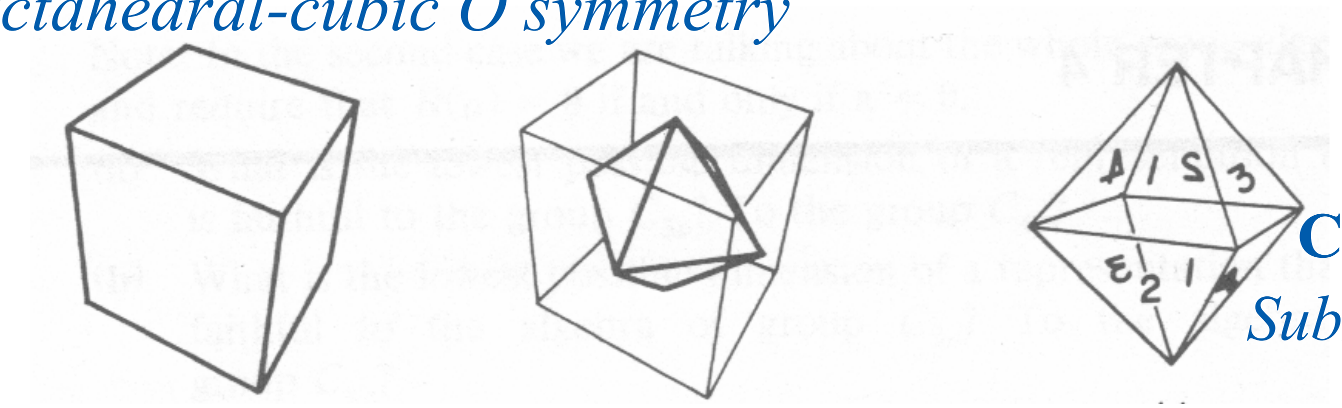
Introduction to octahedral / tetrahedral symmetry $O_h \supset O \sim T_d \supset T$

Octahedral-cubic O symmetry



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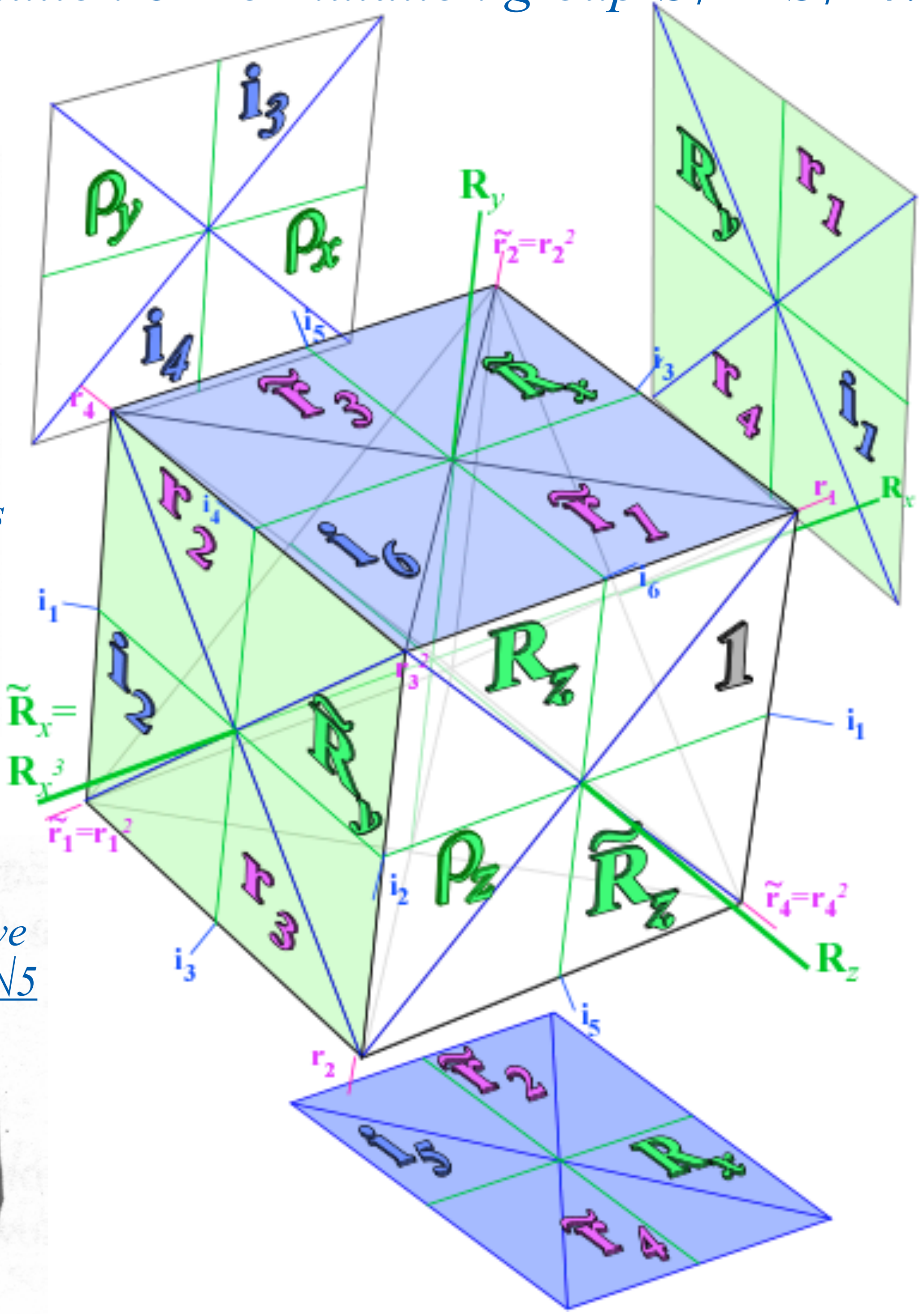
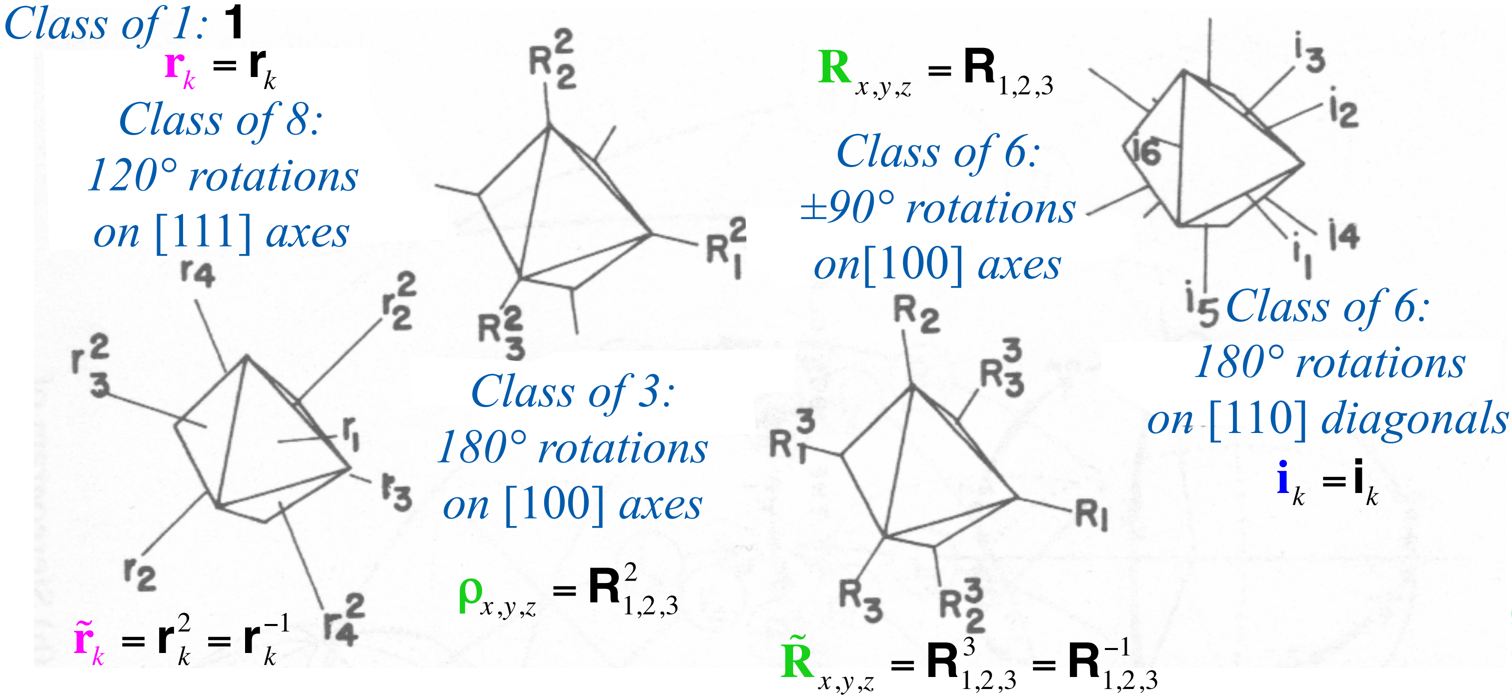


*Octahedral group O **operations***



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

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

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

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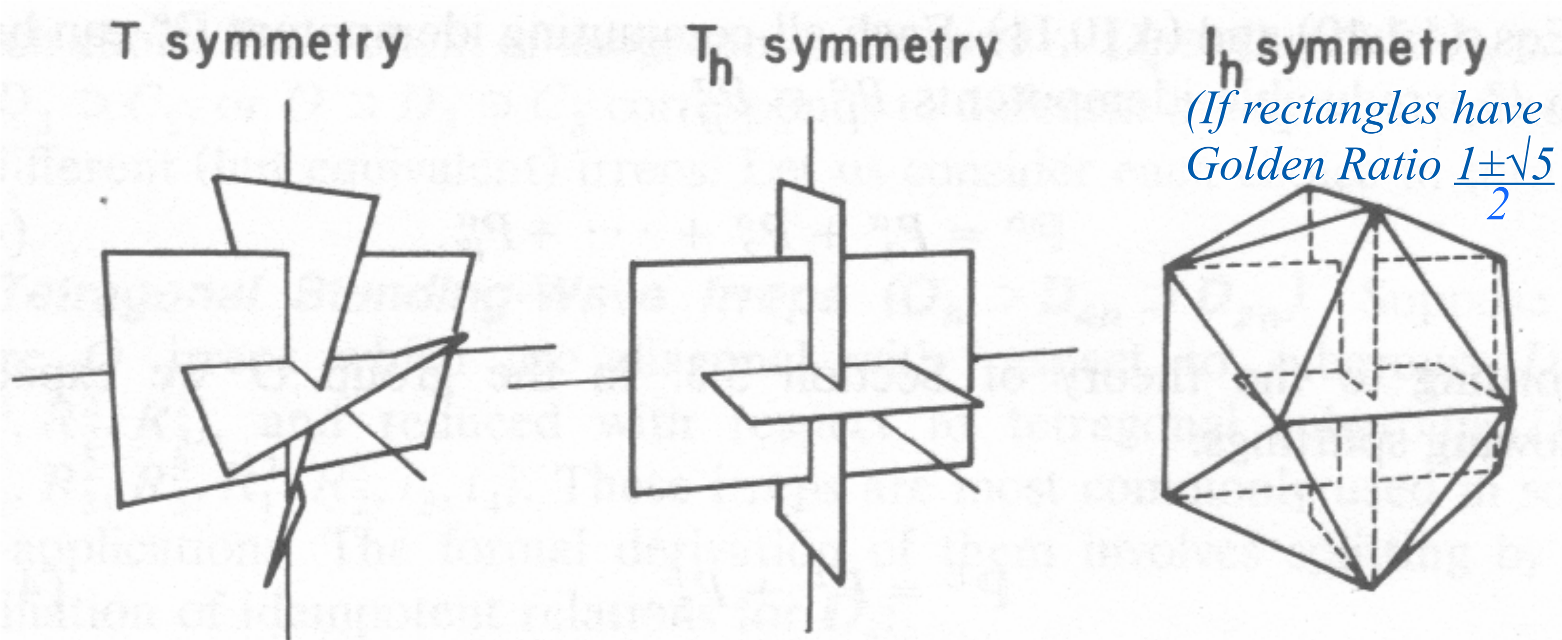
Class of 6:
180° rotations
on [110] diagonals

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

Tetrahedral symmetry becomes Icosahedral



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

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Octahedral-cubic O symmetry and group operations, *O slide-rule*

Tetrahedral symmetry leads to Icosahedral

Octahedral groups $O_h \supset O \sim T_d \supset T$ and its large subgroups. *O_h slide-rule*

Octahedral O and spin-O⊂U(2) nomograms

Tetrahedral T class algebra *minimal equations* *centrum projectors and characters*

Octahedral O class algebra *minimal equations* *centrum projectors and characters*

Characters of full Octahedral symmetry $O_h = O \times C_\mathbf{I} = O \times \{\mathbf{1},\mathbf{I}\}$

Octahedral $O_h \supset O \supset C_\mathbf{I}$ subgroup correlations

Octahedral subgroup correlation *$O_h \supset O \supset D_4$* *$O_h \supset O \supset D_4 \supset C_4$* *and level-splitting*

Comparing $O \supset C_4$ and $O \supset C_3$ and $O \supset C_2$

$R(3) \subset O(3) \supset O_h \supset O$ character analysis: Crystal field splitting *p, d, f,...orbitals*

Cluster structure in SF_6 16um spectra. *Analogy with D_6 band gap structure*

Global vs Local *External LAB splitting vs Internal BODY clustering*

Detailed superfine structure for A_1T_1E cluster *preview of next lecture*

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

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

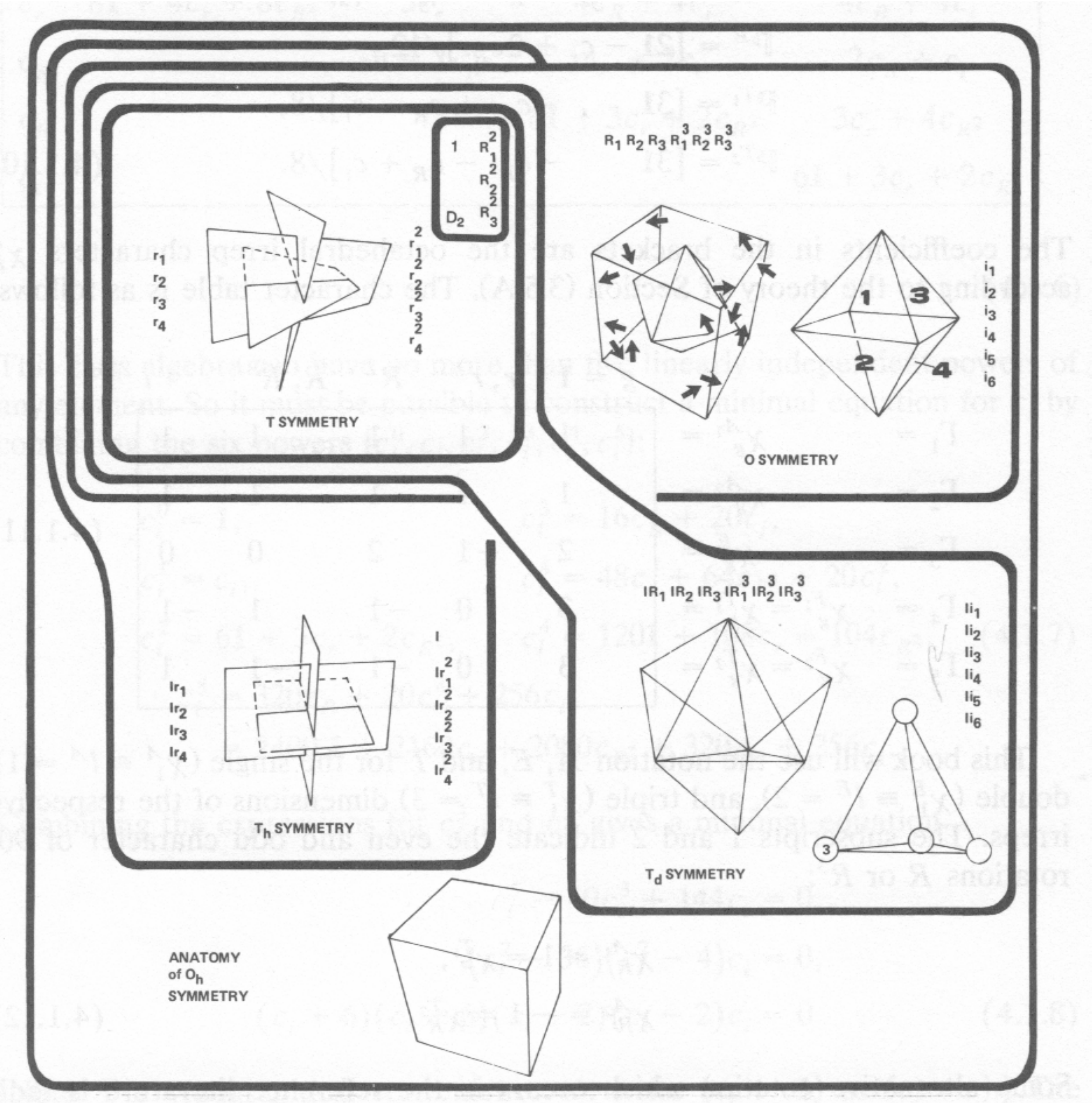


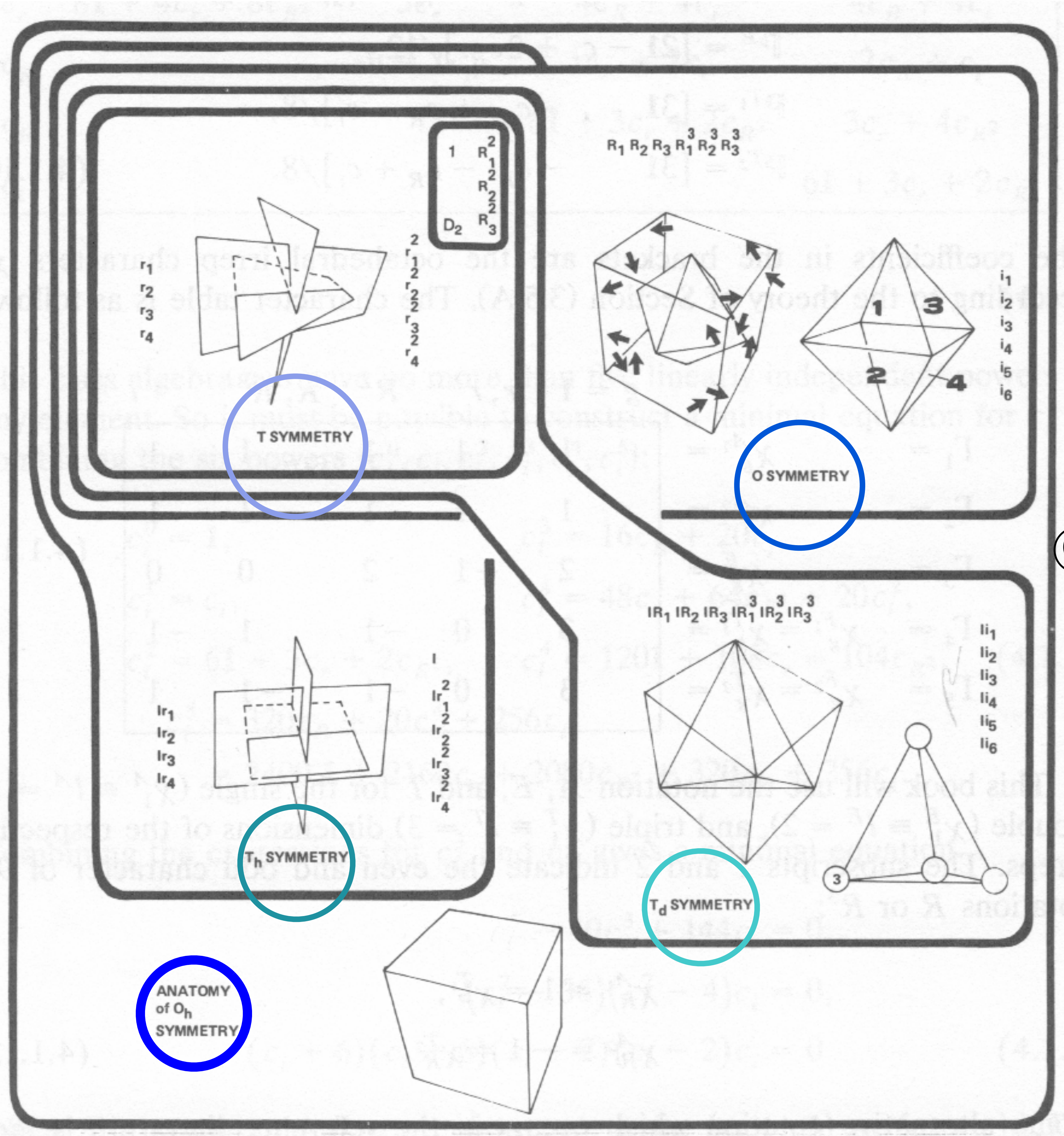
Figure 4.1.5 The full octahedral group (O_h) and four non-Abelian subgroups T, T_h, T_d, and O. The Abelian D_2 subgroup of T is indicated also.

Fig. 4.1.5 from Principles of Symmetry, Dynamics and Spectroscopy

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

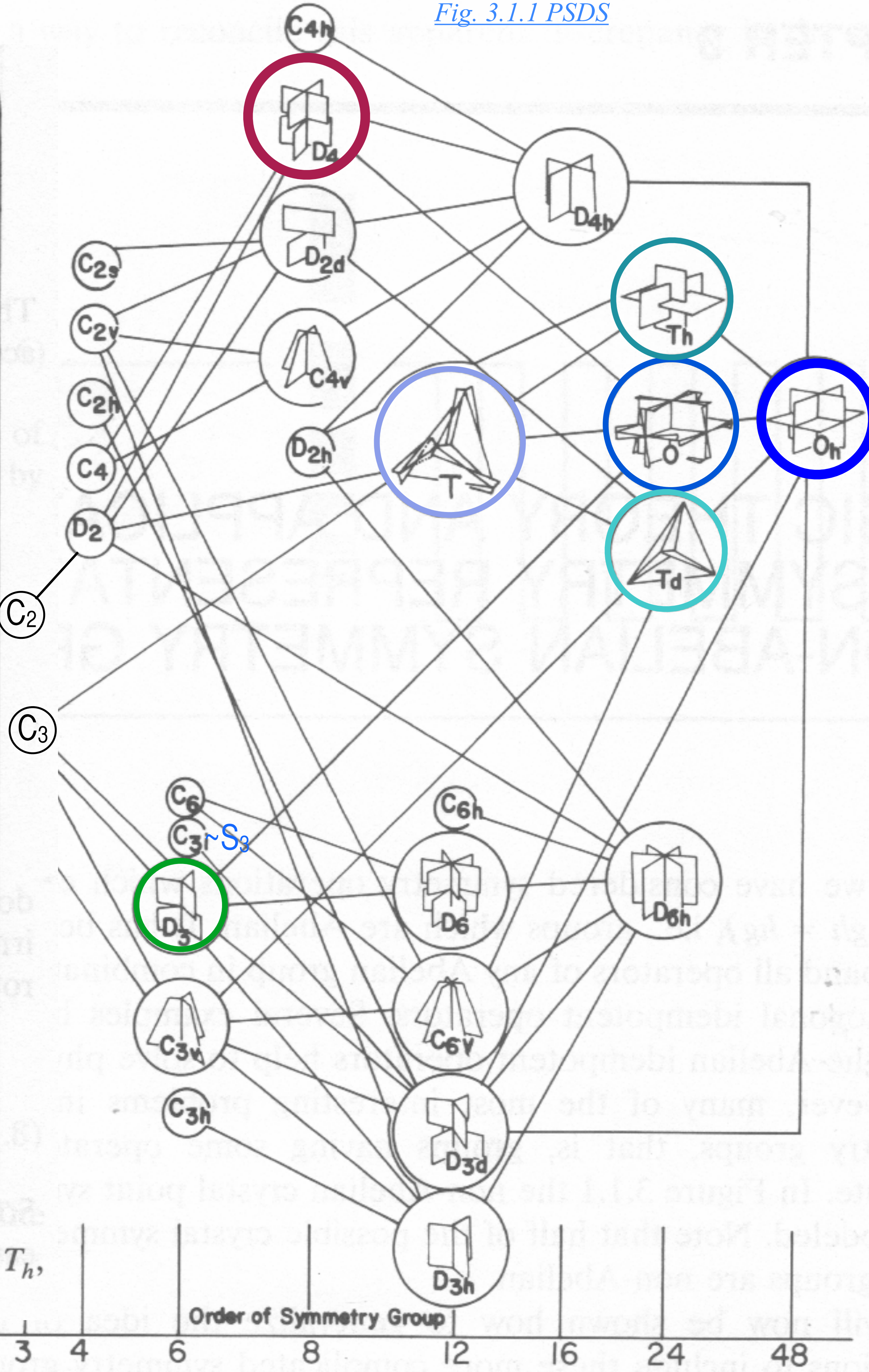
Octahedral groups $O_h \supset O \sim T_d$ and $O_h \supset T_h \supset T$

Fig. 3.1.1 PSDS



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

Fig. 4.1.5 from Principles of Symmetry, Dynamics and Spectroscopy



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

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

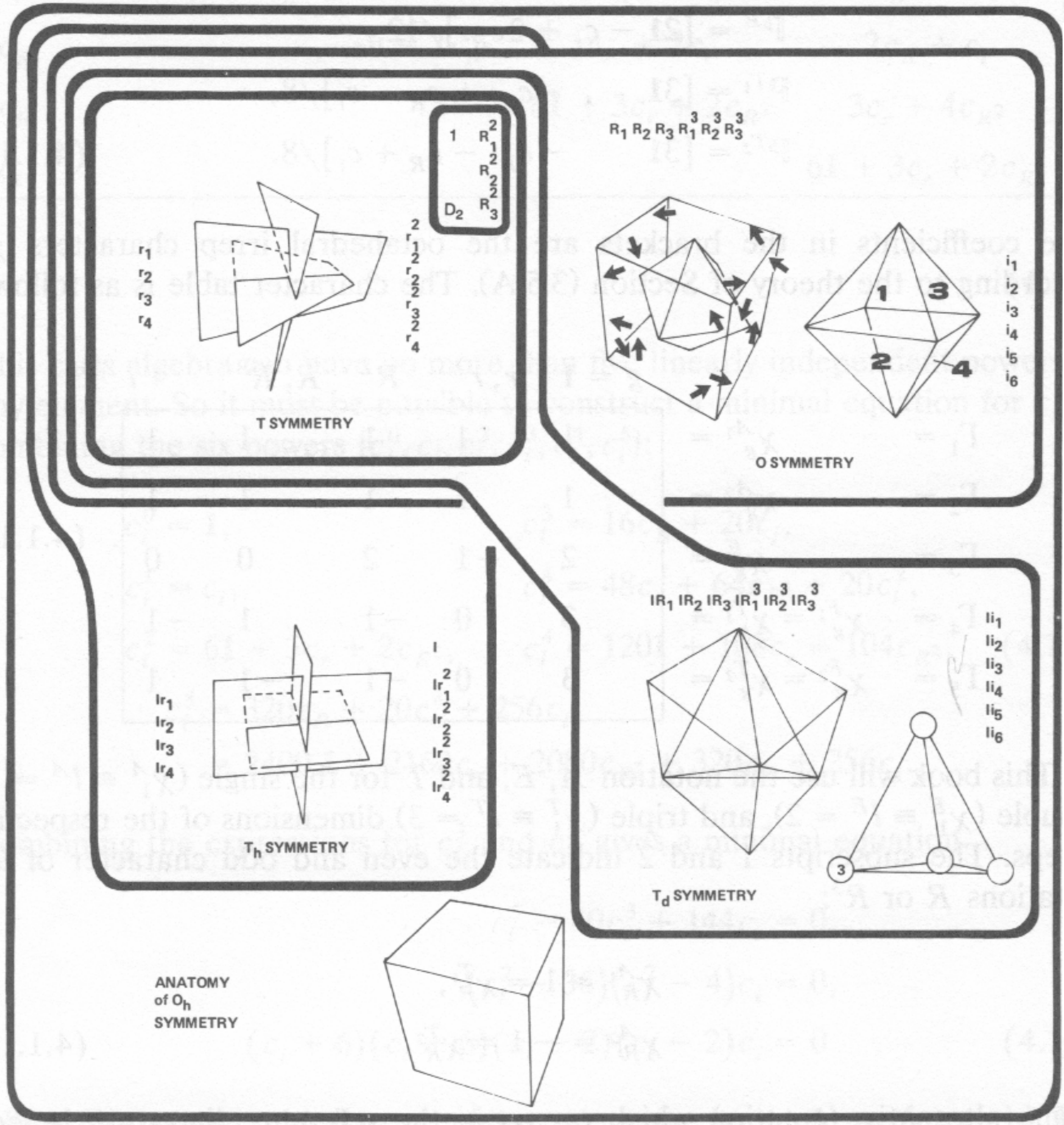


Figure 4.1.5 The full octahedral group (O_h) and four non-Abelian subgroups T, T_h, T_d, and O. The Abelian D_2 subgroup of T is indicated also.

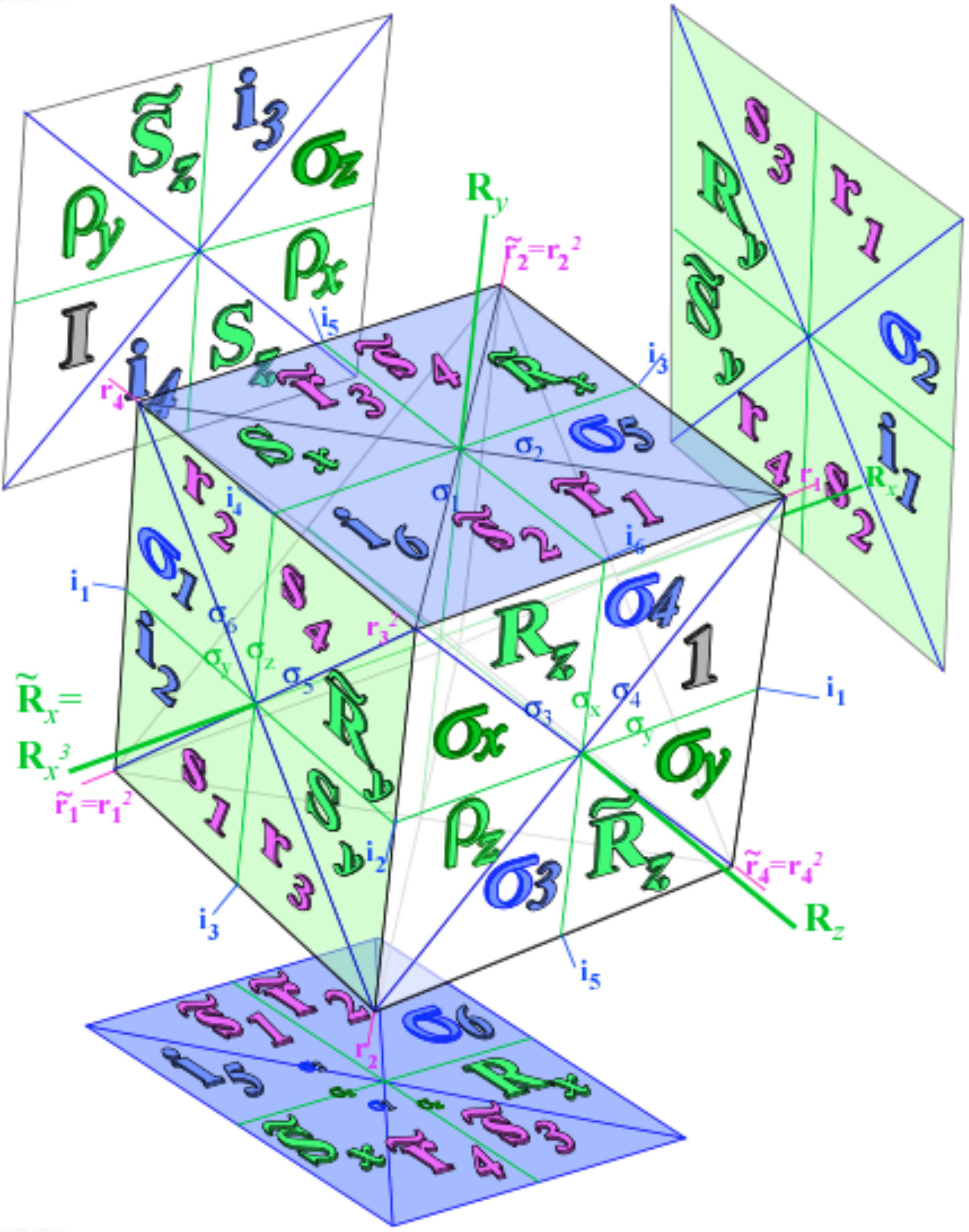


Fig. 4.1.5 from Principles of Symmetry, Dynamics and Spectroscopy

IJMol.Sci.14(2013)p776

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

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

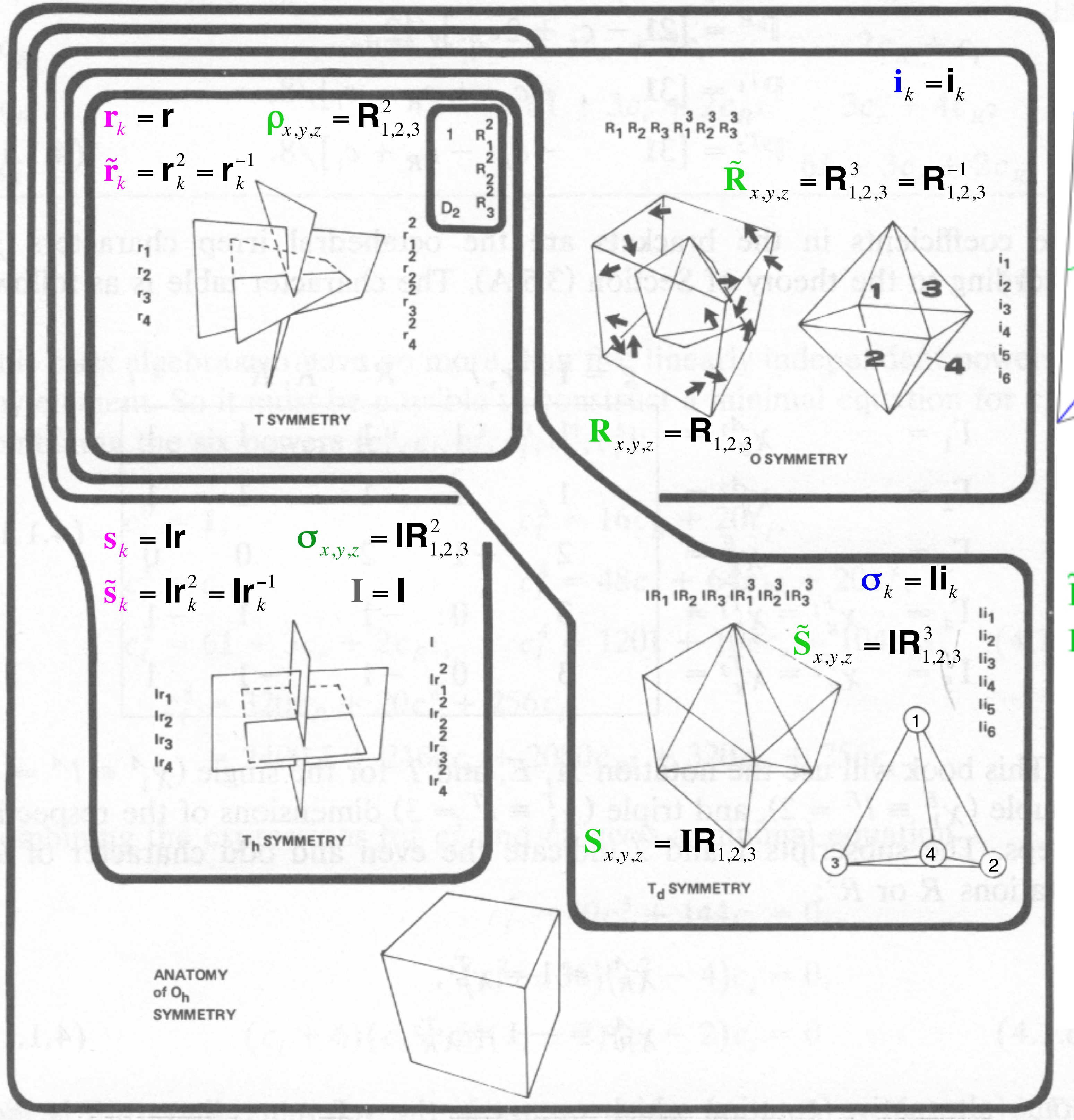
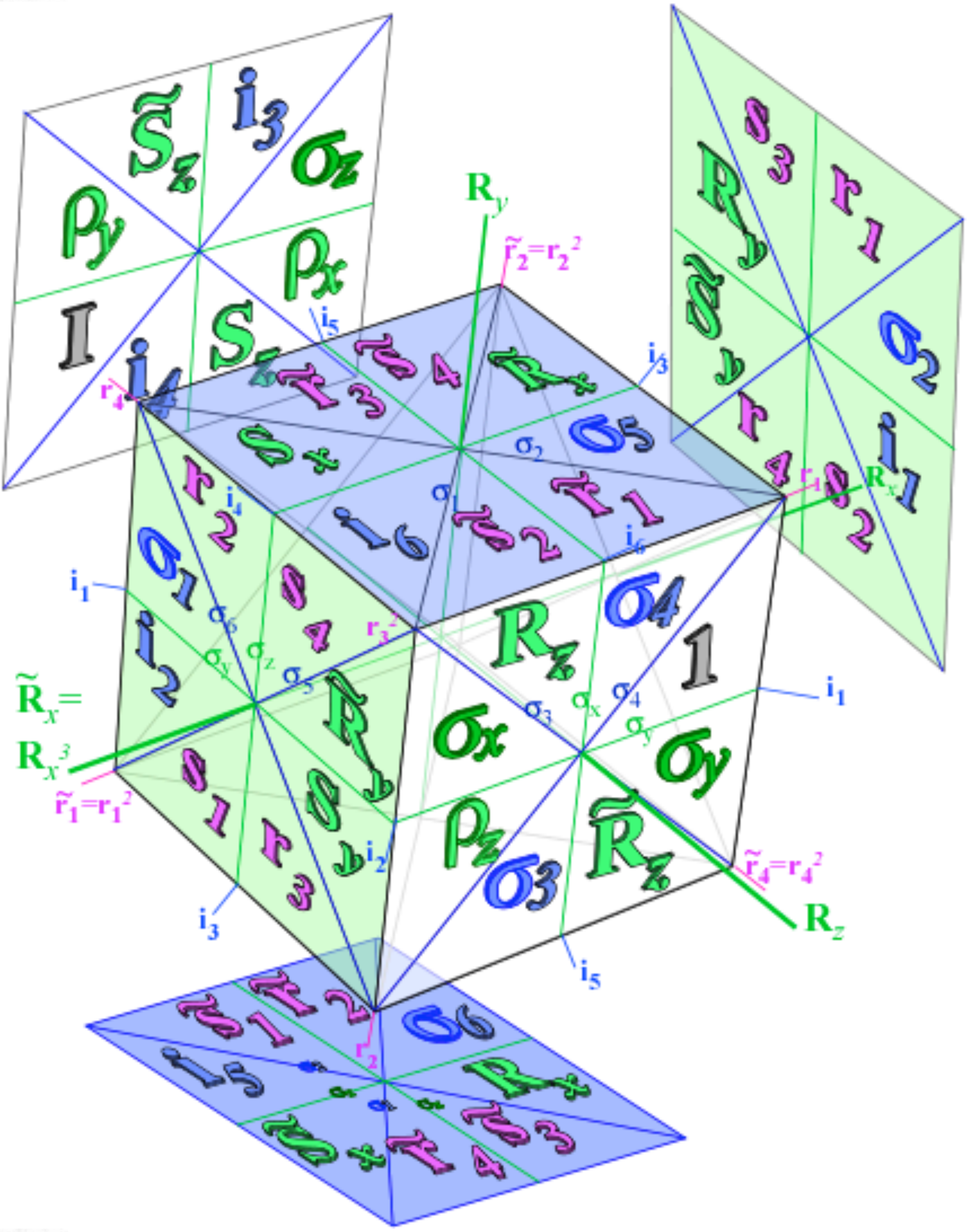


Figure 4.1.5 The full octahedral group (O_h) and four non-Abelian subgroups T, T_h, T_d, and O. The Abelian D_2 subgroup of T is indicated also.

Fig. 4.1.5 from Principles of Symmetry, Dynamics and Spectroscopy



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AMOP reference links on page 2

3.05.18 class 15.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Discrete symmetry subgroups of O(3)⊃(Octahedral O_h⊃O~T_d, Cubic-Tetrahedral T_h⊃T): Characters and subgroup-chain defined ireps, and applications to SF_6 and CF_4 spectra

Review: *General all-commuting class-character-projector formula derivations.* *f^μ derivation 2015 Lect15 p.40-45.*

$\mathbb{P}^\mu$ in χ^μ-terms of $\boldsymbol{\kappa}_\mathbf{g}$　　*$\boldsymbol{\kappa}_\mathbf{g}$ in $\chi^{\mu*}$-terms of $\mathbb{P}^\mu$*　　*Irep frequency f^μ in $\chi^{\mu*}$-terms of Trace$R(\mathbf{g})$*

Introducing octahedral/ tetrahedral symmetry $O_h \supset O \sim T_d \supset T$: relating $D_4 \supset C_4$ and $D_3 \supset C_3$

- *Octahedral-cubic O symmetry and group operations,*　　*O slide-rule*
- *Tetrahedral symmetry leads to Icosahedral*
- *Octahedral groups $O_h \supset O \sim T_d \supset T$ and its large subgroups.*　➡ *O_h slide-rule*
  - ➡ *Octahedral O and spin-O⊂U(2) nomograms*

Tetrahedral T class algebra　　*minimal equations*　　*centrum projectors and characters*

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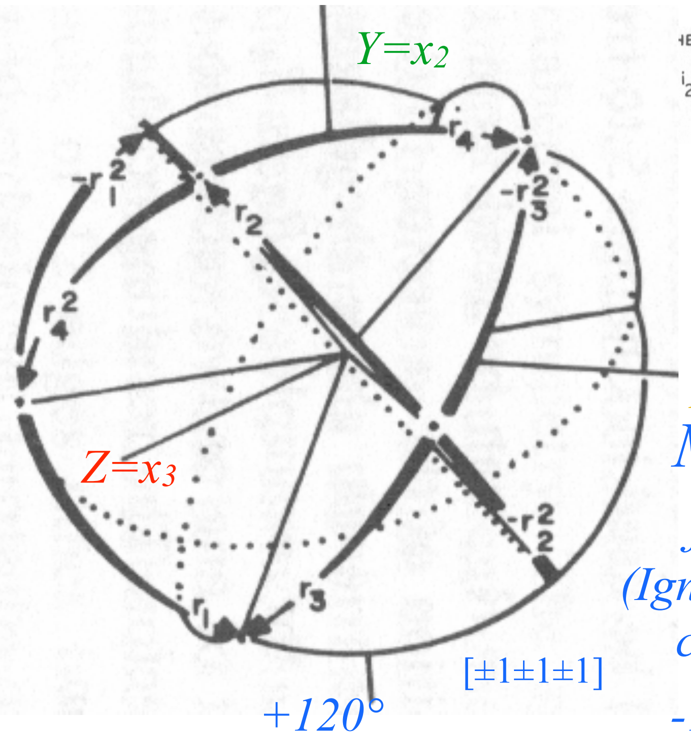
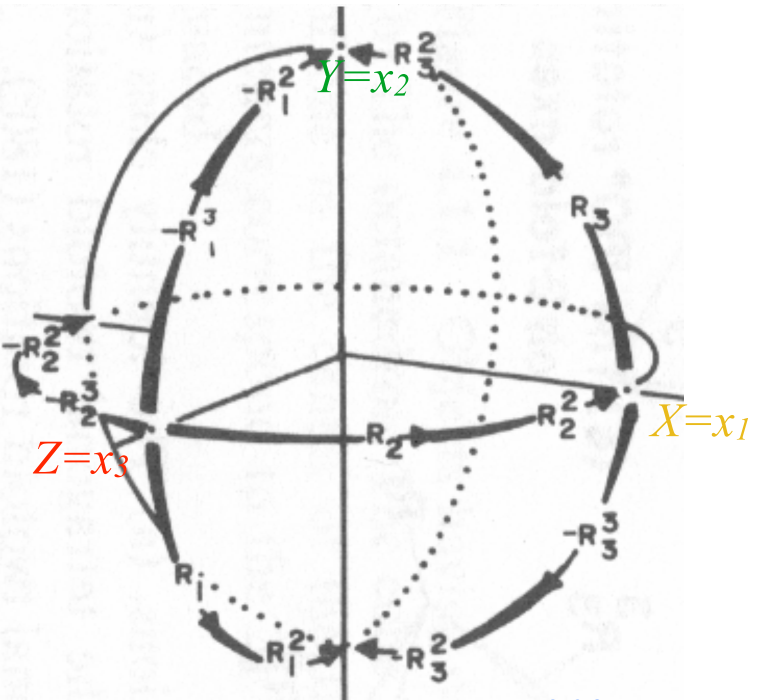
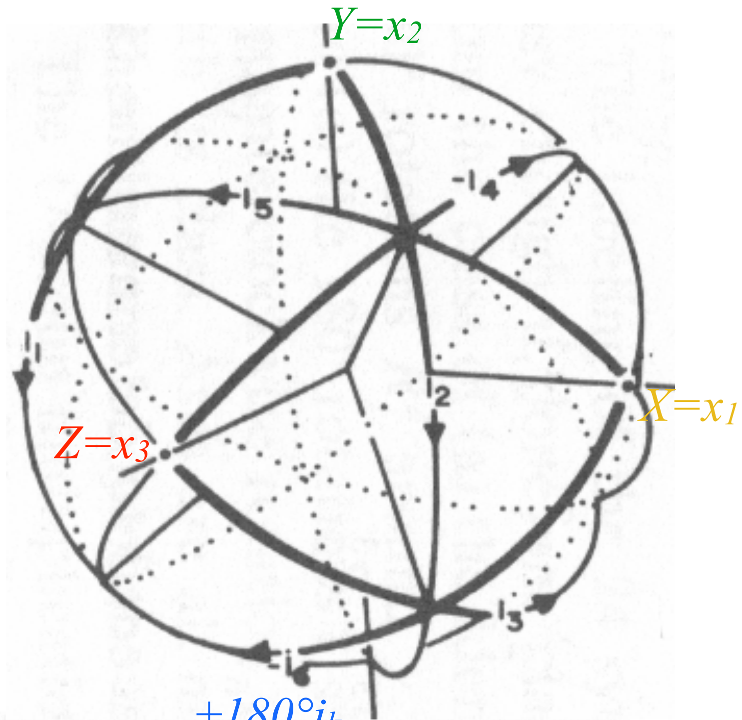
- *Detailed superfine structure for A_1T_1E cluster*　　*preview of next lecture*



IE 180°CLASS
$i_2\, i_3\, i_4\, i_5\, i_6$





Minus (-)signs for Fermions

(Ignore (-) for Bosons or classical particles)

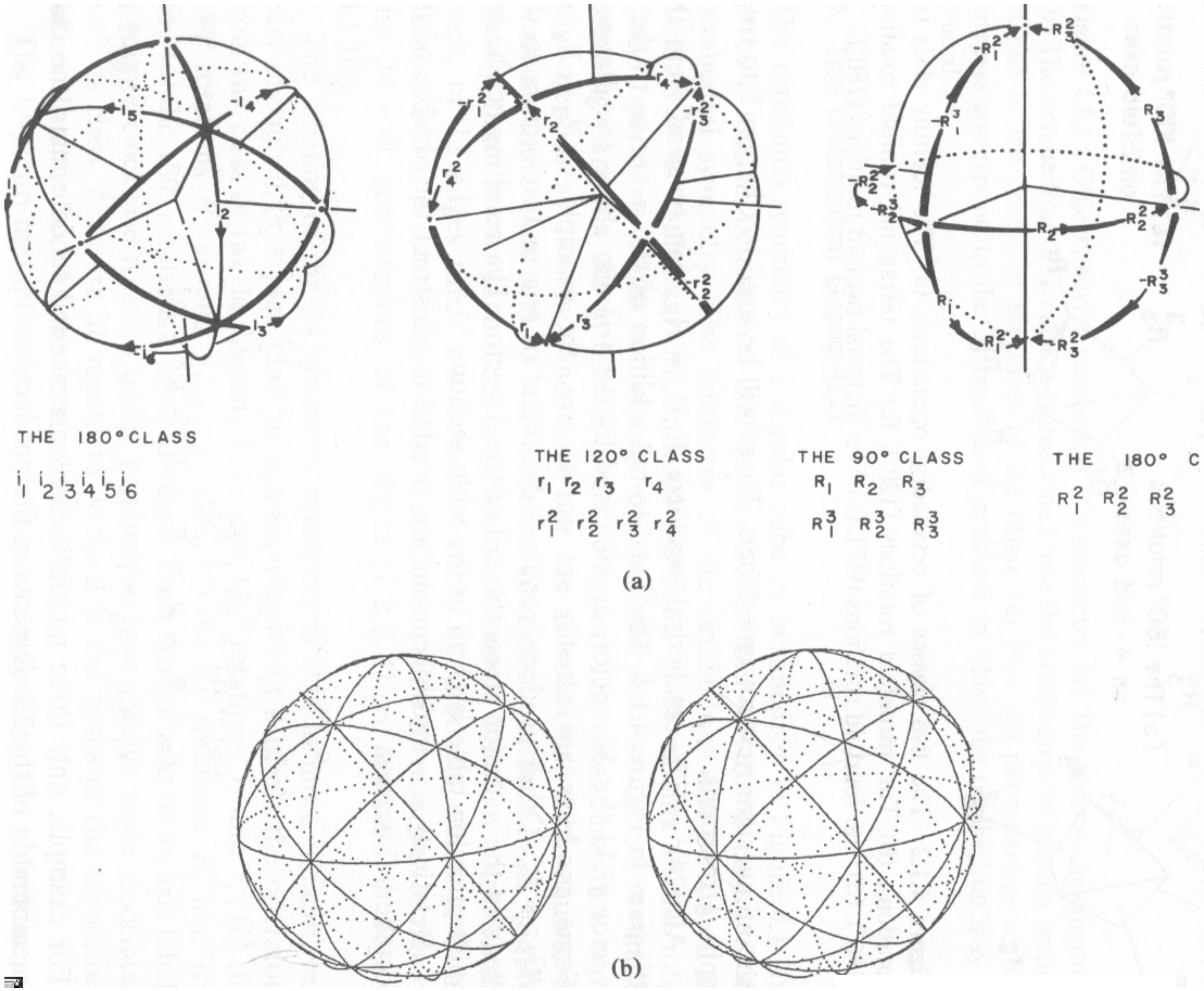
[±1±1±1]

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

	$[1\,1\,1]$	$[\bar1\,\bar1\,1]$	$[1\,\bar1\,\bar1]$	$[\bar1\,1\,\bar1]$	$[\bar1\,\bar1\,\bar1]$	$[1\,1\,\bar1]$	$[\bar1\,1\,1]$	$[1\,\bar1\,1]$	$[1\,0\,0]$	$[0\,1\,0]$	$[0\,0\,1]$	$[1\,0\,0]$	$[0\,1\,0]$	$[0\,0\,1]$	$[\bar1\,0\,0]$	$[0\,\bar1\,0]$	$[0\,0\,\bar1]$	$[1\,0\,1]$	$[1\,0\,\bar1]$	$[1\,1\,0]$	$[1\,\bar1\,0]$	$[0\,1\,\bar1]$	$[0\,1\,1]$
1	r_1	r_2	r_3	r_4	r_1^2	r_2^2	r_3^2	r_4^2	R_1^2	R_2^2	R_3^2	R_1	R_2	R_3	R_1^3	R_2^3	R_3^3	i_1	i_2	i_3	i_4	i_5	i_6
r_1	r_1^2	$-r_4^2$	$-r_2^2$	$-r_3^2$	-1	$-R_2^2$	$-R_3^2$	$-R_1^2$	$-r_2$	$-r_3$	$-r_4$	i_3	i_6	i_1	$-R_3$	$-R_1$	$-R_2$	R_1^3	i_5	R_2^3	i_2	$-i_4$	R_3^3
r_2	$-r_3^2$	r_2^2	$-r_4^2$	$-r_1^2$	R_2^2	-1	R_1^2	$-R_3^2$	r_1	r_4	$-r_3$	R_3	$-R_1^3$	i_2	i_3	$-i_5$	R_2^3	i_6	$-R_1$	R_2	$-i_1$	R_3^3	i_4
r_3	$-r_4^2$	$-r_1^2$	r_3^2	$-r_2^2$	R_3^2	$-R_1^2$	-1	R_2^2	$-r_4$	r_1	r_2	$-i_4$	R_1	$-R_2^3$	R_3^3	i_6	i_2	i_5	$-R_1^3$	i_1	R_2	$-i_3$	R_3
r_4	$-r_2^2$	$-r_3^2$	$-r_1^2$	r_4^2	R_1^2	R_3^2	$-R_2^2$	-1	r_3	$-r_2$	r_1	$-R_3^3$	$-i_5$	R_2	$-i_4$	R_1^3	i_1	R_1	i_6	$-i_2$	R_2^3	R_3	i_3
r_1^2	-1	R_1^2	R_2^2	R_3^2	$-r_1$	r_3	r_4	r_2	r_4^2	r_2^2	r_3^2	R_2^3	R_3^3	R_1^3	$-i_1$	$-i_3$	$-i_6$	$-R_3$	$-i_4$	$-R_1$	i_5	$-i_2$	$-R_2$
r_2^2	$-R_1^2$	-1	R_3^2	$-R_2^2$	r_4	$-r_2$	r_1	r_3	$-r_3^2$	$-r_1^2$	r_4^2	i_2	$-i_3$	$-R_1$	R_2	$-R_3^3$	$-i_5$	i_4	$-R_3$	$-R_1^3$	$-i_6$	R_2^3	$-i_1$
r_3^2	$-R_2^2$	$-R_3^2$	-1	R_1^2	r_2	r_4	$-r_3$	r_1	r_2^2	$-r_4^2$	$-r_1^2$	$-R_2$	$-i_4$	$-i_6$	i_2	R_3	$-R_1^3$	$-i_3$	$-R_3^3$	i_5	R_1	$-i_1$	$-R_2^3$
r_4^2	$-R_3^2$	R_2^2	$-R_1^2$	-1	r_3	r_1	r_2	$-r_4$	$-r_1^2$	r_3^2	$-r_2^2$	$-i_1$	$-R_3$	$-i_5$	$-R_2^3$	$-i_4$	R_1	$-R_3^3$	i_3	$-i_6$	R_1^3	R_2	$-i_2$
R_1^2	$-r_4$	r_3	$-r_2$	r_1	r_2^2	$-r_1^2$	r_4^2	$-r_3^2$	-1	R_3^2	$-R_2^2$	R_1^3	i_1	$-i_4$	$-R_1$	i_2	$-i_3$	$-R_2$	$-R_2^3$	R_3^3	R_3	$-i_6$	i_5
R_2^2	$-r_2$	r_1	r_4	$-r_3$	r_3^2	$-r_4^2$	$-r_1^2$	r_2^2	$-R_3^2$	-1	R_1^2	$-i_5$	R_2^3	i_3	$-i_6$	$-R_2$	$-i_4$	$-i_2$	i_1	$-R_3$	R_3^3	R_1	R_1^3
R_3^2	$-r_3$	$-r_4$	r_1	r_2	r_4^2	r_3^2	$-r_2^2$	$-r_1^2$	R_2^2	$-R_1^2$	-1	i_6	i_2	R_3^3	$-i_5$	$-i_1$	$-R_3$	R_2^3	$-R_2$	i_4	$-i_3$	R_1^3	$-R_1$
R_1	i_1	$-R_2^3$	$-i_2$	R_2	R_3^3	$-i_3$	$-R_3$	i_4	R_1^3	i_6	i_5	R_1^2	r_1	$-r_4^2$	-1	$-r_3$	r_2^2	$-r_4$	r_2	r_1^2	$-r_3^2$	$-R_2^2$	R_3^2
R_2	i_3	R_3	$-R_3^3$	i_4	R_1^3	i_5	$-i_6$	$-R_1$	$-i_2$	R_2^3	i_1	$-r_2^2$	R_2^2	r_1	r_3^2	-1	$-r_4$	R_1^2	R_3^2	$-r_2$	$-r_3$	$-r_4^2$	r_1^2
R_3	i_6	i_5	R_1	$-R_1^3$	R_2^3	$-R_2$	$-i_2$	$-i_1$	i_3	i_4	R_3^3	r_1	$-r_3^2$	R_3^2	$-r_2$	r_4^2	-1	r_1^2	r_2^2	R_2^2	$-R_1^2$	$-r_4$	$-r_3$
R_1^3	$-R_2$	$-i_2$	R_2^3	i_1	$-i_3$	$-R_3^3$	i_4	R_3	$-R_1$	i_5	$-i_6$	-1	$-r_4$	r_3^2	$-R_1^2$	r_2	$-r_1^2$	$-r_1$	r_3	r_2^2	$-r_4^2$	$-R_3^2$	$-R_2^2$
R_2^3	$-R_3$	i_3	i_4	R_3^3	$-i_6$	R_1	$-R_1^3$	i_5	$-i_1$	$-R_2$	$-i_2$	r_4^2	-1	$-r_2$	$-r_1^2$	$-R_2^2$	r_3	$-R_3^2$	R_1^2	$-r_1$	$-r_4$	$-r_2^2$	r_3^2
R_3^3	$-R_1$	R_1^3	i_6	i_5	$-i_1$	$-i_2$	R_2	$-R_2^3$	i_4	$-i_3$	$-R_3$	$-r_3$	r_2^2	-1	r_4	$-r_1^2$	$-R_3^2$	r_4^2	r_3^2	$-R_1^2$	$-R_2^2$	$-r_2$	$-r_1$
i_1	R_3^3	$-i_4$	i_3	R_3	$-R_1$	$-i_6$	$-i_5$	$-R_1^3$	R_2^3	i_2	$-R_2$	r_1^2	R_3^2	$-r_4$	r_4^2	$-R_1^2$	$-r_1$	-1	$-R_2^2$	$-r_3$	r_2	r_3^2	r_2^2
i_2	i_4	R_3^3	R_3	$-i_3$	$-i_5$	R_1^3	R_1	$-i_6$	R_2	$-i_1$	R_2^3	$-r_3^2$	$-R_1^2$	$-r_3$	$-r_2^2$	$-R_3^2$	$-r_2$	R_2^2	-1	r_4	$-r_1$	r_1^2	r_4^2
i_3	R_1^3	R_1	$-i_5$	i_6	$-R_2$	$-R_2^3$	$-i_1$	i_2	$-R_3$	R_3^3	$-i_4$	$-r_2$	r_1^2	R_1^2	$-r_1$	r_2^2	$-R_2^2$	r_3^2	$-r_4^2$	-1	R_3^2	r_3	$-r_4$
i_4	$-i_5$	i_6	$-R_1^3$	$-R_1$	$-i_2$	i_1	$-R_2^3$	$-R_2$	$-R_3^3$	$-R_3$	i_3	r_4	r_4^2	R_2^2	r_3	r_3^2	R_1^2	$-r_2^2$	r_1^2	$-R_3^3$	-1	r_1	$-r_2$
i_5	i_2	$-R_2$	i_1	$-R_2^3$	i_4	$-R_3$	i_3	$-R_3^3$	i_6	$-R_1^3$	$-R_1$	R_3^2	r_2	r_2^2	R_2^2	r_4	r_4^2	$-r_3$	$-r_1$	$-r_3^2$	$-r_1^2$	-1	$-R_1^2$
i_6	R_2^3	i_1	R_2	i_2	$-R_3$	$-i_4$	$-R_3^3$	$-i_3$	$-i_5$	$-R_1$	R_1^3	R_2^2	$-r_3$	r_1^2	$-R_3^2$	$-r_1$	r_3^2	$-r_2$	$-r_4$	r_4^2	r_2^2	R_1^2	-1

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

Octahedral O and spin-O⊂U(2) rotation nomograms



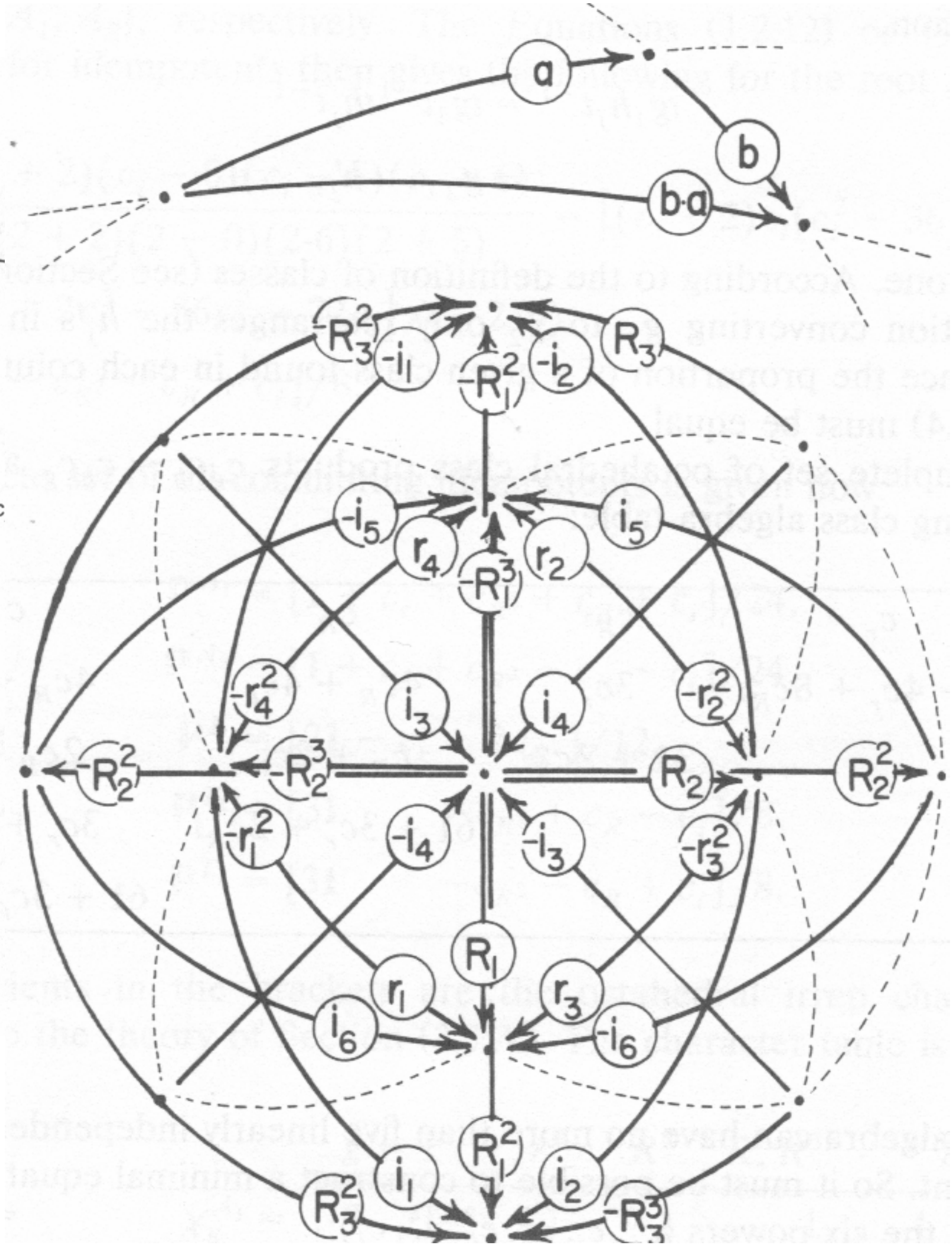


Fig. 4.1.3-4 Principles of Symmetry, Dynamics and Spectroscopy.

AMOP
reference links
on page 2

3.05.18 class 15.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Discrete symmetry subgroups of O(3)$\supset$(Octahedral $O_h \supset O \sim T_d$, Cubic-Tetrahedral $T_h \supset T$): Characters and subgroup-chain defined ireps, and applications to SF_6 and CF_4 spectra

Review: *General all-commuting class-character-projector formula derivations.* *f^μ derivation 2015 Lect15 p.40-45.*

$\mathbb{P}^\mu$ *in* χ^μ*-terms of* $\boldsymbol{\kappa}_\mathbf{g}$ $\boldsymbol{\kappa}_\mathbf{g}$ *in* $\chi^{\mu *}$*-terms of* $\mathbb{P}^\mu$ *Irep frequency* f^μ *in* $\chi^{\mu *}$*-terms of* Trace$R(\mathbf{g})$

Introducing octahedral/ tetrahedral symmetry $O_h \supset O \sim T_d \supset T$ *: relating* $D_4 \supset C_4$ *and* $D_3 \supset C_3$

Octahedral-cubic O symmetry and group operations, *O slide-rule*
Tetrahedral symmetry leads to Icosahedral
Octahedral groups $O_h \supset O \sim T_d \supset T$ *and its large subgroups.* O_h *slide-rule*
Octahedral O and spin-$O \subset U(2)$ *nomograms*

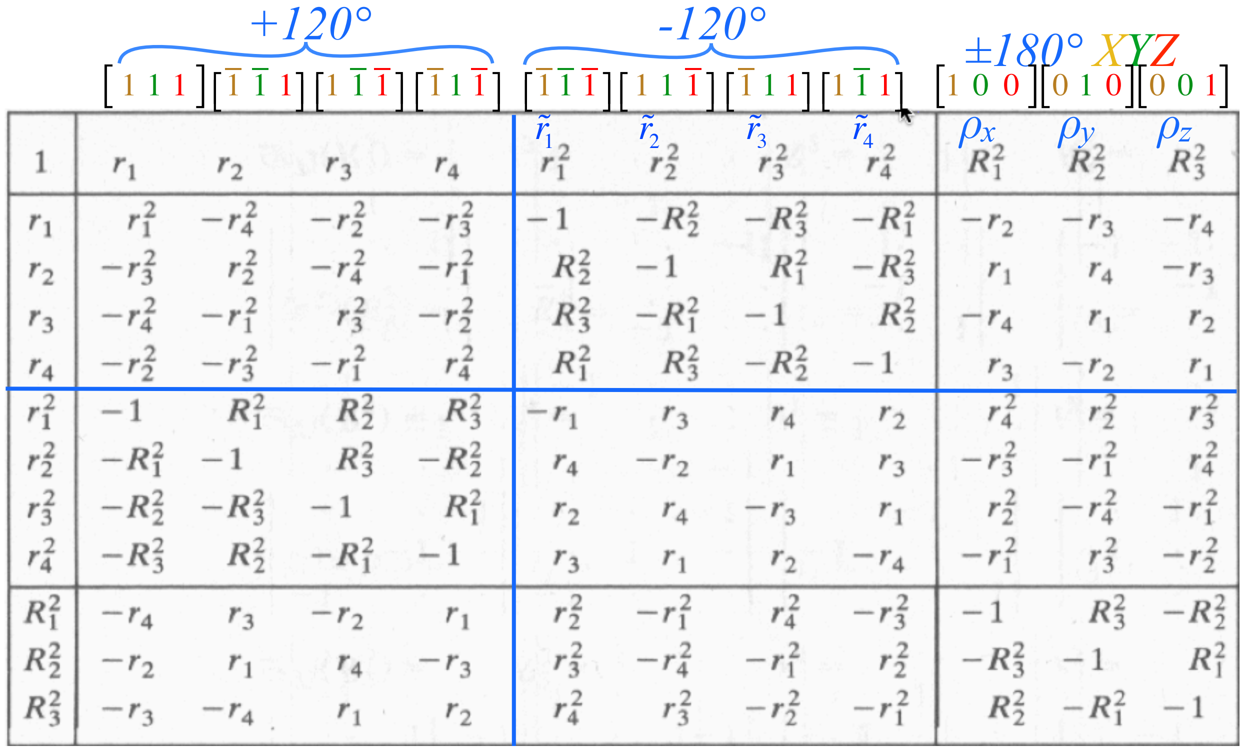
Tetrahedral T class algebra *minimal equations* *centrum projectors and characters*
Octahedral O class algebra *minimal equations* *centrum projectors and characters*

Characters of full Octahedral symmetry $O_h = O \times C_\mathbf{I} = O \times \{\mathbf{1}, \mathbf{I}\}$
Octahedral $O_h \supset O \supset C_\mathbf{I}$ *subgroup correlations*
Octahedral subgroup correlation $O_h \supset O \supset D_4$ $O_h \supset O \supset D_4 \supset C_4$ *and level-splitting*
Comparing $O \supset C_4$ *and* $O \supset C_3$ *and* $O \supset C_2$
$R(3) \subset O(3) \supset O_h \supset O$ *character analysis: Crystal field splitting* *p, d, f,…orbitals*
Cluster structure in SF_6 *16um spectra.* *Analogy with* D_6 *band gap structure*
Global vs Local *External LAB splitting vs Internal BODY clustering*
Detailed superfine structure for $A_1 T_1 E$ *cluster* *preview of next lecture*

Tetrahedral T class algebra

$\mathbf{c}_1=\mathbf{1}$, $\mathbf{c}_r=\mathbf{r}_1+\mathbf{r}_2+\mathbf{r}_3+\mathbf{r}_4$, $\mathbf{c}^\dagger{}_r=\mathbf{r}_1{}^2+\mathbf{r}_2{}^2+\mathbf{r}_3{}^2+\mathbf{r}_4{}^2$, $\mathbf{c}_\rho=\mathbf{R}_1{}^2+\mathbf{R}_2{}^2+\mathbf{R}_3{}^2$,

T group products



	+120°				-120°				±180° XYZ		
	$[1\ 1\ 1]$	$[\bar{1}\ \bar{1}\ 1]$	$[1\ \bar{1}\ \bar{1}]$	$[\bar{1}\ 1\ \bar{1}]$	$[\bar{1}\ \bar{1}\ \bar{1}]$	$[1\ 1\ \bar{1}]$	$[\bar{1}\ 1\ 1]$	$[1\ \bar{1}\ 1]$	$[1\ 0\ 0]$	$[0\ 1\ 0]$	$[0\ 0\ 1]$
					$\tilde{r}_1$	$\tilde{r}_2$	$\tilde{r}_3$	$\tilde{r}_4$	ρ_x	ρ_y	ρ_z
1	r_1	r_2	r_3	r_4	r_1^2	r_2^2	r_3^2	r_4^2	R_1^2	R_2^2	R_3^2
r_1	r_1^2	$-r_4^2$	$-r_2^2$	$-r_3^2$	-1	$-R_2^2$	$-R_3^2$	$-R_1^2$	$-r_2$	$-r_3$	$-r_4$
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	$-r_4^2$	$-r_1^2$	r_3^2	$-r_2^2$	R_3^2	$-R_1^2$	-1	R_2^2	$-r_4$	r_1	r_2
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_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_2^2	$-R_1^2$	-1	R_3^2	$-R_2^2$	r_4	$-r_2$	r_1	r_3	$-r_3^2$	$-r_1^2$	r_4^2
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_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	$-r_2^2$
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_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
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

Minus (-)signs
for Fermions
(Ignore (-) for Bosons or
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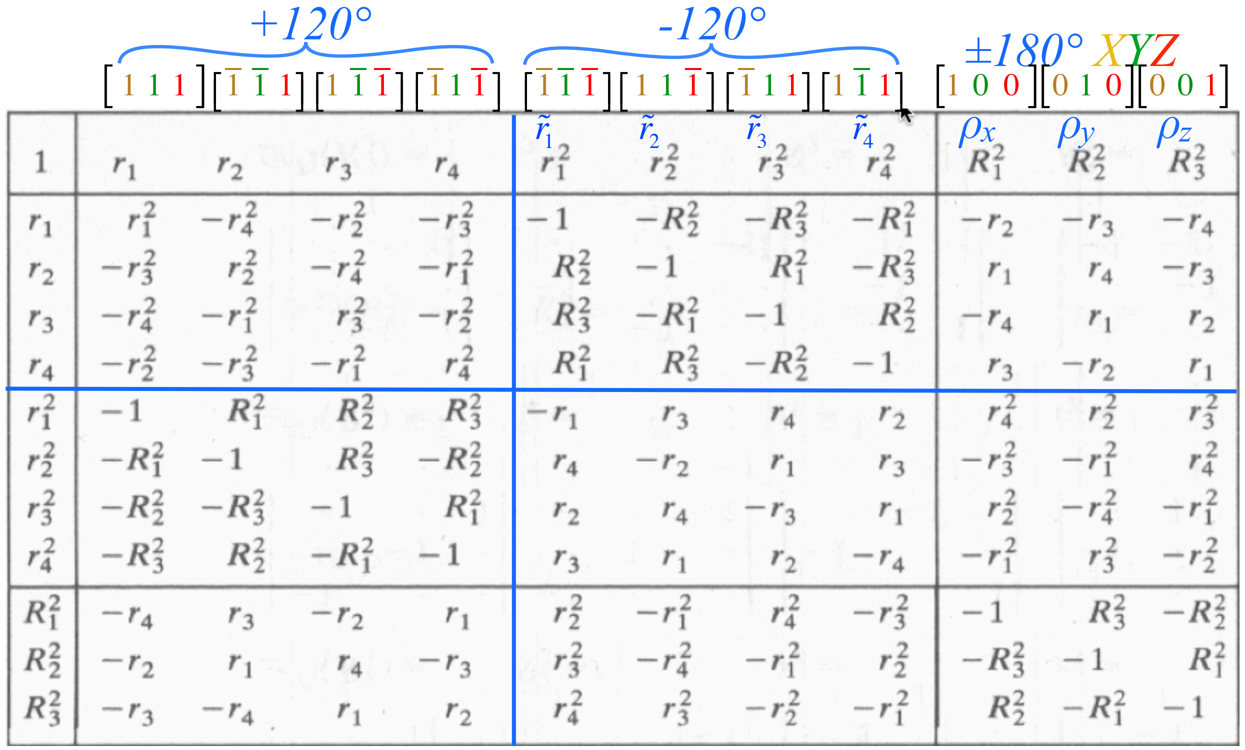
Step-byStep Development of
T-characters
GrpTh Lect.19 start:p.22

GrpTh Lect.19 end:p.50

Tetrahedral T class algebra

$\mathbf{c}_1=\mathbf{1}$, $\mathbf{c}_r=\mathbf{r}_1+\mathbf{r}_2+\mathbf{r}_3+\mathbf{r}_4$, $\mathbf{c}^\dagger_r=\mathbf{r}_1^2+\mathbf{r}_2^2+\mathbf{r}_3^2+\mathbf{r}_4^2$, $\mathbf{c}_\rho=\mathbf{R}_1^2+\mathbf{R}_2^2+\mathbf{R}_3^2$,

T group products



	+120°				-120°				±180° XYZ		
	$[1\,1\,1]$	$[\bar1\,\bar1\,1]$	$[1\,\bar1\,\bar1]$	$[\bar1\,1\,\bar1]$	$[\bar1\,\bar1\,\bar1]$	$[1\,1\,\bar1]$	$[\bar1\,1\,1]$	$[1\,\bar1\,1]$	$[1\,0\,0]$	$[0\,1\,0]$	$[0\,0\,1]$
					$\tilde r_1$	$\tilde r_2$	$\tilde r_3$	$\tilde r_4$	ρ_x	ρ_y	ρ_z
1	r_1	r_2	r_3	r_4	r_1^2	r_2^2	r_3^2	r_4^2	R_1^2	R_2^2	R_3^2
r_1	r_1^2	$-r_4^2$	$-r_2^2$	$-r_3^2$	-1	$-R_2^2$	$-R_3^2$	$-R_1^2$	$-r_2$	$-r_3$	$-r_4$
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	$-r_4^2$	$-r_1^2$	r_3^2	$-r_2^2$	R_3^2	$-R_1^2$	-1	R_2^2	$-r_4$	r_1	r_2
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_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_2^2	$-R_1^2$	-1	R_3^2	$-R_2^2$	r_4	$-r_2$	r_1	r_3	$-r_3^2$	$-r_1^2$	r_4^2
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_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	$-r_2^2$
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_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
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

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$\mathbf{c}_r$	$4\mathbf{c}_r^\dagger$	$4\mathbf{1}+4\mathbf{c}_\rho$	$3\mathbf{c}_r$
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AMOP reference links on page 2

3.05.18 class 15.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

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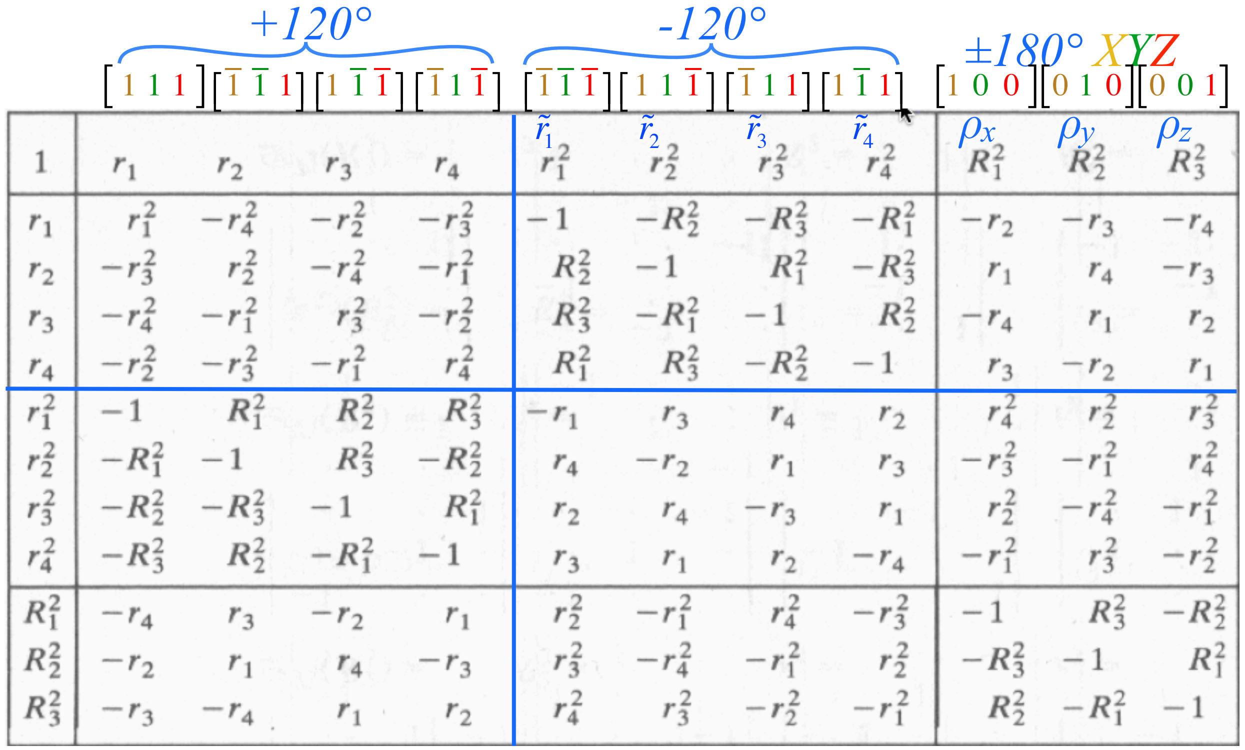

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1	r_1	r_2	r_3	r_4	$\tilde r_1$ r_1^2	$\tilde r_2$ r_2^2	$\tilde r_3$ r_3^2	$\tilde r_4$ r_4^2	ρ_x R_1^2	ρ_y R_2^2	ρ_z R_3^2
r_1	r_1^2	$-r_4^2$	$-r_2^2$	$-r_3^2$	-1	$-R_2^2$	$-R_3^2$	$-R_1^2$	$-r_2$	$-r_3$	$-r_4$
r_2	$-r_3^2$	r_2^2	$-r_4^2$	$-r_1^2$	R_2^2	-1	R_1^2	$-R_3^2$	r_1	r_4	$-r_3$
r_3	$-r_4^2$	$-r_1^2$	r_3^2	$-r_2^2$	R_3^2	$-R_1^2$	-1	R_2^2	$-r_4$	r_1	r_2
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_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_2^2	$-R_1^2$	-1	R_3^2	$-R_2^2$	r_4	$-r_2$	r_1	r_3	$-r_3^2$	$-r_1^2$	r_4^2
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_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	$-r_2^2$
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_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
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

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Step-byStep Development of
T-characters
GrpTh Lect.19 start:p.22

GrpTh Lect.19 end:p.50

Minimal equation for $\mathbf{c}_r$

$$\mathbf{c}_r^2=4\tilde{\mathbf{c}}_r$$

$$\mathbf{c}_r^3=4\tilde{\mathbf{c}}_r\mathbf{c}_r=4(4\cdot\mathbf{1}+4\mathbf{c}_\rho)=16\cdot\mathbf{1}+16\mathbf{c}_\rho$$

$$\mathbf{c}_r^4=16\cdot\mathbf{1}\mathbf{c}_r+16\mathbf{c}_\rho\mathbf{c}_r=16\cdot\mathbf{1}\mathbf{c}_r+16(3\mathbf{c}_r)$$

$$\mathbf{c}_r^4-64\mathbf{c}_r=(\mathbf{c}_r^3-64\cdot\mathbf{1})\mathbf{c}_r=\mathbf{0}$$

$$\boxed{(\mathbf{c}_r-4e^{\frac{+2\pi i}{3}}\mathbf{1})(\mathbf{c}_r-4e^{\frac{-2\pi i}{3}}\mathbf{1})(\mathbf{c}_r-4\mathbf{1})(\mathbf{c}_r-0)=\mathbf{0}}$$

Minimal equation for $\mathbf{c}_\rho$

$$\mathbf{c}_\rho^2=3\cdot\mathbf{1}+2\mathbf{c}_\rho$$

$$\mathbf{c}_\rho^2-2\mathbf{c}_\rho-3\cdot\mathbf{1}=\mathbf{0}$$

$$(\mathbf{c}_\rho-3\cdot\mathbf{1})(\mathbf{c}_\rho+\mathbf{1})=\mathbf{0}$$

AMOP reference links on page 2

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Octahedral subgroup correlation $O_h \supset O \supset D_4$ $O_h \supset O \supset D_4 \supset C_4$ *and level-splitting*

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Global vs Local *External LAB splitting vs Internal BODY clustering*

Detailed superfine structure for $A_1 T_1 E$ *cluster* *preview of next lecture*

Tetrahedral T class characters

$$\boxed{\mathbf{c_g} = \sum_\mu \frac{{}^\circ c_g \chi_g^\mu}{\ell^\mu}\mathbb{P}^\mu}$$

$$\boxed{\mathbb{P}^\mu = \sum_{classes\, c_\mathbf{g}} \frac{\ell^\mu}{{}^\circ G}\chi_g^{\mu *}\mathbf{c_g}} = \frac{\left(\ell^\mu\right)^2}{{}^\circ G}\mathbf{1} + \ldots$$

T class products

$\mathbf{1} = \mathbf{c}_1$	$\mathbf{c}_r$	$\tilde{\mathbf{c}}_r$	$\mathbf{c}_\rho$
$\mathbf{c}_r$	$4\tilde{\mathbf{c}}_r$	$4\mathbf{1}+4\mathbf{c}_\rho$	$3\mathbf{c}_r$
$\tilde{\mathbf{c}}_r$		$4\mathbf{c}_r$	$3\tilde{\mathbf{c}}$
$\mathbf{c}_\rho$			$3\mathbf{1}+2\mathbf{c}_\rho$

Minimal equation for $\mathbf{c}_r : (\mathbf{c}_r - 4\varepsilon\mathbf{1})(\mathbf{c}_r - 4\varepsilon^*\mathbf{1})(\mathbf{c}_r - 4\cdot\mathbf{1})(\mathbf{c}_r - 0) = \mathbf{0}$

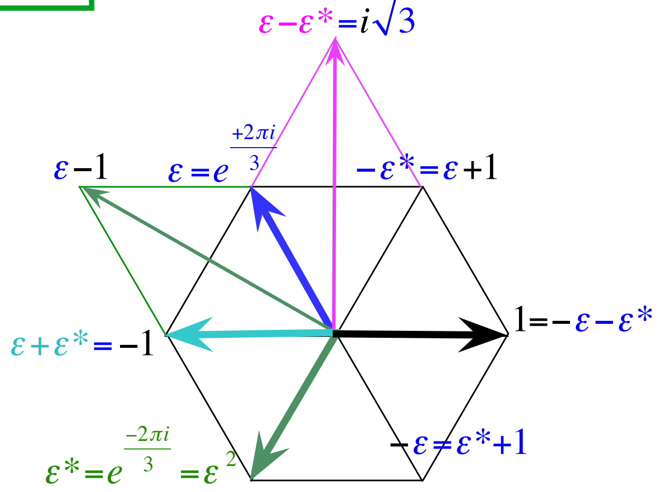
$$\mathbf{P}^{(4\varepsilon)} = \frac{(\mathbf{c}_r - 4\varepsilon^*\mathbf{1})(\mathbf{c}_r - 4\cdot\mathbf{1})(\mathbf{c}_r - 0)}{(4\varepsilon - 4\varepsilon^*)(4\varepsilon - 4)(4\varepsilon - 0)} = \frac{(\mathbf{c}_r^2 - 4(\varepsilon^* + 1)\mathbf{c}_r + 16\cdot\varepsilon^*)\mathbf{c}_r}{64(\varepsilon - \varepsilon^*)(\varepsilon - 1)\varepsilon}$$

$$= \frac{4\tilde{\mathbf{c}}_r\mathbf{c}_r + 4(\varepsilon)4\tilde{\mathbf{c}}_r + 16\cdot\varepsilon^*\mathbf{c}_r}{64i\sqrt{3}(\varepsilon^2 - \varepsilon)} = \frac{16(\mathbf{1} + \mathbf{c}_\rho) + 16\varepsilon\tilde{\mathbf{c}}_r + 16\cdot\varepsilon^*\mathbf{c}_r}{64i\sqrt{3}(-i\sqrt{3})} = \boxed{\frac{\mathbf{1} + \mathbf{c}_\rho + \varepsilon\tilde{\mathbf{c}}_r + \varepsilon^*\mathbf{c}_r}{12}}$$

$$\mathbf{P}^{(4\varepsilon^*)} = \frac{(\mathbf{c}_r - 4\varepsilon\mathbf{1})(\mathbf{c}_r - 4\cdot\mathbf{1})(\mathbf{c}_r - 0)}{(4\varepsilon^* - 4\varepsilon)(4\varepsilon^* - 4)(4\varepsilon^* - 0)} = \boxed{\frac{\mathbf{1} + \mathbf{c}_\rho + \varepsilon^*\tilde{\mathbf{c}}_r + \varepsilon\mathbf{c}_r}{12}}$$

$$\mathbf{P}^{(4)} = \frac{(\mathbf{c}_r - 4\varepsilon\mathbf{1})(\mathbf{c}_r - 4\varepsilon^*\mathbf{1})(\mathbf{c}_r - 0)}{(4 - 4\varepsilon)(4 - 4\varepsilon^*)(4 - 0)} = \frac{(\mathbf{c}_r^2 - 4(\varepsilon + \varepsilon^*)\mathbf{c}_r + 16\mathbf{1})\mathbf{c}_r}{64(1 - (\varepsilon + \varepsilon^*) + 1)}$$

$$= \frac{4\tilde{\mathbf{c}}_r\mathbf{c}_r + 4\cdot 4\tilde{\mathbf{c}}_r + 16\mathbf{c}_r}{64(1 + 1 + 1)} = \frac{16(\mathbf{1} + \mathbf{c}_\rho) + 16\tilde{\mathbf{c}}_r + 16\mathbf{c}_r}{64(1 + 1 + 1)} = \boxed{\frac{\mathbf{1} + \mathbf{c}_\rho + \tilde{\mathbf{c}}_r + \mathbf{c}_r}{12}}$$



$$\mathbf{P}^{(0)} = \frac{(\mathbf{c}_r - 4\varepsilon\mathbf{1})(\mathbf{c}_r - 4\varepsilon^*\mathbf{1})(\mathbf{c}_r - 4\cdot\mathbf{1})}{(0 - 4\varepsilon)(0 - 4\varepsilon^*)(0 - 4)} = \frac{(\mathbf{c}_r^2 - 4(\varepsilon + \varepsilon^*)\mathbf{c}_r + 16\cdot\mathbf{1})(\mathbf{c}_r - 4\cdot\mathbf{1})}{64(-\varepsilon)(-\varepsilon^*)(-1)}$$

$$= \frac{4\tilde{\mathbf{c}}_r + 4\mathbf{c}_r + 16\cdot\mathbf{1})(\mathbf{c}_r - 4\cdot\mathbf{1})}{-64}$$

$$= \frac{4\tilde{\mathbf{c}}_r\mathbf{c}_r + 4\mathbf{c}_r^2 + 16\mathbf{c}_r - 16\tilde{\mathbf{c}}_r - 16\mathbf{c}_r - 64\cdot\mathbf{1})}{-64}$$

$$= \frac{4(4\mathbf{1} + 4\mathbf{c}_\rho) + 16\tilde{\mathbf{c}}_r + 16\mathbf{c}_r - 16\tilde{\mathbf{c}}_r - 16\mathbf{c}_r - 64\cdot\mathbf{1})}{-64} = \frac{-48\cdot\mathbf{1} + 16\mathbf{c}_\rho}{-64} = \boxed{\frac{3}{4}\mathbf{1} - \frac{1}{4}\mathbf{c}_\rho}$$

$T : \mathbf{c}_g =$	$\mathbf{c}_1$	$\mathbf{c}_r$	$\tilde{\mathbf{c}}_r$	$\mathbf{c}_\rho$
$\chi_g^A =$	1	1	1	1
$\chi_g^\varepsilon =$	1	ε^*	ε	1
$\chi_g^{\varepsilon^*} =$	1	ε	ε^*	1
$\chi_g^T =$	3	0	0	−1

Step-byStep Development of
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GrpTh Lect.19 start:p.22

GrpTh Lect.19 end:p.50

AMOP
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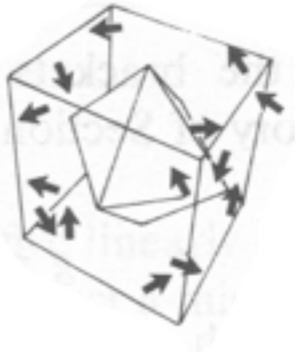
Octahedral O class algebra



$\mathbf{c}_1=\mathbf{1}$, $\mathbf{c}_r=\mathbf{r}_1+\mathbf{r}_2+\mathbf{r}_3+\mathbf{r}_4+\mathbf{r}_1{}^2+\mathbf{r}_2{}^2+\mathbf{r}_3{}^2+\mathbf{r}_4{}^2$, $\mathbf{c}_\rho=\mathbf{R}_1{}^2+\mathbf{R}_2{}^2+\mathbf{R}_3{}^2$,

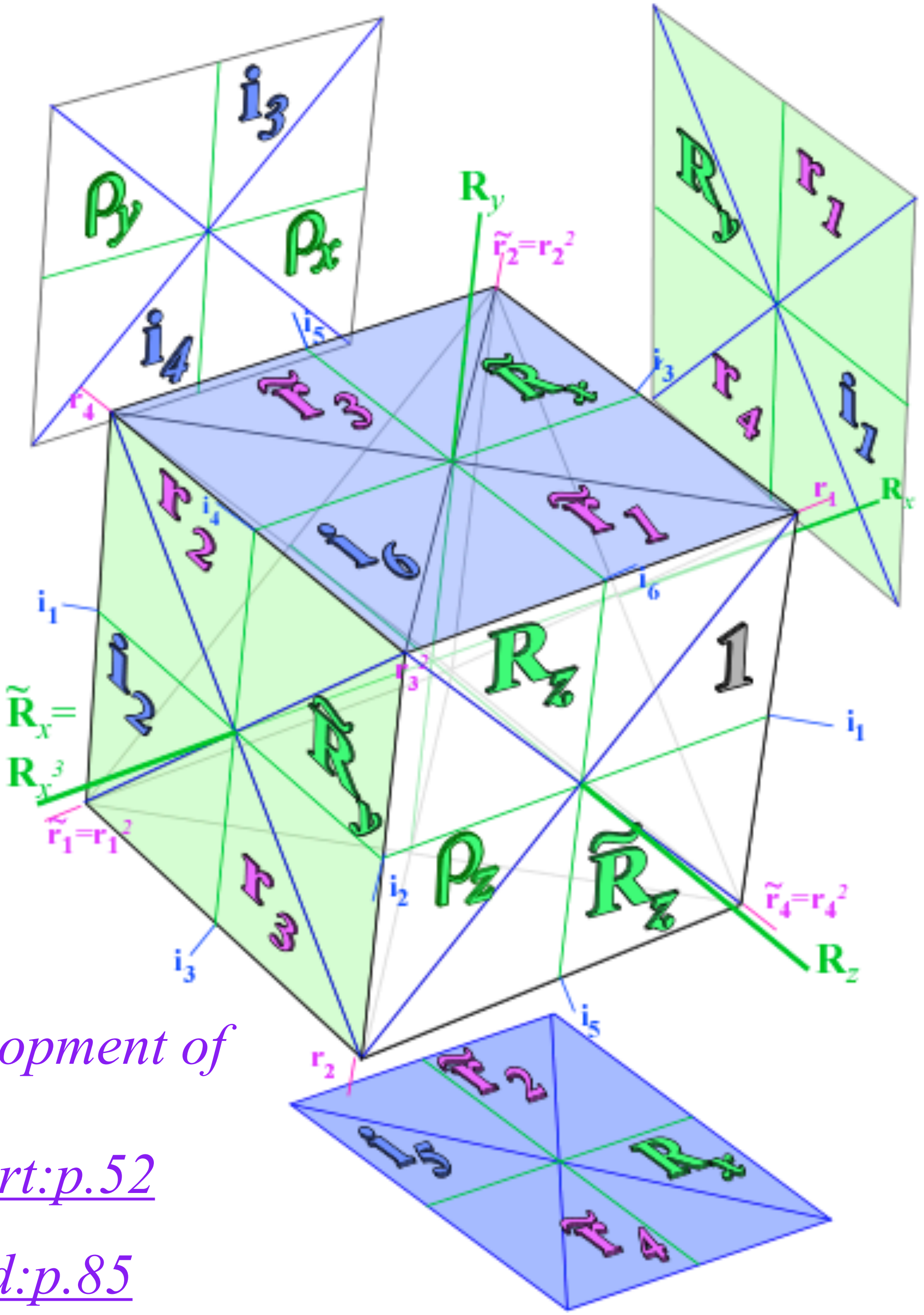
$\mathbf{c}_R=\mathbf{R}_1+\mathbf{R}_2+\mathbf{R}_3+\mathbf{R}_1{}^3+\mathbf{R}_2{}^3+\mathbf{R}_3{}^3$, $\mathbf{c}_i=\mathbf{i}_1+\mathbf{i}_2+\mathbf{i}_3+\mathbf{i}_4+\mathbf{i}_5+\mathbf{i}_6$

O class products

Unnecessary to do $24^2=576$ *products since each row (or column) of* $\mathbf{c}_A\mathbf{c}_B$ *has same class proportion*

For example:

$$\begin{aligned}\mathbf{c}_\rho\mathbf{c}_i = \ &\mathbf{R}_1{}^2\mathbf{i}_1+\ldots.= &&\mathbf{R}_2+\ldots.\\ &+\mathbf{R}_2{}^2\mathbf{i}_1+\ldots. &&+\mathbf{i}_2\ +\ldots.\\ &+\mathbf{R}_3{}^2\mathbf{i}_1+\ldots. &&+\mathbf{R}_2{}^3+\end{aligned}$$

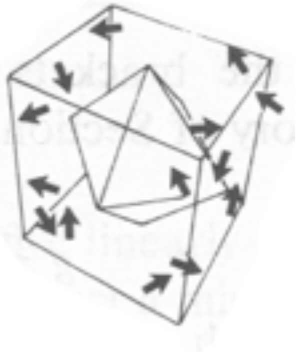


Step-byStep Development of O-characters

GrpTh Lect.19 start:p.52

GrpTh Lect.19 end:p.85

Octahedral O class algebra



$\mathbf{c}_1=\mathbf{1}$, $\mathbf{c}_r=\mathbf{r}_1+\mathbf{r}_2+\mathbf{r}_3+\mathbf{r}_4+\mathbf{r}_1^2+\mathbf{r}_2^2+\mathbf{r}_3^2+\mathbf{r}_4^2$, $\mathbf{c}_\rho=\mathbf{R}_1^2+\mathbf{R}_2^2+\mathbf{R}_3^2$,

$\mathbf{c}_R=\mathbf{R}_1+\mathbf{R}_2+\mathbf{R}_3+\mathbf{R}_1^3+\mathbf{R}_2^3+\mathbf{R}_3^3$, $\mathbf{c}_i=\mathbf{i}_1+\mathbf{i}_2+\mathbf{i}_3+\mathbf{i}_4+\mathbf{i}_5+\mathbf{i}_6$

O class products

Unnecessary to do $24^2=576$ *products since each row (or column) of* $\mathbf{c}_A\mathbf{c}_B$ *has same class proportion*

For example:

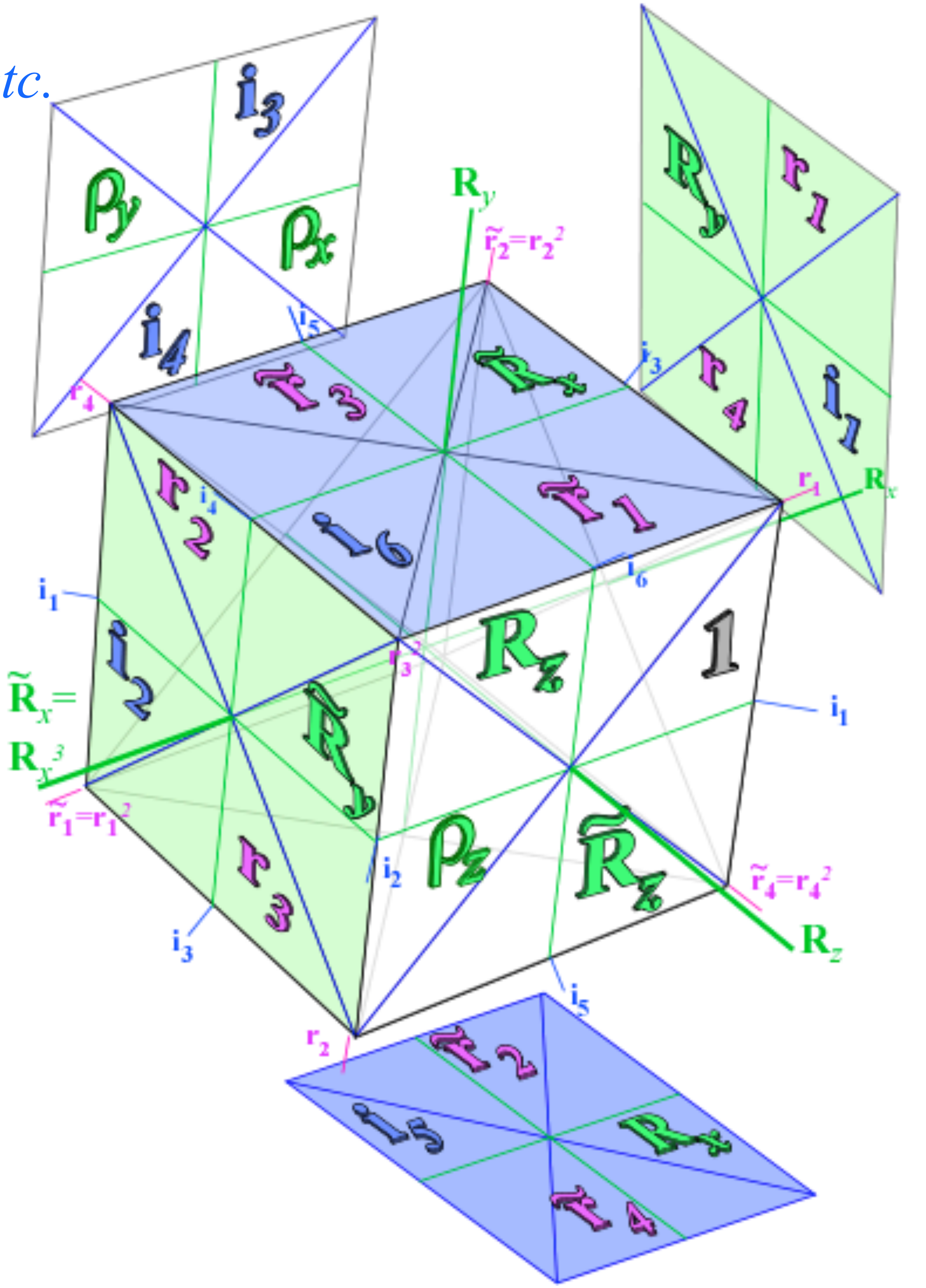
$\mathbf{c}_{R^2}\mathbf{c}_i = \mathbf{R}_1^2\mathbf{i}_1+\ldots = \mathbf{R}_2+\ldots$

$+\mathbf{R}_2^2\mathbf{i}_1+\ldots \quad + \mathbf{i}_2+\ldots$

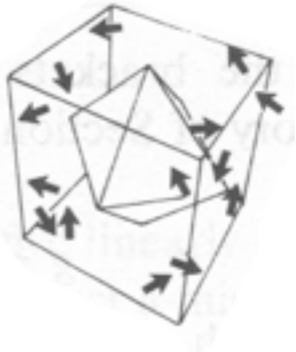
$+\mathbf{R}_3^2\mathbf{i}_1+\ldots \quad + \mathbf{R}_2^3+$

So there are $2\mathbf{c}_R$ *for each* $\mathbf{c}_i$ *:*

$\mathbf{c}_\rho\mathbf{c}_i = 2\mathbf{c}_R+\mathbf{c}_i$ *or:* $4\mathbf{c}_R+2\mathbf{c}_i$ *etc.*



Octahedral O class algebra



$\mathbf{c}_1=\mathbf{1}$, $\mathbf{c}_r=\mathbf{r}_1+\mathbf{r}_2+\mathbf{r}_3+\mathbf{r}_4+\mathbf{r}_1^2+\mathbf{r}_2^2+\mathbf{r}_3^2+\mathbf{r}_4^2$, $\mathbf{c}_\rho=\mathbf{R}_1^2+\mathbf{R}_2^2+\mathbf{R}_3^2$,

$\mathbf{c}_R=\mathbf{R}_1+\mathbf{R}_2+\mathbf{R}_3+\mathbf{R}_1^3+\mathbf{R}_2^3+\mathbf{R}_3^3$, $\mathbf{c}_i=\mathbf{i}_1+\mathbf{i}_2+\mathbf{i}_3+\mathbf{i}_4+\mathbf{i}_5+\mathbf{i}_6$

O class products

Unnecessary to do $24^2=576$ products since each row (or column) of $\mathbf{c}_A\mathbf{c}_B$ has same class proportion

For example: $\mathbf{c}_\rho\mathbf{c}_i=?$

$$\mathbf{c}_{R^2}\mathbf{c}_i = \mathbf{R}_1^2\mathbf{i}_1+\ldots = \mathbf{R}_2+\ldots$$
$$+\mathbf{R}_2^2\mathbf{i}_1+\ldots \quad +\mathbf{i}_2+\ldots$$
$$+\mathbf{R}_3^2\mathbf{i}_1+\ldots \quad +\mathbf{R}_2^3+$$

So there are $2\mathbf{c}_R$ for each $\mathbf{c}_i$ ....in $({}^\circ c_\rho)\cdot({}^\circ c_i)=(3)\cdot(6)=18$ terms

$\mathbf{c}_\rho\mathbf{c}_i=2\mathbf{c}_R+\mathbf{c}_i$ *or:* $4\mathbf{c}_R+2\mathbf{c}_i$ *etc.*

So: $2({}^\circ c_R)+({}^\circ c_i)=2\cdot 6+6=18$

Proof that class proportion cannot vary:

$$\begin{aligned}\mathbf{c}_g\mathbf{c}_h &= \mathbf{g}_1\mathbf{h}_1+\mathbf{g}_2\mathbf{h}_1+\ldots = \mathbf{g}_1\mathbf{h}_1+\mathbf{t}\mathbf{g}_1\mathbf{h}_1\mathbf{t}^{-1}+\ldots = \mathbf{g}_1\mathbf{h}_1+\mathbf{t}\mathbf{g}_1\mathbf{t}^{-1}\mathbf{t}\mathbf{h}_1\mathbf{t}^{-1}+\ldots = \mathbf{g}_1\mathbf{h}_1+\ \mathbf{g}_2\ \ \mathbf{t}\mathbf{h}_1\mathbf{t}^{-1}+\ldots\\ &\quad +\mathbf{g}_1\mathbf{h}_2+\mathbf{g}_2\mathbf{h}_2+\ldots \quad +\mathbf{g}_1\mathbf{h}_2+\mathbf{t}\mathbf{g}_1\mathbf{h}_2\mathbf{t}^{-1}+\ldots \quad +\mathbf{g}_1\mathbf{h}_2+\mathbf{t}\mathbf{g}_1\mathbf{t}^{-1}\mathbf{t}\mathbf{h}_2\mathbf{t}^{-1}+\ldots \quad +\mathbf{g}_1\mathbf{h}_2+\ \mathbf{g}_2\ \ \mathbf{t}\mathbf{h}_2\mathbf{t}^{-1}+\ldots\\ &= \mathbf{g}_1\mathbf{h}_3+\mathbf{g}_2\mathbf{h}_3+\ldots \quad +\mathbf{g}_1\mathbf{h}_2+\mathbf{t}\mathbf{g}_1\mathbf{h}_3\mathbf{t}^{-1}+\ldots \quad +\mathbf{g}_1\mathbf{h}_2+\mathbf{t}\mathbf{g}_1\mathbf{t}^{-1}\mathbf{t}\mathbf{h}_3\mathbf{t}^{-1}+\ldots \quad +\mathbf{g}_1\mathbf{h}_2+\ \mathbf{g}_2\ \ \mathbf{t}\mathbf{h}_3\mathbf{t}^{-1}+\ldots\end{aligned}$$

O class product table

$\mathbf{1}=c_1$	$\mathbf{c}_r$	$\mathbf{c}_\rho$	$\mathbf{c}_R$	$\mathbf{c}_i$
$\mathbf{c}_r$	$8\mathbf{1}+4\mathbf{c}_r+8\mathbf{c}_\rho$	$3\mathbf{c}_r$	$4\mathbf{c}_R+4\mathbf{c}_i$	$4\mathbf{c}_R+4\mathbf{c}_i$
$\mathbf{c}_\rho$		$3\mathbf{1}+2\mathbf{c}_\rho$	$\mathbf{c}_R+2\mathbf{c}_i$	$2\mathbf{c}_R+\mathbf{c}_i$
$\mathbf{c}_R$			$6\mathbf{1}+3\mathbf{c}_r+2\mathbf{c}_\rho$	$3\mathbf{c}_r+4\mathbf{c}_\rho$
$\mathbf{c}_i$				$6\mathbf{1}+3\mathbf{c}_r+2\mathbf{c}_\rho$

Minimal equation for $\mathbf{c}_\rho$

$\mathbf{c}_\rho^2=3\mathbf{1}+2\mathbf{c}_\rho$

$\mathbf{c}_\rho^2-2\mathbf{c}_\rho-3\mathbf{1}=\mathbf{0}$

$(\mathbf{c}_\rho-3\mathbf{1})(\mathbf{c}_\rho+\mathbf{1})=\mathbf{0}$

Step-byStep Development of
O-characters
GrpTh Lect.19 start:p.52

GrpTh Lect.19 end:p.85

AMOP reference links on page 2

3.05.18 class 15.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Discrete symmetry subgroups of O(3)⊃(Octahedral O_h⊃O~T_d, Cubic-Tetrahedral T_h⊃T): Characters and subgroup-chain defined ireps, and applications to SF_6 and CF_4 spectra

Review: *General all-commuting class-character-projector formula derivations.*

$\mathbb{P}^\mu$ in χ^μ-terms of κ_g *κ_g in $\chi^{\mu *}$-terms of $\mathbb{P}^\mu$* *Irep frequency f^μ in $\chi^{\mu *}$-terms of Trace$R(\mathbf{g})$*

Introducing octahedral/ tetrahedral symmetry $O_h \supset O \sim T_d \supset T$: relating $D_4 \supset C_4$ and $D_3 \supset C_3$

Octahedral-cubic O symmetry and group operations, *O slide-rule*

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➡ *Octahedral O class algebra* ➡ *minimal equations* *centrum projectors and characters*

Characters of full Octahedral symmetry $O_h = O \times C_{\mathbf{I}} = O \times \{\mathbf{1},\mathbf{I}\}$

Octahedral $O_h \supset O \supset C_{\mathbf{I}}$ subgroup correlations

Octahedral subgroup correlation *$O_h \supset O \supset D_4$* *$O_h \supset O \supset D_4 \supset C_4$* *and level-splitting*

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R(3)⊂O(3)⊃O_h⊃O character analysis: Crystal field splitting *p, d, f,…orbitals*

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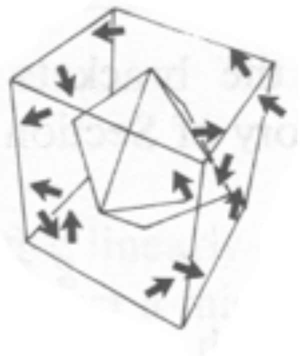
Global vs Local *External LAB splitting vs Internal BODY clustering*

Detailed superfine structure for A_1T_1E cluster *preview of next lecture*

Octahedral O class minimal equations



$$\boxed{\mathbf{c_g} = \sum_{\mu} \frac{{}^{\circ}c_g \chi^{\mu}_{g}}{\ell^{\mu}} \mathbb{P}^{\mu}}$$

$$\boxed{\mathbb{P}^{\mu} = \sum_{classes\, c_{\mathbf{g}}} \frac{\ell^{\mu}}{{}^{\circ}G} \chi^{\mu *}_{g} \mathbf{c_g}}$$

O class product table

$\mathbf{1} = c_1$	$\mathbf{c}_r$	$\mathbf{c}_\rho$	$\mathbf{c}_R$	$\mathbf{c}_i$
$\mathbf{c}_r$	$8\mathbf{1}+4\mathbf{c}_r+8\mathbf{c}_\rho$	$3\mathbf{c}_r$	$4\mathbf{c}_R+4\mathbf{c}_i$	$4\mathbf{c}_R+4\mathbf{c}_i$
$\mathbf{c}_\rho$		$3\mathbf{1}+2\mathbf{c}_\rho$	$\mathbf{c}_R+2\mathbf{c}_i$	$2\mathbf{c}_R+\mathbf{c}_i$
$\mathbf{c}_R$			$6\mathbf{1}+3\mathbf{c}_r+2\mathbf{c}_\rho$	$3\mathbf{c}_r+4\mathbf{c}_\rho$
$\mathbf{c}_i$				$6\mathbf{1}+3\mathbf{c}_r+2\mathbf{c}_\rho$

Minimal equation for $\mathbf{c}_i$

$$\mathbf{c}_i^2 = 6\cdot\mathbf{1} + 3\mathbf{c}_r + 2\mathbf{c}_\rho$$

$$\mathbf{c}_i^3 = 6\cdot\mathbf{1}\mathbf{c}_i + 3\mathbf{c}_r\mathbf{c}_i + 2\mathbf{c}_\rho\mathbf{c}_i$$
$$= 6\mathbf{c}_i + 3(4\mathbf{c}_R + 4\mathbf{c}_i) + 2(2\mathbf{c}_R + \mathbf{c}_i)$$
$$\mathbf{c}_i^3 = 16\mathbf{c}_R + 20\mathbf{c}_i$$

$$\mathbf{c}_i^4 = 16\mathbf{c}_R\mathbf{c}_i + 20\mathbf{c}_i\mathbf{c}_i$$
$$= 16(3\mathbf{c}_r + 4\mathbf{c}_\rho) + 20(6\cdot\mathbf{1} + 3\mathbf{c}_r + 2\mathbf{c}_\rho)$$
$$= 48\mathbf{c}_r + 64\mathbf{c}_\rho + 120\cdot\mathbf{1} + 60\mathbf{c}_r + 40\mathbf{c}_\rho)$$
$$= 120\cdot\mathbf{1} + 108\mathbf{c}_r + 104\mathbf{c}_\rho$$

Step-byStep Development of
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GrpTh Lect.19 start:p.52

GrpTh Lect.19 end:p.85

$$\mathbf{c}_i^5 = 120\mathbf{c}_i + 108\mathbf{c}_r\mathbf{c}_i + 104\mathbf{c}_\rho\mathbf{c}_i$$
$$= 120\mathbf{c}_i + 108(4\mathbf{c}_R + 4\mathbf{c}_i) + 104(2\mathbf{c}_R + \mathbf{c}_i)$$
$$= 640\mathbf{c}_R + 656\mathbf{c}_i$$

$$40\mathbf{c}_i^3 = 640\mathbf{c}_R + 800\mathbf{c}_i$$

$$\mathbf{c}_i^5 - 40\mathbf{c}_i^3 + 144\mathbf{c}_i = \mathbf{0} = (\mathbf{c}_i^2 - 36\cdot\mathbf{1})(\mathbf{c}_i^2 - 4\cdot\mathbf{1})(\mathbf{c}_i - 0\cdot\mathbf{1})$$

800
-656
144

Minimal equation for $\mathbf{c}_i$

$$\boxed{\mathbf{0} = (\mathbf{c}_i + 6\cdot\mathbf{1})(\mathbf{c}_i - 6\cdot\mathbf{1})(\mathbf{c}_i + 2\cdot\mathbf{1})(\mathbf{c}_i - 2\cdot\mathbf{1})(\mathbf{c}_i - 0\cdot\mathbf{1})}$$

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Global vs Local *External LAB splitting vs Internal BODY clustering*

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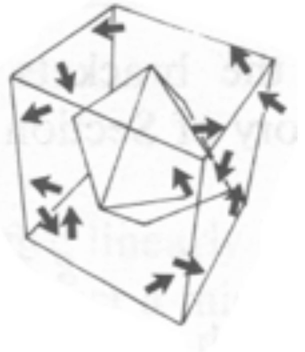
Octahedral O projector algebra

Begin with minimal equation: $\mathbf{0} = (\mathbf{c}_i + 2\cdot\mathbf{1})\cancel{(\mathbf{c}_i - 2\cdot\mathbf{1})}(\mathbf{c}_i + 6\cdot\mathbf{1})(\mathbf{c}_i - 6\cdot\mathbf{1})(\mathbf{c}_i - 0\cdot\mathbf{1})$



$$\mathbf{c_g} = \sum_{\mu} \frac{{}^{\circ}c_g \chi_g^{\mu}}{\ell^{\mu}} \mathbb{P}^{\mu}$$

$$\mathbb{P}^{\mu} = \sum_{classes\, c_\mathbf{g}} \frac{\ell^{\mu}}{{}^{\circ}G} \chi_g^{\mu *} \mathbf{c_g}$$

$$\mathbf{P}^{(2)} = \frac{(\mathbf{c}_i + 2\cdot\mathbf{1})(\mathbf{c}_i - 6\cdot\mathbf{1})(\mathbf{c}_i + 6\cdot\mathbf{1})(\mathbf{c}_i - 0)}{(2+2)(2-6)(2+6)(2-0)} = \frac{(\mathbf{c}_i + 2\cdot\mathbf{1})(\mathbf{c}_i^2 - 36\cdot\mathbf{1})\mathbf{c}_i}{-256} = \frac{\mathbf{c}_i^4 + 2\cdot\mathbf{c}_i^3 - 36\,\mathbf{c}_i^2 - 72\,\mathbf{c}_i}{-256}$$

Expanding $\mathbf{P}^{(2)}$

$\mathbf{c}_i^4 = 120\cdot\mathbf{1} + 108\mathbf{c}_r + 104\mathbf{c}_\rho$

$\mathbf{c}_i^3 = \qquad + 16\mathbf{c}_R + 20\mathbf{c}_i$

$\mathbf{c}_i^2 = \quad 6\cdot\mathbf{1} + 3\mathbf{c}_r + 2\mathbf{c}_\rho$

$\mathbf{c}_i = \qquad + \quad \mathbf{c}_i$

$$\begin{aligned} \mathbf{c}_i^4 &= 120\cdot\mathbf{1} + 108\mathbf{c}_r + 104\mathbf{c}_\rho \\ +2\mathbf{c}_i^3 &= \qquad\qquad\qquad\qquad + 32\mathbf{c}_R + 40\mathbf{c}_i \\ -36\mathbf{c}_i^2 &= -216\cdot\mathbf{1} - 108\mathbf{c}_r \quad -72\mathbf{c}_\rho \\ -72\mathbf{c}_i &= \qquad\qquad\qquad\qquad\qquad\qquad -72\mathbf{c}_i \\ \hline -256\mathbf{P}^{(2)} &= -96\cdot\mathbf{1} + 0\,\mathbf{c}_r + 32\mathbf{c}_\rho + 32\mathbf{c}_R - \; 32\mathbf{c}_i \end{aligned}$$

$$\mathbf{P}^{(2)} = \boxed{\frac{3}{8}\mathbf{1} - \frac{0}{8}\mathbf{c}_r + \frac{1}{8}\mathbf{c}_\rho - \frac{1}{8}\mathbf{c}_R + \frac{1}{8}\mathbf{c}_i}$$

O class product table

$\mathbf{1} = c_1$	$\mathbf{c}_r$	$\mathbf{c}_\rho$	$\mathbf{c}_R$	$\mathbf{c}_i$
$\mathbf{c}_r$	$8\mathbf{1}+4\mathbf{c}_r+8\mathbf{c}_\rho$	$3\mathbf{c}_r$	$4\mathbf{c}_R+4\mathbf{c}_i$	$4\mathbf{c}_R+4\mathbf{c}_i$
$\mathbf{c}_\rho$		$3\mathbf{1}+2\mathbf{c}_\rho$	$\mathbf{c}_R+2\mathbf{c}_i$	$2\mathbf{c}_R+\mathbf{c}_i$
$\mathbf{c}_R$			$6\mathbf{1}+3\mathbf{c}_r+2\mathbf{c}_\rho$	$3\mathbf{c}_r+4\mathbf{c}_\rho$
$\mathbf{c}_i$				$6\mathbf{1}+3\mathbf{c}_r+2\mathbf{c}_\rho$

Step-byStep Development of O-characters

GrpTh Lect.19 start:p.52

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Octahedral O projector algebra

Begin with minimal equation: $\mathbf{0}= (\mathbf{c}_i +2\cdot\mathbf{1})(\mathbf{c}_i -2\cdot\mathbf{1})(\mathbf{c}_i+6\cdot\mathbf{1})\cancel{(\mathbf{c}_i-6\cdot\mathbf{1})}(\mathbf{c}_i-0\cdot\mathbf{1})$

$$\boxed{\mathbf{c_g} = \sum_{\mu} \frac{{}^\circ c_g \chi^\mu_g}{\ell^\mu} \mathbb{P}^\mu}$$

$$\boxed{\mathbb{P}^\mu = \sum_{classes\, c_{\mathbf{g}}} \frac{\ell^\mu}{{}^\circ G} \chi^{\mu *}_g \mathbf{c_g}}$$

$$\mathbf{P}^{(2)} = \frac{(\mathbf{c}_i+2\mathbf{1})(\mathbf{c}_i-6\mathbf{1})(\mathbf{c}_i+6\mathbf{1})(\mathbf{c}_i-0)}{(2+2)(2-6)(2+6)(2-0)} = \frac{(\mathbf{c}_i+2\mathbf{1})(\mathbf{c}_i^2-36\mathbf{1})\mathbf{c}_i}{-256} = \frac{\mathbf{c}_i^4+2\mathbf{c}_i^3-36\mathbf{c}_i^2-72\mathbf{c}_i}{-256}$$

$\mathbf{c}_i^4=120\cdot\mathbf{1}+108\mathbf{c}_r+104\mathbf{c}_\rho$

$\mathbf{c}_i^3= \qquad\qquad +16\mathbf{c}_R+20\mathbf{c}_i$

$\mathbf{c}_i^2= \quad 6\cdot\mathbf{1}+3\mathbf{c}_r+2\mathbf{c}_\rho$

$\mathbf{c}_i = \qquad\qquad + \quad \mathbf{c}_i$

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$\mathbf{c}_i^4 =120\cdot\mathbf{1}+108\mathbf{c}_r+104\mathbf{c}_\rho$

$+2\mathbf{c}_i^3 = \qquad\qquad +32\mathbf{c}_R+40\mathbf{c}_i$

$-36\mathbf{c}_i^2=-216\cdot\mathbf{1}-108\mathbf{c}_r \;\; -72\mathbf{c}_\rho$

$-72\mathbf{c}_i = \qquad\qquad -72\mathbf{c}_i$

$-256\mathbf{P}^{(2)} =-96\cdot\mathbf{1}+ 0\, \mathbf{c}_r+32\mathbf{c}_\rho +32\mathbf{c}_R- 32\mathbf{c}_i$

$$\mathbf{P}^{(2)} = \boxed{\frac{3}{8}\mathbf{1}+\frac{0}{8}\mathbf{c}_r-\frac{1}{8}\mathbf{c}_\rho-\frac{1}{8}\mathbf{c}_R+\frac{1}{8}\mathbf{c}_i}$$

Expansion of $\mathbf{P}^{(-2)}$ has (-)sign on last 2 terms...

$$\mathbf{P}^{(-2)} = \boxed{\frac{3}{8}\mathbf{1}+\frac{0}{8}\mathbf{c}_r-\frac{1}{8}\mathbf{c}_\rho+\frac{1}{8}\mathbf{c}_R-\frac{1}{8}\mathbf{c}_i}$$

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$\mathbf{c}_R$			$6\mathbf{1}+3\mathbf{c}_r+2\mathbf{c}_\rho$	$3\mathbf{c}_r+4\mathbf{c}_\rho$
$\mathbf{c}_i$				$6\mathbf{1}+3\mathbf{c}_r+2\mathbf{c}_\rho$

Octahedral O characters

χ^μ_g	$\mathbf{g}=\mathbf{1}$	$\mathbf{r}_{1\ldots4}$	$\boldsymbol{\rho}_{xyz}$	$\mathbf{R}_{xyz}$	$\mathbf{i}_{1\ldots6}$
χ^{A_1}	1	1	1	1	1
χ^{A_2}	1	1	1	−1	−1
χ^{E}	2	−1	2	0	0
χ^{T_1}	3	0	−1	1	−1
χ^{T_2}	3	0	−1	−1	1

(Remaining character derivations left as an exercise)

AMOP
reference links
on page 2

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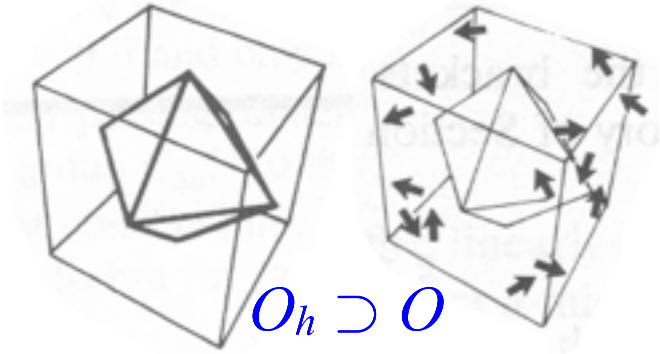


$O_h \supset O$ symmetry

	χ_g^μ	$\mathbf{g} = \mathbf{1}$	$\mathbf{r}_{1\ldots4}$	$\boldsymbol{\rho}_{xyz}$	$\mathbf{R}_{xyz}$	$\mathbf{i}_{1\ldots6}$
A_{1g}	$\chi^{A_{1g}}$	1	1	1	1	1
A_{2g}	$\chi^{A_{2g}}$	1	1	1	−1	−1
E_g	χ^{E_g}	2	−1	2	0	0
T_{1g}	$\chi^{T_{1g}}$	3	0	−1	1	−1
T_{2g}	$\chi^{T_{2g}}$	3	0	−1	−1	1

EVEN
parity
(gerade)

3D – Inversion

$$\langle \mathbf{I} \rangle = \begin{pmatrix} -1 & \cdot & \cdot \\ \cdot & -1 & \cdot \\ \cdot & \cdot & -1 \end{pmatrix}$$

$C_\mathbf{I}$-symmetry

1	**I**
I	1

$C_\mathbf{I}$-characters

$C_\mathbf{I}$	1	**I**
g	*1*	*1*
u	*1*	*-1*

±
Parity P
(gerade)
(ungerade)

O class product table

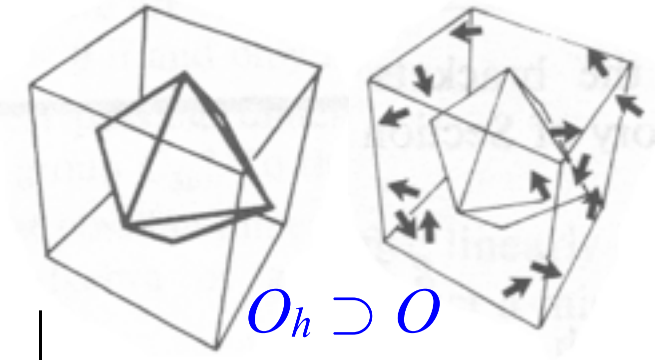
$\mathbf{1} = c_1$	$\mathbf{c}_r$	$\mathbf{c}_\rho$	$\mathbf{c}_R$	$\mathbf{c}_i$
$\mathbf{c}_r$	$8\mathbf{1}+4\mathbf{c}_r+8\mathbf{c}_\rho$	$3\mathbf{c}_r$	$4\mathbf{c}_R+4\mathbf{c}_i$	$4\mathbf{c}_R+4\mathbf{c}_i$
$\mathbf{c}_\rho$		$3\mathbf{1}+2\mathbf{c}_\rho$	$\mathbf{c}_R+2\mathbf{c}_i$	$2\mathbf{c}_R+\mathbf{c}_i$
$\mathbf{c}_R$			$6\mathbf{1}+3\mathbf{c}_r+2\mathbf{c}_\rho$	$3\mathbf{c}_r+4\mathbf{c}_\rho$
$\mathbf{c}_i$				$6\mathbf{1}+3\mathbf{c}_r+2\mathbf{c}_\rho$

Octahedral O characters

χ_g^μ	$\mathbf{g} = \mathbf{1}$	$\mathbf{r}_{1\ldots4}$	$\boldsymbol{\rho}_{xyz}$	$\mathbf{R}_{xyz}$	$\mathbf{i}_{1\ldots6}$
χ^{A_1}	1	1	1	1	1
χ^{A_2}	1	1	1	−1	−1
χ^{E}	2	−1	2	0	0
χ^{T_1}	3	0	−1	1	−1
χ^{T_2}	3	0	−1	−1	1

(Remaining character derivations left as an exercise)

Octahedral $O_h = O \times \{\mathbf{1},\mathbf{I}\}$ characters of $O \times C_{\mathbf{I}} \supset O$



$O_h \supset O$ symmetry

		χ^{μ}_{g}	$\mathbf{g=1}$	$\mathbf{r}_{1...4}$	$\boldsymbol{\rho}_{xyz}$	$\mathbf{R}_{xyz}$	$\mathbf{i}_{1...6}$	$\mathbf{g=I}$	$\mathbf{Ir}_{1...4}$	$\mathbf{I}\boldsymbol{\rho}_{xyz}$	$\mathbf{IR}_{xyz}$	$\mathbf{Ii}_{1...6}$
	A_{1g}	$\chi^{A_{1g}}$	1	1	1	1	1	1	1	1	1	1
	A_{2g}	$\chi^{A_{2g}}$	1	1	1	−1	−1	1	1	1	−1	−1
EVEN parity *(gerade)*	E_g	χ^{E_g}	2	−1	2	0	0	2	−1	2	0	0
	T_{1g}	$\chi^{T_{1g}}$	3	0	−1	1	−1	3	0	−1	1	−1
	T_{2g}	$\chi^{T_{2g}}$	3	0	−1	−1	1	3	0	−1	−1	1

3D – Inversion

$$\langle \mathbf{I} \rangle = \begin{pmatrix} -1 & \cdot & \cdot \\ \cdot & -1 & \cdot \\ \cdot & \cdot & -1 \end{pmatrix}$$

$C_{\mathbf{I}}$-symmetry

1	**I**
I	1

$C_{\mathbf{I}}$-characters

$C_{\mathbf{I}}$	1	**I**	± Parity P
g	*1*	*1*	*(gerade)*
u	*1*	*-1*	*(ungerade)*

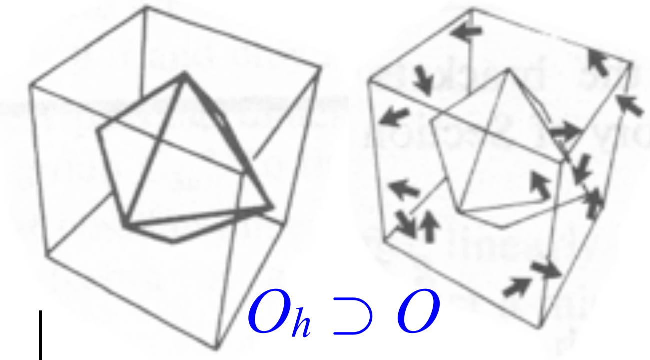
O class product table

$\mathbf{1}=c_1$	$\mathbf{c}_r$	$\mathbf{c}_\rho$	$\mathbf{c}_R$	$\mathbf{c}_i$
$\mathbf{c}_r$	$8\mathbf{1}+4\mathbf{c}_r+8\mathbf{c}_\rho$	$3\mathbf{c}_r$	$4\mathbf{c}_R+4\mathbf{c}_i$	$4\mathbf{c}_R+4\mathbf{c}_i$
$\mathbf{c}_\rho$		$3\mathbf{1}+2\mathbf{c}_\rho$	$\mathbf{c}_R+2\mathbf{c}_i$	$2\mathbf{c}_R+\mathbf{c}_i$
$\mathbf{c}_R$			$6\mathbf{1}+3\mathbf{c}_r+2\mathbf{c}_\rho$	$3\mathbf{c}_r+4\mathbf{c}_\rho$
$\mathbf{c}_i$				$6\mathbf{1}+3\mathbf{c}_r+2\mathbf{c}_\rho$

Octahedral O characters

χ^{μ}_{g}	$\mathbf{g=1}$	$\mathbf{r}_{1...4}$	$\boldsymbol{\rho}_{xyz}$	$\mathbf{R}_{xyz}$	$\mathbf{i}_{1...6}$
χ^{A_1}	1	1	1	1	1
χ^{A_2}	1	1	1	−1	−1
χ^{E}	2	−1	2	0	0
χ^{T_1}	3	0	−1	1	−1
χ^{T_2}	3	0	−1	−1	1

Octahedral $O_h = O \times \{\mathbf{1}, \mathbf{I}\}$ characters of $O \times C_\mathbf{I} \supset O$



$O_h \supset O$ symmetry

		χ^{μ}_{g}	$\mathbf{g=1}$	$\mathbf{r}_{1...4}$	$\boldsymbol{\rho}_{xyz}$	$\mathbf{R}_{xyz}$	$\mathbf{i}_{1...6}$	$\mathbf{g=I}$	$\mathbf{Ir}_{1...4}$	$\mathbf{I\rho}_{xyz}$	$\mathbf{IR}_{xyz}$	$\mathbf{Ii}_{1...6}$
EVEN parity *(gerade)*	A_{1g}	$\chi^{A_{1g}}$	1	1	1	1	1	1	1	1	1	1
	A_{2g}	$\chi^{A_{2g}}$	1	1	1	−1	−1	1	1	1	−1	−1
	E_{g}	$\chi^{E_{g}}$	2	−1	2	0	0	2	−1	2	0	0
	T_{1g}	$\chi^{T_{1g}}$	3	0	−1	1	−1	3	0	−1	1	−1
	T_{2g}	$\chi^{T_{2g}}$	3	0	−1	−1	1	3	0	−1	−1	1
ODD parity *(ungerade)*	A_{1u}	$\chi^{A_{1u}}$	1	1	1	1	1					
	A_{2u}	$\chi^{A_{2u}}$	1	1	1	−1	−1					
	E_{u}	$\chi^{E_{u}}$	2	−1	2	0	0					
	T_{1u}	$\chi^{T_{1u}}$	3	0	−1	1	−1					
	T_{2u}	$\chi^{T_{2u}}$	3	0	−1	−1	1					

3D – Inversion

$$\langle \mathbf{I} \rangle = \begin{pmatrix} -1 & \cdot & \cdot \\ \cdot & -1 & \cdot \\ \cdot & \cdot & -1 \end{pmatrix}$$

$C_\mathbf{I}$-symmetry

1	**I**
I	1

$C_\mathbf{I}$-characters

$C_\mathbf{I}$	1	**I**	± Parity P
g	*1*	*1*	*(gerade)*
u	*1*	*-1*	*(ungerade)*

O class product table

$\mathbf{1} = c_1$	$\mathbf{c}_r$	$\mathbf{c}_\rho$	$\mathbf{c}_R$	$\mathbf{c}_i$
$\mathbf{c}_r$	$8\mathbf{1}+4\mathbf{c}_r+8\mathbf{c}_\rho$	$3\mathbf{c}_r$	$4\mathbf{c}_R+4\mathbf{c}_i$	$4\mathbf{c}_R+4\mathbf{c}_i$
$\mathbf{c}_\rho$		$3\mathbf{1}+2\mathbf{c}_\rho$	$\mathbf{c}_R+2\mathbf{c}_i$	$2\mathbf{c}_R+\mathbf{c}_i$
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Octahedral O characters

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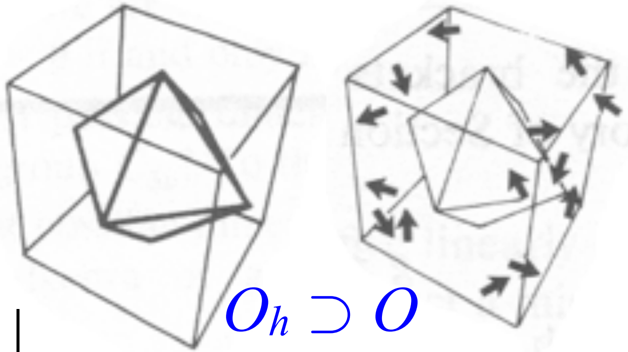
Octahedral $O_h = O \times \{\mathbf{1},\mathbf{I}\}$ *characters of* $O \times C_{\mathbf{I}} \supset O$

O_h easily derived from those of O and $C_{\mathbf{I}}$!



$O_h \supset O$ symmetry

		χ_g^μ	$\mathbf{g=1}$	$\mathbf{r}_{1\ldots4}$	$\boldsymbol{\rho}_{xyz}$	$\mathbf{R}_{xyz}$	$\mathbf{i}_{1\ldots6}$	$\mathbf{g=I}$	$\mathbf{Ir}_{1\ldots4}$	$\mathbf{I}\boldsymbol{\rho}_{xyz}$	$\mathbf{IR}_{xyz}$	$\mathbf{Ii}_{1\ldots6}$
EVEN parity *(gerade)*	A_{1g}	$\chi^{A_{1g}}$	1	1	1	1	1	1	1	1	1	1
	A_{2g}	$\chi^{A_{2g}}$	1	1	1	−1	−1	1	1	1	−1	−1
	E_g	χ^{E_g}	2	−1	2	0	0	2	−1	2	0	0
	T_{1g}	$\chi^{T_{1g}}$	3	0	−1	1	−1	3	0	−1	1	−1
	T_{2g}	$\chi^{T_{2g}}$	3	0	−1	−1	1	3	0	−1	−1	1
ODD parity *(ungerade)*	A_{1u}	$\chi^{A_{1u}}$	1	1	1	1	1	−1	−1	−1	−1	−1
	A_{2u}	$\chi^{A_{2u}}$	1	1	1	−1	−1	−1	−1	−1	+1	+1
	E_u	χ^{E_u}	2	−1	2	0	0	−2	+1	−2	0	0
	T_{1u}	$\chi^{T_{1u}}$	3	0	−1	1	−1	−3	0	+1	−1	+1
	T_{2u}	$\chi^{T_{2u}}$	3	0	−1	−1	1	−3	0	+1	+1	−1

3D – Inversion

$$\langle \mathbf{I} \rangle = \begin{pmatrix} -1 & \cdot & \cdot \\ \cdot & -1 & \cdot \\ \cdot & \cdot & -1 \end{pmatrix}$$

$C_{\mathbf{I}}$-symmetry

1	**I**
I	1

$C_{\mathbf{I}}$-characters

$C_{\mathbf{I}}$	1	**I**
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± Parity P

(gerade)

(ungerade)

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$\mathbf{c}_\rho$		$3\mathbf{1}+2\mathbf{c}_\rho$	$\mathbf{c}_R+2\mathbf{c}_i$	$2\mathbf{c}_R+\mathbf{c}_i$
$\mathbf{c}_R$			$6\mathbf{1}+3\mathbf{c}_r+2\mathbf{c}_\rho$	$3\mathbf{c}_r+4\mathbf{c}_\rho$
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Octahedral O characters

χ_g^μ	$\mathbf{g=1}$	$\mathbf{r}_{1\ldots4}$	$\boldsymbol{\rho}_{xyz}$	$\mathbf{R}_{xyz}$	$\mathbf{i}_{1\ldots6}$
χ^{A_1}	1	1	1	1	1
χ^{A_2}	1	1	1	−1	−1
χ^{E}	2	−1	2	0	0
χ^{T_1}	3	0	−1	1	−1
χ^{T_2}	3	0	−1	−1	1

AMOP reference links on page 2

3.05.18 class 15.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Discrete symmetry subgroups of O(3)⊃(Octahedral O_h⊃O~T_d, Cubic-Tetrahedral T_h⊃T): Characters and subgroup-chain defined ireps, and applications to SF_6 and CF_4 spectra

Review: *General all-commuting class-character-projector formula derivations.*

$\mathbb{P}^{\mu}$ *in* χ^{μ}*-terms of* $\boldsymbol{\kappa}_{\mathbf{g}}$ $\boldsymbol{\kappa}_{\mathbf{g}}$ *in* $\chi^{\mu *}$*-terms of* $\mathbb{P}^{\mu}$ *Irep frequency* f^{μ} *in* $\chi^{\mu *}$*-terms of* Trace$R(\mathbf{g})$

Introducing octahedral/ tetrahedral symmetry $O_h \supset O \sim T_d \supset T$ *: relating* $D_4 \supset C_4$ *and* $D_3 \supset C_3$

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$R(3) \subset O(3) \supset O_h \supset O$ *character analysis: Crystal field splitting* *p, d, f,…orbitals*

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Detailed superfine structure for $A_1 T_1 E$ *cluster* *preview of next lecture*

Octahedral $O_h \supset O$ subgroup correlations

χ^{μ}_{g}	$\mathbf{g=1}$	$\mathbf{r}_{1...4}$	$\boldsymbol{\rho}_{xyz}$	$\mathbf{R}_{xyz}$	$\mathbf{i}_{1...6}$
χ^{A_1}	1	1	1	1	1
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χ^{T_1}	3	0	−1	1	−1
χ^{T_2}	3	0	−1	−1	1

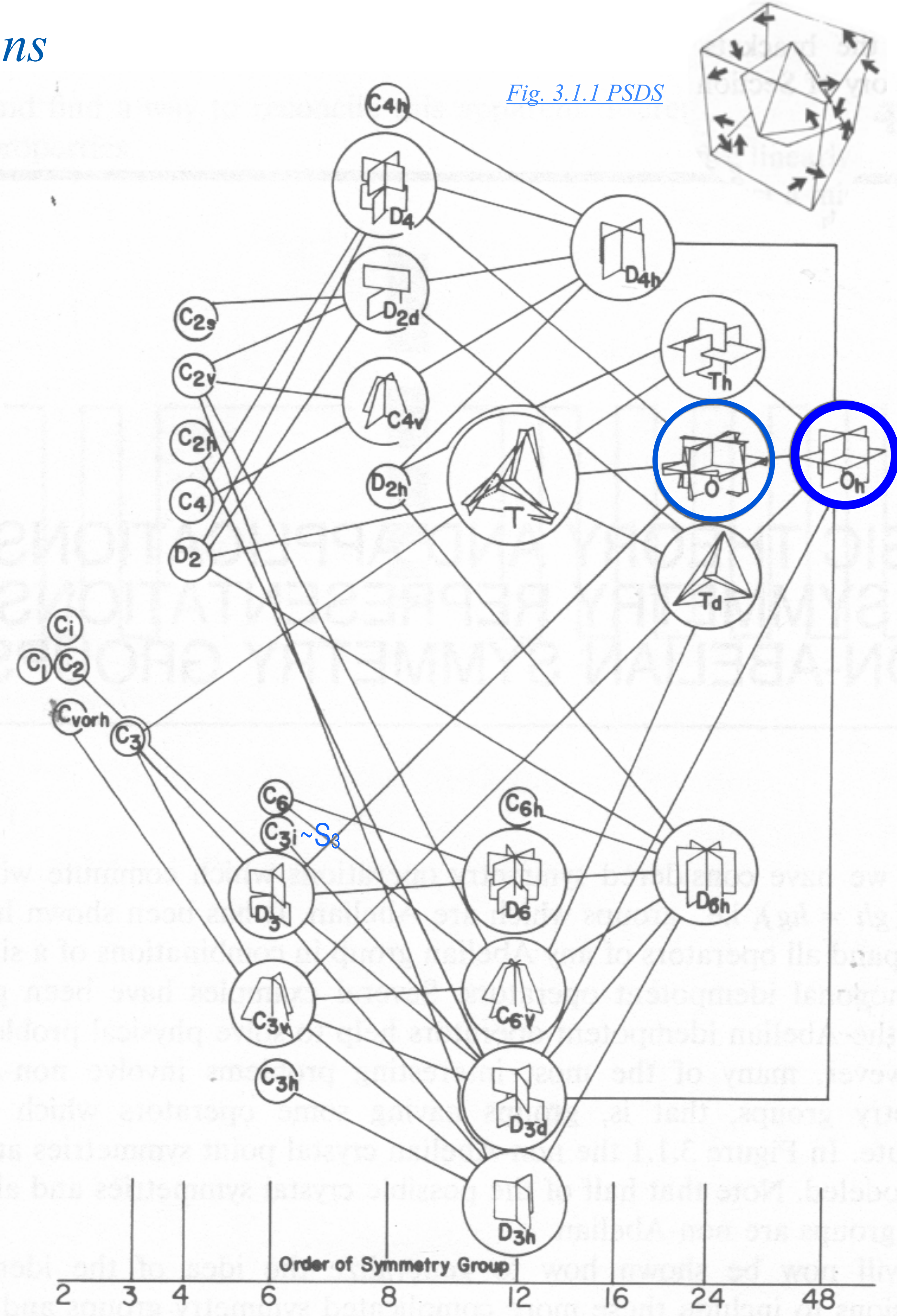

Fig. 3.1.1 PSDS

Octahedral $O_h \supset O$ subgroup correlations

$\chi_g^{\mu_p}$	$\mathbf{1}$	$\mathbf{r}_{1...4}$	$\boldsymbol{\rho}_{xyz}$	$\mathbf{R}_{xyz}$	$\mathbf{i}_{1...6}$	$\mathbf{I}$	$\mathbf{Ir}=$ $\mathbf{s}_{1...4}$	$\mathbf{I\rho}=$ $\boldsymbol{\sigma}_{xyz}$	$\mathbf{IR}=$ $\mathbf{S}_{xyz}$	$\mathbf{Ii}=$ $\boldsymbol{\sigma}_{1...6}$
$\chi^{A_{1g}}$	1	1	1	1	1	1	1	1	1	1
$\chi^{A_{2g}}$	1	1	1	−1	−1	1	1	1	−1	−1
χ^{E_g}	2	−1	2	0	0	2	−1	2	0	0
$\chi^{T_{1g}}$	3	0	−1	1	−1	3	0	−1	1	−1
$\chi^{T_{2g}}$	3	0	−1	−1	1	3	0	−1	−1	1
$\chi^{A_{1u}}$	1	1	1	1	1	−1	−1	−1	−1	−1
$\chi^{A_{2u}}$	1	1	1	−1	−1	−1	−1	−1	1	1
χ^{E_u}	2	−1	2	0	0	−2	1	−2	0	0
$\chi^{T_{1u}}$	3	0	−1	1	−1	−3	0	1	−1	1
$\chi^{T_{2u}}$	3	0	−1	−1	1	−3	0	1	1	−1

$O_h \supset O$	A_1	A_2	E	T_1	T_2
A_{1g}	1	·	·	·	·
A_{2g}	·	1	·	·	·
E_g	·	·	1	·	·
T_{1g}	·	·	·	1	·
T_{2g}	·	·	·	·	1
A_{1u}	1	·	·	·	·
A_{2u}	·	1	·	·	·
E_u	·	·	1	·	·
T_{1u}	·	·	·	1	·
T_{2u}	·	·	·	·	1

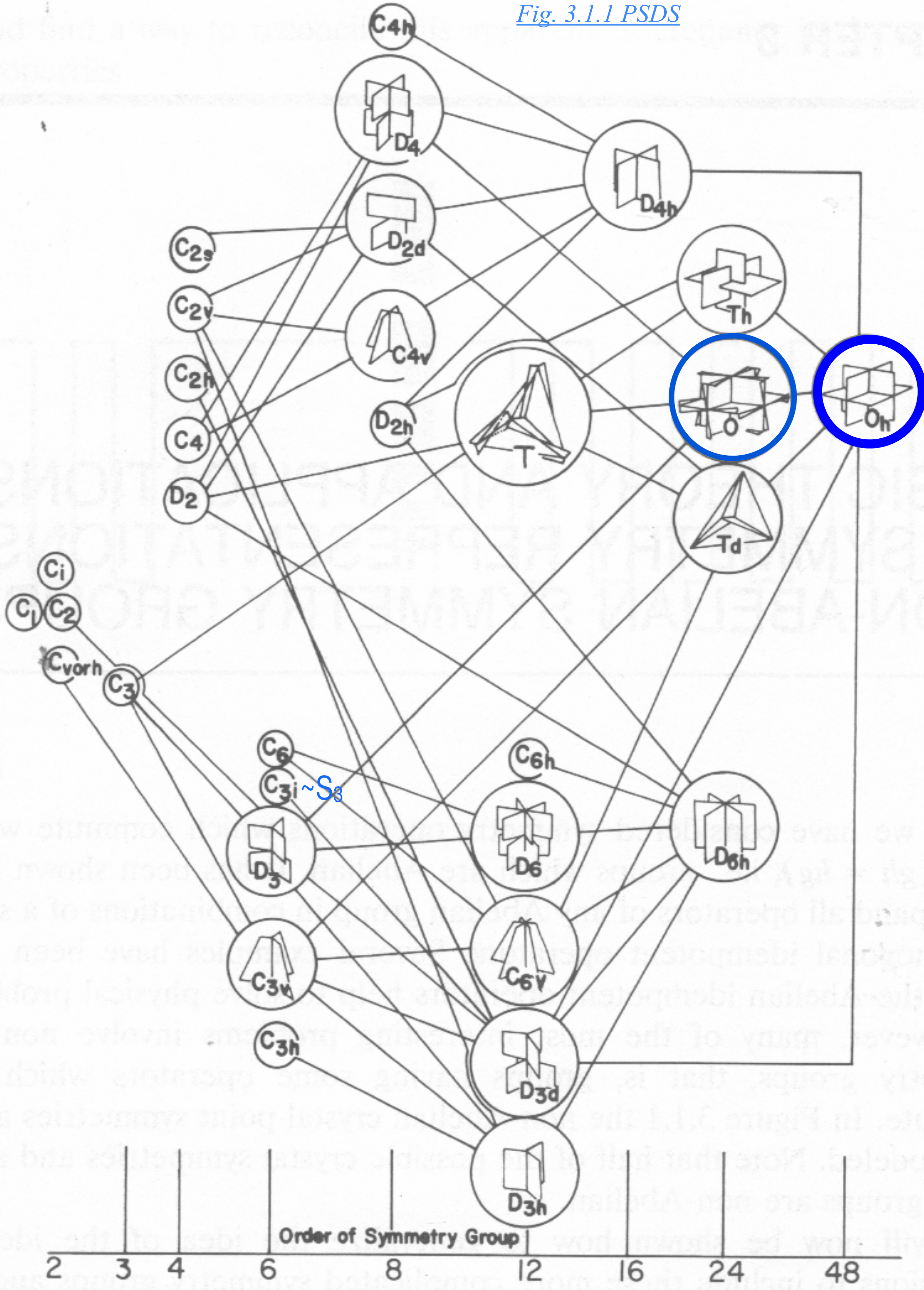

Fig. 3.1.1 PSDS

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Review: *General all-commuting class-character-projector formula derivations.* f^{μ} *derivation 2015 Lect15 p.40-45.*

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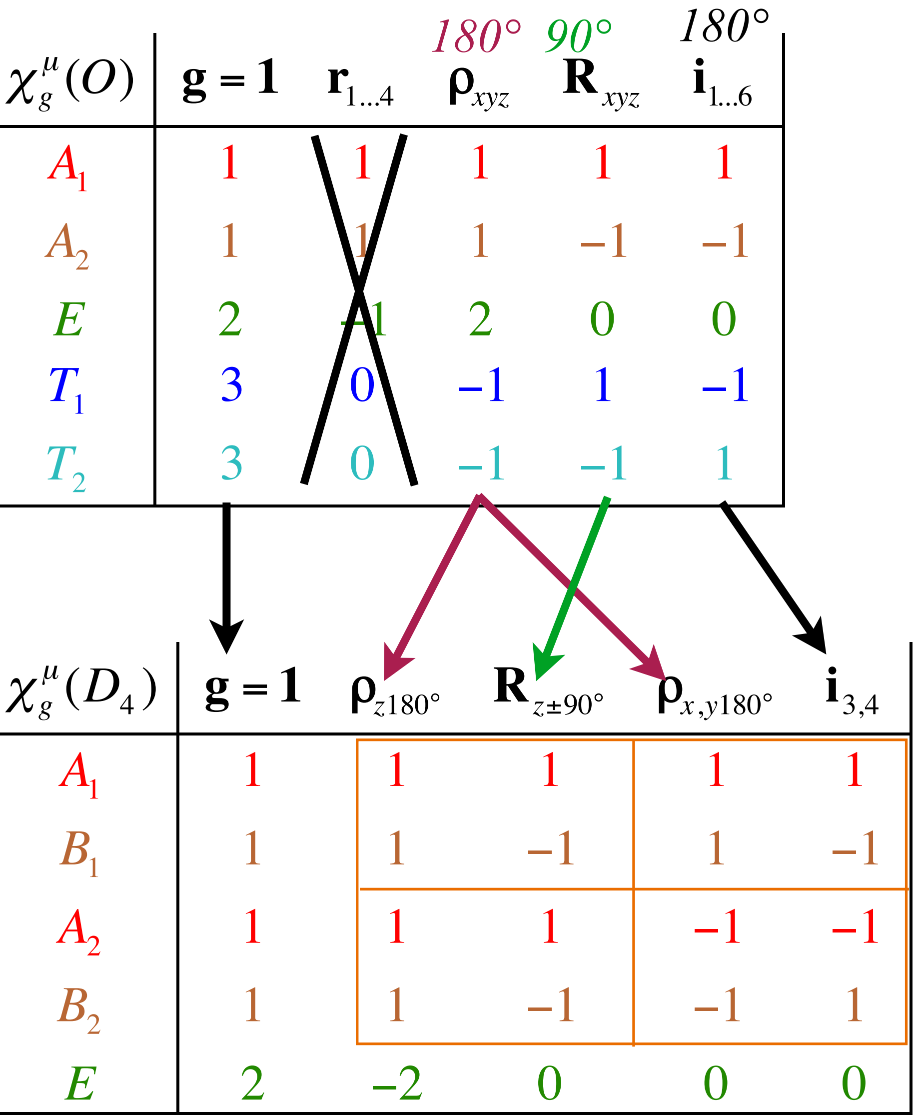
Detailed superfine structure for A_1T_1E *cluster* *preview of next lecture*

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

O↓D_4 subduction

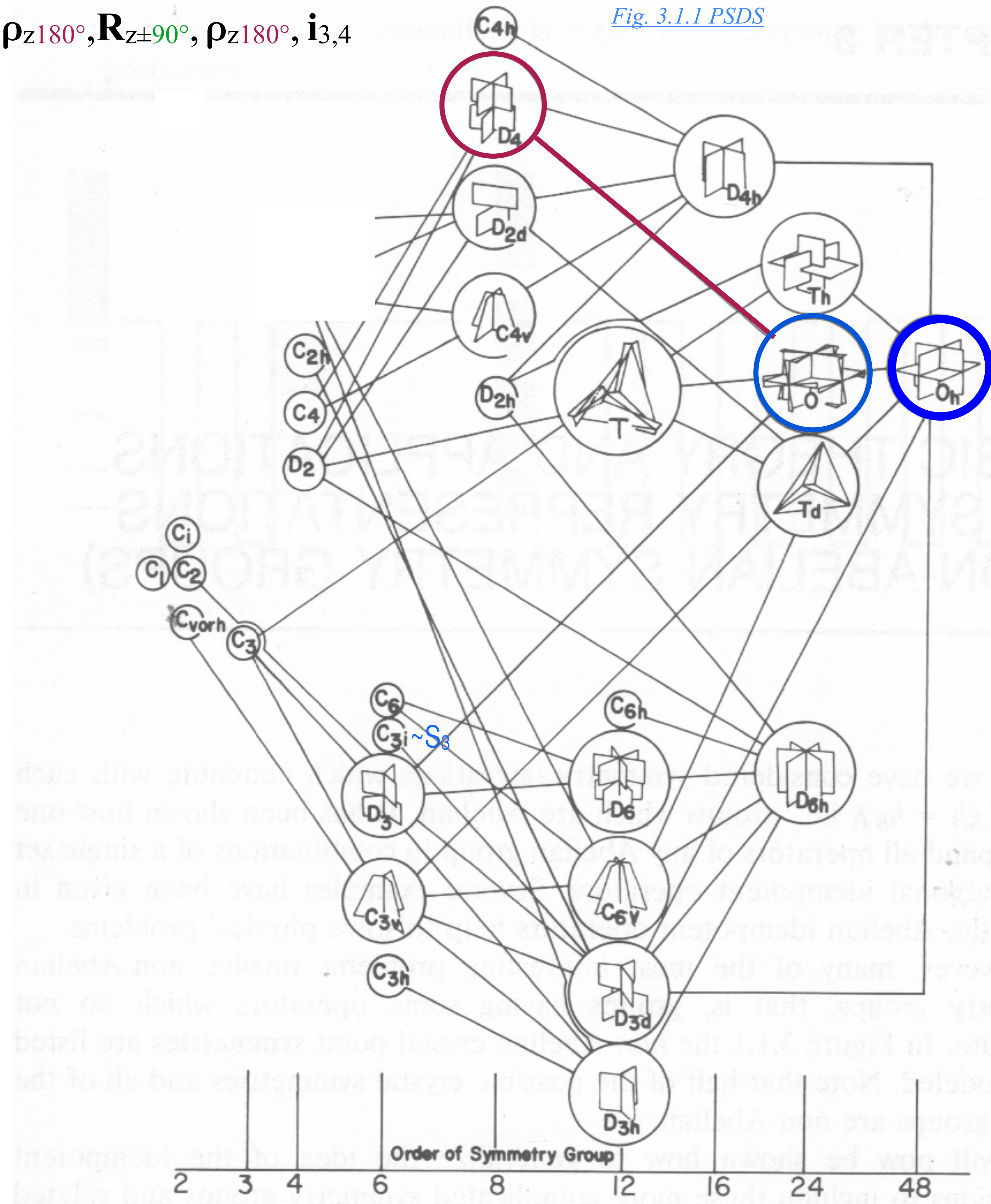
D_4: $\mathbf{1}, \boldsymbol{\rho}_{z180°}, \mathbf{R}_{z\pm 90°}, \boldsymbol{\rho}_{z180°}, \mathbf{i}_{3,4}$



$\chi^{\mu}_{g}(O)$	$\mathbf{g=1}$	~~$\mathbf{r}_{1\ldots4}$~~	180° $\boldsymbol{\rho}_{xyz}$	90° $\mathbf{R}_{xyz}$	180° $\mathbf{i}_{1\ldots6}$
A_1	1	~~1~~	1	1	1
A_2	1	~~1~~	1	−1	−1
E	2	~~−1~~	2	0	0
T_1	3	~~0~~	−1	1	−1
T_2	3	~~0~~	−1	−1	1

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

Fig. 3.1.1 PSDS



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

$O \downarrow D_4$ subduction

D_4: $\mathbf{1}, \rho_{z180°}, \mathbf{R}_{z\pm 90°}, \rho_{x,y180°}, \mathbf{i}_{3,4}$

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

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

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

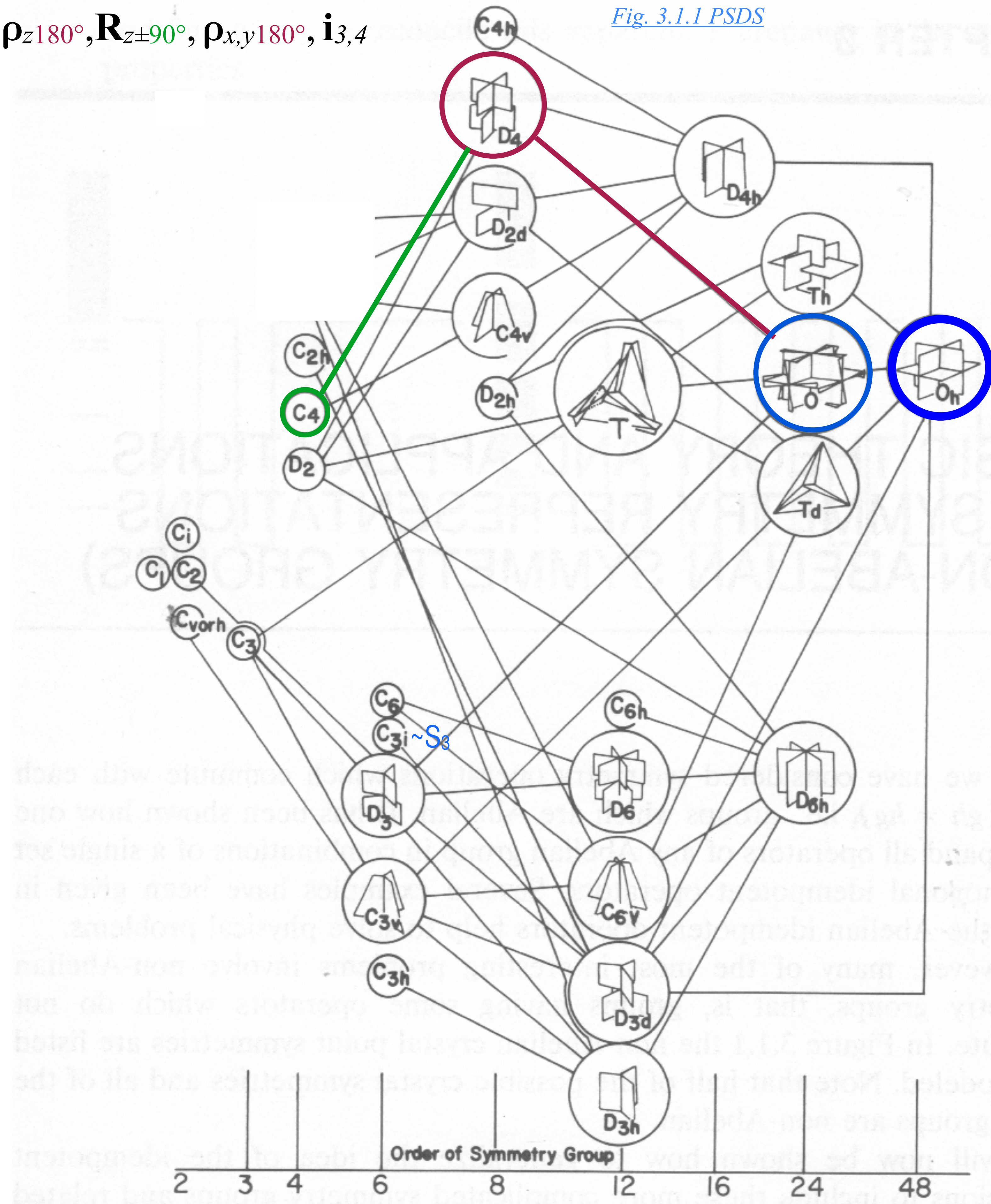


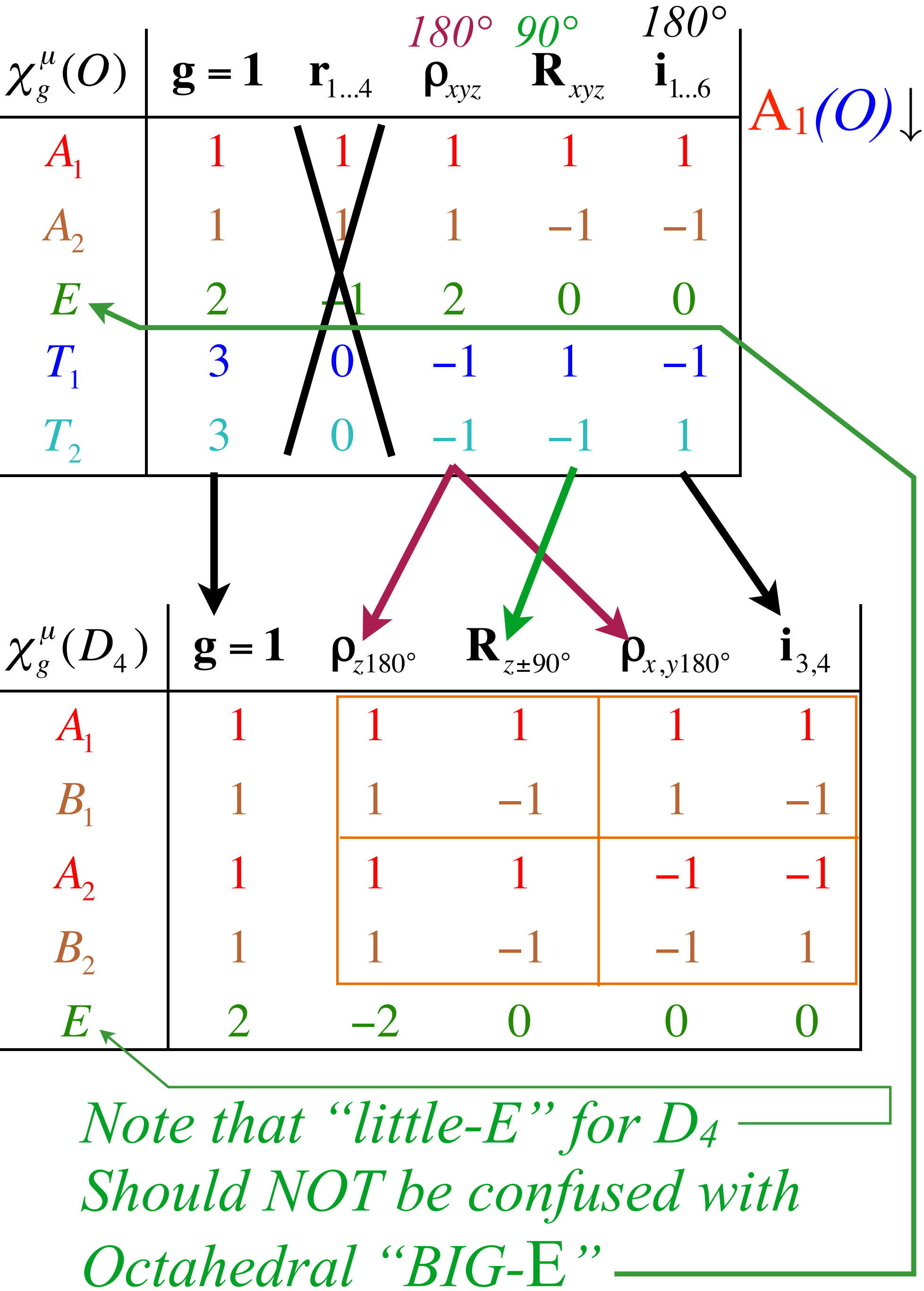
Fig. 3.1.1 PSDS

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

$O\downarrow D_4$ subduction

D_4: $\mathbf{1}, \rho_{z180°}, \mathbf{R}_{z\pm 90°}, \rho_{x,y180°}, \mathbf{i}_{3,4}$

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



$\chi_g^\mu(O)$	$\mathbf{g}=\mathbf{1}$	$\mathbf{r}_{1\ldots4}$	180° ρ_{xyz}	90° $\mathbf{R}_{xyz}$	180° $\mathbf{i}_{1\ldots6}$
A_1	1	~~1~~	1	1	1
A_2	1	~~1~~	1	−1	−1
E	2	~~−1~~	2	0	0
T_1	3	~~0~~	−1	1	−1
T_2	3	~~0~~	−1	−1	1

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

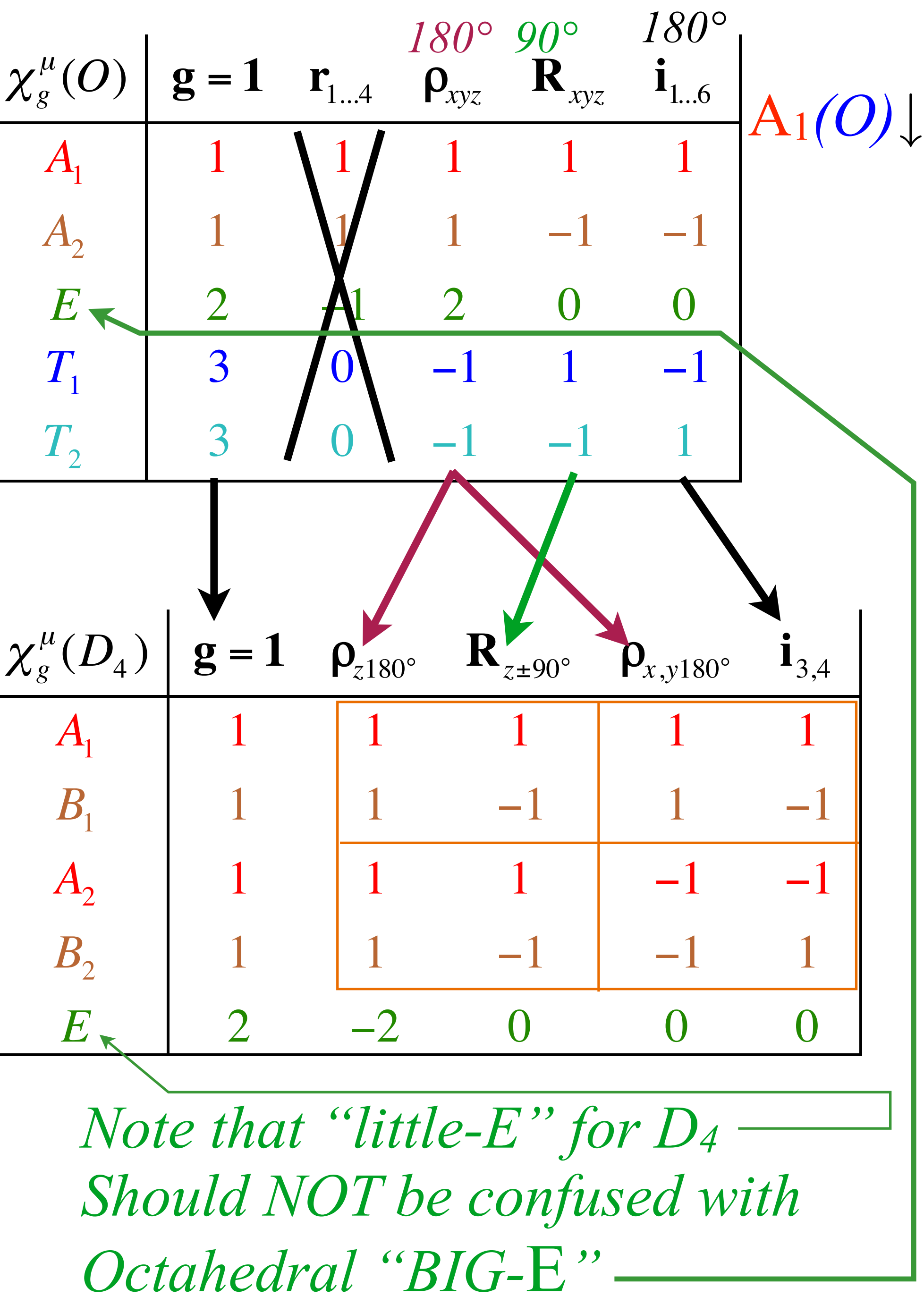
Note that "little-E" for D_4
Should NOT be confused with
Octahedral "BIG-E"

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

$O \downarrow D_4$ subduction

D_4: $\mathbf{1}, \rho_{z180°}, \mathbf{R}_{z\pm 90°}, \rho_{x,y180°}, \mathbf{i}_{3,4}$

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

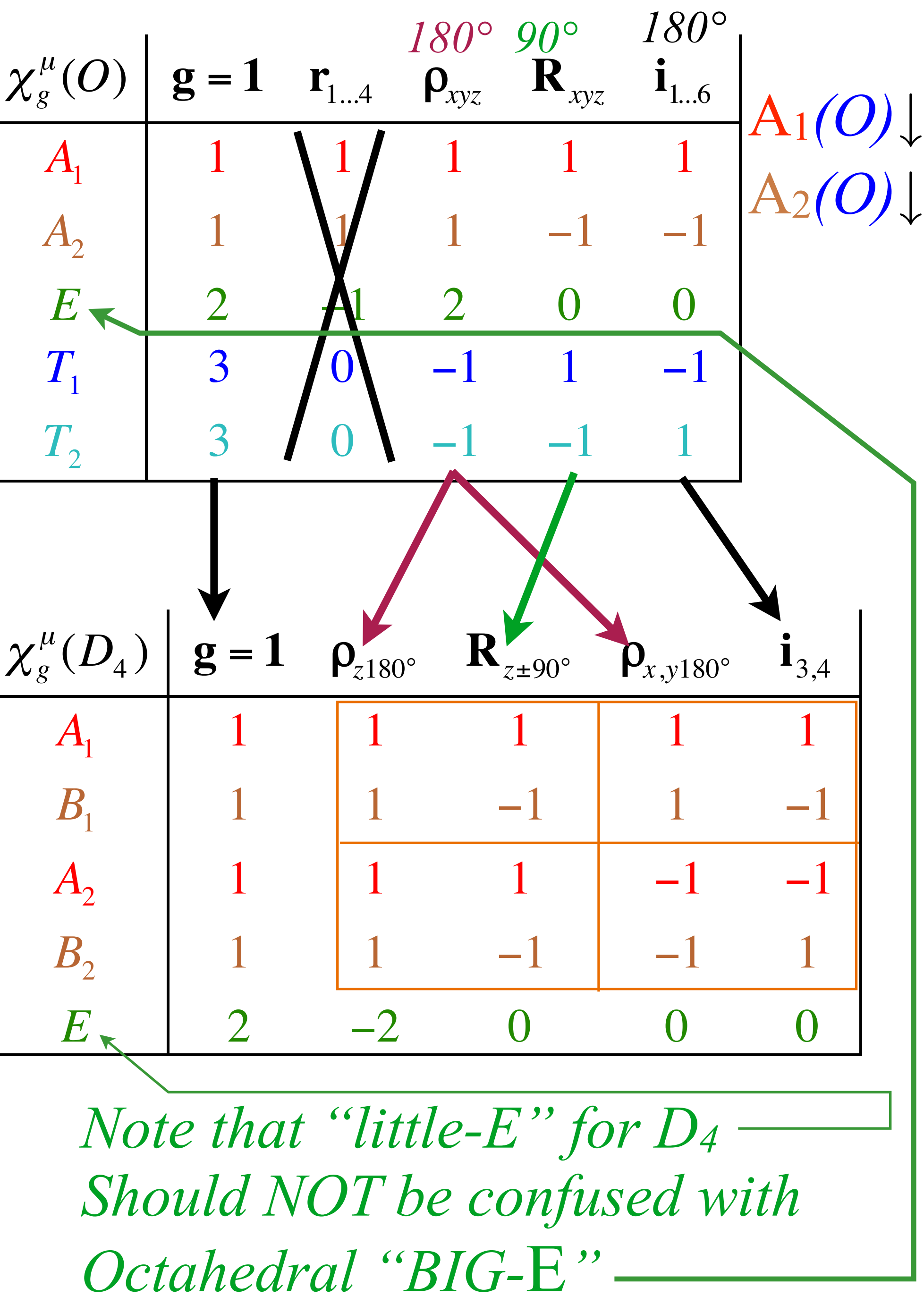


$\chi^{\mu}_{g}(O)$	$\mathbf{g=1}$	~~$\mathbf{r}_{1...4}$~~	180° ρ_{xyz}	90° $\mathbf{R}_{xyz}$	180° $\mathbf{i}_{1...6}$
A_1	1	~~1~~	1	1	1
A_2	1	~~1~~	1	−1	−1
E	2	~~−1~~	2	0	0
T_1	3	~~0~~	−1	1	−1
T_2	3	~~0~~	−1	−1	1

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

Note that "little-E" for D_4
Should NOT be confused with
Octahedral "BIG-E"

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



$\chi_g^\mu(O)$	$\mathbf{g=1}$	$\mathbf{r}_{1\ldots4}$	180° $\boldsymbol{\rho}_{xyz}$	90° $\mathbf{R}_{xyz}$	180° $\mathbf{i}_{1\ldots6}$
A_1	1	1	1	1	1
A_2	1	1	1	−1	−1
E	2	−1	2	0	0
T_1	3	0	−1	1	−1
T_2	3	0	−1	−1	1

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

Note that "little-E" for D_4
Should NOT be confused with
Octahedral "BIG-E"

$O{\downarrow}D_4$ *subduction*

D_4: $\mathbf{1}, \boldsymbol{\rho}_{z180°}, \mathbf{R}_{z\pm90°}, \boldsymbol{\rho}_{x,y180°}, \mathbf{i}_{3,4}$

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

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

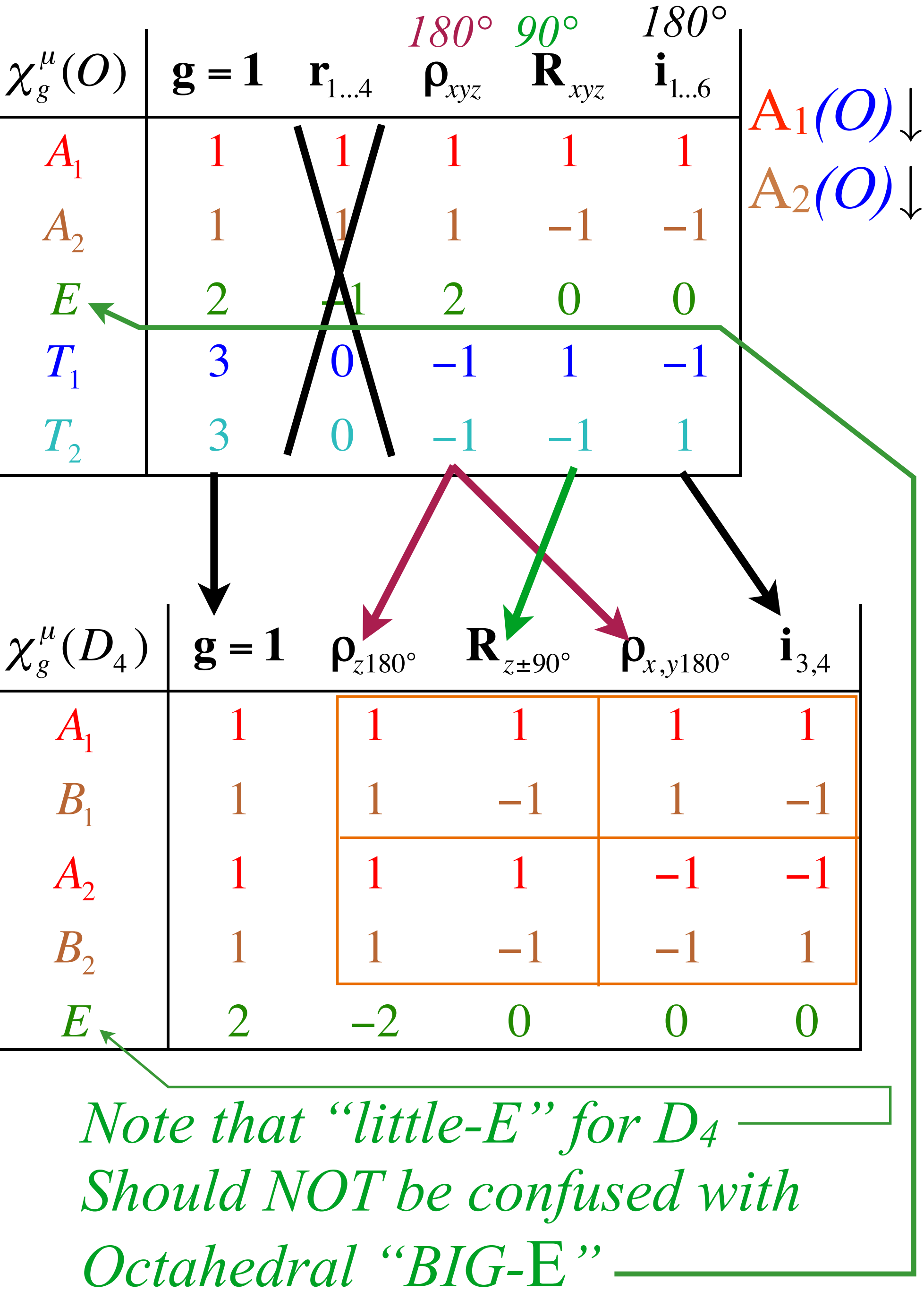
Octahedral $O_h \supset O \supset D_4 \supset C_4$ subgroup correlations

$O \downarrow D_4$ subduction

D_4: $\mathbf{1}, \rho_{z180°}, \mathbf{R}_{z\pm 90°}, \rho_{x,y180°}, \mathbf{i}_{3,4}$

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

$A_2(O) \downarrow D_4 = 1, \quad 1, \quad -1, \quad 1, \quad -1\ .\quad A_2(O) \downarrow D_4 = B_1(D_4)$

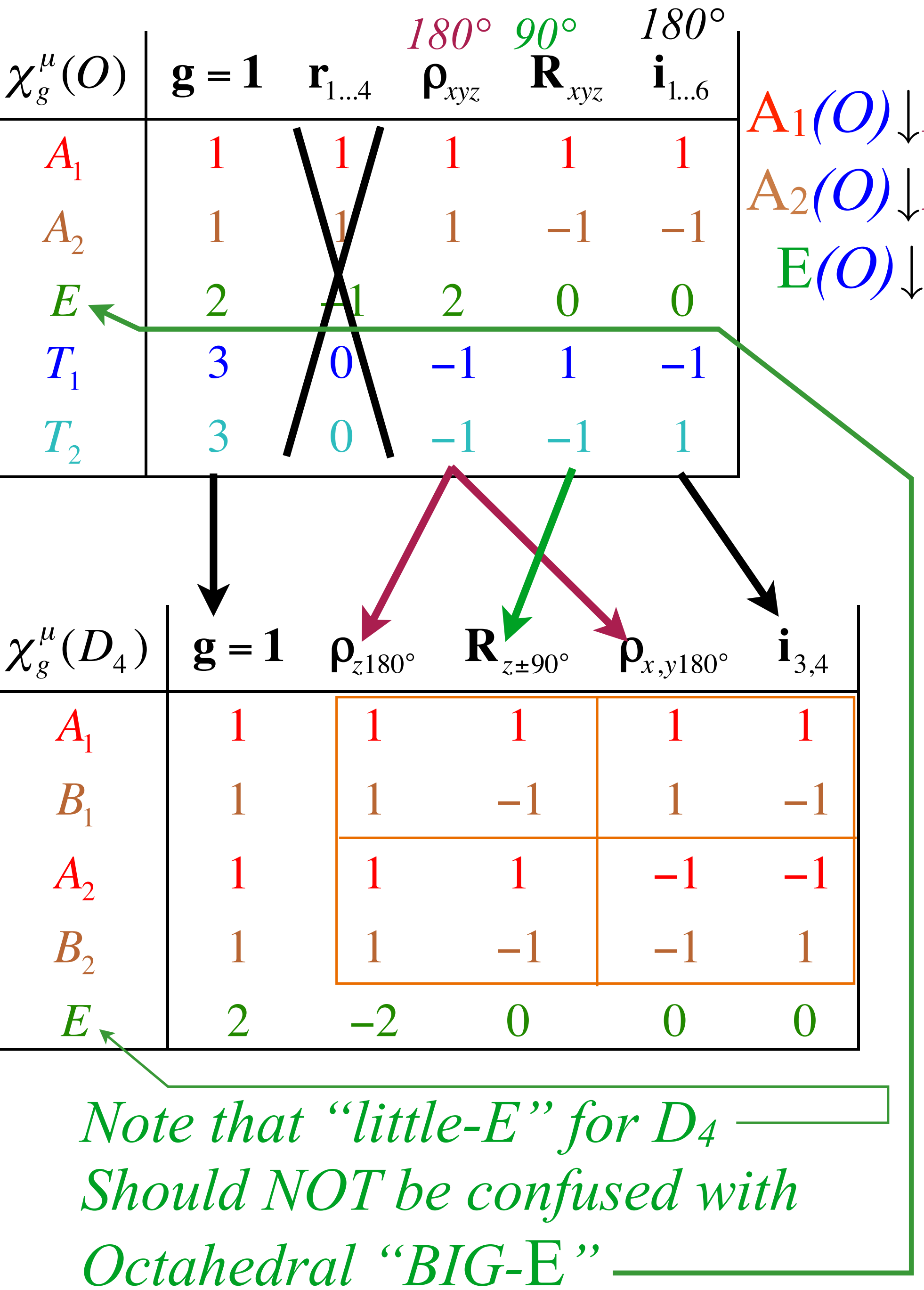


$\chi_g^\mu(O)$	$\mathbf{g}=\mathbf{1}$	$\mathbf{r}_{1\ldots4}$	180° ρ_{xyz}	90° $\mathbf{R}_{xyz}$	180° $\mathbf{i}_{1\ldots6}$
A_1	1	1	1	1	1
A_2	1	1	1	−1	−1
E	2	−1	2	0	0
T_1	3	0	−1	1	−1
T_2	3	0	−1	−1	1

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

Note that "little-E" for D_4
Should NOT be confused with
Octahedral "BIG-E"

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



$\chi^{\mu}_{g}(O)$	$\mathbf{g=1}$	$\mathbf{r}_{1\ldots4}$	180° $\boldsymbol{\rho}_{xyz}$	90° $\mathbf{R}_{xyz}$	180° $\mathbf{i}_{1\ldots6}$
A_1	1	~~1~~	1	1	1
A_2	1	~~1~~	1	−1	−1
E	2	~~−1~~	2	0	0
T_1	3	~~0~~	−1	1	−1
T_2	3	~~0~~	−1	−1	1

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

Note that "little-E" for D_4
Should NOT be confused with
Octahedral "BIG-E"

$O{\downarrow}D_4$ *subduction*

D_4: $\mathbf{1}, \boldsymbol{\rho}_{z180°}, \mathbf{R}_{z\pm90°}, \boldsymbol{\rho}_{x,y180°}, \mathbf{i}_{3,4}$

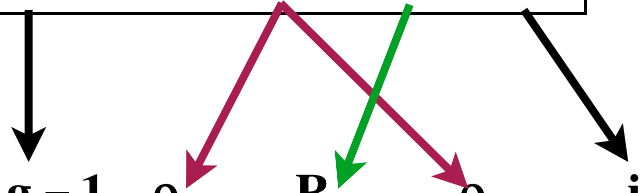
$A_1(O){\downarrow}D_4 = 1,\ 1,\ 1,\ 1,\ 1\ .\quad A_1(O){\downarrow}D_4 = A_1(D_4)$

$A_2(O){\downarrow}D_4 = 1,\ 1,\ -1,\ 1,\ -1\ .\quad A_2(O){\downarrow}D_4 = B_1(D_4)$

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

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

$\chi^{\mu}_{g}(O)$	$\mathbf{g=1}$	$\mathbf{r}_{1\ldots4}$	180° $\boldsymbol{\rho}_{xyz}$	90° $\mathbf{R}_{xyz}$	180° $\mathbf{i}_{1\ldots6}$
A_1	1	1	1	1	1
A_2	1	1	1	−1	−1
E	2	−1	2	0	0
T_1	3	0	−1	1	−1
T_2	3	0	−1	−1	1



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

$O{\downarrow}D_4$ subduction

D_4: $\mathbf{1}, \boldsymbol{\rho}_{z180°}, \mathbf{R}_{z\pm90°}, \boldsymbol{\rho}_{x,y180°}, \mathbf{i}_{3,4}$

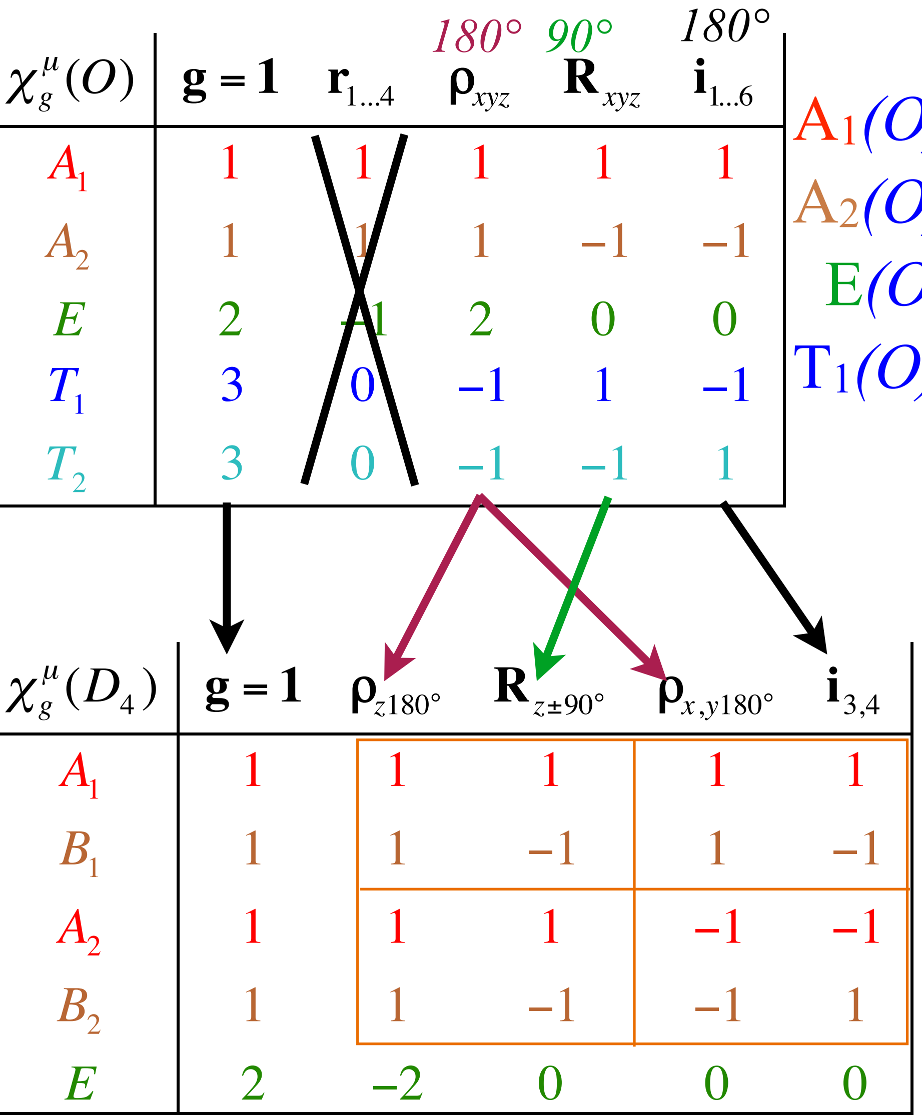
$A_1(O){\downarrow}D_4 = 1,\quad 1,\quad 1,\quad 1,\quad 1\ .$ $A_1(O){\downarrow}D_4 = A_1(D_4)$

$A_2(O){\downarrow}D_4 = 1,\quad 1,\quad -1,\quad 1,\quad -1\ .$ $A_2(O){\downarrow}D_4 = B_1(D_4)$

$E(O){\downarrow}D_4 = 2,\quad 2,\quad 0,\quad 2,\quad 0\ .$ $E(O){\downarrow}D_4 = A_1 \oplus B_1(D_4)$

Note that "little-E" for D₄
Should NOT be confused with
*Octahedral "BIG-*E*"*

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



			180°	90°	180°
$\chi_g^\mu(O)$	$\mathbf{g=1}$	$\mathbf{r}_{1\ldots4}$	$\boldsymbol{\rho}_{xyz}$	$\mathbf{R}_{xyz}$	$\mathbf{i}_{1\ldots6}$
A_1	1	1	1	1	1
A_2	1	1	1	−1	−1
E	2	−1	2	0	0
T_1	3	0	−1	1	−1
T_2	3	0	−1	−1	1

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

$O\downarrow D_4$ subduction

D_4: $\mathbf{1}, \boldsymbol{\rho}_{z180°}, \mathbf{R}_{z\pm90°}, \boldsymbol{\rho}_{x,y180°}, \mathbf{i}_{3,4}$

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

$A_2(O)\downarrow D_4 = 1,\ 1,\ -1,\ 1,\ -1\ .$ $A_2(O)\downarrow D_4 = B_1(D_4)$

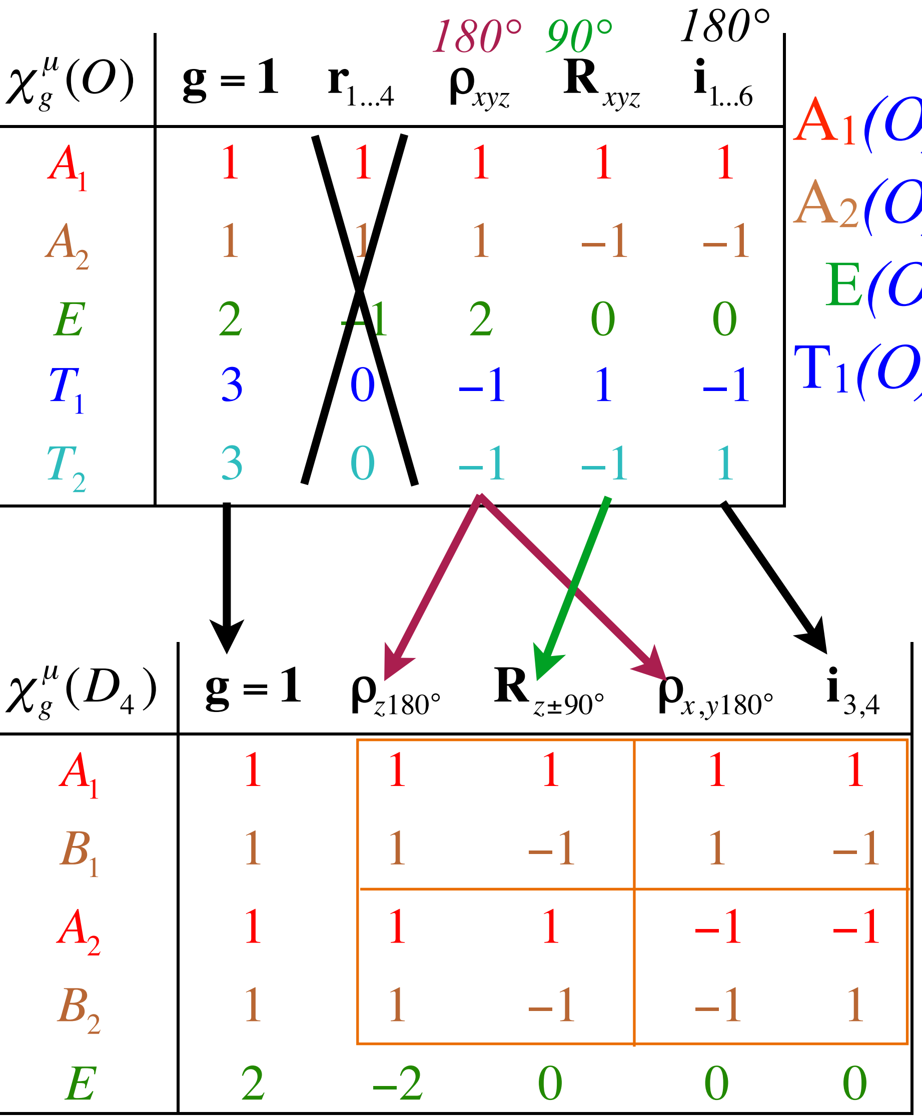
$E(O)\downarrow D_4 = 2,\ 2,\ 0,\ 2,\ 0\ .$ $E(O)\downarrow D_4 = A_1 \oplus B_1(D_4)$

$T_1(O)\downarrow D_4 = 3,\ -1,\ 1,\ -1,\ -1\ .$

Note that "little-E" for D_4
Should NOT be confused with
Octahedral "BIG-E"

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

$O \downarrow D_4$ subduction



$\chi^{\mu}_{g}(O)$	$\mathbf{g=1}$	$\mathbf{r}_{1\ldots4}$	180° $\boldsymbol{\rho}_{xyz}$	90° $\mathbf{R}_{xyz}$	180° $\mathbf{i}_{1\ldots6}$
A_1	1	1	1	1	1
A_2	1	1	1	−1	−1
E	2	−1	2	0	0
T_1	3	0	−1	1	−1
T_2	3	0	−1	−1	1

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

D_4: $\mathbf{1}, \boldsymbol{\rho}_{z180°}, \mathbf{R}_{z\pm90°}, \boldsymbol{\rho}_{x,y180°}, \mathbf{i}_{3,4}$

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

$A_2(O)\downarrow D_4 = 1,\ 1,\ -1,\ 1,\ -1\ .$ $A_2(O)\downarrow D_4 = B_1(D_4)$

$E(O)\downarrow D_4 = 2,\ 2,\ 0,\ 2,\ 0\ .$ $E(O)\downarrow D_4 = A_1 \oplus B_1(D_4)$

$T_1(O)\downarrow D_4 = 3,\ -1,\ 1,\ -1,\ -1\ .$ $T_1(O)\downarrow D_4 = E \oplus A_2(D_4)$

Note that "little-E" for D_4
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Octahedral "BIG-E"

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

$O \downarrow D_4$ subduction

D_4: $\mathbf{1}, \boldsymbol{\rho}_{z180°}, \mathbf{R}_{z\pm 90°}, \boldsymbol{\rho}_{x,y180°}, \mathbf{i}_{3,4}$

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

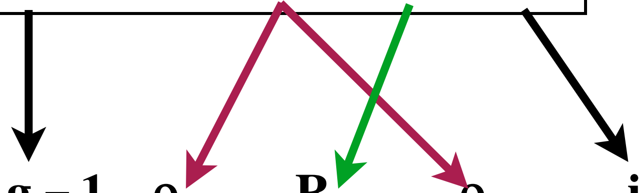
$A_2(O)\downarrow D_4 = 1, \quad 1, \quad -1, \quad 1, \quad -1 .$ $\quad A_2(O)\downarrow D_4 = B_1(D_4)$

$E(O)\downarrow D_4 = 2, \quad 2, \quad 0, \quad 2, \quad 0 .$ $\quad E(O)\downarrow D_4 = A_1 \oplus B_1(D_4)$

$T_1(O)\downarrow D_4 = 3, \quad -1, \quad 1, \quad -1, \quad -1 .$ $\quad T_1(O)\downarrow D_4 = E \oplus A_2(D_4)$

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

$\chi_g^\mu(O)$	$\mathbf{g}=\mathbf{1}$	$\mathbf{r}_{1\ldots4}$	180° $\boldsymbol{\rho}_{xyz}$	90° $\mathbf{R}_{xyz}$	180° $\mathbf{i}_{1\ldots6}$
A_1	1	~~1~~	1	1	1
A_2	1	~~1~~	1	−1	−1
E	2	~~−1~~	2	0	0
T_1	3	~~0~~	−1	1	−1
T_2	3	~~0~~	−1	−1	1



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

Note that "little-E" for D_4
Should NOT be confused with
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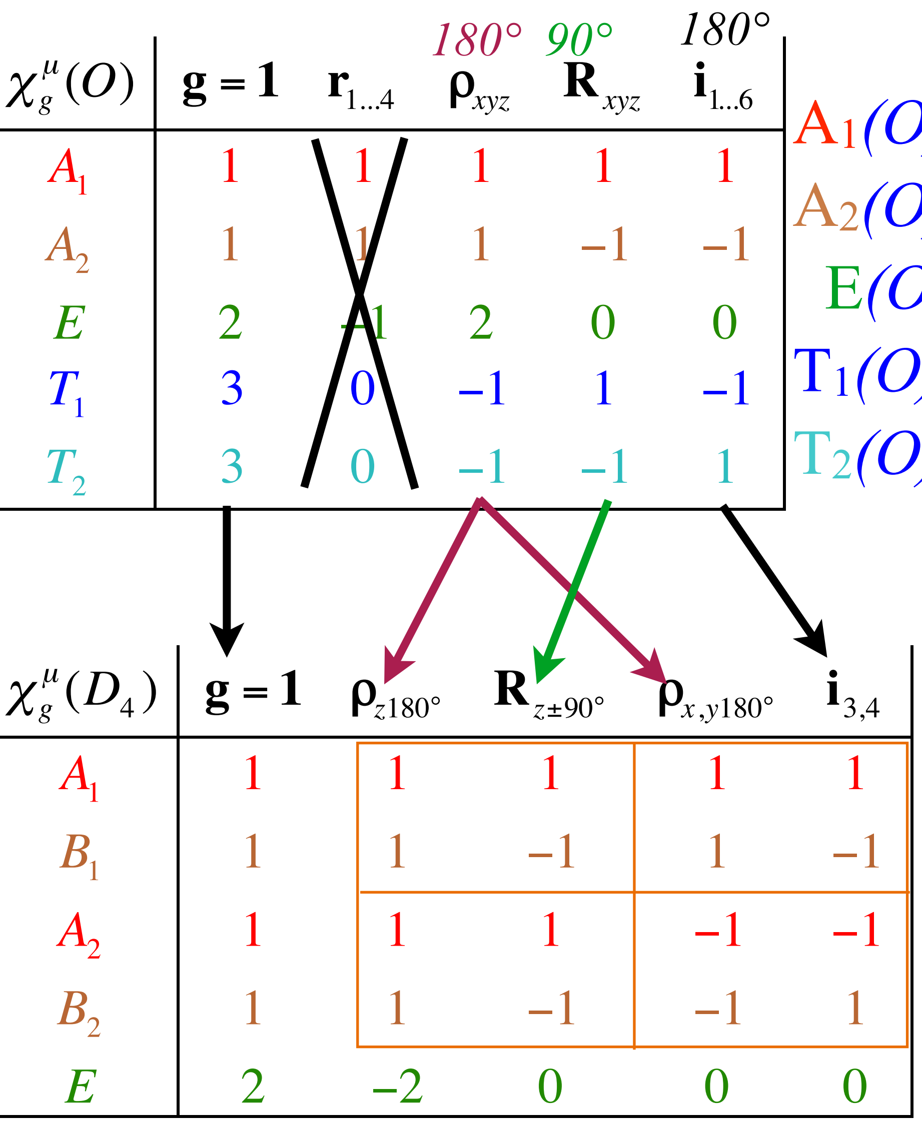
Octahedral $O_h \supset O \supset D_4 \supset C_4$ subgroup correlations



$\chi_g^\mu(O)$	$\mathbf{g=1}$	~~$\mathbf{r}_{1\ldots4}$~~	180° $\boldsymbol{\rho}_{xyz}$	90° $\mathbf{R}_{xyz}$	180° $\mathbf{i}_{1\ldots6}$
A_1	1	~~1~~	1	1	1
A_2	1	~~1~~	1	−1	−1
E	2	~~−1~~	2	0	0
T_1	3	~~0~~	−1	1	−1
T_2	3	~~0~~	−1	−1	1

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

Note that "little-E" for D_4
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Octahedral "BIG-E"

$O{\downarrow}D_4$ subduction

D_4: $\mathbf{1}, \boldsymbol{\rho}_{z180°}, \mathbf{R}_{z\pm90°}, \boldsymbol{\rho}_{x,y180°}, \mathbf{i}_{3,4}$

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

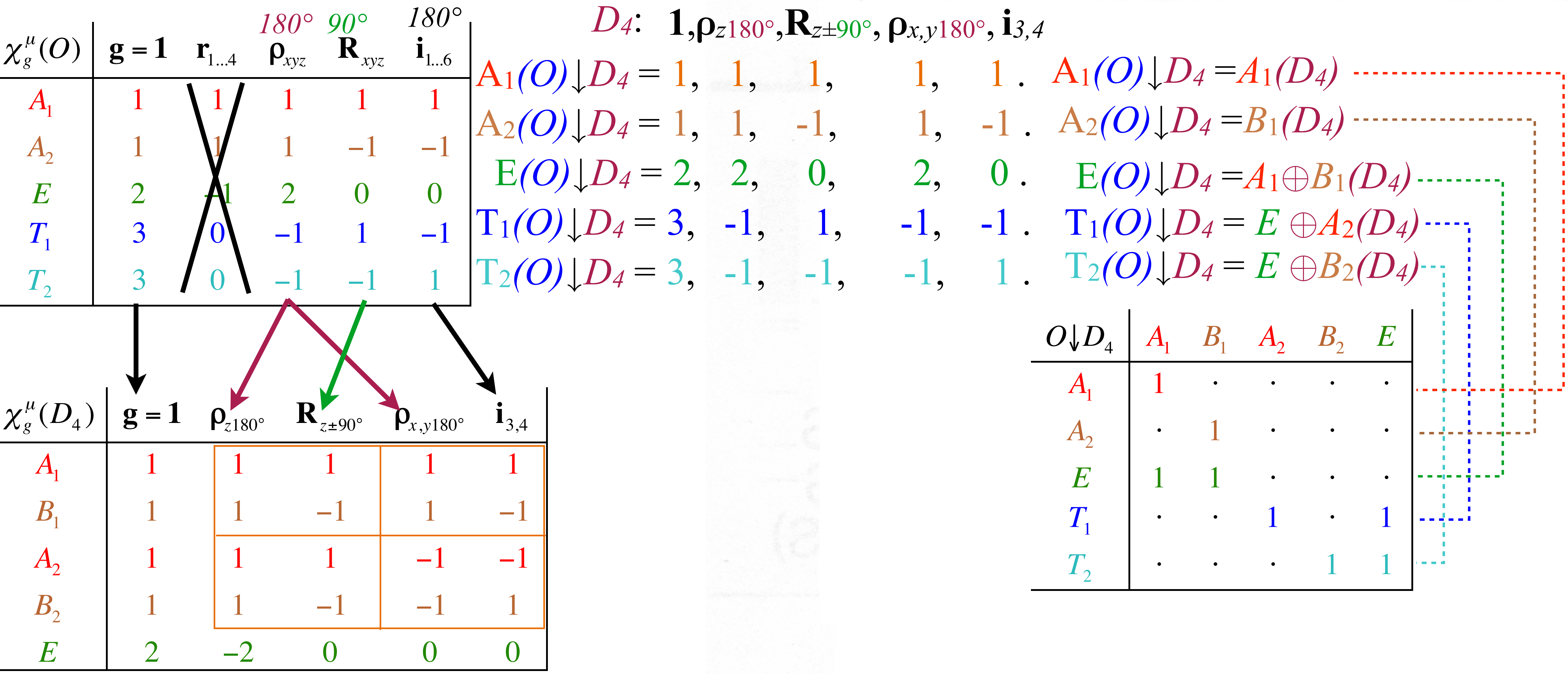
$A_2(O){\downarrow}D_4 = 1,\ 1,\ -1,\ 1,\ -1\ .$ $A_2(O){\downarrow}D_4 = B_1(D_4)$

$E(O){\downarrow}D_4 = 2,\ 2,\ 0,\ 2,\ 0\ .$ $E(O){\downarrow}D_4 = A_1 \oplus B_1(D_4)$

$T_1(O){\downarrow}D_4 = 3,\ -1,\ 1,\ -1,\ -1\ .$ $T_1(O){\downarrow}D_4 = E \oplus A_2(D_4)$

$T_2(O){\downarrow}D_4 = 3,\ -1,\ -1,\ -1,\ 1\ .$ $T_2(O){\downarrow}D_4 = E \oplus B_2(D_4)$

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



$O\downarrow D_4$ subduction

D_4: $\mathbf{1}, \boldsymbol{\rho}_{z180°}, \mathbf{R}_{z\pm 90°}, \boldsymbol{\rho}_{x,y180°}, \mathbf{i}_{3,4}$

$\chi^{\mu}_{g}(O)$	$\mathbf{g}=\mathbf{1}$	$\mathbf{r}_{1\ldots4}$	180° $\boldsymbol{\rho}_{xyz}$	90° $\mathbf{R}_{xyz}$	180° $\mathbf{i}_{1\ldots6}$
A_1	1	1	1	1	1
A_2	1	1	1	−1	−1
E	2	−1	2	0	0
T_1	3	0	−1	1	−1
T_2	3	0	−1	−1	1

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

$A_2(O)\downarrow D_4 = 1, \; 1, \; -1, \; 1, \; -1 \,.$ $\quad A_2(O)\downarrow D_4 = B_1(D_4)$

$E(O)\downarrow D_4 = 2, \; 2, \; 0, \; 2, \; 0 \,.$ $\quad E(O)\downarrow D_4 = A_1 \oplus B_1(D_4)$

$T_1(O)\downarrow D_4 = 3, \; -1, \; 1, \; -1, \; -1 \,.$ $\quad T_1(O)\downarrow D_4 = E \oplus A_2(D_4)$

$T_2(O)\downarrow D_4 = 3, \; -1, \; -1, \; -1, \; 1 \,.$ $\quad T_2(O)\downarrow D_4 = E \oplus B_2(D_4)$

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

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

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Should NOT be confused with
Octahedral "BIG-E"

AMOP reference links on page 2

3.05.18 class 15.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Discrete symmetry subgroups of $O(3)\supset$(Octahedral $O_h\supset O\sim T_d$, Cubic-Tetrahedral $T_h\supset T$): Characters and subgroup-chain defined ireps, and applications to SF_6 and CF_4 spectra

Review: *General all-commuting class-character-projector formula derivations.* *f^μ derivation 2015 Lect15 p.40-45.*

$\mathbb{P}^\mu$ in χ^μ-terms of $\boldsymbol{\kappa}_\mathbf{g}$ *$\boldsymbol{\kappa}_\mathbf{g}$ in $\chi^{\mu *}$-terms of $\mathbb{P}^\mu$* *Irep frequency f^μ in $\chi^{\mu *}$-terms of Trace$R(\mathbf{g})$*

Introducing octahedral/ tetrahedral symmetry $O_h\supset O\sim T_d\supset T$: relating $D_4\supset C_4$ and $D_3\supset C_3$

Octahedral-cubic O symmetry and group operations, *O slide-rule*

Tetrahedral symmetry leads to Icosahedral

Octahedral groups $O_h\supset O\sim T_d\supset T$ and its large subgroups. *O_h slide-rule*

Octahedral O and spin-$O\subset U(2)$ nomograms

Tetrahedral T class algebra *minimal equations* *centrum projectors and characters*

Octahedral O class algebra *minimal equations* *centrum projectors and characters*

Characters of full Octahedral symmetry $O_h=O\times C_\mathbf{I}=O\times\{\mathbf{1},\mathbf{I}\}$

Octahedral $O_h\supset O\supset C_\mathbf{I}$ subgroup correlations

➡ *Octahedral subgroup correlation* ➡ *$O_h\supset O\supset D_4$* *$O_h\supset O\supset D_4\supset C_4$* ➡ *and level-splitting*

Comparing $O\supset C_4$ and $O\supset C_3$ and $O\supset C_2$

$R(3)\subset O(3)\supset O_h\supset O$ character analysis: Crystal field splitting *p, d, f,…orbitals*

Cluster structure in SF_6 16um spectra. *Analogy with D_6 band gap structure*

Global vs Local *External LAB splitting vs Internal BODY clustering*

Detailed superfine structure for A_1T_1E cluster *preview of next lecture*

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

$O{\downarrow}D_4$ subduction

D_4: $\mathbf{1}, \boldsymbol{\rho}_{z180°}, \mathbf{R}_{z\pm 90°}, \boldsymbol{\rho}_{x,y180°}, \mathbf{i}_{3,4}$

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

$A_2(O){\downarrow}D_4 = 1,\ \ 1,\ \ -1,\ \ 1,\ \ -1\ .$ $\quad A_2(O){\downarrow}D_4 = B_1(D_4)$

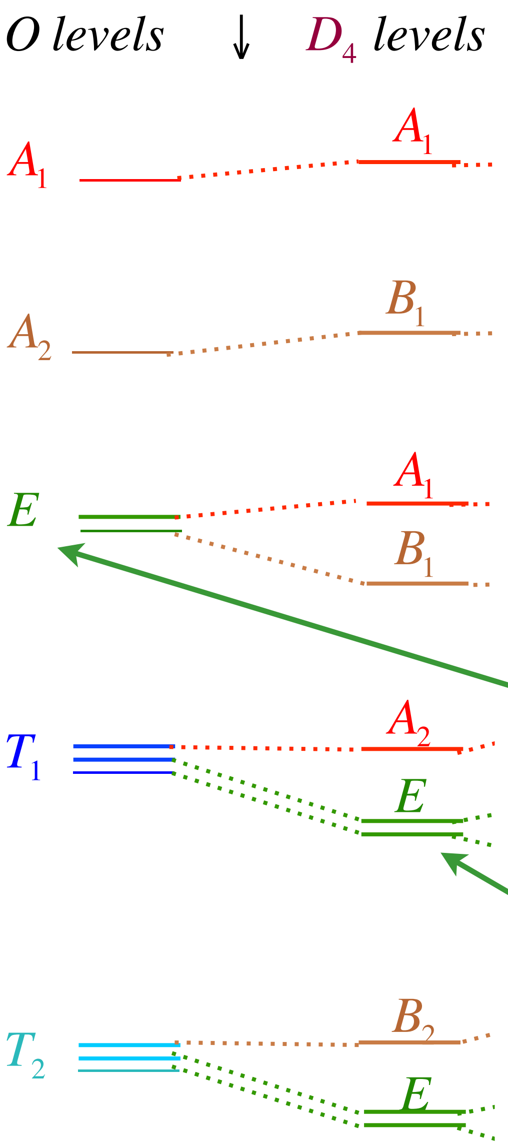
$E(O){\downarrow}D_4 = 2,\ \ 2,\ \ 0,\ \ 2,\ \ 0\ .$ $\quad E(O){\downarrow}D_4 = A_1 \oplus B_1(D_4)$

$T_1(O){\downarrow}D_4 = 3,\ \ -1,\ \ 1,\ \ -1,\ \ -1\ .$ $\quad T_1(O){\downarrow}D_4 = E \oplus A_2(D_4)$

$T_2(O){\downarrow}D_4 = 3,\ \ -1,\ \ -1,\ \ -1,\ \ 1\ .$ $\quad T_2(O){\downarrow}D_4 = E \oplus B_2(D_4)$

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

$O \supset D_4 \supset C_4$ subgroup and level-splitting/relabeling correlations



Note that "BIG-E" for O is NOT to be confused with "little-E" for D_4

AMOP reference links on page 2

3.05.18 class 15.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Discrete symmetry subgroups of O(3)⊃(Octahedral O_h⊃O~T_d, Cubic-Tetrahedral T_h⊃T): Characters and subgroup-chain defined ireps, and applications to SF_6 and CF_4 spectra

Review: *General all-commuting class-character-projector formula derivations.* *f^μ derivation 2015 Lect15 p.40-45.*

$\mathbb{P}^\mu$ in χ^μ-terms of $\boldsymbol{\kappa}_\mathbf{g}$ *$\boldsymbol{\kappa}_\mathbf{g}$ in $\chi^{\mu*}$-terms of $\mathbb{P}^\mu$* *Irep frequency f^μ in $\chi^{\mu*}$-terms of Trace$R(\mathbf{g})$*

Introducing octahedral/ tetrahedral symmetry $O_h \supset O \sim T_d \supset T$: relating $D_4 \supset C_4$ and $D_3 \supset C_3$

Octahedral-cubic O symmetry and group operations, *O slide-rule*

Tetrahedral symmetry leads to Icosahedral

Octahedral groups $O_h \supset O \sim T_d \supset T$ and its large subgroups. *O_h slide-rule*

Octahedral O and spin-$O \subset U(2)$ nomograms

Tetrahedral T class algebra *minimal equations* *centrum projectors and characters*

Octahedral O class algebra *minimal equations* *centrum projectors and characters*

Characters of full Octahedral symmetry $O_h = O \times C_\mathbf{I} = O \times \{\mathbf{1},\mathbf{I}\}$

Octahedral $O_h \supset O \supset C_\mathbf{I}$ subgroup correlations

Octahedral subgroup correlation *$O_h \supset O \supset D_4$ → $O_h \supset O \supset D_4 \supset C_4$* *and level-splitting*

Comparing $O \supset C_4$ and $O \supset C_3$ and $O \supset C_2$

$R(3) \subset O(3) \supset O_h \supset O$ character analysis: Crystal field splitting *p, d, f,…orbitals*

Cluster structure in SF_6 16um spectra. *Analogy with D_6 band gap structure*

Global vs Local *External LAB splitting vs Internal BODY clustering*

Detailed superfine structure for A_1T_1E cluster *preview of next lecture*

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

$\chi^{\mu}_{g}(O)$	$\mathbf{g=1}$	$\mathbf{r}_{1\ldots4}$	180° $\boldsymbol{\rho}_{xyz}$	90° $\mathbf{R}_{xyz}$	180° $\mathbf{i}_{1\ldots6}$
A_1	1	~~1~~	1	1	1
A_2	1	~~1~~	1	-1	-1
E	2	~~-1~~	2	0	0
T_1	3	~~0~~	-1	1	-1
T_2	3	~~0~~	-1	-1	1

$O{\downarrow}D_4$ subduction

D_4: $\mathbf{1}, \rho_{z180°}, \mathbf{R}_{z\pm 90°}, \rho_{x,y180°}, \mathbf{i}_{3,4}$

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

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

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

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

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

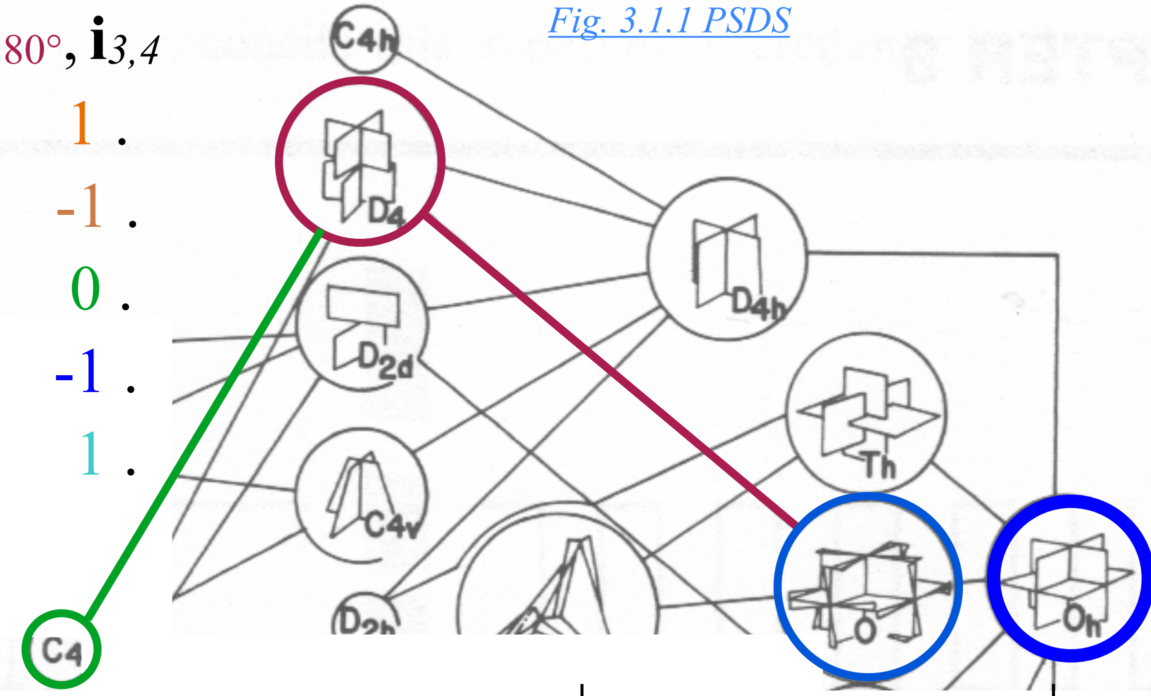


Fig. 3.1.1 PSDS

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

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

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

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

$\chi^{\mu}_{g}(O)$	$\mathbf{g}=\mathbf{1}$	$\mathbf{r}_{1\ldots4}$	180° $\boldsymbol{\rho}_{xyz}$	90° $\mathbf{R}_{xyz}$	180° $\mathbf{i}_{1\ldots6}$
A_1	1	1	1	1	1
A_2	1	1	1	−1	−1
E	2	−1	2	0	0
T_1	3	0	−1	1	−1
T_2	3	0	−1	−1	1

O↓D₄ subduction

D_4: $\mathbf{1}, \boldsymbol{\rho}_{z180°}, \mathbf{R}_{z\pm90°}, \boldsymbol{\rho}_{x,y180°}, \mathbf{i}_{3,4}$

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

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

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

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

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

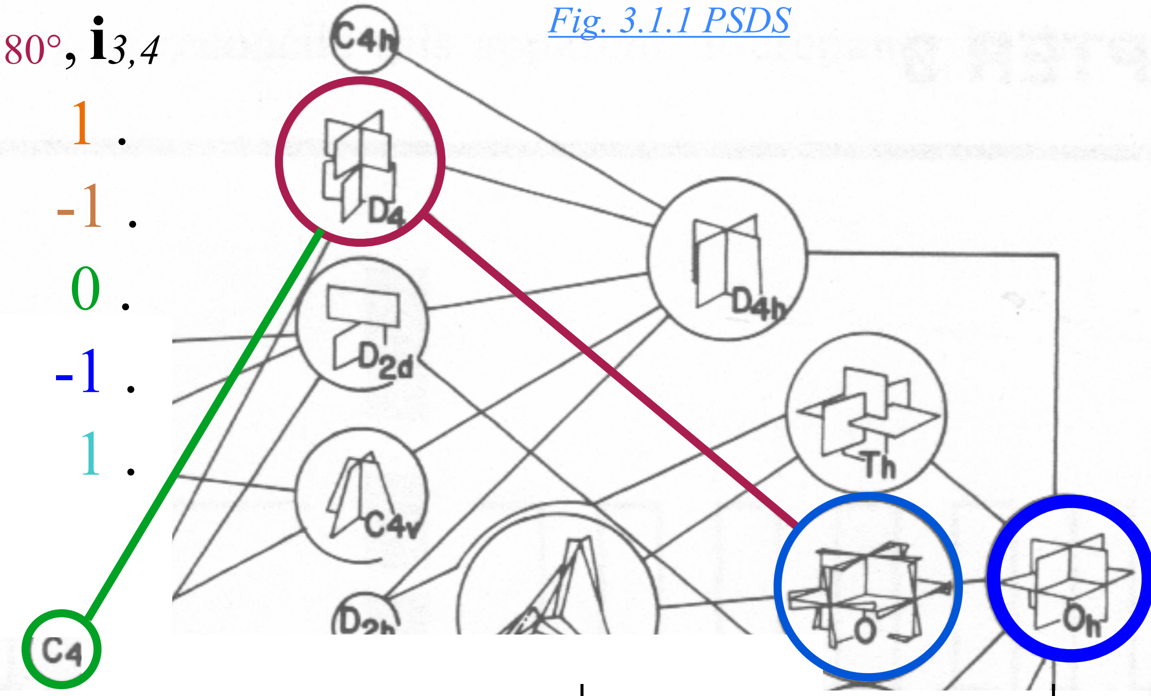


Fig. 3.1.1 PSDS

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

D₄↓C₄ subduction

C_4: $\mathbf{1}, \mathbf{R}_{z+90°}, \boldsymbol{\rho}_{z180°}, \mathbf{R}_{z-90°}$

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

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

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

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

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

O↓D₄ subduction

D_4: $\mathbf{1}, \boldsymbol{\rho}_{z180°}, \mathbf{R}_{z\pm 90°}, \boldsymbol{\rho}_{x,y180°}, \mathbf{i}_{3,4}$

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

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

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

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

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

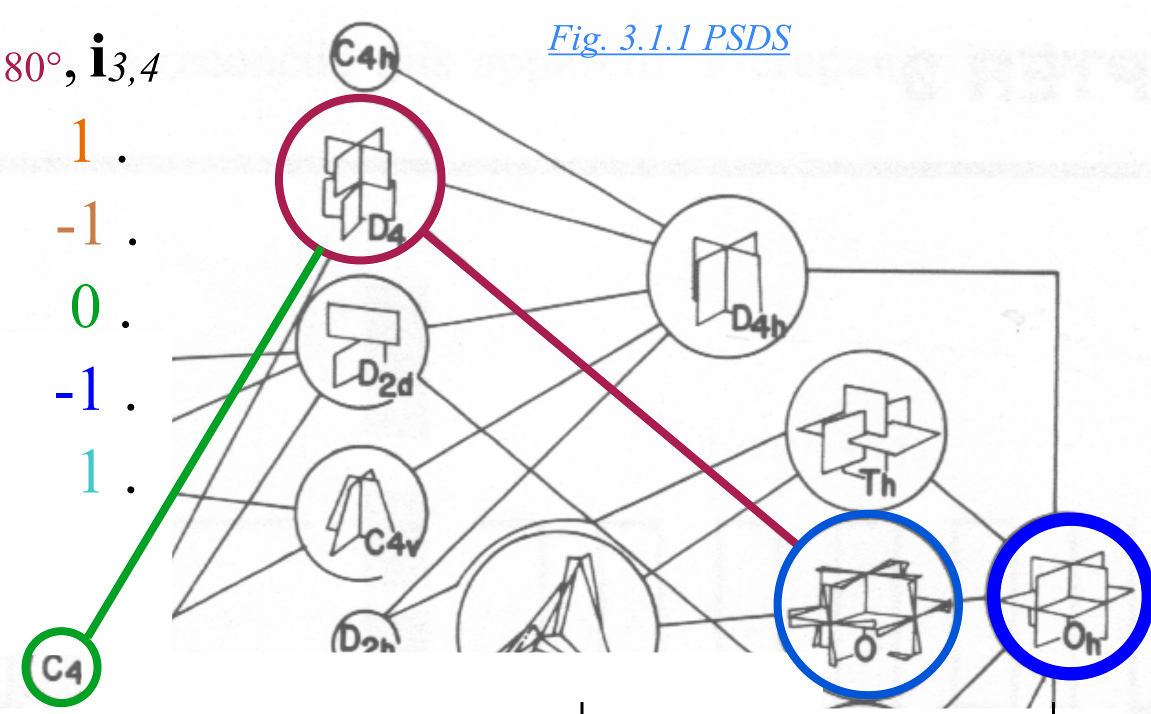


Fig. 3.1.1 PSDS

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

D₄↓C₄ subduction

C_4: $\mathbf{1}, \mathbf{R}_{z+90°}, \boldsymbol{\rho}_{z180°}, \mathbf{R}_{z-90°}$

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

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

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

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

$\chi^{\mu}_{g}(O)$	$\mathbf{g=1}$	$\mathbf{r}_{1\ldots4}$	180° $\boldsymbol{\rho}_{xyz}$	90° $\mathbf{R}_{xyz}$	180° $\mathbf{i}_{1\ldots6}$
A_1	1	$\cancel{1}$	1	1	1
A_2	1	$\cancel{1}$	1	−1	−1
E	2	$\cancel{-1}$	2	0	0
T_1	3	$\cancel{0}$	−1	1	−1
T_2	3	$\cancel{0}$	−1	−1	1

$O\downarrow D_4$ subduction

D_4: $\mathbf{1}, \boldsymbol{\rho}_{z180°}, \mathbf{R}_{z\pm90°}, \boldsymbol{\rho}_{x,y180°}, \mathbf{i}_{3,4}$

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

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

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

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

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

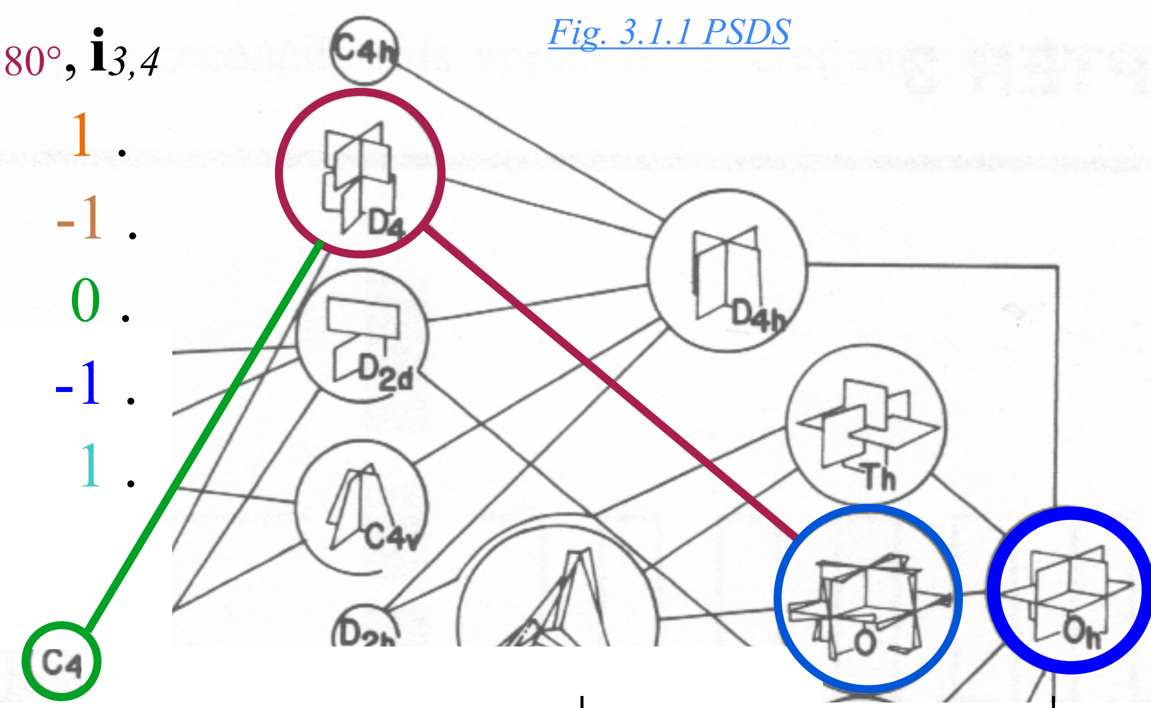


Fig. 3.1.1 PSDS

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

$D_4\downarrow C_4$ subduction

C_4: $\mathbf{1}, \mathbf{R}_{z+90°}, \boldsymbol{\rho}_{z180°}, \mathbf{R}_{z-90°}$

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

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

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

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

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

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

O↓D₄ subduction

D_4: $\mathbf{1}, \boldsymbol{\rho}_{z180°}, \mathbf{R}_{z\pm 90°}, \boldsymbol{\rho}_{x,y180°}, \mathbf{i}_{3,4}$

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

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

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

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

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

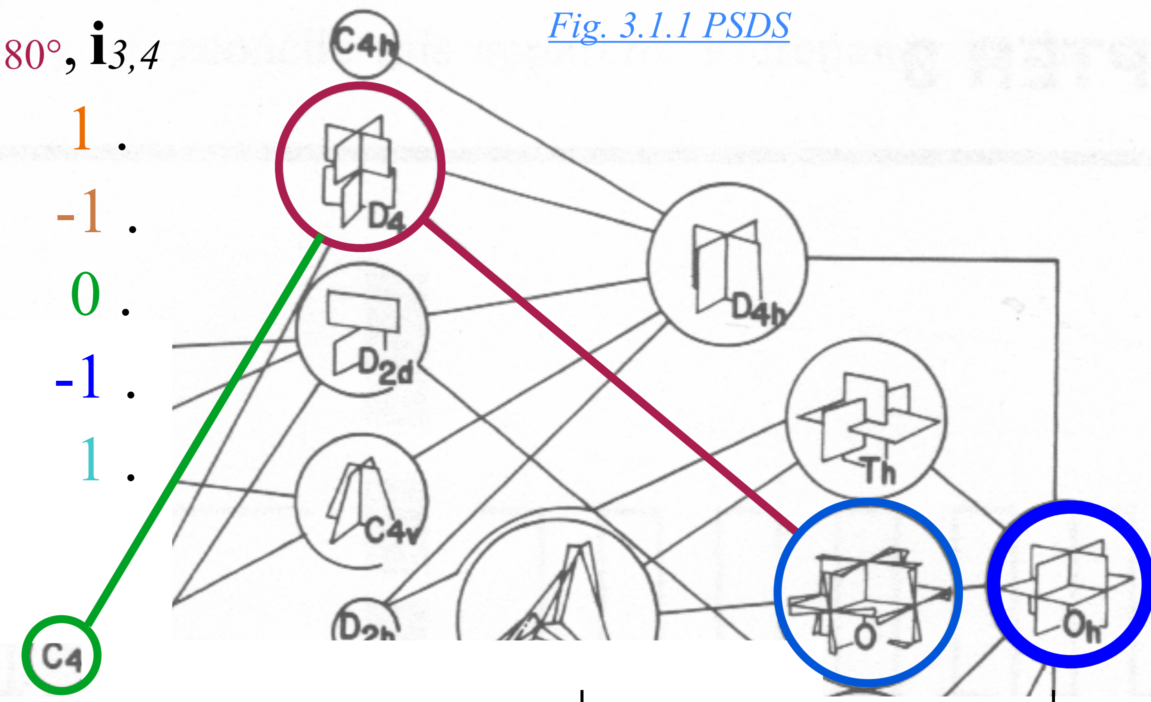


Fig. 3.1.1 PSDS

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

D₄↓C₄ subduction

C_4: $\mathbf{1}, \mathbf{R}_{z+90°}, \boldsymbol{\rho}_{z180°}, \mathbf{R}_{z-90°}$

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

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

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

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

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

$\chi_g^\mu(O)$	$\mathbf{g}=\mathbf{1}$	$\mathbf{r}_{1\ldots4}$	180° ρ_{xyz}	90° $\mathbf{R}_{xyz}$	180° $\mathbf{i}_{1\ldots6}$
A_1	1	1	1	1	1
A_2	1	1	1	−1	−1
E	2	−1	2	0	0
T_1	3	0	−1	1	−1
T_2	3	0	−1	−1	1

$O\downarrow D_4$ subduction

D_4: $\mathbf{1}, \rho_{z180°}, \mathbf{R}_{z\pm90°}, \rho_{x,y180°}, \mathbf{i}_{3,4}$

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

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

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

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

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

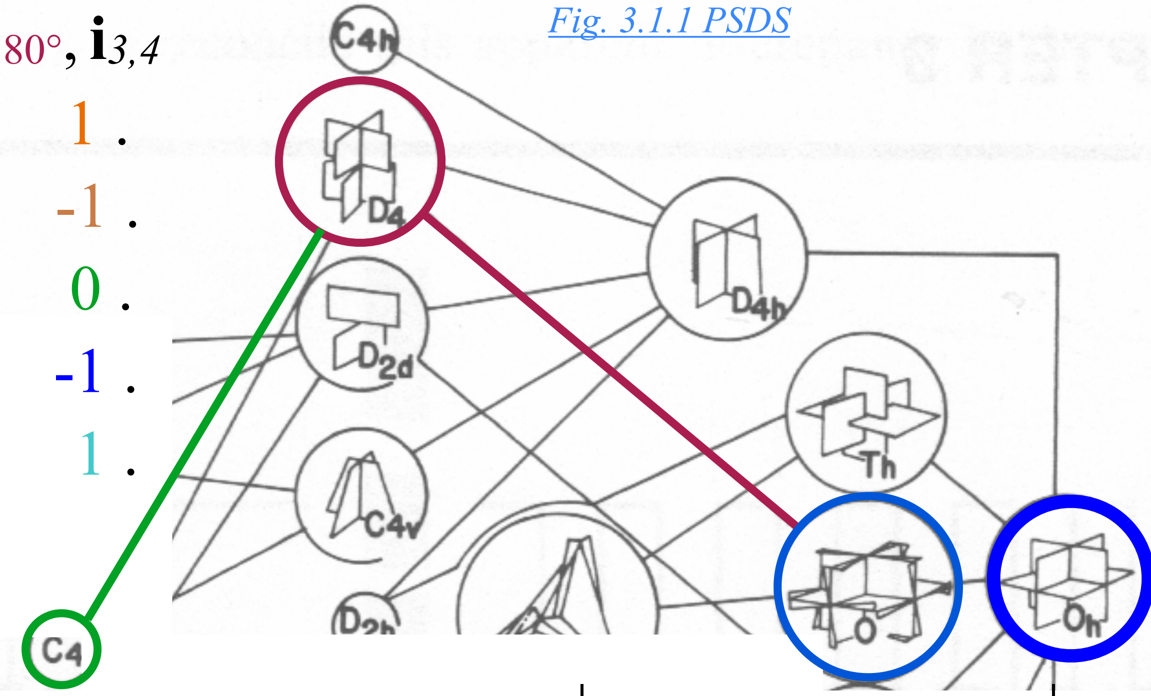


Fig. 3.1.1 PSDS

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

$D_4\downarrow C_4$ subduction

C_4 : $\mathbf{1}, \mathbf{R}_{z+90°}, \rho_{z180°}, \mathbf{R}_{z-90°}$

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

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

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

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

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

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

$\chi_g^\mu(O)$	$\mathbf{g}=\mathbf{1}$	$\mathbf{r}_{1\ldots4}$	180° $\boldsymbol{\rho}_{xyz}$	90° $\mathbf{R}_{xyz}$	180° $\mathbf{i}_{1\ldots6}$
A_1	1	~~1~~	1	1	1
A_2	1	~~1~~	1	−1	−1
E	2	~~−1~~	2	0	0
T_1	3	~~0~~	−1	1	−1
T_2	3	~~0~~	−1	−1	1

$O{\downarrow}D_4$ subduction

D_4: $\mathbf{1}, \boldsymbol{\rho}_{z180°}, \mathbf{R}_{z\pm90°}, \boldsymbol{\rho}_{x,y180°}, \mathbf{i}_{3,4}$

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

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

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

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

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

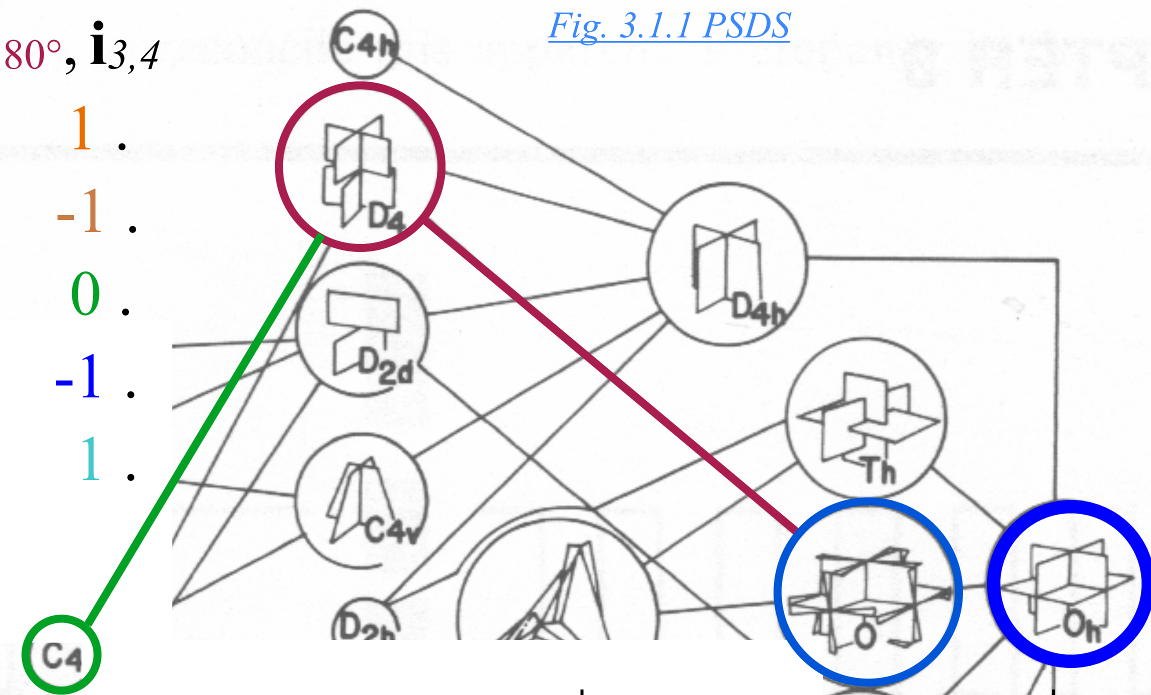


Fig. 3.1.1 PSDS

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

$D_4{\downarrow}C_4$ subduction

C_4: $\mathbf{1}, \mathbf{R}_{Z+90°}, \boldsymbol{\rho}_{Z180°}, \mathbf{R}_{Z-90°}$

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

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

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

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

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

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

$\chi^{\mu}_{g}(O)$	$\mathbf{g=1}$	$\mathbf{r}_{1\ldots4}$	180° $\boldsymbol{\rho}_{xyz}$	90° $\mathbf{R}_{xyz}$	180° $\mathbf{i}_{1\ldots6}$
A_1	1	1	1	1	1
A_2	1	1	1	−1	−1
E	2	−1	2	0	0
T_1	3	0	−1	1	−1
T_2	3	0	−1	−1	1

$O\downarrow D_4$ subduction

D_4: $\mathbf{1}, \boldsymbol{\rho}_{z180°}, \mathbf{R}_{z\pm90°}, \boldsymbol{\rho}_{x,y180°}, \mathbf{i}_{3,4}$

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

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

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

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

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

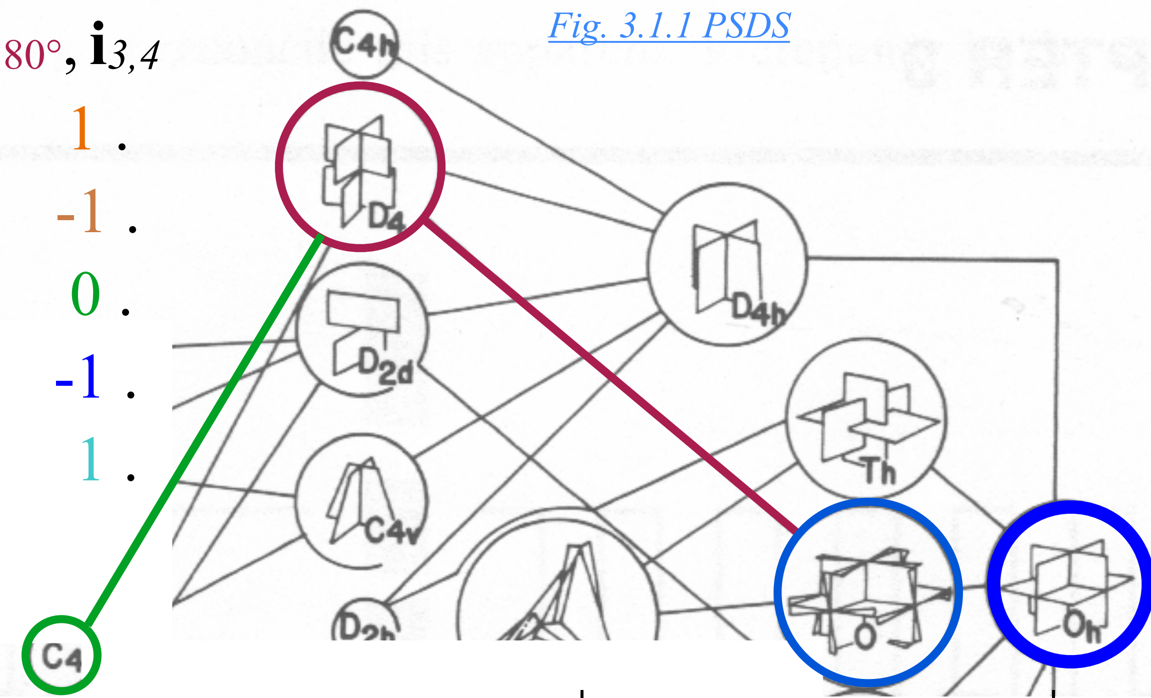


Fig. 3.1.1 PSDS

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

$D_4\downarrow C_4$ subduction

C_4 : $\mathbf{1}, \mathbf{R}_{z+90°}, \boldsymbol{\rho}_{z180°}, \mathbf{R}_{z-90°}$

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

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

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

$B_2(D_4)\downarrow C_4 = 1, \; -1, \; 1, \; -1.$

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

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

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

$\chi^{\mu}_{g}(O)$	$\mathbf{g=1}$	$\mathbf{r}_{1\ldots4}$	180° $\boldsymbol{\rho}_{xyz}$	90° $\mathbf{R}_{xyz}$	180° $\mathbf{i}_{1\ldots6}$
A_1	1	$\cancel{1}$	1	1	1
A_2	1	$\cancel{1}$	1	−1	−1
E	2	$\cancel{-1}$	2	0	0
T_1	3	$\cancel{0}$	−1	1	−1
T_2	3	$\cancel{0}$	−1	−1	1

$O{\downarrow}D_4$ subduction

D_4: $\mathbf{1}, \boldsymbol{\rho}_{z180°}, \mathbf{R}_{z\pm90°}, \boldsymbol{\rho}_{x,y180°}, \mathbf{i}_{3,4}$

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

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

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

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

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

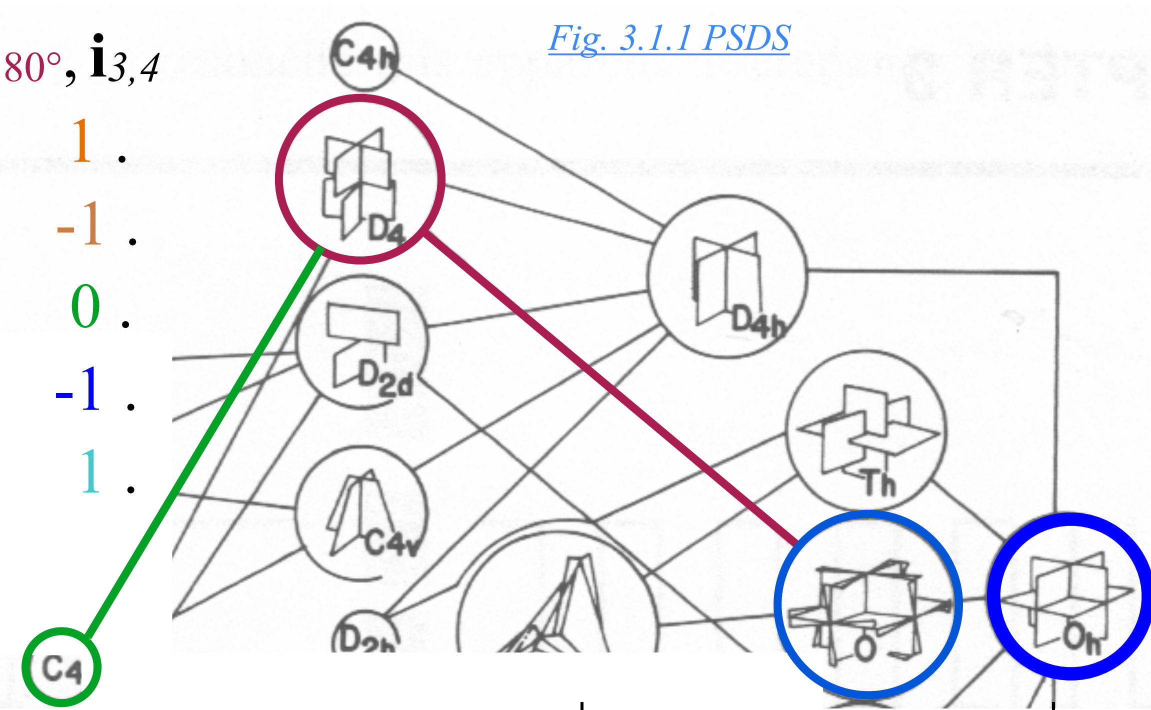


Fig. 3.1.1 PSDS

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

$D_4{\downarrow}C_4$ subduction

C_4: $\mathbf{1}, \mathbf{R}_{z+90°}, \boldsymbol{\rho}_{z180°}, \mathbf{R}_{z-90°}$

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

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

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

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

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

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

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

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

$O{\downarrow}D_4$ subduction

D_4: $\mathbf{1}, \boldsymbol{\rho}_{z180°}, \mathbf{R}_{z\pm 90°}, \boldsymbol{\rho}_{x,y180°}, \mathbf{i}_{3,4}$

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

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

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

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

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

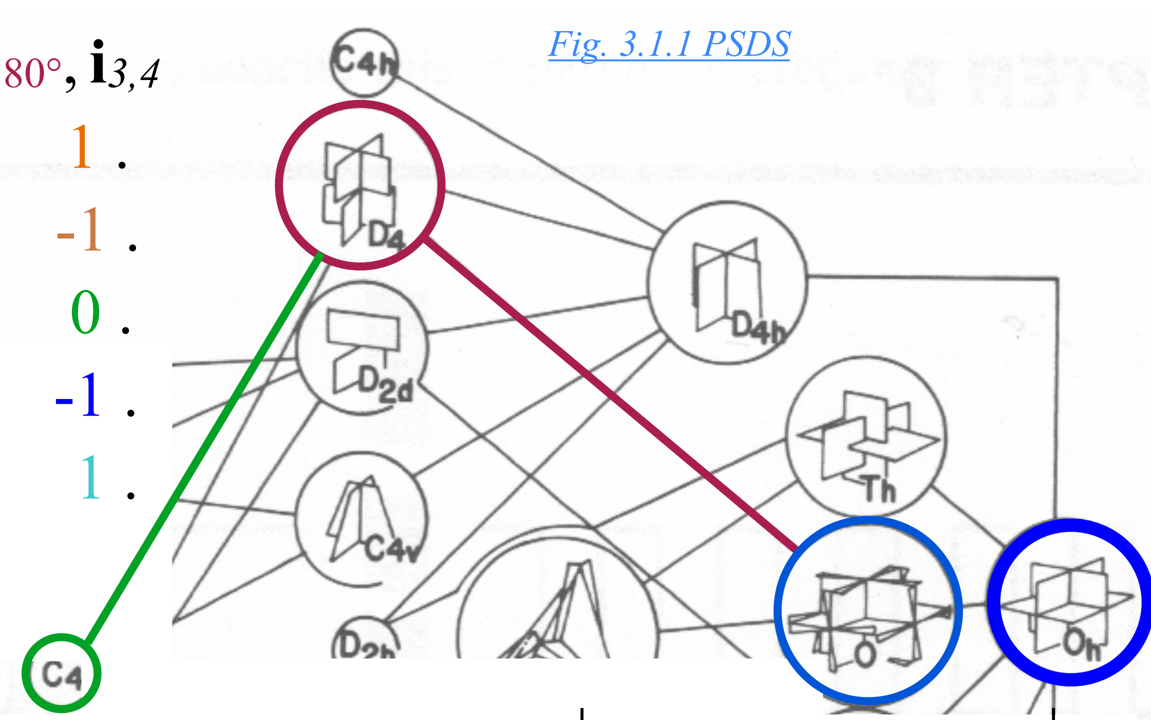


Fig. 3.1.1 PSDS

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

$D_4{\downarrow}C_4$ subduction

C_4 : $\mathbf{1}, \mathbf{R}_{z+90°}, \boldsymbol{\rho}_{z180°}, \mathbf{R}_{z-90°}$

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

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

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

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

$E(D_4){\downarrow}C_4 = 2,\ 0,\ -2,\ 0\ .$

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

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

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

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

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

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

O↓D₄ subduction

D_4: $\mathbf{1}, \boldsymbol{\rho}_{z180°}, \mathbf{R}_{z\pm90°}, \boldsymbol{\rho}_{x,y180°}, \mathbf{i}_{3,4}$

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

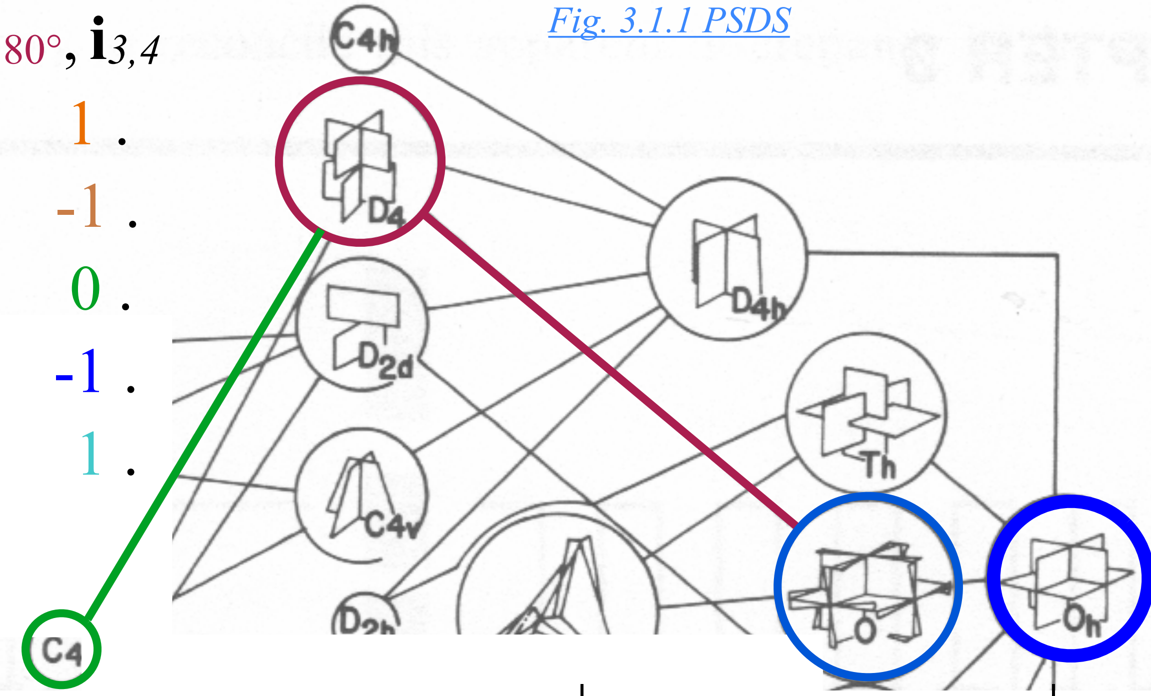
$A_2(O)\downarrow D_4 = 1,\ 1,\ -1,\ 1,\ -1\ .$

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

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

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

Fig. 3.1.1 PSDS



D₄↓C₄ subduction

C_4: $\mathbf{1}, \mathbf{R}_{z+90°}, \boldsymbol{\rho}_{z180°}, \mathbf{R}_{z-90°}$

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

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

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

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

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

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

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

$\chi^{\mu}_{g}(O)$	$\mathbf{g=1}$	$\cancel{\mathbf{r}_{1\ldots4}}$	180° $\boldsymbol{\rho}_{xyz}$	90° $\mathbf{R}_{xyz}$	180° $\mathbf{i}_{1\ldots6}$
A_1	1	1	1	1	1
A_2	1	1	1	−1	−1
E	2	−1	2	0	0
T_1	3	0	−1	1	−1
T_2	3	0	−1	−1	1

O↓D₄ subduction

D_4: $\mathbf{1}, \boldsymbol{\rho}_{z180°}, \mathbf{R}_{z\pm90°}, \boldsymbol{\rho}_{x,y180°}, \mathbf{i}_{3,4}$

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

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

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

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

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

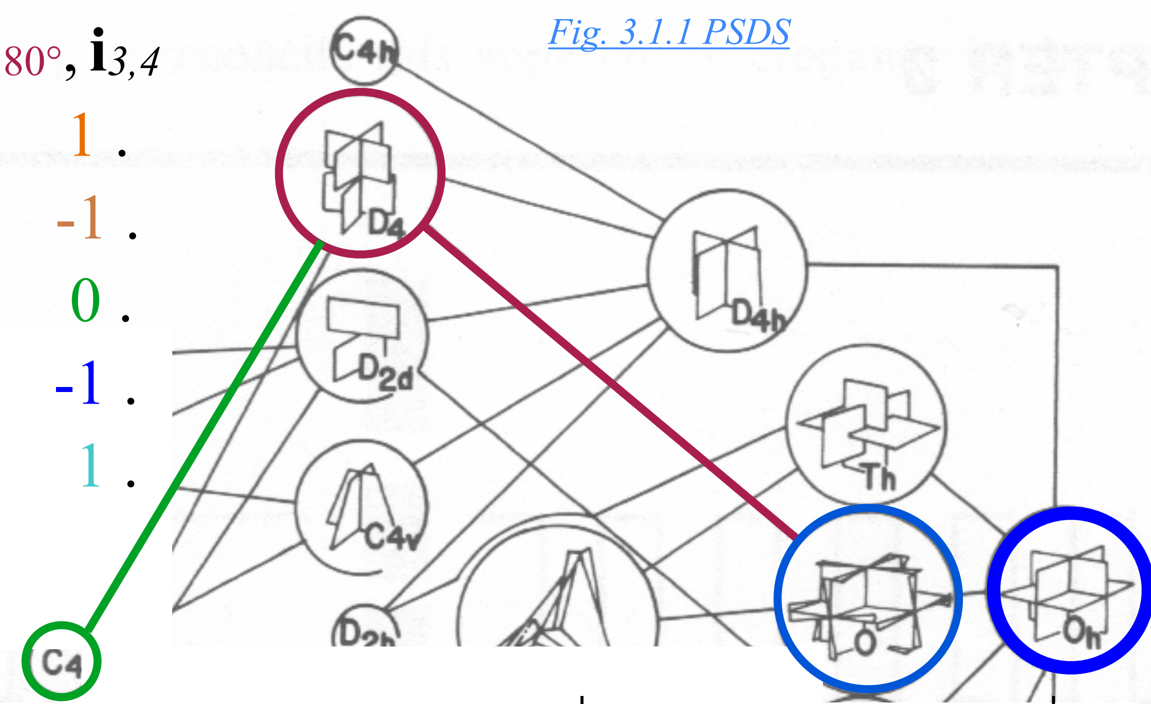


Fig. 3.1.1 PSDS

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

D₄↓C₄ subduction

C_4: $\mathbf{1}, \mathbf{R}_{z+90°}, \boldsymbol{\rho}_{z180°}, \mathbf{R}_{z-90°}$

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

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

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

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

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

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

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

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

AMOP
reference links
on page 2

3.05.18 class 15.0: *Symmetry Principles for*
Advanced Atomic-Molecular-Optical-Physics

William G. Harter - University of Arkansas

Discrete symmetry subgroups of $O(3)\supset$(Octahedral $O_h\supset O\sim T_d$, Cubic-Tetrahedral $T_h\supset T$): Characters and subgroup-chain defined ireps, and applications to SF_6 and CF_4 spectra

Review: *General all-commuting class-character-projector formula derivations.* *f^μ derivation 2015 Lect15 p.40-45.*

$\mathbb{P}^\mu$ in χ^μ-terms of $\boldsymbol{\kappa}_\mathbf{g}$ *$\boldsymbol{\kappa}_\mathbf{g}$ in $\chi^{\mu *}$-terms of $\mathbb{P}^\mu$* *Irep frequency f^μ in $\chi^{\mu *}$-terms of Trace$R(\mathbf{g})$*

Introducing octahedral/ tetrahedral symmetry $O_h\supset O\sim T_d\supset T$: relating $D_4\supset C_4$ and $D_3\supset C_3$

Octahedral-cubic O symmetry and group operations, *O slide-rule*

Tetrahedral symmetry leads to Icosahedral

Octahedral groups $O_h\supset O\sim T_d\supset T$ and its large subgroups. *O_h slide-rule*

Octahedral O and spin-$O\subset U(2)$ nomograms

Tetrahedral T class algebra *minimal equations* *centrum projectors and characters*

Octahedral O class algebra *minimal equations* *centrum projectors and characters*

Characters of full Octahedral symmetry $O_h=O\times C_\mathbf{I}=O\times\{\mathbf{1},\mathbf{I}\}$

Octahedral $O_h\supset O\supset C_\mathbf{I}$ subgroup correlations

➡ *Octahedral subgroup correlation* *$O_h\supset O\supset D_4$* ➡ *$O_h\supset O\supset D_4\supset C_4$* ➡ *and level-splitting*

Comparing $O\supset C_4$ and $O\supset C_3$ and $O\supset C_2$

$R(3)\subset O(3)\supset O_h\supset O$ character analysis: Crystal field splitting *p, d, f,…orbitals*

Cluster structure in SF_6 16um spectra. *Analogy with D_6 band gap structure*

Global vs Local *External LAB splitting vs Internal BODY clustering*

Detailed superfine structure for A_1T_1E cluster *preview of next lecture*

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

$O\downarrow D_4$ subduction

D_4: $\mathbf{1}, \boldsymbol{\rho}_{z180°}, \mathbf{R}_{z\pm 90°}, \boldsymbol{\rho}_{x,y180°}, \mathbf{i}_{3,4}$

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

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

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

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

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

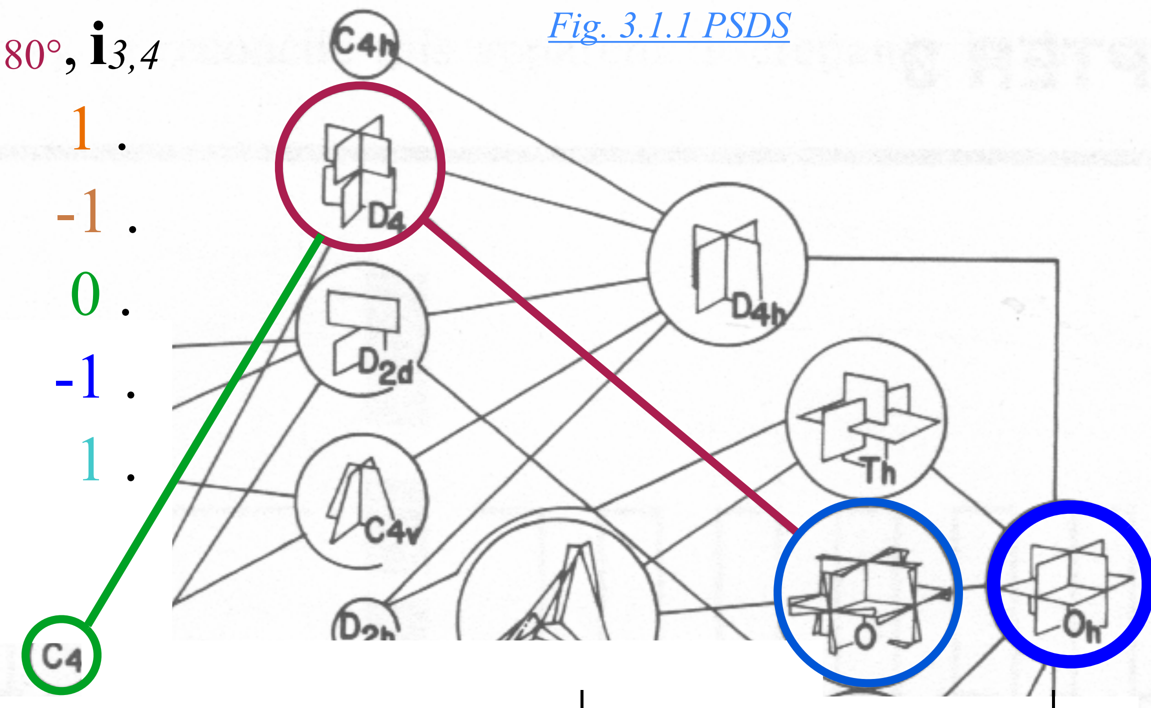
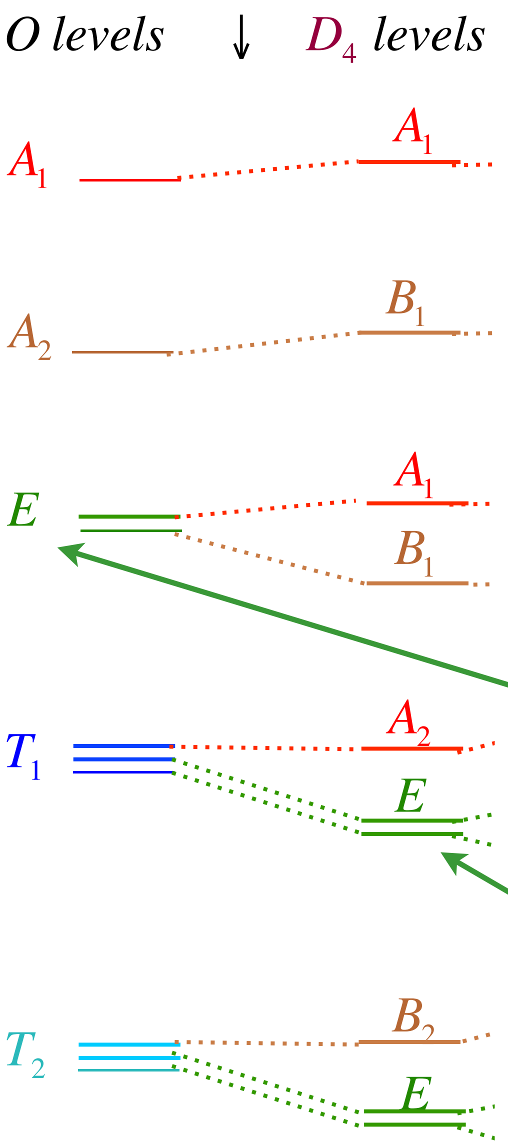


Fig. 3.1.1 PSDS

$O \supset D_4 \supset C_4$ subgroup and level-splitting/relabeling correlations



$D_4\downarrow C_4$ subduction

C_4: $\mathbf{1}, \mathbf{R}_{z+90°}, \boldsymbol{\rho}_{z180°}, \mathbf{R}_{z-90°}$

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

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

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

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

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

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

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

Note that "BIG-E" for O is NOT to be confused with "little-E" for D_4

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

$O\downarrow D_4$ subduction

D_4: $\mathbf{1}, \rho_{z180°}, \mathbf{R}_{z\pm 90°}, \rho_{x,y180°}, \mathbf{i}_{3,4}$

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

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

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

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

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

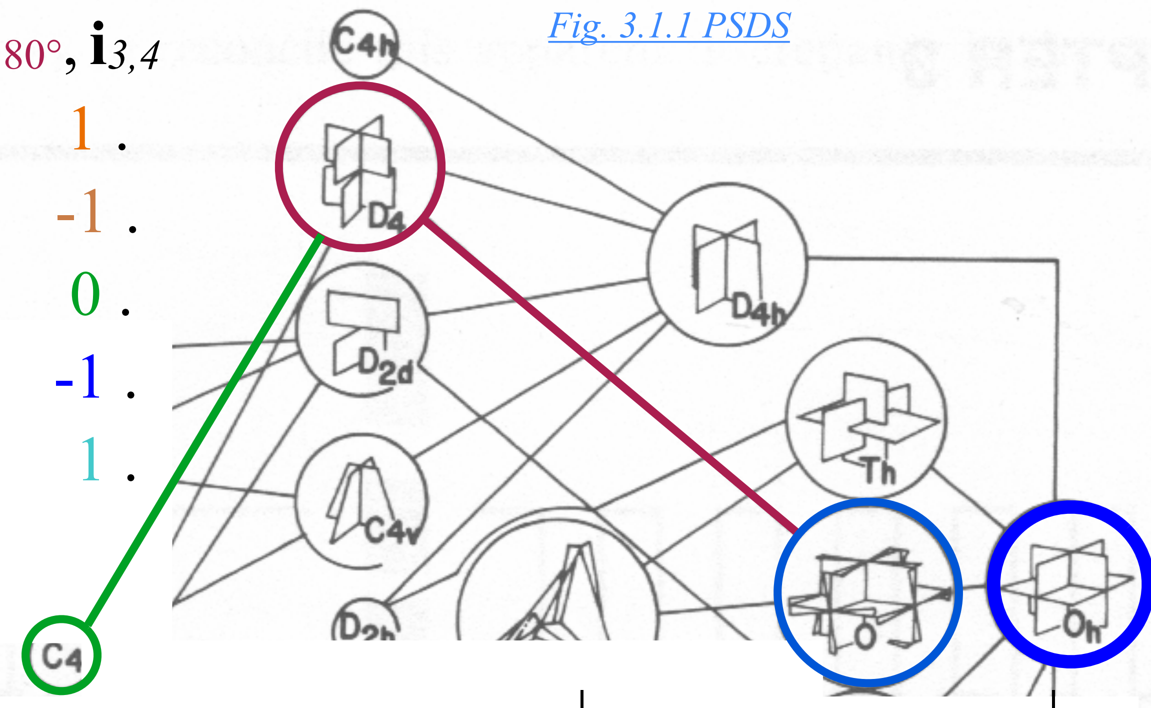
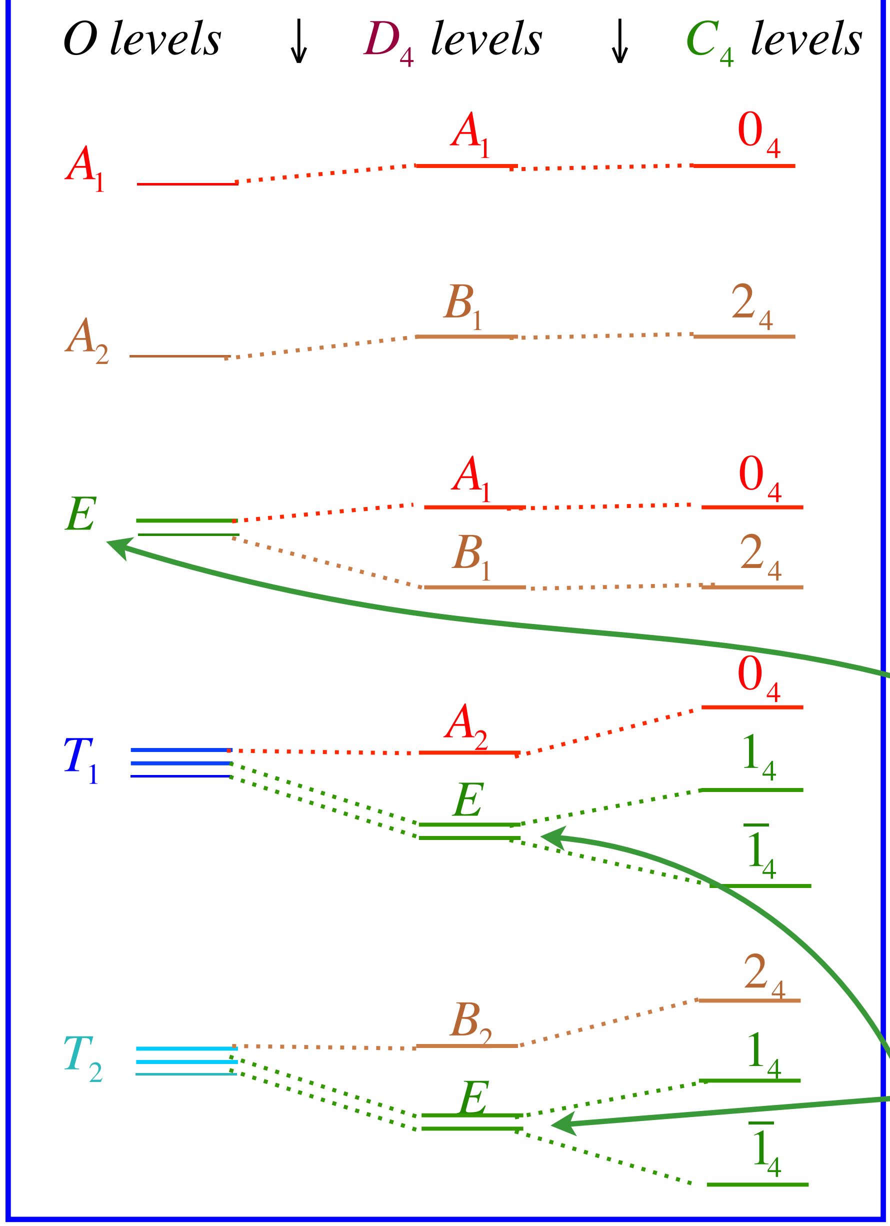


Fig. 3.1.1 PSDS

$O \supset D_4 \supset C_4$ subgroup and level-splitting/relabeling correlations



Note that "BIG-E" for O is NOT to be confused with "little-E" for D_4

$D_4\downarrow C_4$ subduction

C_4 : $\mathbf{1}, \mathbf{R}_{z+90°}, \rho_{z180°}, \mathbf{R}_{z-90°}$

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

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

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

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

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

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

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

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

$O \downarrow D_4$ subduction

D_4: $\mathbf{1}, \boldsymbol{\rho}_{z180°}, \mathbf{R}_{z\pm 90°}, \boldsymbol{\rho}_{x,y180°}, \mathbf{i}_{3,4}$

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

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

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

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

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

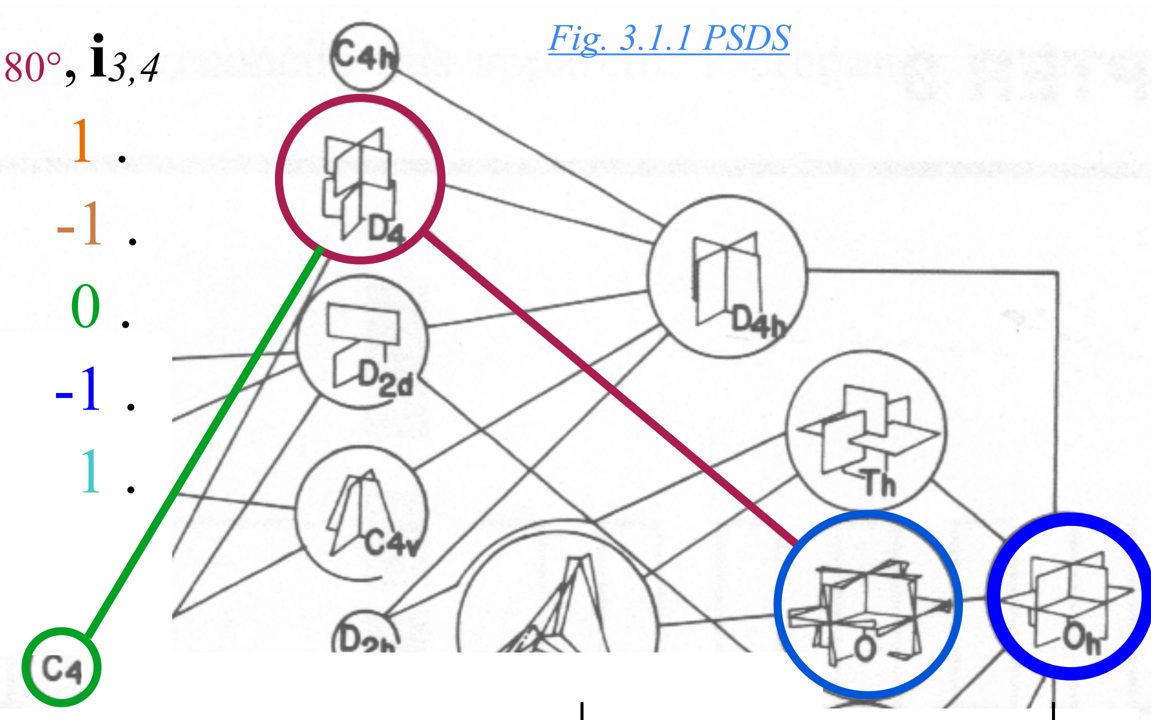
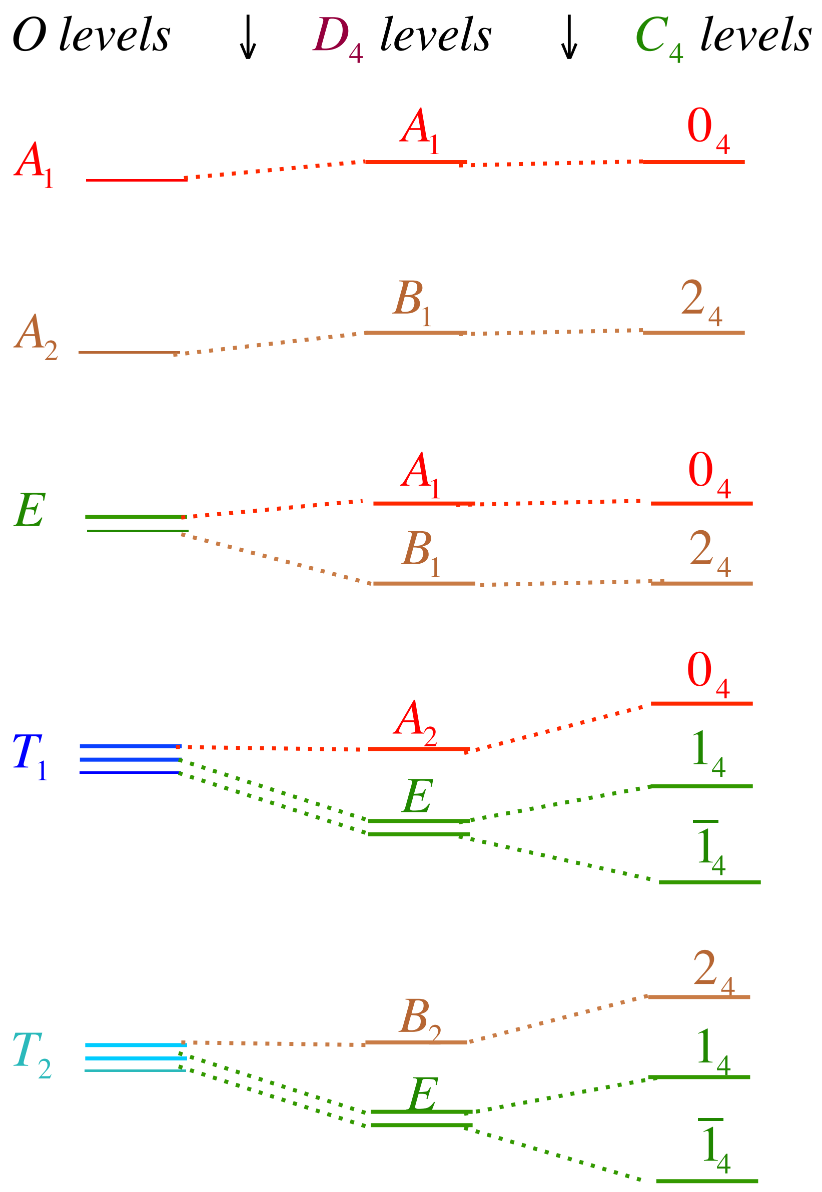


Fig. 3.1.1 PSDS

$O \supset D_4 \supset C_4$ subgroup and level-splitting/relabeling correlations



$D_4 \downarrow C_4$ subduction

C_4 : $\mathbf{1}, \mathbf{R}_{z+90°}, \boldsymbol{\rho}_{z180°}, \mathbf{R}_{z-90°}$

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

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

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

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

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

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

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

$O \downarrow C_4$ subduction

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

AMOP reference links on page 2

3.05.18 class 15.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Discrete symmetry subgroups of O(3)⊃(Octahedral O_h⊃O~T_d, Cubic-Tetrahedral T_h⊃T): Characters and subgroup-chain defined ireps, and applications to SF_6 and CF_4 spectra

Review: *General all-commuting class-character-projector formula derivations.* *f^μ derivation 2015 Lect15 p.40-45.*

$\mathbb{P}^\mu$ in χ^μ-terms of $\boldsymbol{\kappa}_\mathbf{g}$ *$\boldsymbol{\kappa}_\mathbf{g}$ in $\chi^{\mu *}$-terms of $\mathbb{P}^\mu$* *Irep frequency f^μ in $\chi^{\mu *}$-terms of Trace$R(\mathbf{g})$*

Introducing octahedral/ tetrahedral symmetry $O_h \supset O \sim T_d \supset T$: relating $D_4 \supset C_4$ and $D_3 \supset C_3$

Octahedral-cubic O symmetry and group operations, *O slide-rule*

Tetrahedral symmetry leads to Icosahedral

Octahedral groups $O_h \supset O \sim T_d \supset T$ and its large subgroups. *O_h slide-rule*

Octahedral O and spin-O⊂U(2) nomograms

Tetrahedral T class algebra *minimal equations* *centrum projectors and characters*

Octahedral O class algebra *minimal equations* *centrum projectors and characters*

Characters of full Octahedral symmetry $O_h = O \times C_\mathbf{I} = O \times \{\mathbf{1},\mathbf{I}\}$

Octahedral $O_h \supset O \supset C_\mathbf{I}$ subgroup correlations

Octahedral subgroup correlation *$O_h \supset O \supset D_4$* *$O_h \supset O \supset D_4 \supset C_4$* *and level-splitting*

Comparing $O \supset C_4$ and $O \supset C_3$ and $O \supset C_2$

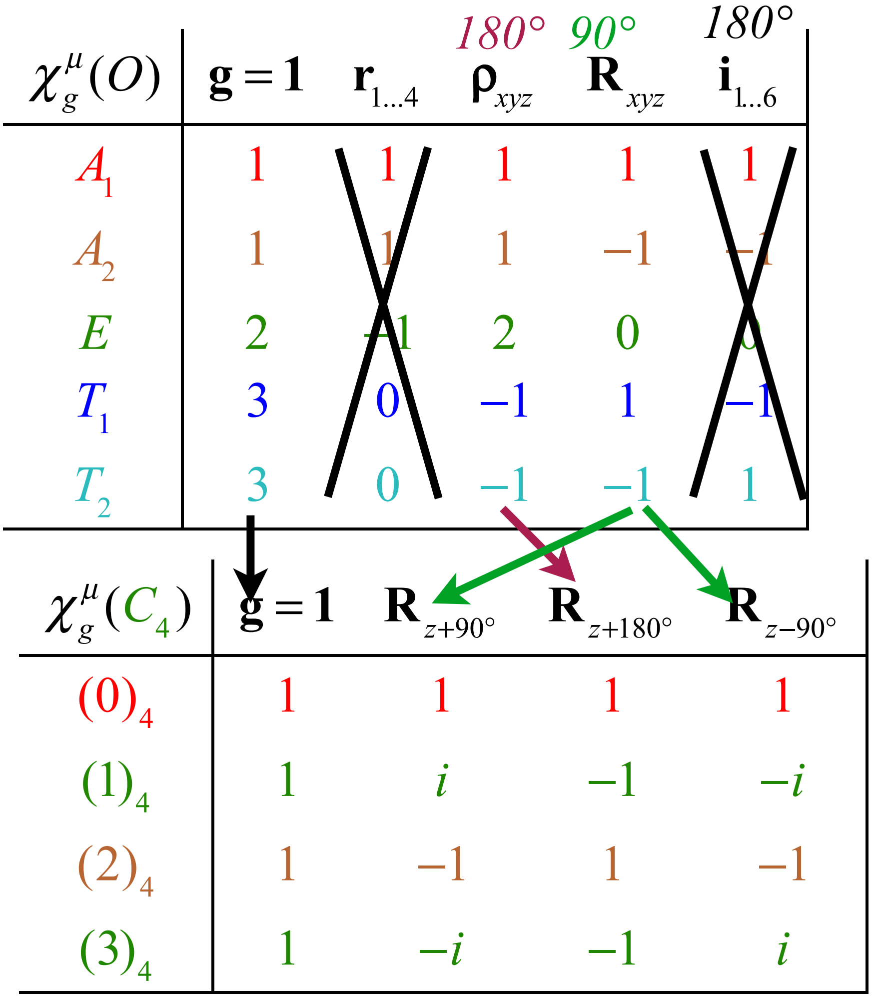
$R(3) \subset O(3) \supset O_h \supset O$ character analysis: Crystal field splitting *p, d, f,…orbitals*

Cluster structure in SF_6 16um spectra. *Analogy with D_6 band gap structure*

Global vs Local *External LAB splitting vs Internal BODY clustering*

Detailed superfine structure for A_1T_1E cluster *preview of next lecture*

Octahedral O⊃C_4 subgroup correlations



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

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

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

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

$A_2(O)\downarrow C_4 = 1,\ -1,\ 1,\ -1.\quad =(2)_4$

$E(O)\downarrow C_4 = 2,\ 0,\ 2,\ 0.\quad =(0)_4\oplus(2)_4$

$T_1(O)\downarrow C_4 = 3,\ 1,\ -1,\ 1.\quad =(0)_4\oplus(1)_4\oplus(3)_4$

$T_2(O)\downarrow C_4 = 3,\ -1,\ -1,\ -1\ .\quad =(2)_4\oplus(1)_4\oplus(3)_4$

O↓C_4 subduction

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

Octahedral O⊃C₄ subgroup correlations

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

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

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

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

$A_2(O)\downarrow C_4 = 1,\ -1,\ 1,\ -1.\quad =(2)_4$

$E(O)\downarrow C_4 = 2,\ 0,\ 2,\ 0.\quad =(0)_4\oplus(2)_4$

$T_1(O)\downarrow C_4 = 3,\ 1,\ -1,\ 1.\quad =(0)_4\oplus(1)_4\oplus(3)_4$

$T_2(O)\downarrow C_4 = 3,\ -1,\ -1,\ -1.\quad =(2)_4\oplus(1)_4\oplus(3)_4$

O↓C₄ subduction

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

Octahedral O⊃C₃ subgroup correlations

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

$\chi^{\mu}_{g}(C_3)$	$\mathbf{g}=\mathbf{1}$	$r_{z+120°}$	$r_{z-120°}$
$(0)_3$	1	1	1
$(1)_3$	1	$e^{i2\pi/3}$	$e^{-i2\pi/3}$
$(2)_3$	1	$e^{-i2\pi/3}$	$e^{i2\pi/3}$

1, $\mathbf{r}_{z+120°}$, $\mathbf{r}_{z-120°}$, $\mathbf{R}_{z-90°}$

$A_1(O)\downarrow C_3 = 1,\ 1,\ 1.\quad =(0)_3$

$A_2(O)\downarrow C_3 = 1,\ 1,\ 1.\quad =(0)_3$

$E(O)\downarrow C_3 = 2,\ -1,\ -1.\quad =(1)_3\oplus(3)_3$

$T_1(O)\downarrow C_3 = 3,\ 0,\ 0.\quad =(0)_3\oplus(1)_3\oplus(3)_3$

$T_2(O)\downarrow C_3 = 3,\ 0,\ 0.\quad =(0)_3\oplus(1)_3\oplus(3)_3$

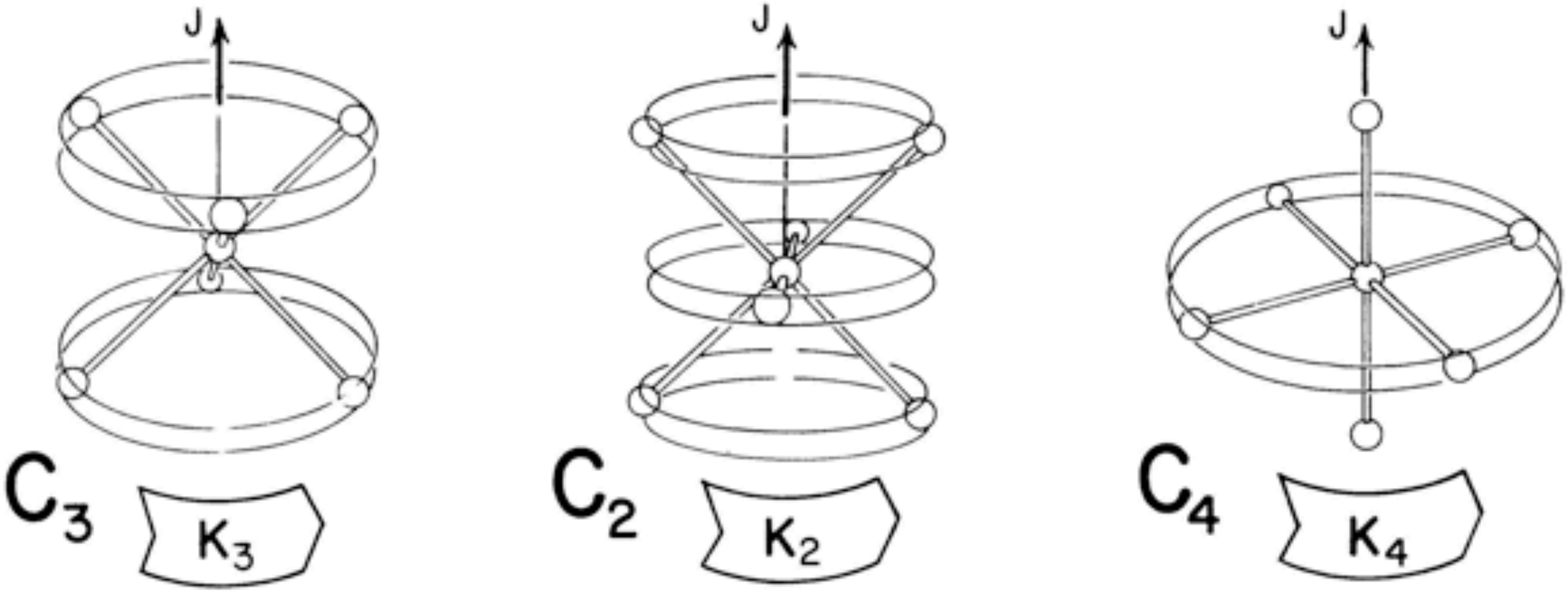
O↓C₃ subduction

$O\downarrow C_3$	0_3	1_3	$2_3=\bar{1}_3$
A_1	1	·	·
A_2	1	·	·
E	·	1	1
T_1	1	1	1
T_2	1	1	1

Octahedral $O\supset C_3$ is 2nd most common local symmetry

Octahedral $O\supset C_2$ is an unusual local symmetry

Octahedral $O\supset C_4$ is most common local symmetry



	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

	0_2	1_2
A_1	1	·
A_2	·	1
E	1	1
T_1	1	2
T_2	2	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

Fig. 25.4.7 *Different choices of rotation axes for octahedral rotor corresponding to local symmetry C_3, C_2, and C_4. Tables correlate global octahedral symmetry species with the local ones.*

PSDS Ch. 7. Fig. 7.4.7.

QTforCA Unit 8. Ch. 25 Fig. 25.4.7.

AMOP reference links on page 2

3.05.18 class 15.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

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Global vs Local   *External LAB splitting vs Internal BODY clustering*

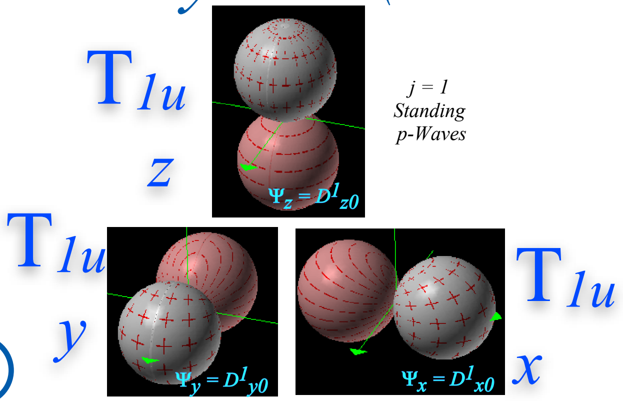
Detailed superfine structure for $A_1 T_1 E$ cluster   *preview of next lecture*

$R(3) \subset O(3) \supset O_h \supset O$ character analysis

(From Principles of Symmetry Dynamics & Spectroscopy Ch.5 p.391)

Frequency of O Irreps

	f^{A_1}	f^{A_2}	f^{E}	f^{T_1}	f^{T_2}	
$l = 0$	1	·	·	·	·	A_{1g}
1	·	·	·	1	·	T_{1u}
2	·	·	1	·	1	$E_g + T_{2g}$
3	·	1	·	1	1	$A_{2u} + T_{1u} + T_{2u}$
4	1	·	1	1	1	$A_{1g} + E_g + T_{1g} + T_{2g}$

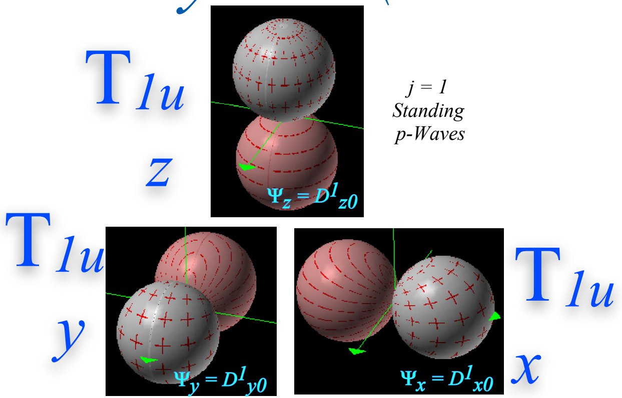


$R(3)\subset O(3)\supset O_h\supset O$ character analysis

(From Principles of Symmetry Dynamics & Spectroscopy Ch.5 p.391)

Frequency of O Irreps

	f^{A_1}	f^{A_2}	f^{E}	f^{T_1}	f^{T_2}	
$l=0$	1	·	·	·	·	A_{1g}
1	·	·	·	1	·	T_{1u}
2	·	·	1	·	1	$E_g + T_{2g}$
3	·	1	·	1	1	$A_{2u} + T_{1u} + T_{2u}$
4	1	·	1	1	1	$A_{1g} + E_g + T_{1g} + T_{2g}$



E_g

T_{2g}

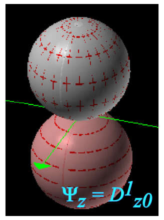
$R(3)\subset O(3)\supset O_h\supset O$ character analysis

(*From Principles of Symmetry Dynamics & Spectroscopy Ch.5 p.391*)

Frequency of O Irreps

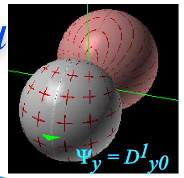
	f^{A_1}	f^{A_2}	f^{E}	f^{T_1}	f^{T_2}	
$l=0$	1	·	·	·	·	A_{1g}
1	·	·	·	1	·	T_{1u}
2	·	·	1	·	1	$E_g + T_{2g}$
3	·	1	·	1	1	$A_{2u} + T_{1u} + T_{2u}$
4	1	·	1	1	1	$A_{1g} + E_g + T_{1g} + T_{2g}$

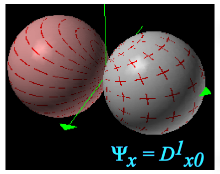
T_{1u}
z



j = 1
Standing
p-Waves

T_{1u}
y





T_{1u}
x

E_g
x^2-y^2

E_g

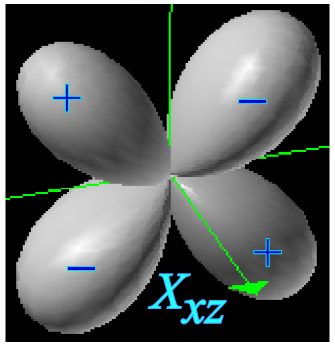
T_{2g}
xy

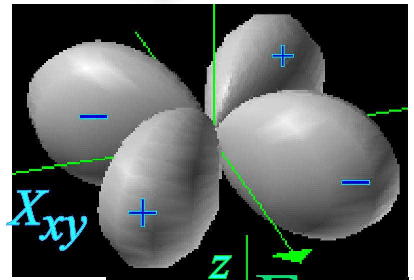
T_{2g}

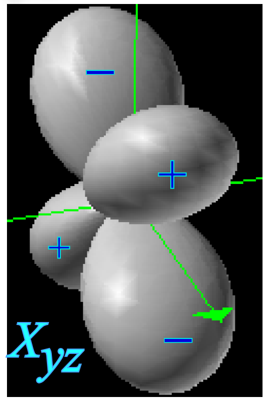
T_{2g}
xz

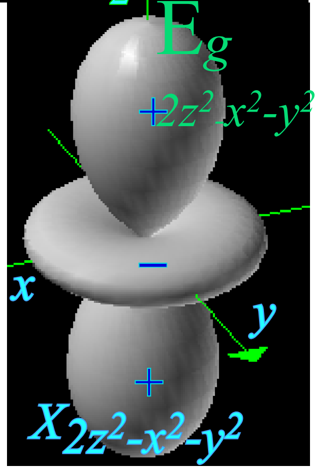
T_{2g}
xy

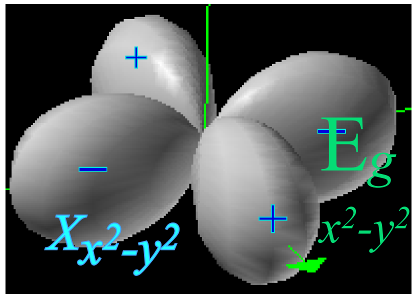
T_{2g}
yz











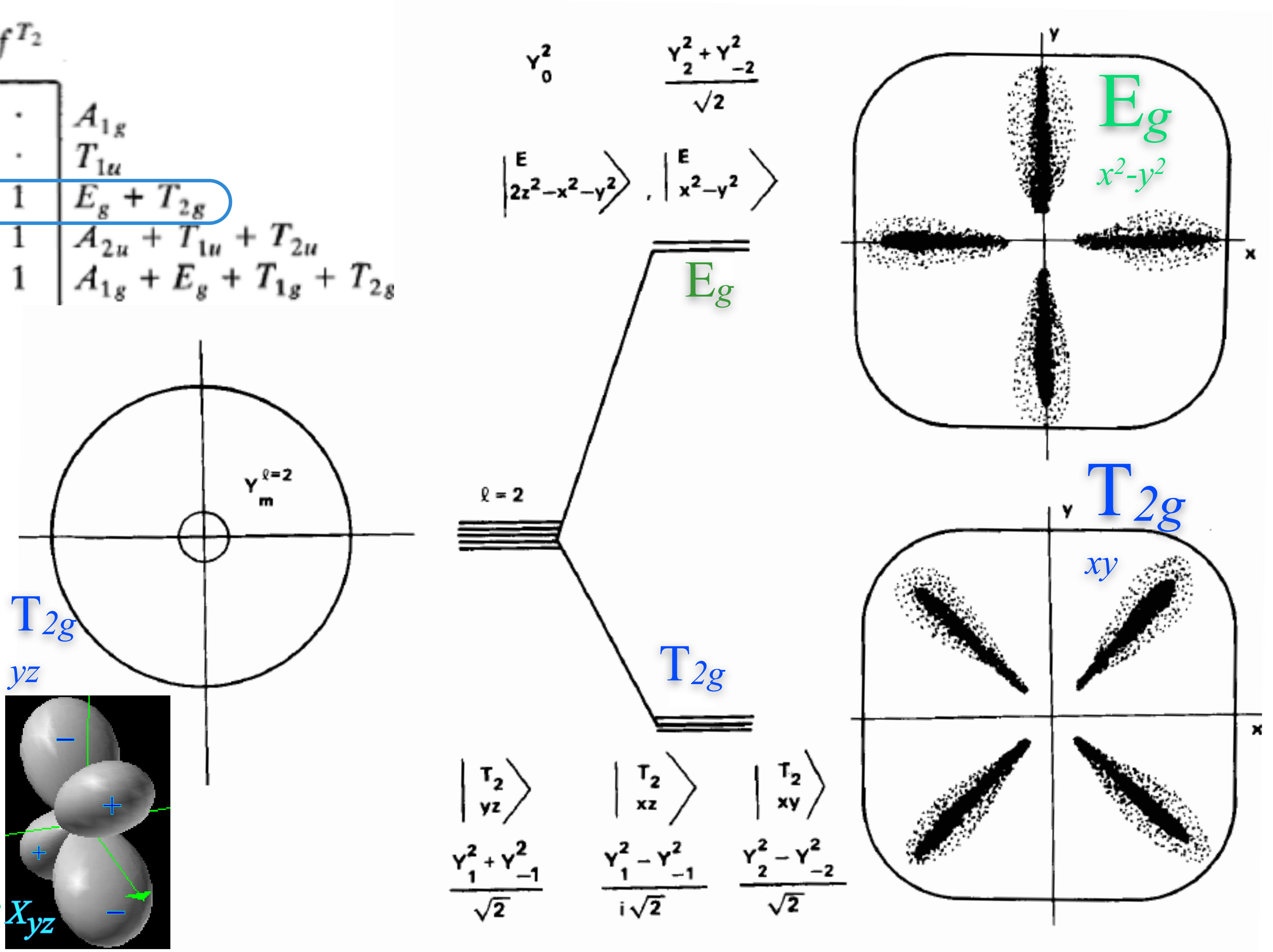
j = 2
Standing
d-Waves

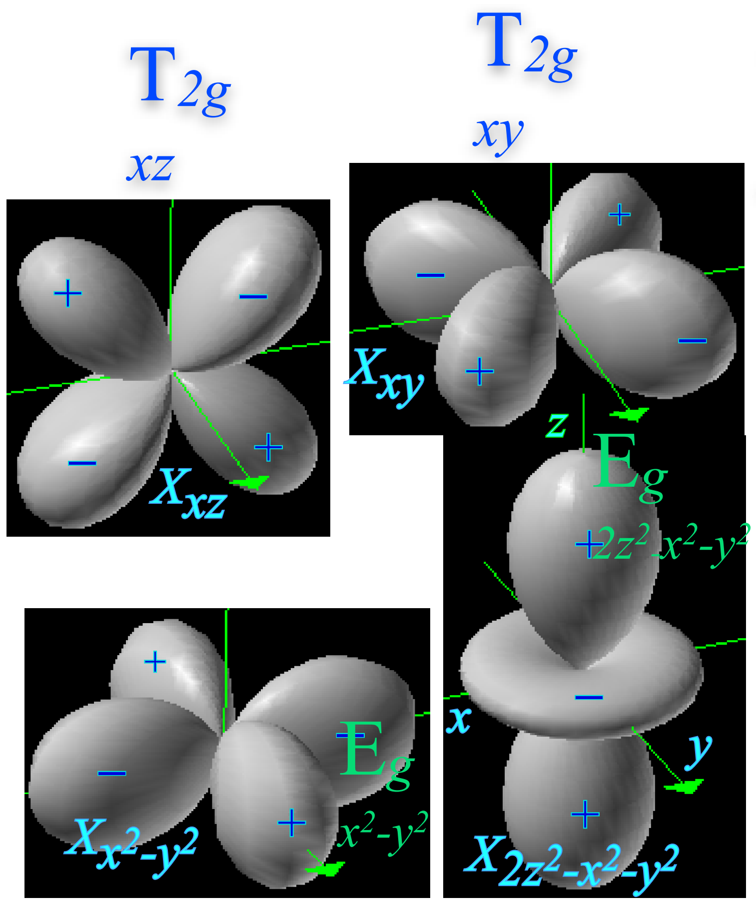
$R(3) \subset O(3) \supset O_h \supset O$ character analysis

(From Principles of Symmetry Dynamics & Spectroscopy Ch.5 p.391)

Frequency of O Irreps

	f^{A_1}	f^{A_2}	f^{E}	f^{T_1}	f^{T_2}	
$l = 0$	1	·	·	·	·	A_{1g}
1	·	·	·	1	·	T_{1u}
2	·	·	1	·	1	$E_g + T_{2g}$
3	·	1	·	1	1	$A_{2u} + T_{1u} + T_{2u}$
4	1	·	1	1	1	$A_{1g} + E_g + T_{1g} + T_{2g}$





$j = 2$
Standing
d-Waves

Figure 5.6.3 Detailed sketch of octahedral splitting of a d orbital. The wave functions $\left\langle \middle| {E \atop 2} \right\rangle$ and $\left\langle \middle| {T_2 \atop 3} \right\rangle$ are sketched inside the equipotential contour $x^4 + y^4 = \text{constant}$ $(z = 0)$.

$R(3) \subset O(3) \supset O_h \supset O$ character analysis

(From Principles of Symmetry Dynamics & Spectroscopy Ch.5 p.385)

	Trace $\mathscr{D}^l(\omega 00)$				
	$\omega = 0°$	$\omega = 120°$	$\omega = 180°$	$\omega = 90°$	$\omega = 180°$
$l = 0$	1	1	1	1	1
1	3	0	−1	1	−1
2	5	−1	1	−1	1
3	7	1	−1	−1	−1
4	9	0	1	1	1
5	11	−1	−1	1	−1
6	13	1	1	−1	1
7	15	0	−1	−1	−1
8	17	−1	1	1	1
9	19	1	−1	1	−1
10	21	0	1	−1	1
11	23	−1	−1	−1	−1
12	25	1	1	1	1
13	27	0	−1	1	−1
14	29	−1	1	−1	1
15	31	1	−1	−1	−1
16	33	0	1	1	1
17	35	−1	−1	1	−1
18	37	1	1	−1	1
19	39	0	−1	−1	−1
20	41	−1	1	1	1

(5.6.5a)

Single Electron Orbital Spectroscopic Labeling		Frequency of O Irreps					
		f^{A_1}	f^{A_2}	f^{E}	f^{T_1}	f^{T_2}	
s_g *"sharp"*	$l = 0$	1	·	·	·	·	A_{1g}
P_u *"principal"*	1	·	·	·	1	·	T_{1u}
d_g *"diffuse"*	2	·	·	1	·	1	$E_g + T_{2g}$
f_u *"fine"*	3	·	1	·	1	1	$A_{2u} + T_{1u} + T_{2u}$
g_g *"gothcha?"*	4	1	·	1	1	1	$A_{1g} + E_g + T_{1g} + T_{2g}$
h_u *"hell knows??"*	5	·	·	1	2	1	
i_g *"I dunnow!"*	6	1	1	1	1	2	
k_u *"kant'tell!"*	7	·	1	1	2	2	
l_g	8	1	·	2	2	2	
m_u	9	1	1	1	3	2	
n_g	10	1	1	2	2	3	
o_u	11	·	1	2	3	3	
q_g	12	2	1	2	3	3	
r_u	13	1	1	2	4	3	
t_g	14	1	1	3	3	4	
u_u	15	1	2	2	4	4	
	16	2	1	3	4	4	
	17	1	1	3	5	4	
	18	2	2	3	4	5	
	19	1	2	3	5	5	
	20	2	1	4	5	5	

(5.6.5b)

R(3) characters

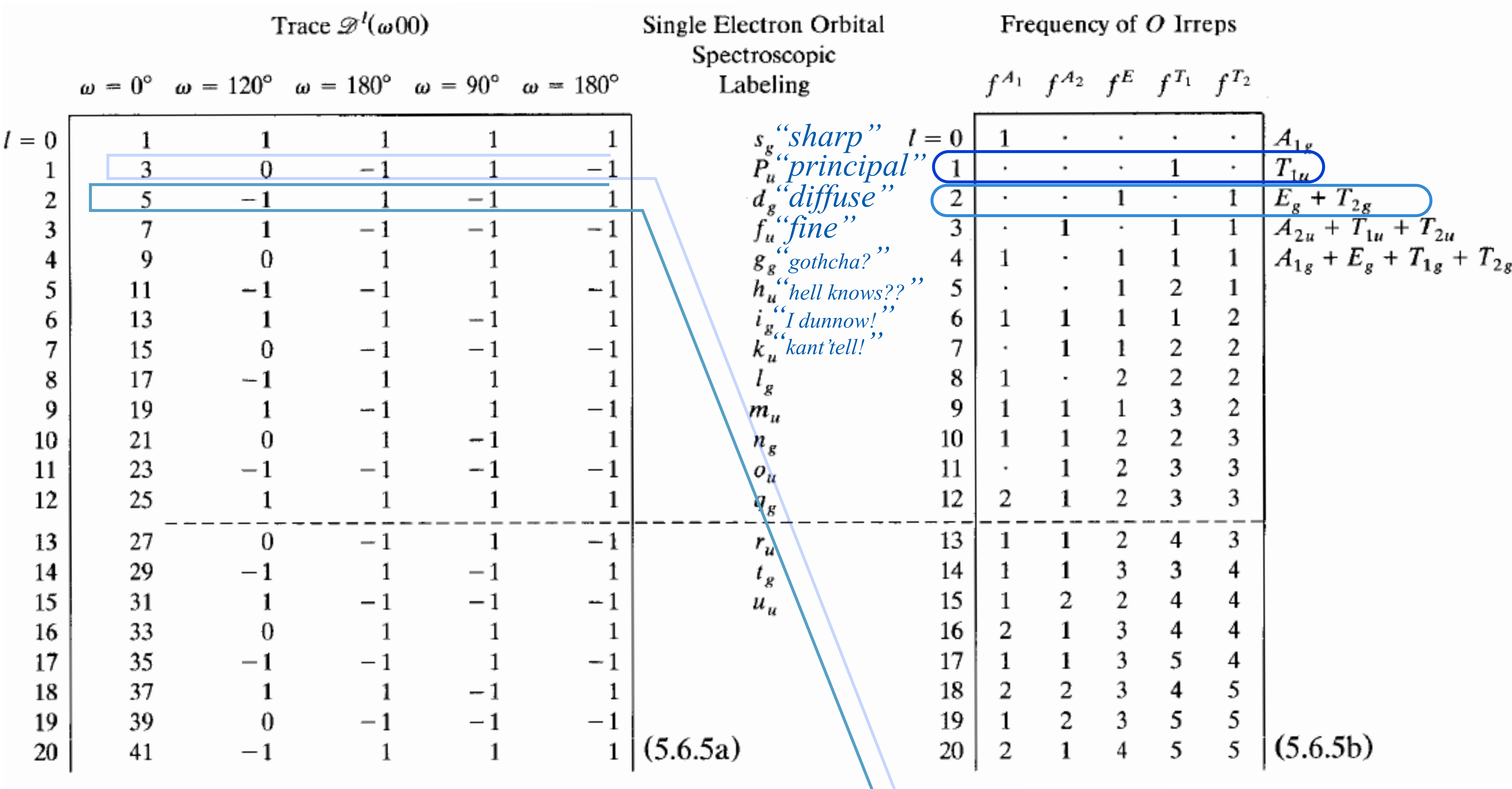
$$\chi^{\ell}(\Theta) = \frac{\sin(\ell + \frac{1}{2})\Theta}{\sin\frac{\Theta}{2}}$$

O characters

O	$\mathbf{1}$	$\mathbf{r}$	$\mathbf{R}^2$	$\mathbf{R}^3$	$\mathbf{i}_k$
A_1	1	1	1	1	1
A_2	1	1	1	-1	-1
E	2	-1	2	0	0
T_1	3	0	-1	1	-1
T_2	3	0	-1	-1	1

$R(3)\subset O(3)\supset O_h\supset O$ character analysis

(From Principles of Symmetry Dynamics & Spectroscopy Ch.5 p.385)



	Trace $\mathscr{D}^l(\omega 00)$					Single Electron Orbital Spectroscopic Labeling		Frequency of O Irreps					
	$\omega = 0°$	$\omega = 120°$	$\omega = 180°$	$\omega = 90°$	$\omega = 180°$			f^{A_1}	f^{A_2}	f^{E}	f^{T_1}	f^{T_2}	
$l = 0$	1	1	1	1	1	s_g "sharp"	$l = 0$	1	·	·	·	·	A_{1g}
1	3	0	−1	1	−1	P_u "principal"	1	·	·	·	1	·	T_{1u}
2	5	−1	1	−1	1	d_g "diffuse"	2	·	·	1	·	1	$E_g + T_{2g}$
3	7	1	−1	−1	−1	f_u "fine"	3	·	1	·	1	1	$A_{2u} + T_{1u} + T_{2u}$
4	9	0	1	1	1	g_g "gothcha?"	4	1	·	1	1	1	$A_{1g} + E_g + T_{1g} + T_{2g}$
5	11	−1	−1	1	−1	h_u "hell knows??"	5	·	·	1	2	1	
6	13	1	1	−1	1	i_g "I dunnow!"	6	1	1	1	1	2	
7	15	0	−1	−1	−1	k_u "kant'tell!"	7	·	1	1	2	2	
8	17	−1	1	1	1	l_g	8	1	·	2	2	2	
9	19	1	−1	1	−1	m_u	9	1	1	1	3	2	
10	21	0	1	−1	1	n_g	10	1	1	2	2	3	
11	23	−1	−1	−1	−1	o_u	11	·	1	2	3	3	
12	25	1	1	1	1	q_g	12	2	1	2	3	3	
13	27	0	−1	1	−1	r_u	13	1	1	2	4	3	
14	29	−1	1	−1	1	t_g	14	1	1	3	3	4	
15	31	1	−1	−1	−1	u_u	15	1	2	2	4	4	
16	33	0	1	1	1		16	2	1	3	4	4	
17	35	−1	−1	1	−1		17	1	1	3	5	4	
18	37	1	1	−1	1		18	2	2	3	4	5	
19	39	0	−1	−1	−1		19	1	2	3	5	5	
20	41	−1	1	1	1		20	2	1	4	5	5	

(5.6.5a) (5.6.5b)

R(3) characters

$$\chi^{\ell}(\Theta) = \frac{\sin(\ell + \frac{1}{2})\Theta}{\sin\frac{\Theta}{2}}$$

O characters

O	**1**	**r**	$\mathbf{R}^2$	$\mathbf{R}^3$	$\mathbf{i}_k$
A_1	1	1	1	1	1
A_2	1	1	1	-1	-1
E	2	-1	2	0	0
T_1	3	0	-1	1	-1
T_2	3	0	-1	-1	1

AMOP reference links on page 2

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$R(3)\subset O(3)\supset O_h\supset O$ cluster structure

(From Principles of Symmetry Dynamics & Spectroscopy Ch.5 p.403)

ROTATIONAL LEVEL SPLITTING IN FINITE SYMMETRY 403

$(A_1\ T_1\ E)_{0_4}\ (T_2\ T_1)_{3_4}\ (E\ T_2\ A_2)_{2_4}\ (T_2\ T_1)_{1_4}\ldots(A_2\ T_2\ T_1\ A_1)_{0_3}\ (T_1\ E\ T_2)_{1_3}\ (T_1\ E\ T_2)_{2_3}\ \ldots$

Bands or "Clusters"
of levels maintain order
but change spacing as
they adapt to varying
local symmetries by
crossing separatrices
in their phase space
(see p. 73-77)

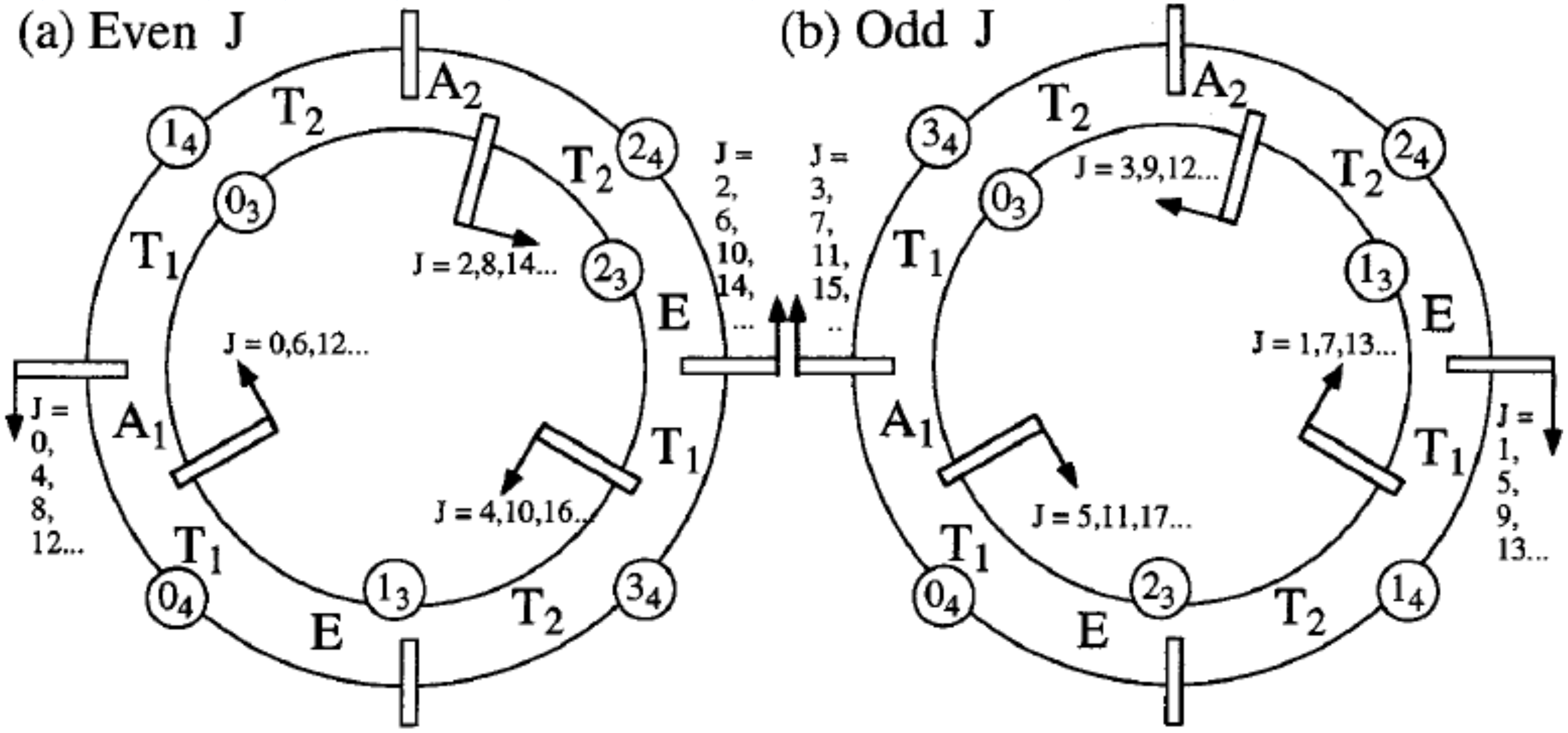
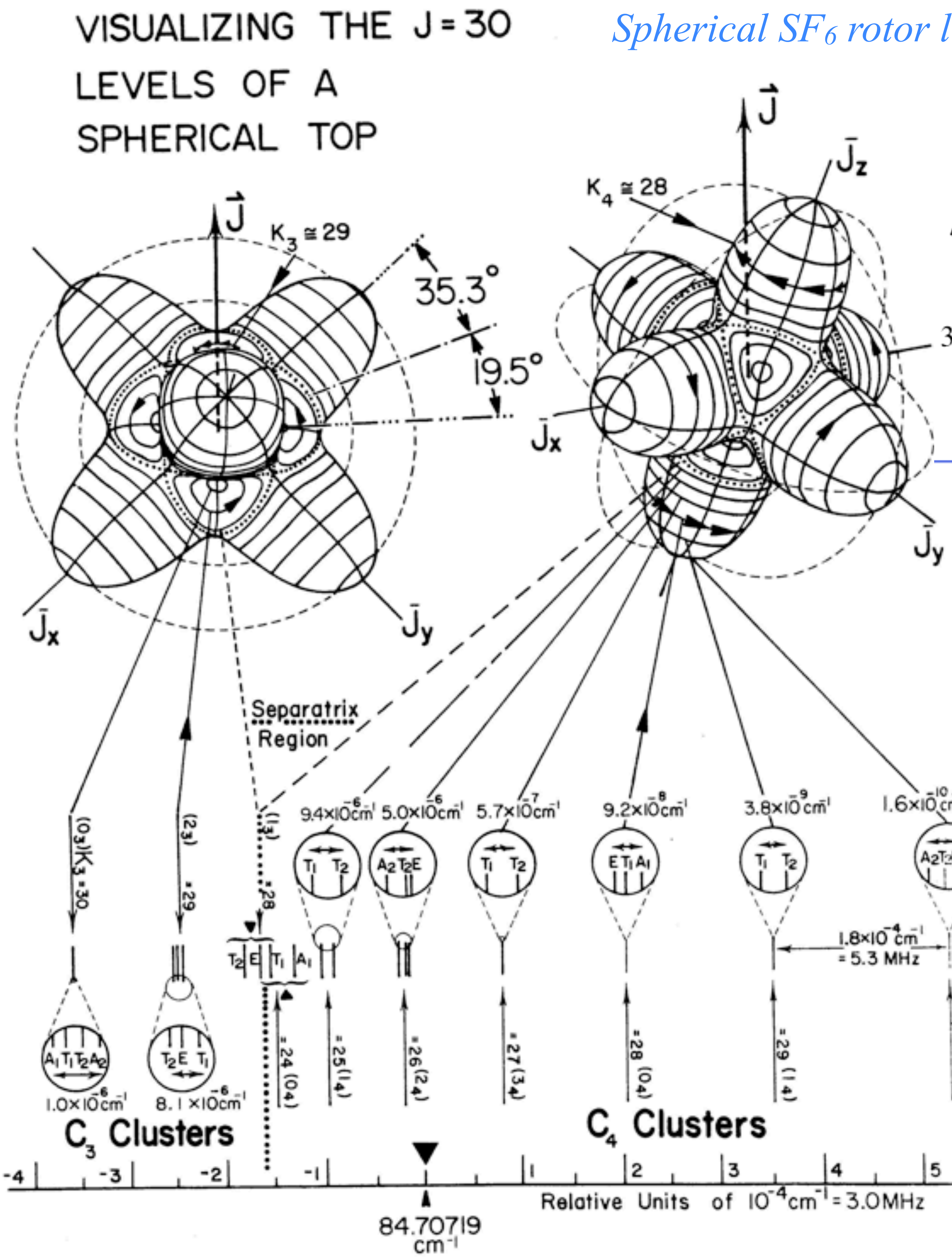
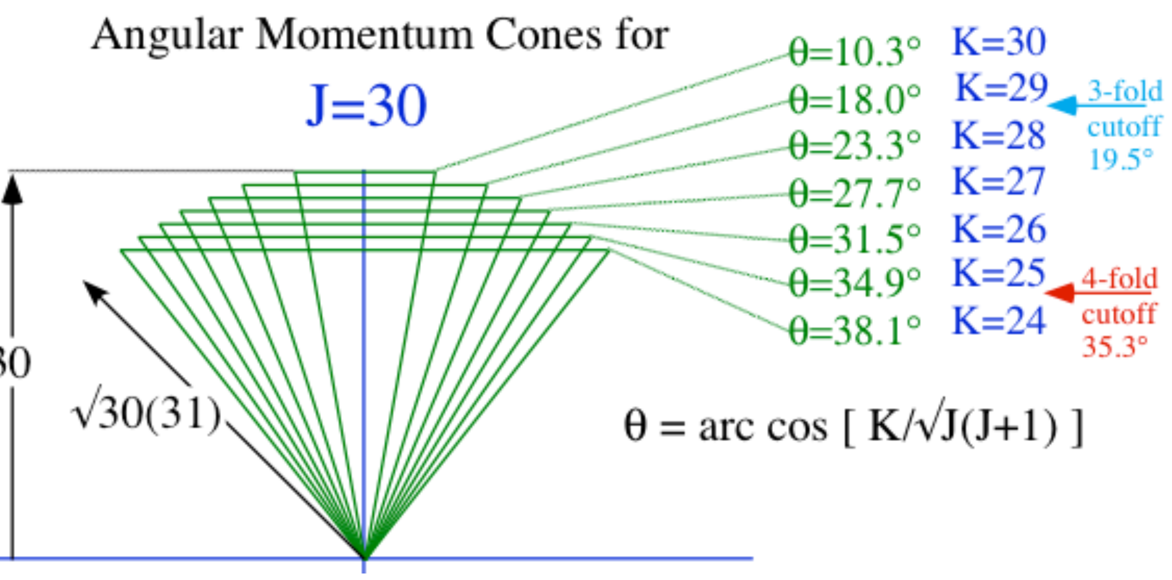
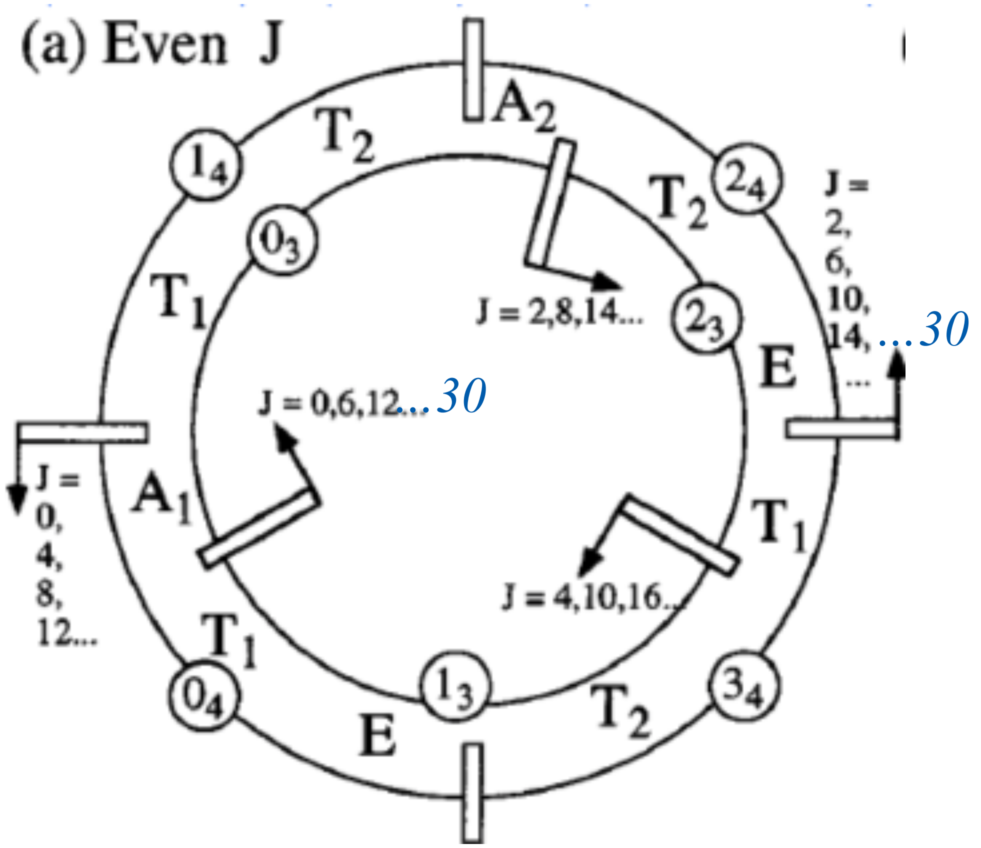


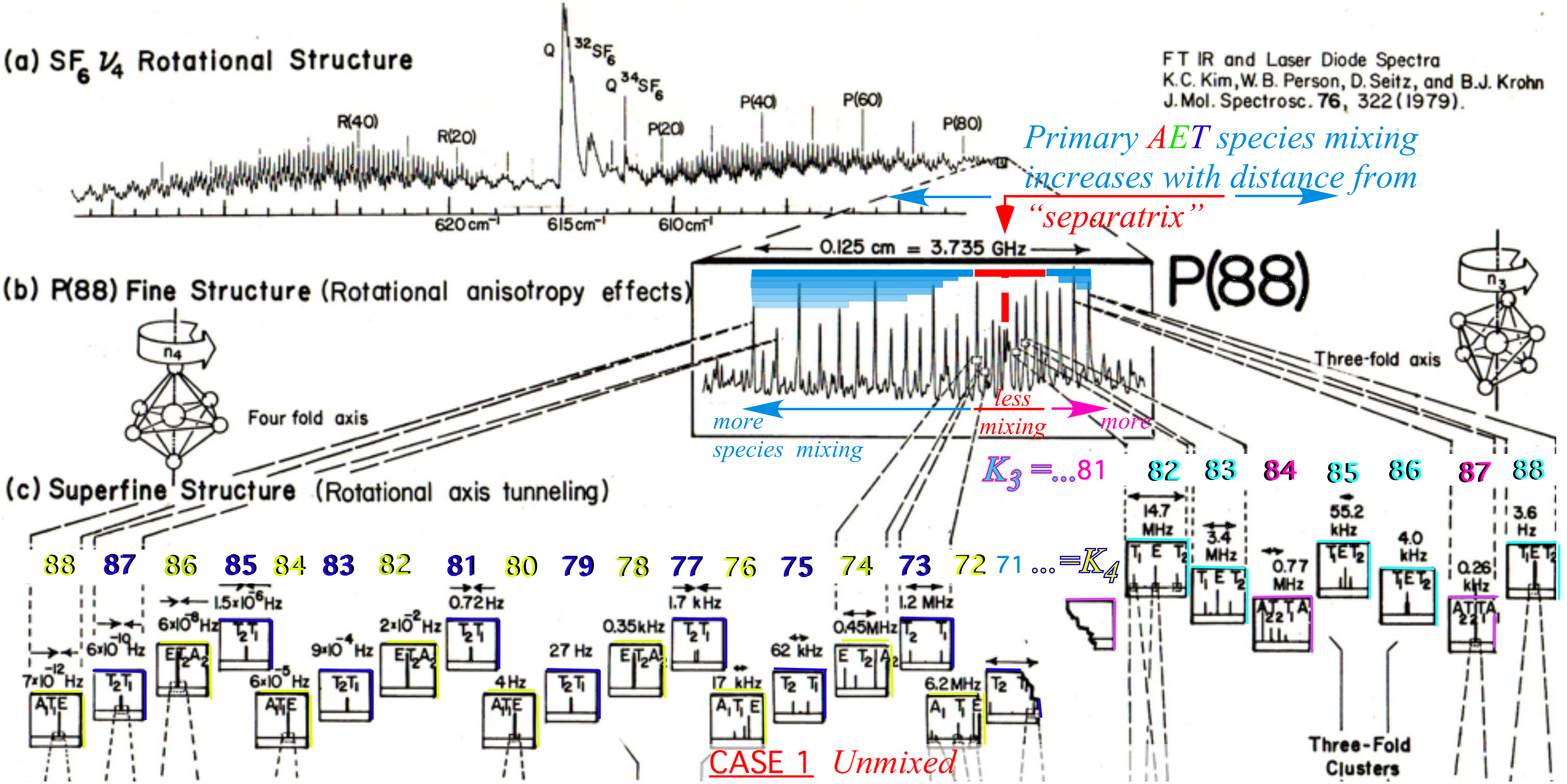
Figure 5.6.9 Mnemonic wheels for octahedral-*O* orbital. Splitting of *J* levels for (a) even *J* and (b) odd *J*.

Spherical SF$_6$ rotor levels









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

more species mixing

less mixing

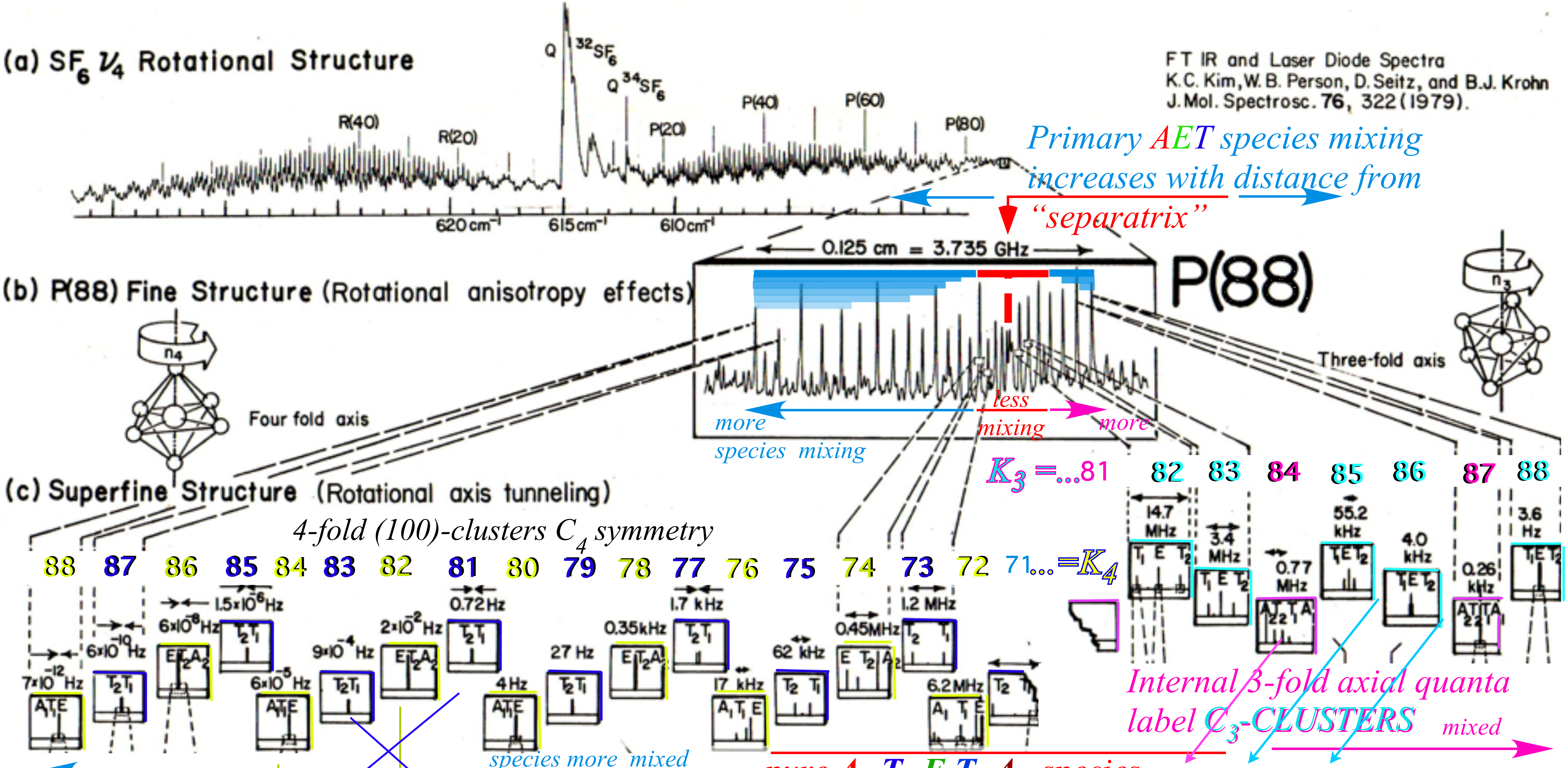
more

CASE 1 *Unmixed*

PQR structure due to Coriolis scalar interaction between vibrational angular momentum ℓ and total momentum $\mathbf{J} = \ell + \mathbf{N}$ *of rotating nuclei*

P(N)=P(88) structure due to tensor centrifugal/Coriolis due to vibrational ℓ and total momentum $\mathbf{J} = \ell + \mathbf{N}$

Superfine structure modeled by **J***-tunneling in body frame (Underlying* F*-spin-permutation symmetry is involved, too.)*



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

more species mixing

less mixing

more

4-fold (100)-clusters C_4 symmetry

species more mixed

pure A_1 T_1 E T_2 A_2 species

Internal 3-fold axial quanta label C_3-CLUSTERS

mixed

Cubic Octahedral symmetry O

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

3 modulo 4 equals -1 modulo 4 (and 83 mod 4)

83=84-1

4-fold (1oo) C_4 symmetry clusters

3-fold (111) C_3 symmetry clusters

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

(2 modulo 3 equals -1 modulo 3 and 86 mod 3)

86=88-1

Spin-rotor S_N-tableau super-hyperfine theory: see p. 11 of Lecture 29

AMOP
reference links
on page 2

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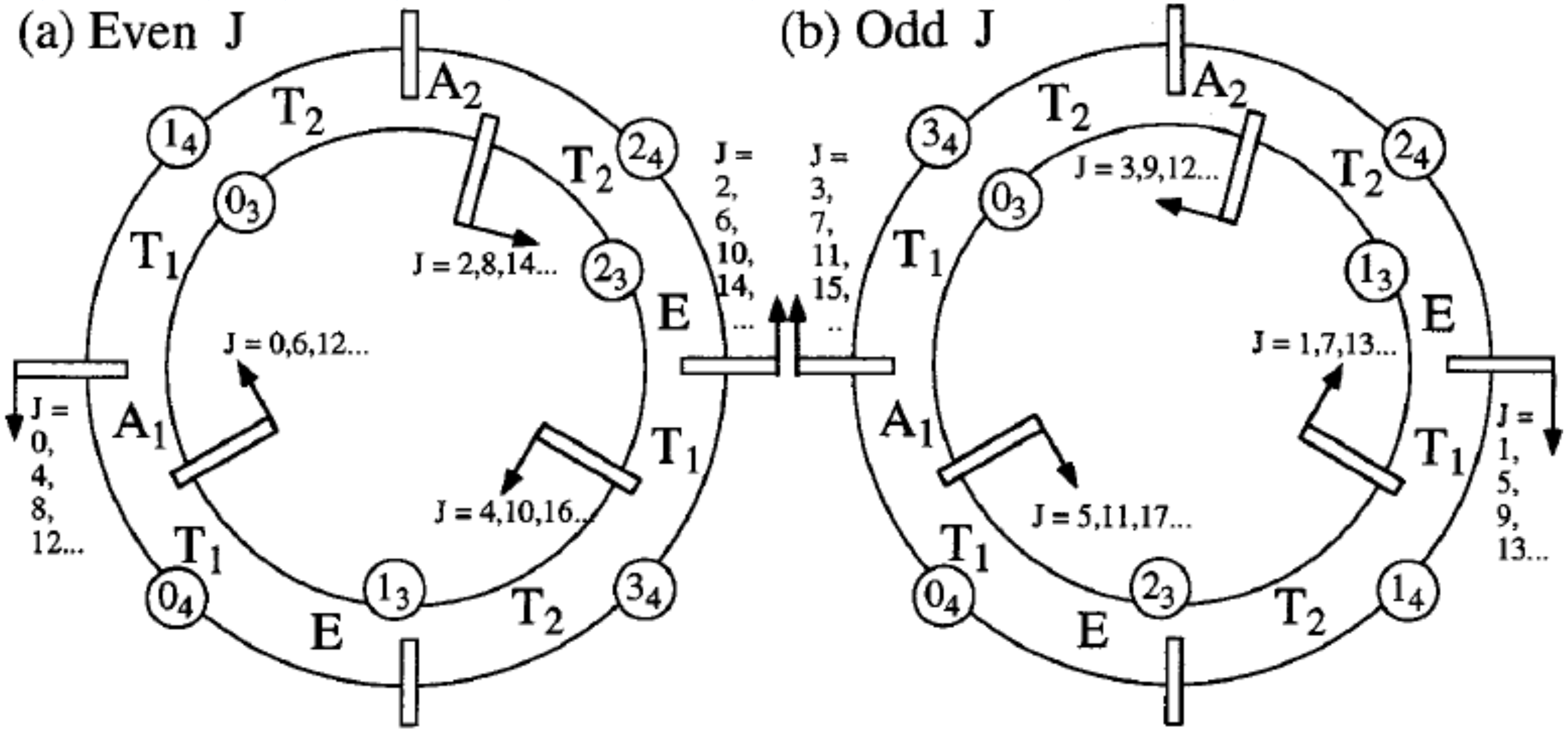
Bands or "Clusters" of levels maintain order but change spacing as they adapt to varying local symmetries and separatrix crossing in their phase space (see p. 73-77)

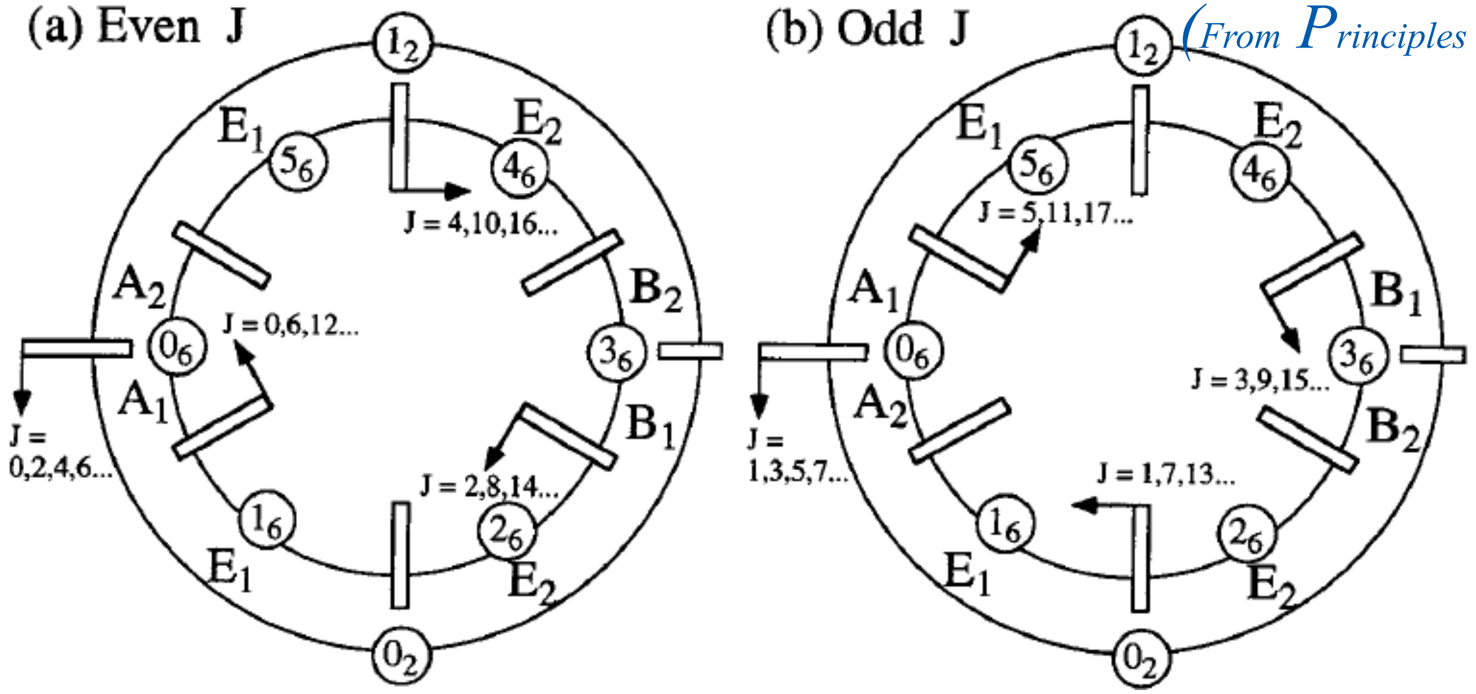
ROTATIONAL LEVEL SPLITTING IN FINITE SYMMETRY 403



$O(3)\supset D_6$ band clusters

$(A_1\ E_1\ E_2\ B_1)_{0_2}\ (B_2\ E_2\ E_1\ A_2)_{1_2}\ldots(A_2A_1)_{0_6}\ (E_1)_{1_6}\ (E_2)_{2_6}\ (B_1\ B_2)_{3_6}(E_2)_{4_6}\ (E_1)_{5_6}\ldots$

(*From Principles of Symmetry Dynamics & Spectroscopy Ch.5 p.402*)

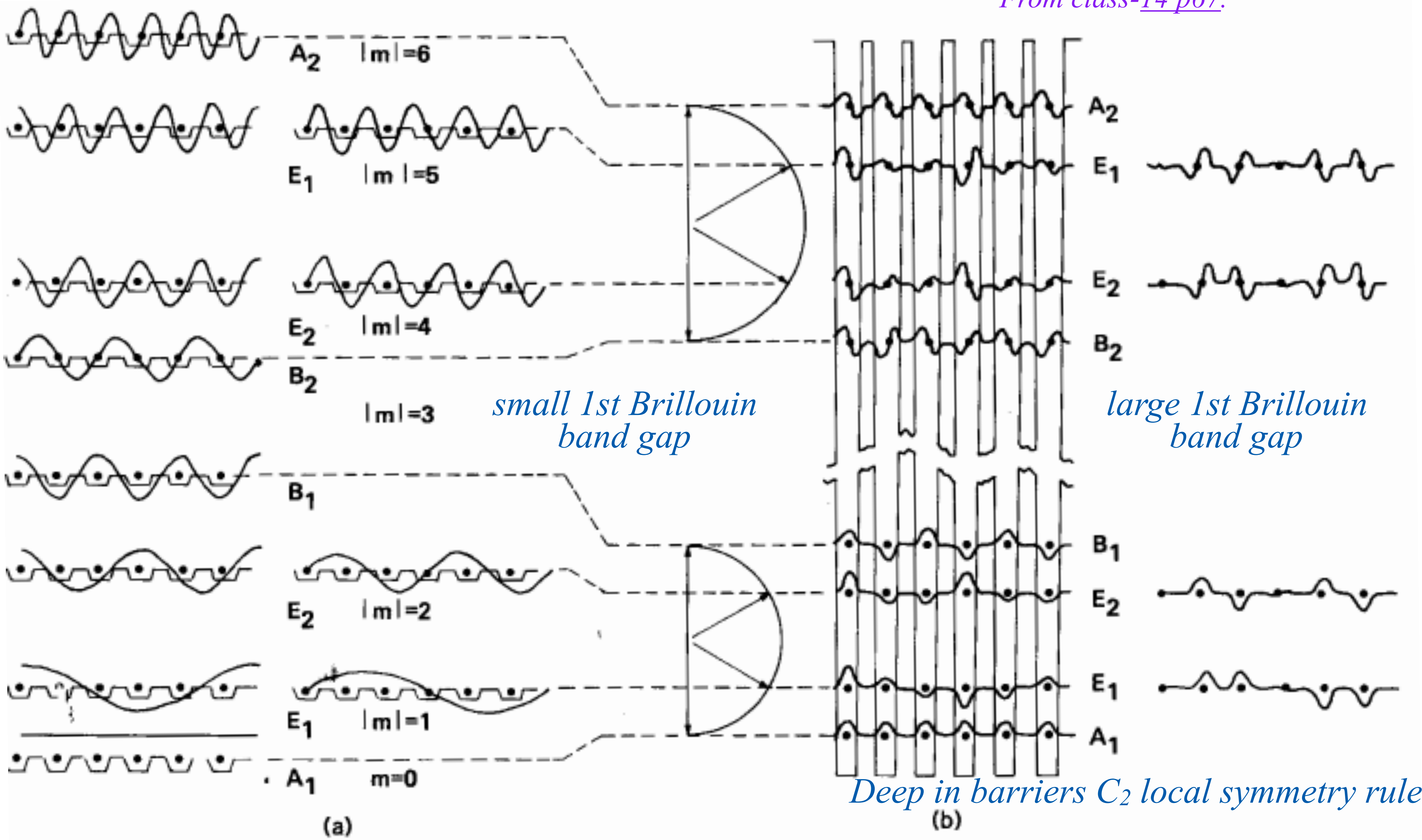


(see the following two pages where "band" and "gap" spacing varies with energy)

D_6 Band structure and related Global vs Local induced representations

High above low barriers $D_6 \supset C_6$ global symmetry rules

From class-14 p67.



small 1st Brillouin band gap

large 1st Brillouin band gap

Deep in barriers C_2 local symmetry rules

Figure 3.6.5 One-dimensional Bohr and Bloch waves in D_6 symmetry. (a) Weak D_6 potential. (b) Strong D_6 potential.

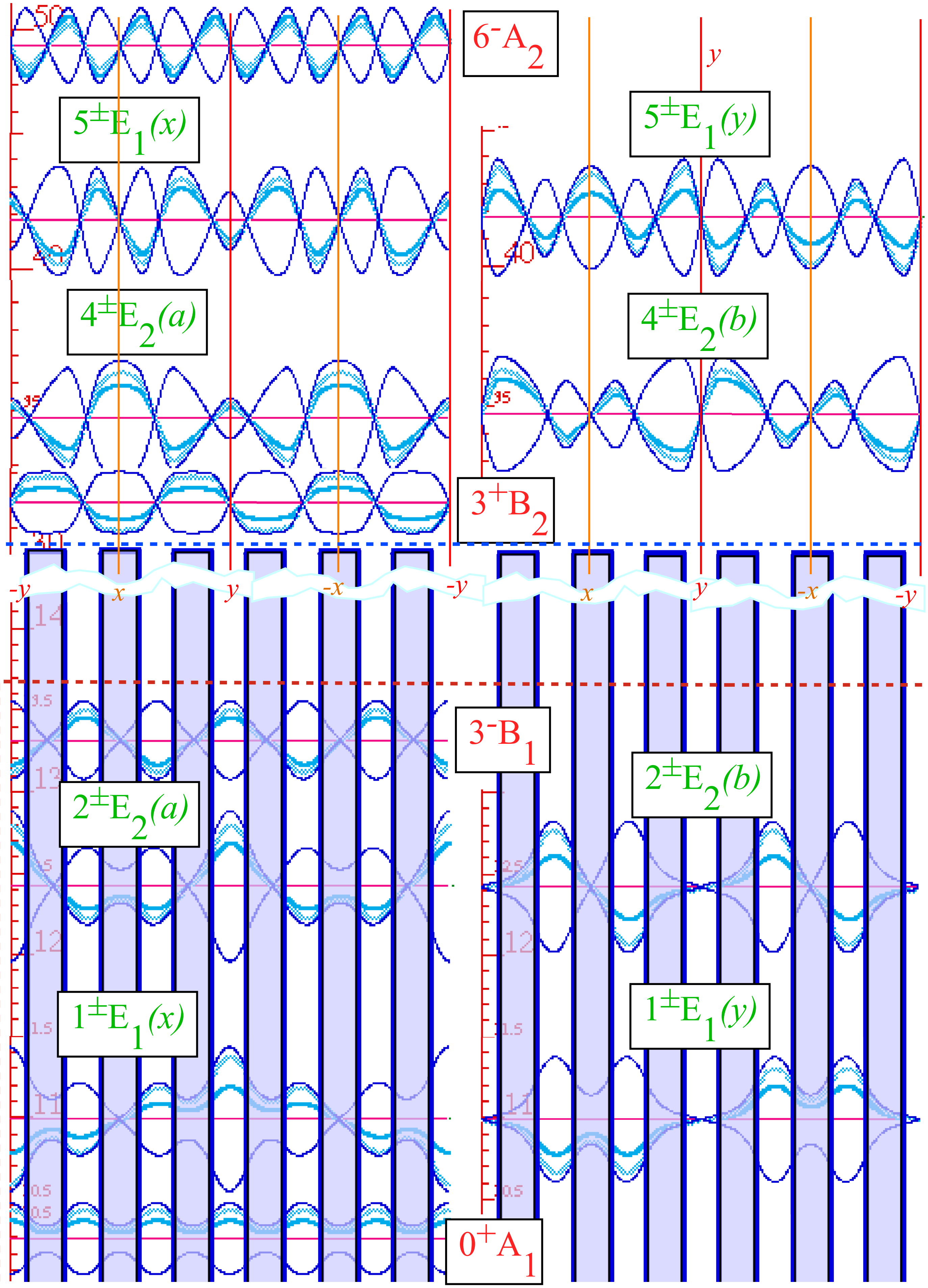
PSDS Ch.3 p 50.

D_6
Band structure and related Global vs Local induced representations

(BohrIt Mac OS-9)

D_6
Band structure
QTCA
Unit 5
p96

From class-14 p68.



Low barrier->D_6 global symm.
m_6 still valid quantum number

$D_6 \supset C_6(h)$	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

$1_2 \uparrow D_6 \sim A_2 \oplus E_2 \oplus E_1 \oplus B_2$

Odd Band or Cluster

$0_2 \uparrow D_6 \sim A_1 \oplus E_1 \oplus E_2 \oplus B_1$

Even Band or Cluster

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

AMOP reference links on page 2

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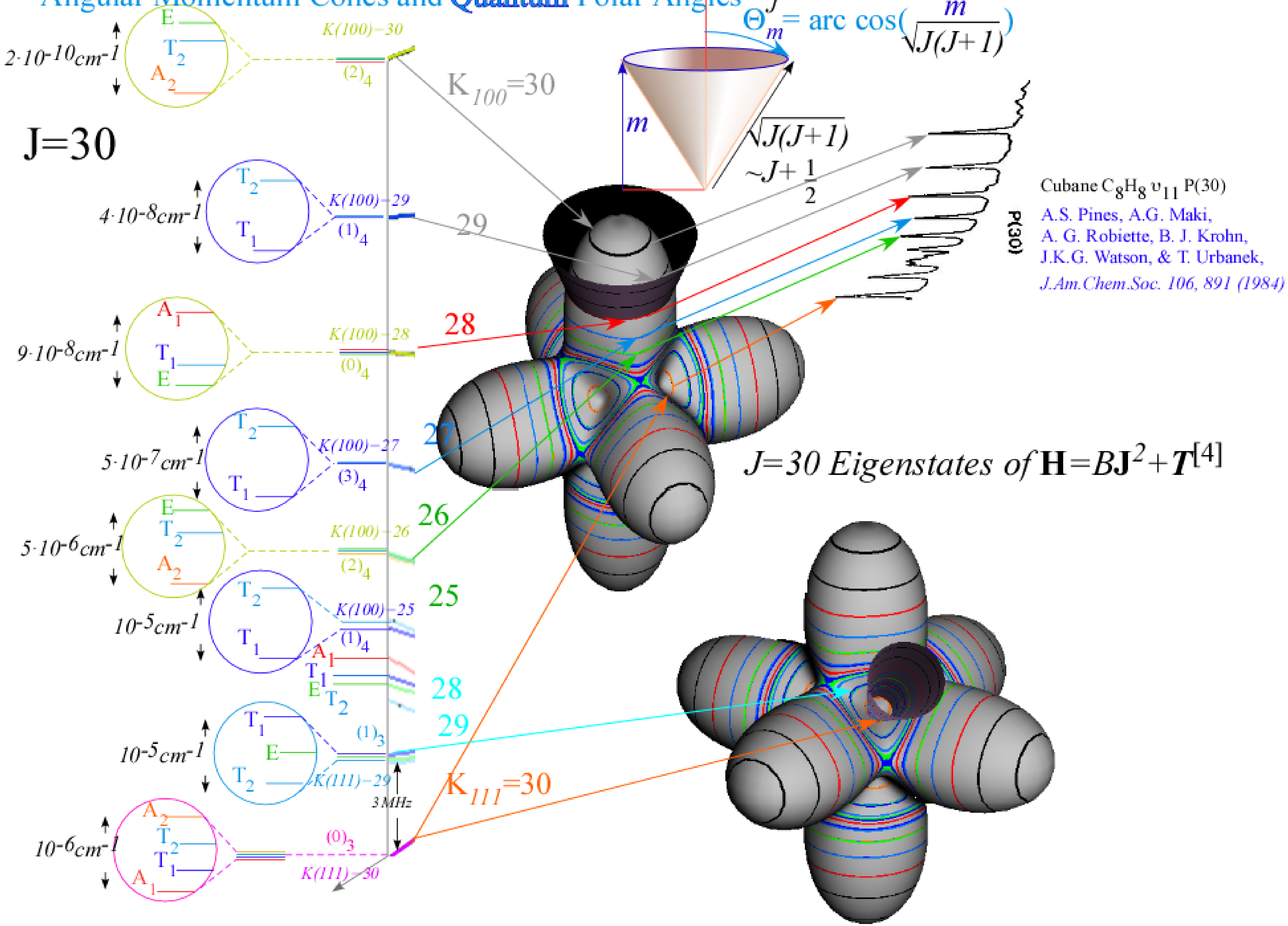
Angular Momentum Cones and Quantum Polar Angles

$$\Theta^J_m = \arccos\left(\frac{m}{\sqrt{J(J+1)}}\right)$$



Cubane C_8H_8 υ_{11} P(30)
A.S. Pines, A.G. Maki,
A. G. Robiette, B. J. Krohn,
J.K.G. Watson, & T. Urbanek,
J.Am.Chem.Soc. 106, 891 (1984)

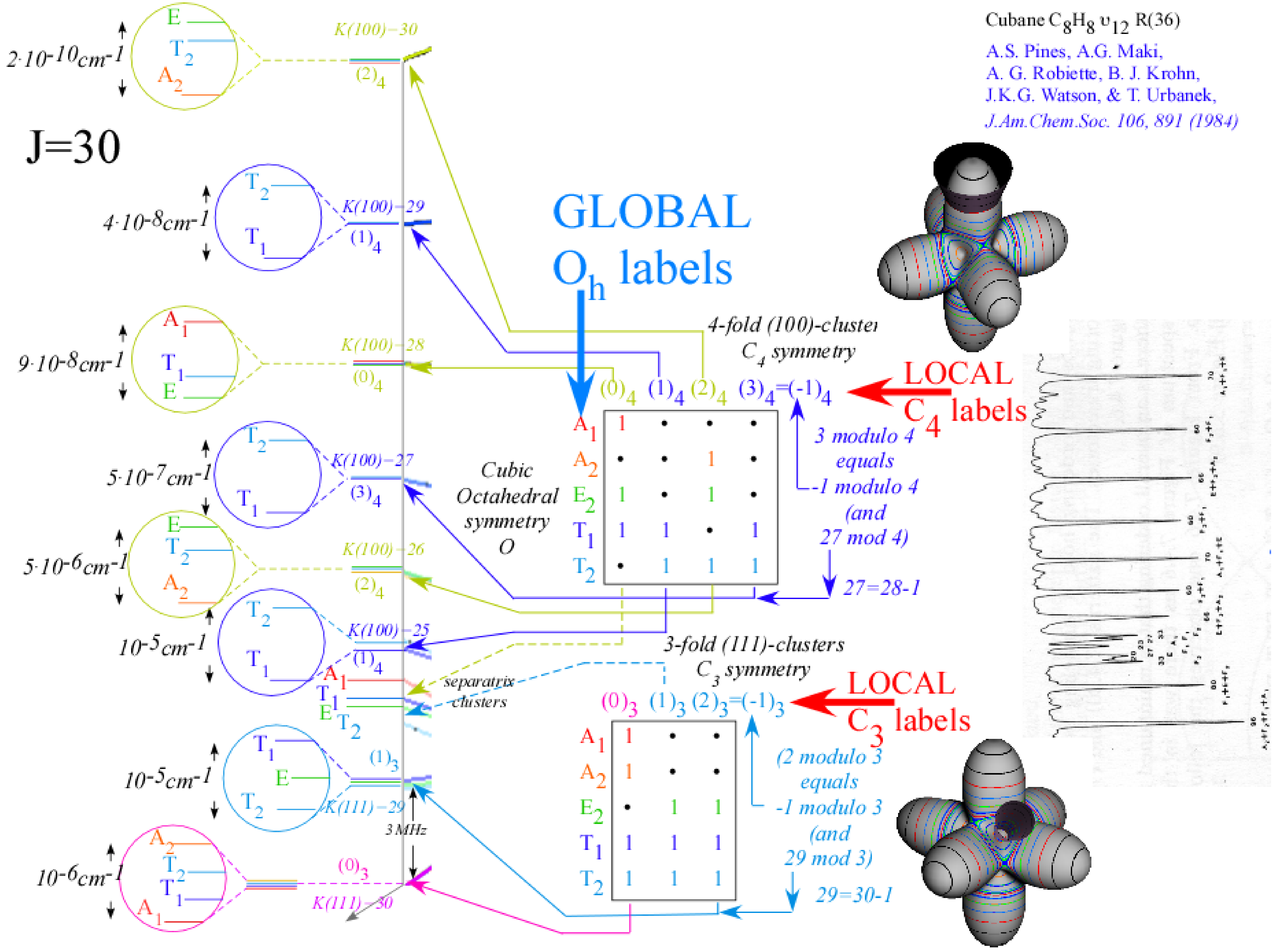
J=30 Eigenstates of $\mathbf{H}=B\mathbf{J}^2+T^{[4]}$

"Tunable Laser Spectra of the Infrared-Active Fundamentals of Cubane" J. Am. Chem. Soc. 106, 891 (1984)

Review: Spherical rotor levels and spectra

Cubane C_8H_8 υ_{12} R(36)

A.S. Pines, A.G. Maki,
A. G. Robiette, B. J. Krohn,
J.K.G. Watson, & T. Urbanek,
J.Am.Chem.Soc. 106, 891 (1984)



	$(0)_4$	$(1)_4$	$(2)_4$	$(3)_4=(-1)_4$
A_1	1	•	•	•
A_2	•	•	1	•
E_2	1	•	1	•
T_1	1	1	•	1
T_2	•	1	1	1

	$(0)_3$	$(1)_3$	$(2)_3=(-1)_3$
A_1	1	•	•
A_2	1	•	•
E_2	•	1	1
T_1	1	1	1
T_2	1	1	1

"Tunable Laser Spectra of the Infrared-Active Fundamentals of Cubane" J. Am. Chem. Soc. 106, 891 (1984)

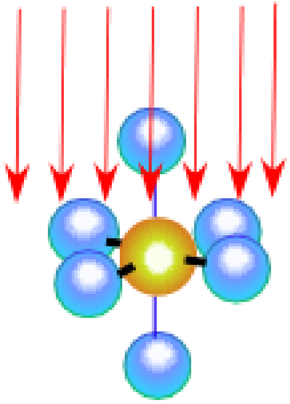
Duality: The "Flip Side" of Symmetry Analysis.

LAB versus BODY, STATE versus PARTICLE,

boils down to :

OUTSIDE versus INSIDE

OUTSIDE or LAB
Symmetry reduction
results in
Level or Spectral
SPLITTING
External B-field
does Zeeman splitting

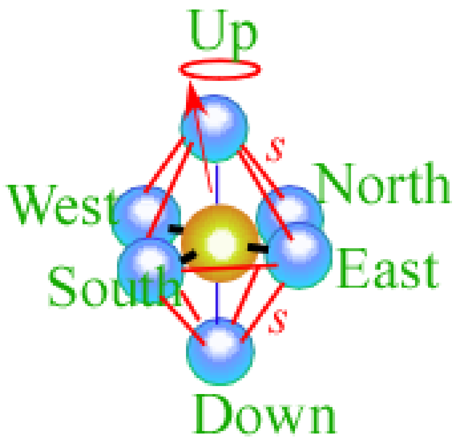


Example:
Cubic-Octahedral O
reduced to
Tetragonal C_4

C_4	0_4	1_4	2_4	3_4
A_1	1	.	.	.
A_2	.	.	1	.
E	1.	.	1	.
T_1	1	1	.	1
T_2	.	1	1	1

INSIDE or BODY
Symmetry reduction
results in
Level or Spectral
UN-SPLITTING
("clustering")

*Internal **J** gets "stuck" on RES axes*
Must "tunnel" axis-to-axis at rate s



$$\begin{array}{cccccc}
|U\rangle & |D\rangle & |E\rangle & |W\rangle & |N\rangle & |S\rangle \\
H & 0 & s & s & s & s \\
0 & H & s & s & s & s \\
s & s & H & 0 & s & s \\
s & s & 0 & H & s & s \\
s & s & s & s & H & 0 \\
s & s & s & s & 0 & H
\end{array}$$

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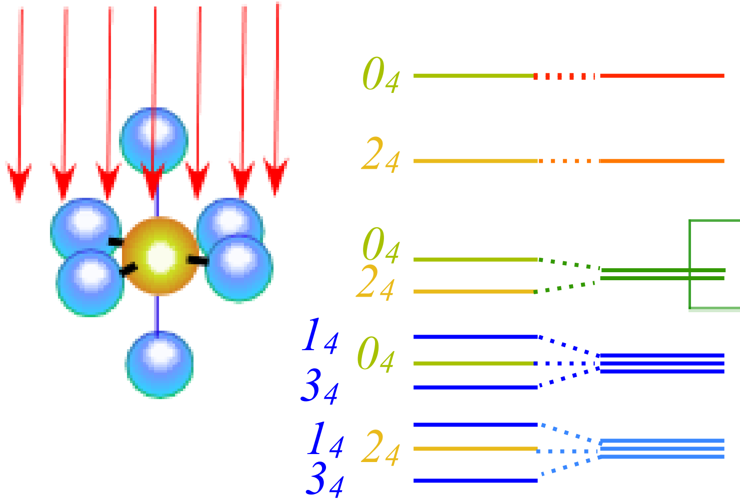
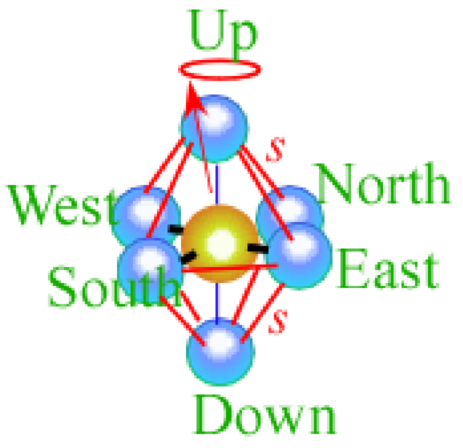


C_4	0_4	1_4	2_4	3_4
A_1	1	.	.	.
A_2	.	.	1	.
E	1.	.	1	.
T_1	1	1	.	1
T_2	.	1	1	1

Internal ***J*** gets "stuck" on RES axes
Must "tunnel" axis-to-axis at rate s



$$\begin{array}{cccccc} |U\rangle & |D\rangle & |E\rangle & |W\rangle & |N\rangle & |S\rangle \\ H & 0 & s & s & s & s \\ 0 & H & s & s & s & s \\ s & s & H & 0 & s & s \\ s & s & 0 & H & s & s \\ s & s & s & s & H & 0 \\ s & s & s & s & 0 & H \end{array}$$

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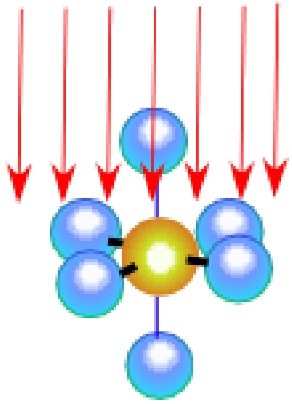

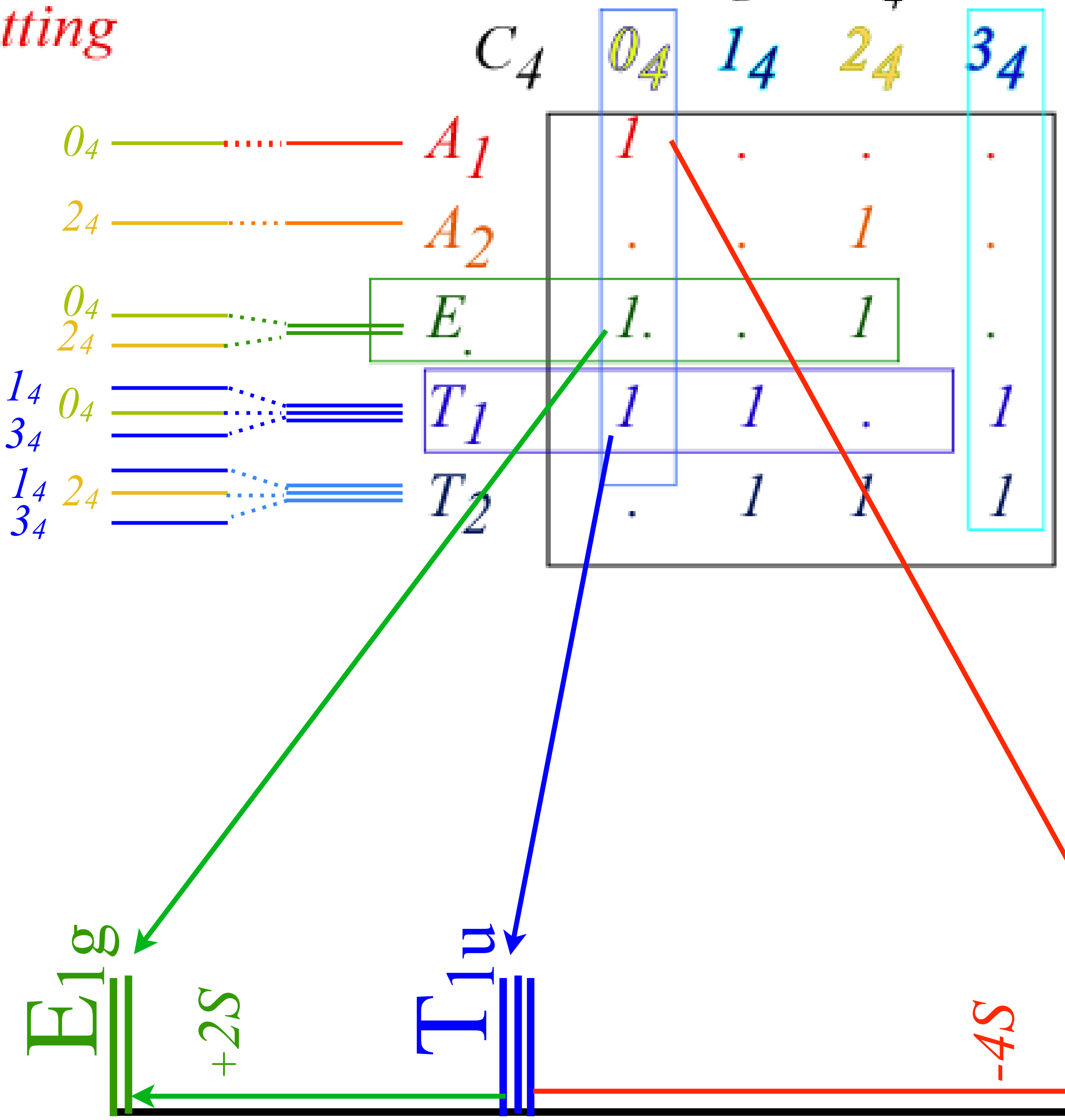

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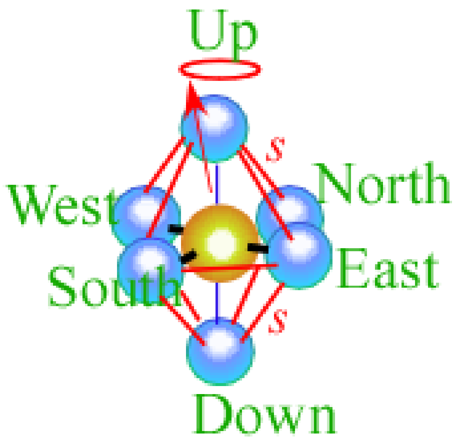
A_1	1	.	.	.
A_2	.	.	1	.
E	1.	.	1	.
T_1	1	1	.	1
T_2	.	1	1	1



|U>	|D>	|E>	|W>	|N>	|S>
H	0	s	s	s	s
0	H	s	s	s	s
s	s	H	0	s	s
s	s	0	H	s	s
s	s	s	s	H	0
s	s	s	s	0	H

Tunneling (s) between axes
*splits the **0_4** cluster*

AMOP
reference links
on page 2

3.05.18 class 15.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Discrete symmetry subgroups of O(3)⊃(Octahedral O_h⊃O~T_d, Cubic-Tetrahedral T_h⊃T): Characters and subgroup-chain defined ireps, and applications to SF_6 and CF_4 spectra

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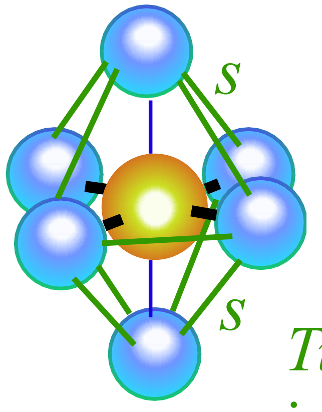
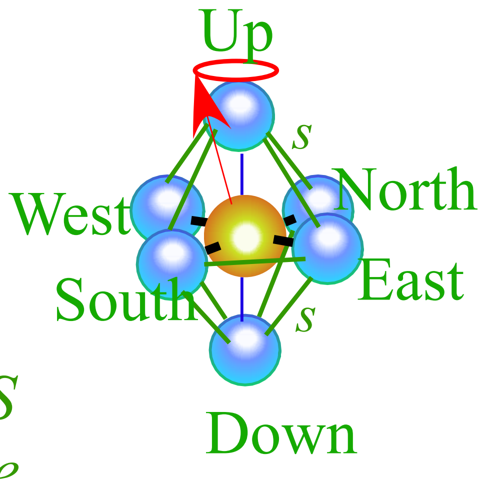
*Internal **J** gets "stuck" on RES axes*
Must "tunnel" axis-to-axis at rate s



Tunneling s=-S
is negative here

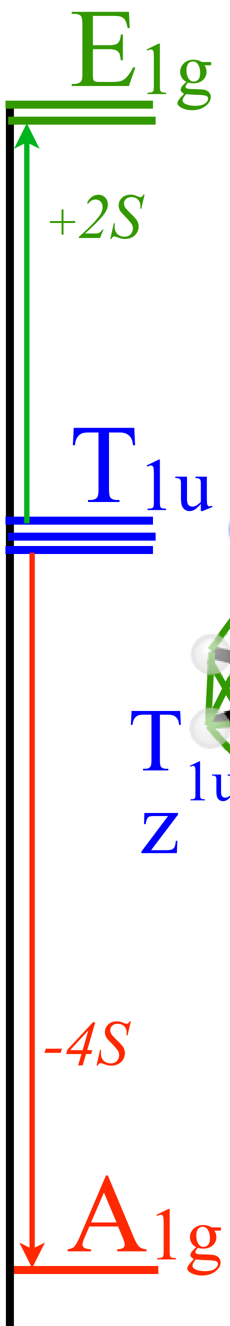


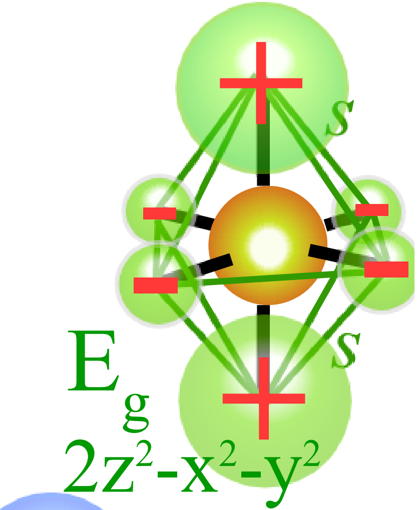
$$\begin{array}{cccccc}
|U\rangle & |D\rangle & |E\rangle & |W\rangle & |N\rangle & |S\rangle \\
\hline
H & 0 & s & s & s & s \\
0 & H & s & s & s & s \\
s & s & H & 0 & s & s \\
s & s & 0 & H & s & s \\
s & s & s & s & H & 0 \\
s & s & s & s & 0 & H
\end{array}$$

$$\left|\begin{matrix} H & 0 & s & s & s & s \\ 0 & H & s & s & s & s \\ s & s & H & 0 & s & s \\ s & s & 0 & H & s & s \\ s & s & s & s & H & 0 \\ s & s & s & s & 0 & H \end{matrix}\right\| \left|\begin{matrix} +2 \\ +2 \\ -1 \\ -1 \\ -1 \\ -1 \end{matrix}\right| \frac{1}{\sqrt{12}} = (H-2s) \left|\begin{matrix} +2 \\ +2 \\ -1 \\ -1 \\ -1 \\ -1 \end{matrix}\right| \frac{1}{\sqrt{12}}$$

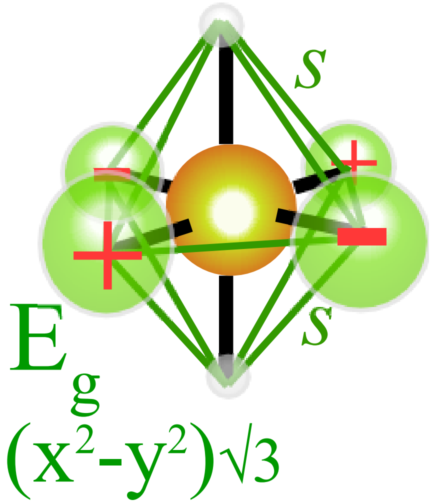
$$\left|\begin{matrix} H & 0 & s & s & s & s \\ 0 & H & s & s & s & s \\ s & s & H & 0 & s & s \\ s & s & 0 & H & s & s \\ s & s & s & s & H & 0 \\ s & s & s & s & 0 & H \end{matrix}\right\| \left|\begin{matrix} +1 \\ -1 \\ 0 \\ 0 \\ 0 \\ 0 \end{matrix}\right| \frac{1}{\sqrt{2}} = (H+0) \left|\begin{matrix} +1 \\ -1 \\ 0 \\ 0 \\ 0 \\ 0 \end{matrix}\right| \frac{1}{\sqrt{2}}$$

$$\left|\begin{matrix} H & 0 & s & s & s & s \\ 0 & H & s & s & s & s \\ s & s & H & 0 & s & s \\ s & s & 0 & H & s & s \\ s & s & s & s & H & 0 \\ s & s & s & s & 0 & H \end{matrix}\right\| \left|\begin{matrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{matrix}\right| \frac{1}{\sqrt{6}} = (H+4s) \left|\begin{matrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{matrix}\right| \frac{1}{\sqrt{6}}$$

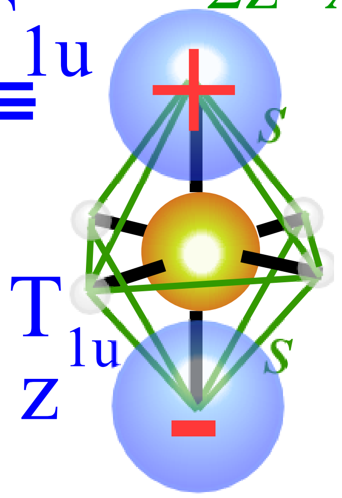




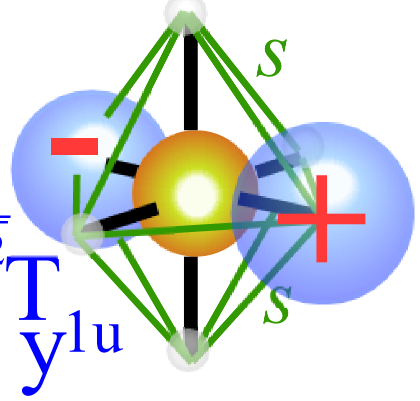
$$\left|\begin{matrix} +2 \\ +2 \\ -1 \\ -1 \\ -1 \\ -1 \end{matrix}\right| \frac{1}{\sqrt{12}}$$

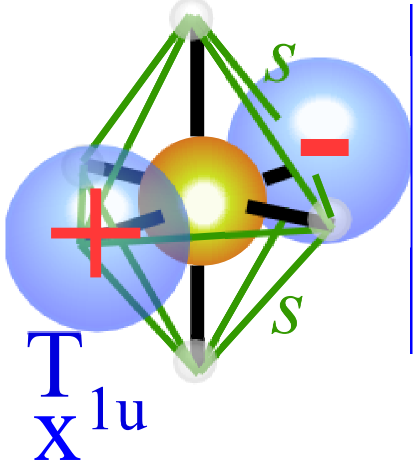


$$\left|\begin{matrix} 0 \\ 0 \\ -1 \\ -1 \\ +1 \\ +1 \end{matrix}\right| \frac{1}{2}$$

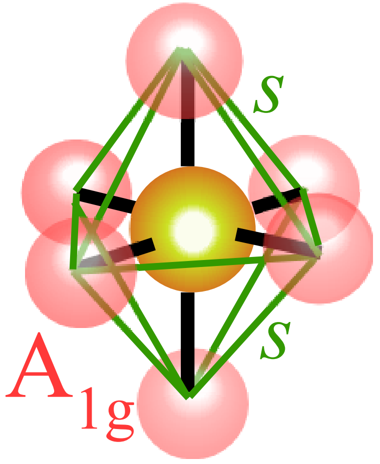


$$\left|\begin{matrix} 0 \\ 0 \\ +1 \\ -1 \\ 0 \\ 0 \end{matrix}\right| \frac{1}{\sqrt{2}}$$





$$\left|\begin{matrix} 0 \\ 0 \\ 0 \\ 0 \\ -1 \\ +1 \end{matrix}\right| \frac{1}{\sqrt{2}}$$



$$\left|\begin{matrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{matrix}\right| \frac{1}{\sqrt{6}}$$

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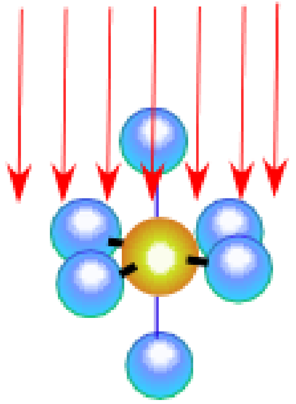
Duality: The “Flip Side” of Symmetry Analysis.

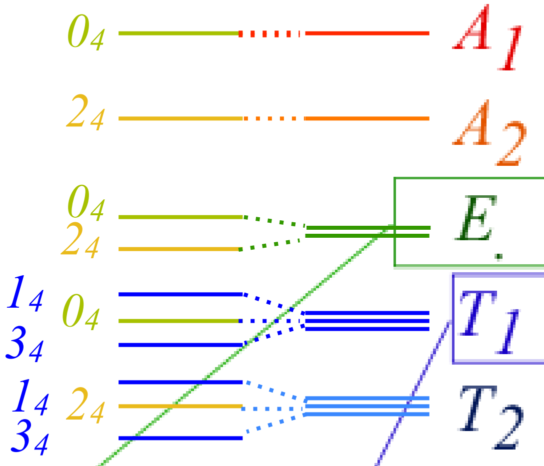
LAB versus BODY, STATE versus PARTICLE,

boils down to :

OUTSIDE versus INSIDE

OUTSIDE or LAB
Symmetry reduction
results in
Level or Spectral
SPLITTING
External B-field
does Zeeman splitting



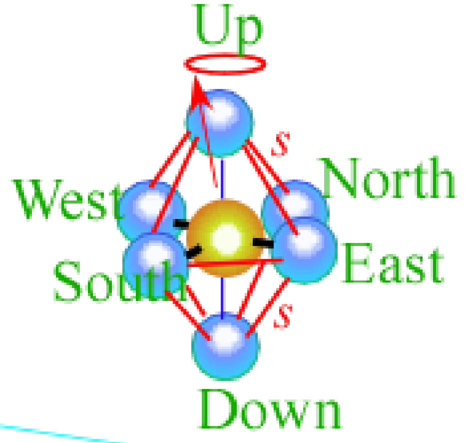


Example:
Cubic-Octahedral O
reduced to
Tetragonal C_4

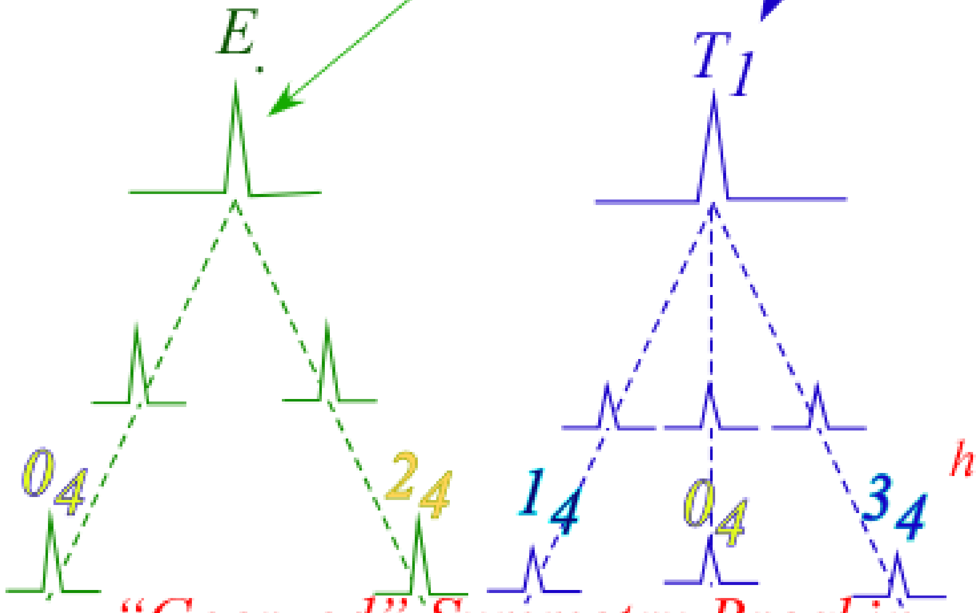
C_4	0_4	1_4	2_4	3_4
A_1	1	.	.	.
A_2	.	.	1	.
E	1.	.	1	.
T_1	1	1	.	1
T_2	.	1	1	1

INSIDE or BODY
Symmetry reduction
results in
Level or Spectral
<u>UN</u>-SPLITTING
(“clustering”)

Internal ***J*** gets “stuck” on RES axes
Must “tunnel” axis-to-axis at rate s



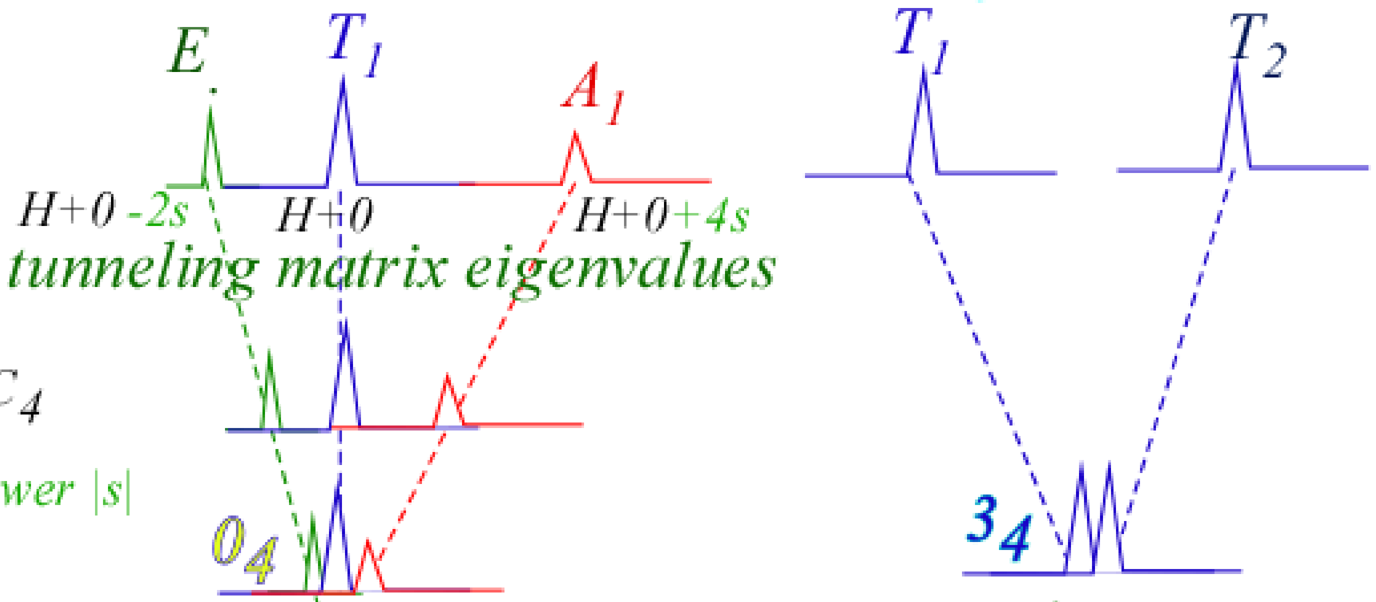
$$\begin{array}{cccccc}
|U\rangle & |D\rangle & |E\rangle & |W\rangle & |N\rangle & |S\rangle \\
H & 0 & s & s & s & s \\
0 & H & s & s & s & s \\
s & s & H & 0 & s & s \\
s & s & 0 & H & s & s \\
s & s & s & s & H & 0 \\
s & s & s & s & 0 & H
\end{array}$$



“Coerced” Symmetry Breaking

Stronger C_4

higher |***B***| lower |s|

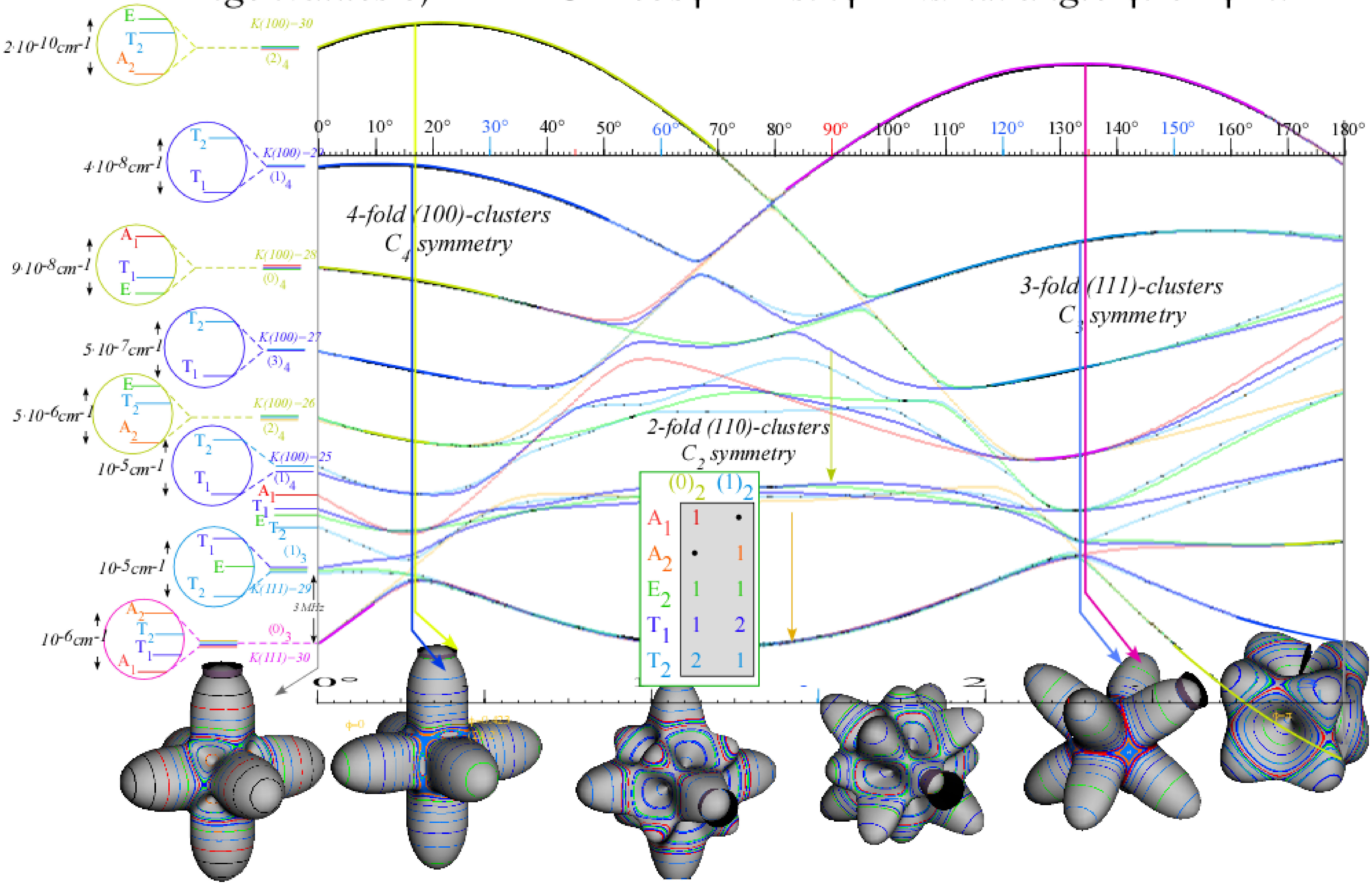


tunneling matrix eigenvalues

“Spontaneous” Symmetry Breaking

J=30 multiplet variation due to adding $\mathbf{T}^{[6]}$ *to* $\mathbf{T}^{[4]}$

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



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

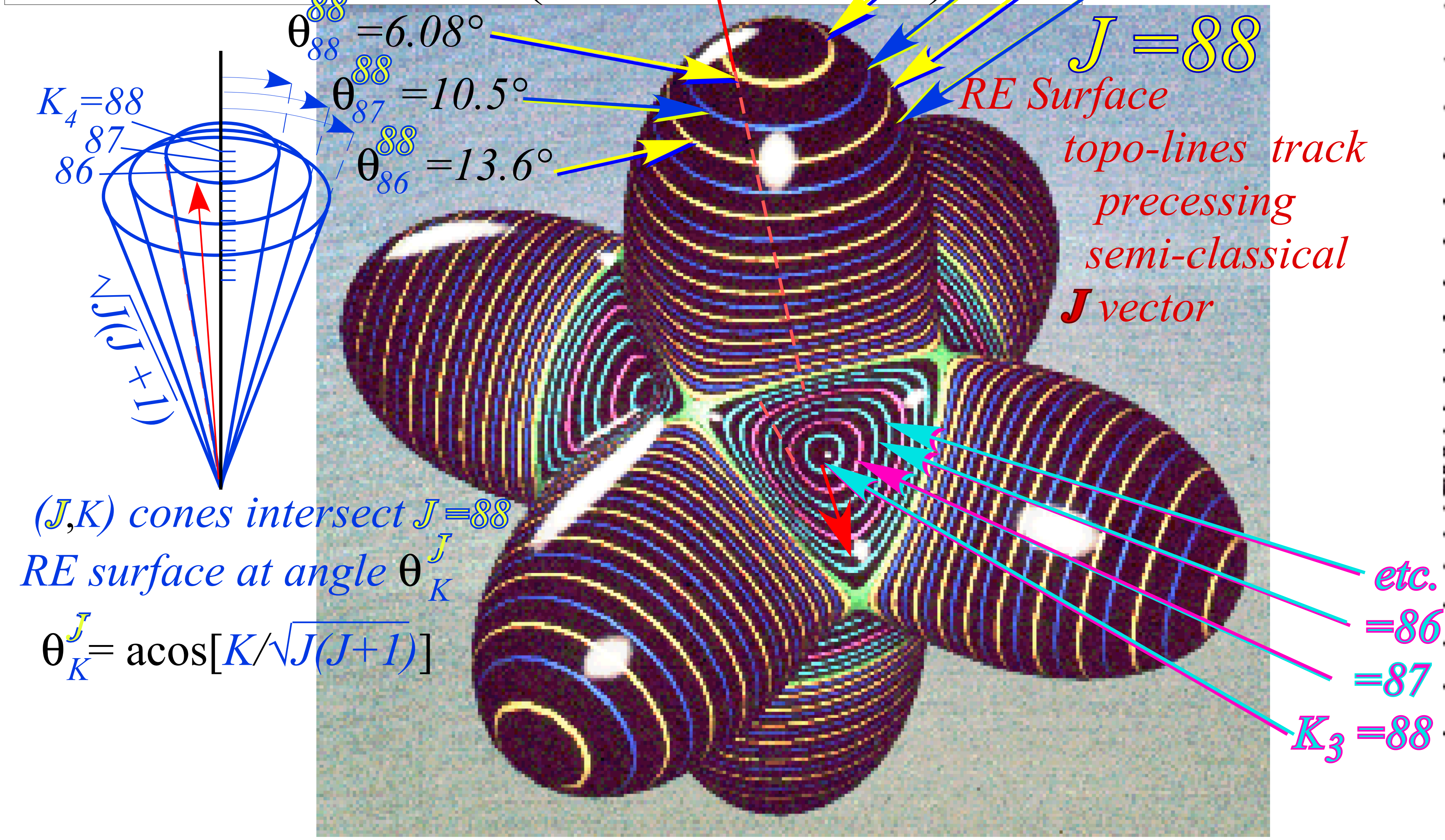
after: Int.J.Molecular Science 14.(2013) Fig.6 p.742 and Fig. 29 p.791

$$\langle H\rangle \sim \nu_{vib} + BJ(J+1) + \langle H^{Scalar\ Coriolis}\rangle + \langle H^{Tensor\ Centrifugal}\rangle + \langle H^{Tensor\ Coriolis}\rangle + \langle H^{Nuclear\ Spin}\rangle + \ldots$$

***O_h or T_d Spherical Top:** (Hecht CH_4 Hamiltonian 1960)*

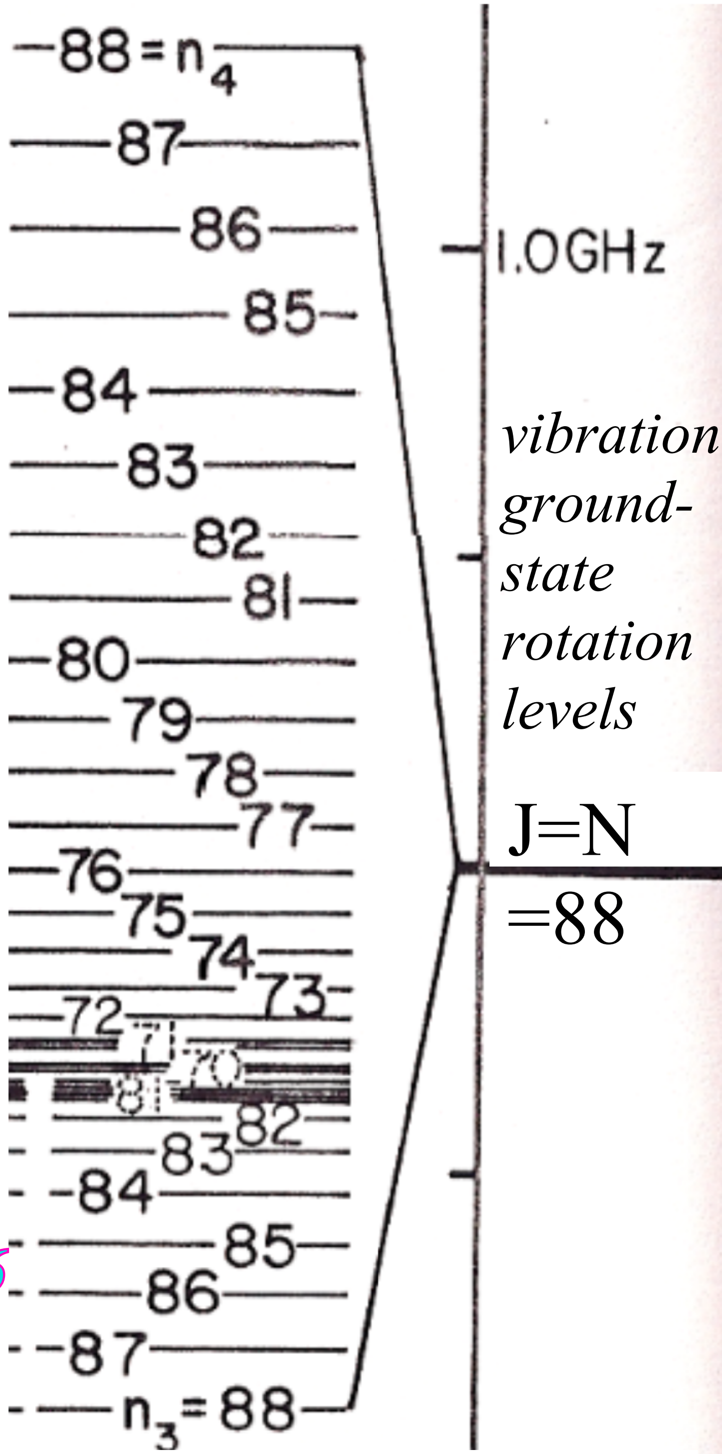
$$\mathbf{H} = B\left(\mathbf{J}_x^2 + \mathbf{J}_y^2 + \mathbf{J}_z^2\right) + t_{440}\left(\mathbf{J}_x^4 + \mathbf{J}_y^4 + \mathbf{J}_z^4 - \frac{3}{5}J^4\right) + \cdots$$

$$= \quad B\mathbf{J}^2 \quad + t_{440}\left(\mathbf{T}_0^4 + \sqrt{\frac{5}{14}}\left[\mathbf{T}_4^4 + \mathbf{T}_{-4}^4\right]\right) + \cdots$$

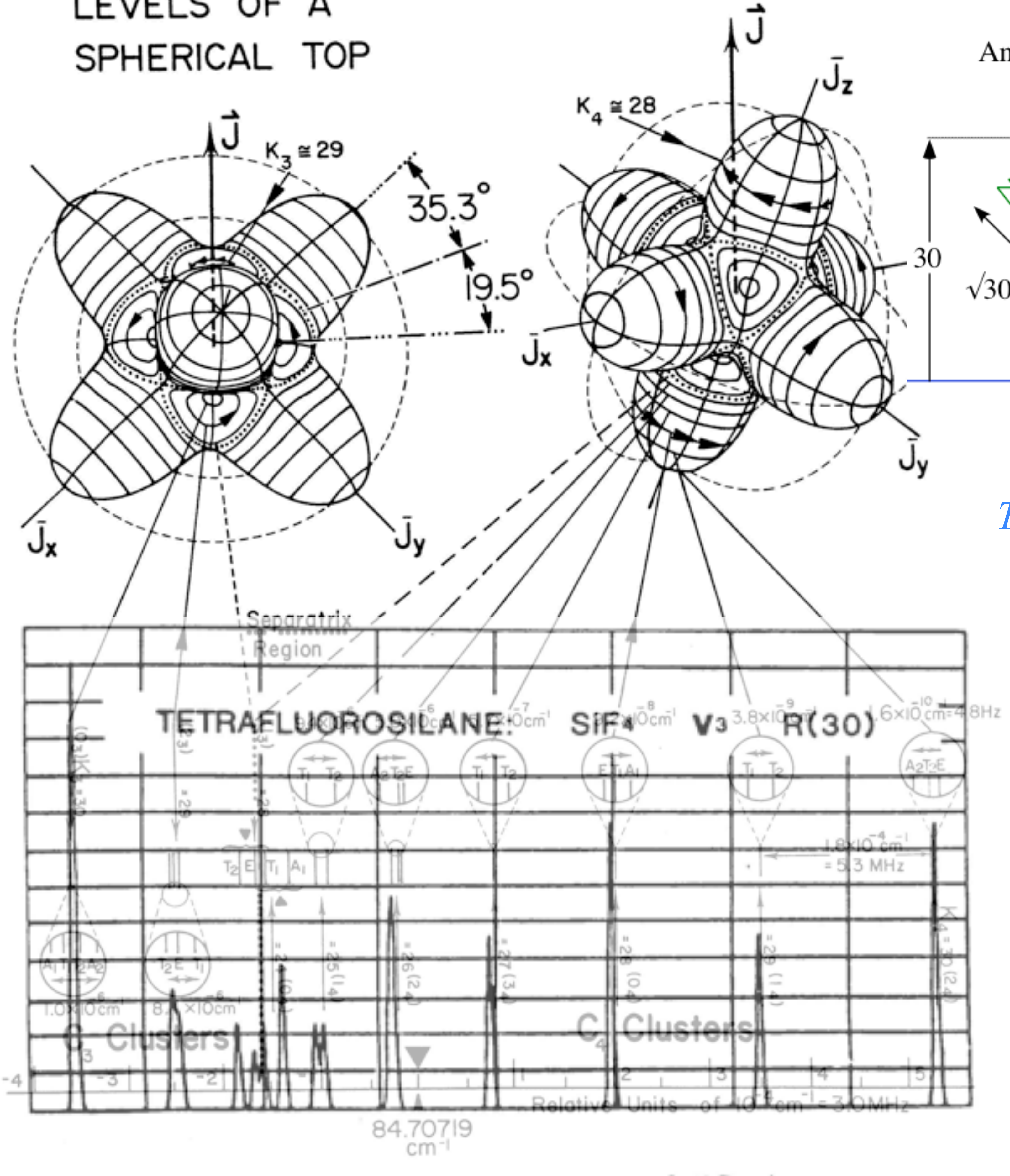


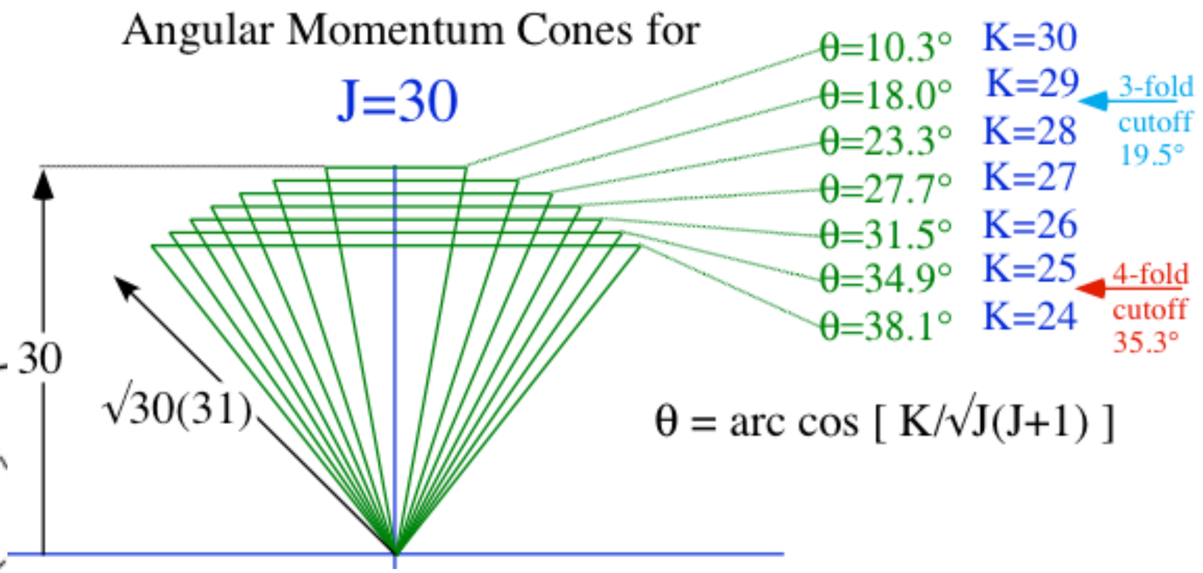
(J,K) cones intersect J=88
RE surface at angle θ^J_K

$$\theta^J_K = \mathrm{acos}[K/\sqrt{J(J+1)}]$$



VISUALIZING THE J = 30 LEVELS OF A SPHERICAL TOP





Two molecular examples: SiF_4 and C_8H_8