Magnetic Refinement: Tutorial (Symmetry)

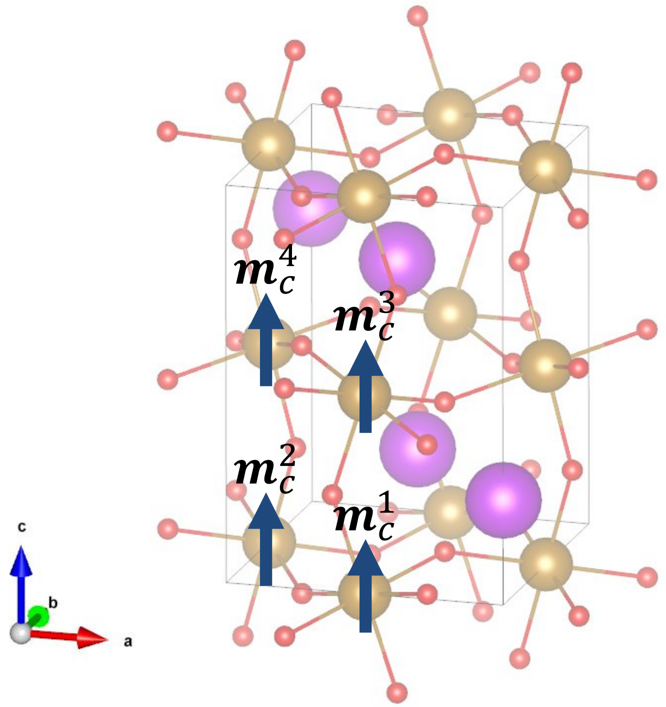
Roger Johnson

Example: Orthoferrites

- Space group *Pbnm*

- Consider a vector space $V_c = \{\boldsymbol{m}_c^1, \boldsymbol{m}_c^2, \boldsymbol{m}_c^3, \boldsymbol{m}_c^4\}$

- Assume **k**=(0,0,0)



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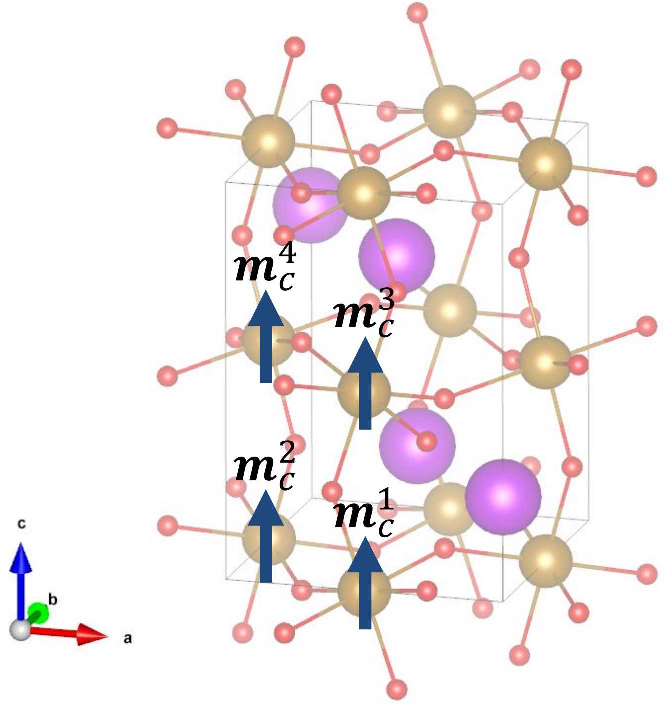


$$1: \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \qquad \bar{1}: \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \qquad \underset{[0.5,0,0]}{2_{100}}: \begin{pmatrix} 0 & \bar{1} & 0 & 0 \\ \bar{1} & 0 & 0 & 0 \\ 0 & 0 & 0 & \bar{1} \\ 0 & 0 & \bar{1} & 0 \end{pmatrix}$$

$$\underset{[0,0.5,0]}{2_{010}}: \begin{pmatrix} 0 & 0 & 0 & \bar{1} \\ 0 & 0 & \bar{1} & 0 \\ 0 & \bar{1} & 0 & 0 \\ \bar{1} & 0 & 0 & 0 \end{pmatrix} \qquad \underset{[0,0,0.5]}{2_{001}}: \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \qquad \underset{[0,0.5,0]}{m_{100}}: \begin{pmatrix} 0 & \bar{1} & 0 & 0 \\ \bar{1} & 0 & 0 & 0 \\ 0 & 0 & 0 & \bar{1} \\ 0 & 0 & \bar{1} & 0 \end{pmatrix} \qquad \underset{[0.5,0,0.5]}{m_{010}}: \begin{pmatrix} 0 & 0 & 0 & \bar{1} \\ 0 & 0 & \bar{1} & 0 \\ 0 & \bar{1} & 0 & 0 \\ \bar{1} & 0 & 0 & 0 \end{pmatrix} \qquad m_{001}: \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$$

Example: Orthoferrites

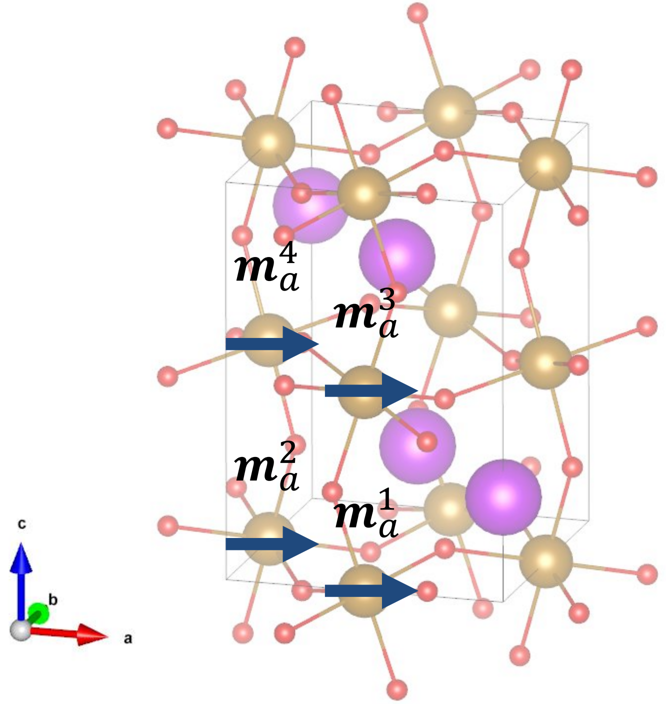
$$\Gamma_{V_p} = \sum_{ij} a_i^j \Gamma_i^j \qquad a_i^j = \frac{1}{h}\sum_g \chi_{\Gamma_{V_p}}(g)\chi_{\Gamma_i^j}(g)$$

$$\boxed{\Gamma_{V_c} = m\Gamma_1^+ + m\Gamma_2^+ + m\Gamma_3^+ + m\Gamma_4^+}$$

	1	**2_{100}**	**2_{001}**	**2_{010}**	**$\bar{1}$**	**m_{100}**	**m_{001}**	**m_{010}**	
Γ_{V_c}	4	0	0	0	4	0	0	0	
$m\Gamma_1^+$	1	1	1	1	1	1	1	1	*Pbnm*
$m\Gamma_1^-$	1	1	1	1	-1	-1	-1	-1	*Pb'n'm'*
$m\Gamma_2^+$	1	1	-1	-1	1	1	-1	-1	*Pbn'm'*
$m\Gamma_2^-$	1	1	-1	-1	-1	-1	1	1	*Pb'nm*
$m\Gamma_3^+$	1	-1	-1	1	1	-1	-1	1	*Pb'nm'*
$m\Gamma_3^-$	1	-1	-1	1	-1	1	1	-1	*Pbn'm*
$m\Gamma_4^+$	1	-1	1	-1	1	-1	1	-1	*Pb'n'm*
$m\Gamma_4^-$	1	-1	1	-1	-1	1	-1	1	*Pbnm'*

Example: Orthoferrites

- Space group *Pbnm*
- Consider a vector space $V_a = \{\boldsymbol{m}_a^1, \boldsymbol{m}_a^2, \boldsymbol{m}_a^3, \boldsymbol{m}_a^4\}$
- Assume **k**=(0,0,0)
- Write down the matrix representations



Example: Orthoferrites

$$\Gamma_{V_p} = \sum_{ij} a_i^j \Gamma_i^j \qquad a_i^j = \frac{1}{h}\sum_g \chi_{\Gamma_{V_p}}(g)\chi_{\Gamma_i^j}(g)$$

$$\boxed{\Gamma_{V_a} = m\Gamma_1^+ + m\Gamma_2^+ + m\Gamma_3^+ + m\Gamma_4^+}$$

	1	2_{100}	2_{001}	2_{010}	$\bar{1}$	m_{100}	m_{001}	m_{010}	
Γ_{V_c}	4	0	0	0	4	0	0	0	
Γ_{V_a}	4	0	0	0	4	0	0	0	
$m\Gamma_1^+$	1	1	1	1	1	1	1	1	*Pbnm*
$m\Gamma_1^-$	1	1	1	1	-1	-1	-1	-1	*Pb’n’m’*
$m\Gamma_2^+$	1	1	-1	-1	1	1	-1	-1	*Pbn’m’*
$m\Gamma_2^-$	1	1	-1	-1	-1	-1	1	1	*Pb’nm*
$m\Gamma_3^+$	1	-1	-1	1	1	-1	-1	1	*Pb’nm’*
$m\Gamma_3^-$	1	-1	-1	1	-1	1	1	-1	*Pbn’m*
$m\Gamma_4^+$	1	-1	1	-1	1	-1	1	-1	*Pb’n’m*
$m\Gamma_4^-$	1	-1	1	-1	-1	1	-1	1	*Pbnm’*

Example: Orthoferrites

$$\Gamma_{V_p} = \sum_{ij} a_i^j \Gamma_i^j \qquad a_i^j = \frac{1}{h}\sum_g \chi_{\Gamma_{V_p}}(g)\chi_{\Gamma_i^j}(g)$$

$$\boxed{\Gamma_{V_b} = m\Gamma_1^+ + m\Gamma_2^+ + m\Gamma_3^+ + m\Gamma_4^+}$$

	1	2_{100}	2_{001}	2_{010}	$\bar{1}$	m_{100}	m_{001}	m_{010}	
Γ_{V_c}	4	0	0	0	4	0	0	0	
Γ_{V_a}	4	0	0	0	4	0	0	0	
Γ_{V_b}	4	0	0	0	4	0	0	0	
$m\Gamma_1^+$	1	1	1	1	1	1	1	1	*Pbnm*
$m\Gamma_1^-$	1	1	1	1	-1	-1	-1	-1	*Pb’n’m’*
$m\Gamma_2^+$	1	1	-1	-1	1	1	-1	-1	*Pbn’m’*
$m\Gamma_2^-$	1	1	-1	-1	-1	-1	1	1	*Pb’nm*
$m\Gamma_3^+$	1	-1	-1	1	1	-1	-1	1	*Pb’nm’*
$m\Gamma_3^-$	1	-1	-1	1	-1	1	1	-1	*Pbn’m*
$m\Gamma_4^+$	1	-1	1	-1	1	-1	1	-1	*Pb’n’m*
$m\Gamma_4^-$	1	-1	1	-1	-1	1	-1	1	*Pbnm’*

Example: Orthoferrites

$$\Gamma_{V_c} = m\Gamma_1^+ + m\Gamma_2^+ + m\Gamma_3^+ + m\Gamma_4^+$$

$$P_j = \frac{d_j}{h} \sum_i \chi_j(g_i) g_i(V)$$

V_c:

$$P_{m\Gamma_1^+}: \frac{1}{4} \begin{pmatrix} 1 & \bar{1} & 1 & \bar{1} \\ \bar{1} & 1 & \bar{1} & 1 \\ 1 & \bar{1} & 1 & \bar{1} \\ \bar{1} & 1 & \bar{1} & 1 \end{pmatrix}$$

$$\boldsymbol{\phi} = (\boldsymbol{m}_c^1, -\boldsymbol{m}_c^2, \boldsymbol{m}_c^3, -\boldsymbol{m}_c^4)$$

$$P_{m\Gamma_2^+}: \frac{1}{4} \begin{pmatrix} 1 & \bar{1} & \bar{1} & 1 \\ \bar{1} & 1 & 1 & \bar{1} \\ \bar{1} & 1 & 1 & \bar{1} \\ 1 & \bar{1} & \bar{1} & 1 \end{pmatrix}$$

$$\boldsymbol{\phi} = (\boldsymbol{m}_c^1, -\boldsymbol{m}_c^2, -\boldsymbol{m}_c^3, \boldsymbol{m}_c^4)$$

$$P_{m\Gamma_3^+}: \frac{1}{4} \begin{pmatrix} 1 & 1 & \bar{1} & \bar{1} \\ 1 & 1 & \bar{1} & \bar{1} \\ \bar{1} & \bar{1} & 1 & 1 \\ \bar{1} & \bar{1} & 1 & 1 \end{pmatrix}$$

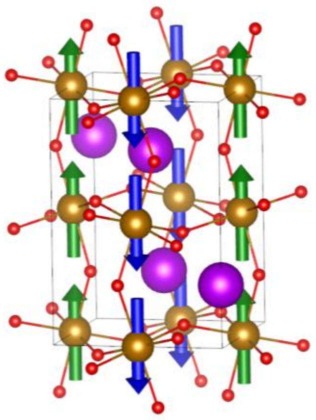
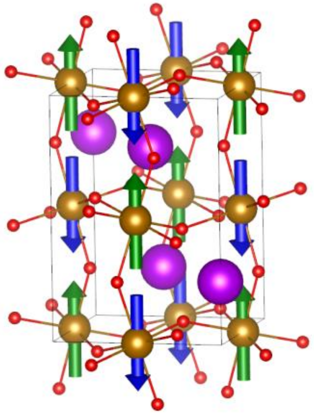
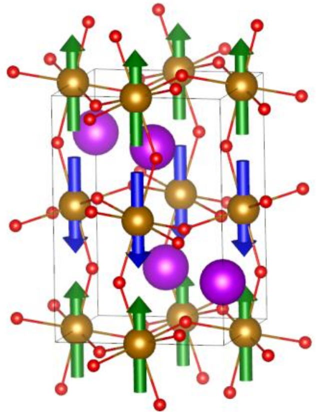
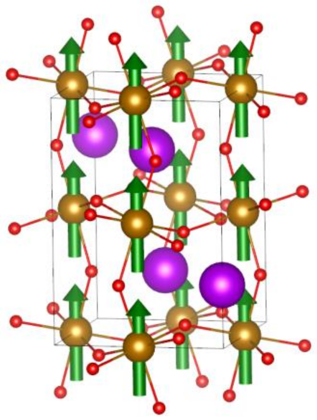
$$\boldsymbol{\phi} = (\boldsymbol{m}_c^1, \boldsymbol{m}_c^2, -\boldsymbol{m}_c^3, -\boldsymbol{m}_c^4)$$

$$P_{m\Gamma_4^+}: \frac{1}{4} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix}$$

$$\boldsymbol{\phi} = (\boldsymbol{m}_c^1, \boldsymbol{m}_c^2, \boldsymbol{m}_c^3, \boldsymbol{m}_c^4)$$

Example: Orthoferrites

$$\Gamma_{V_i} = m\Gamma_1^+ + m\Gamma_2^+ + m\Gamma_3^+ + m\Gamma_4^+$$

	$m\Gamma_1^+$ *Pbnm*	$m\Gamma_2^+$ *Pbn’m’*	$m\Gamma_3^+$ *Pb’nm’*	$m\Gamma_4^+$ *Pb’n’m*
V_c	C_c $(\boldsymbol{m}_c^1, -\boldsymbol{m}_c^2, \boldsymbol{m}_c^3, -\boldsymbol{m}_c^4)$ 	G_c $(\boldsymbol{m}_c^1, -\boldsymbol{m}_c^2, -\boldsymbol{m}_c^3, \boldsymbol{m}_c^4)$ 	A_c $(\boldsymbol{m}_c^1, \boldsymbol{m}_c^2, -\boldsymbol{m}_c^3, -\boldsymbol{m}_c^4)$ 	F_c $(\boldsymbol{m}_c^1, \boldsymbol{m}_c^2, \boldsymbol{m}_c^3, \boldsymbol{m}_c^4)$ 

Example: Orthoferrites

$$\Gamma_{V_a} = m\Gamma_1^+ + m\Gamma_2^+ + m\Gamma_3^+ + m\Gamma_4^+$$

$$P_j = \frac{d_j}{h}\sum_i \chi_j(g_i)g_i(V)$$

V_a:

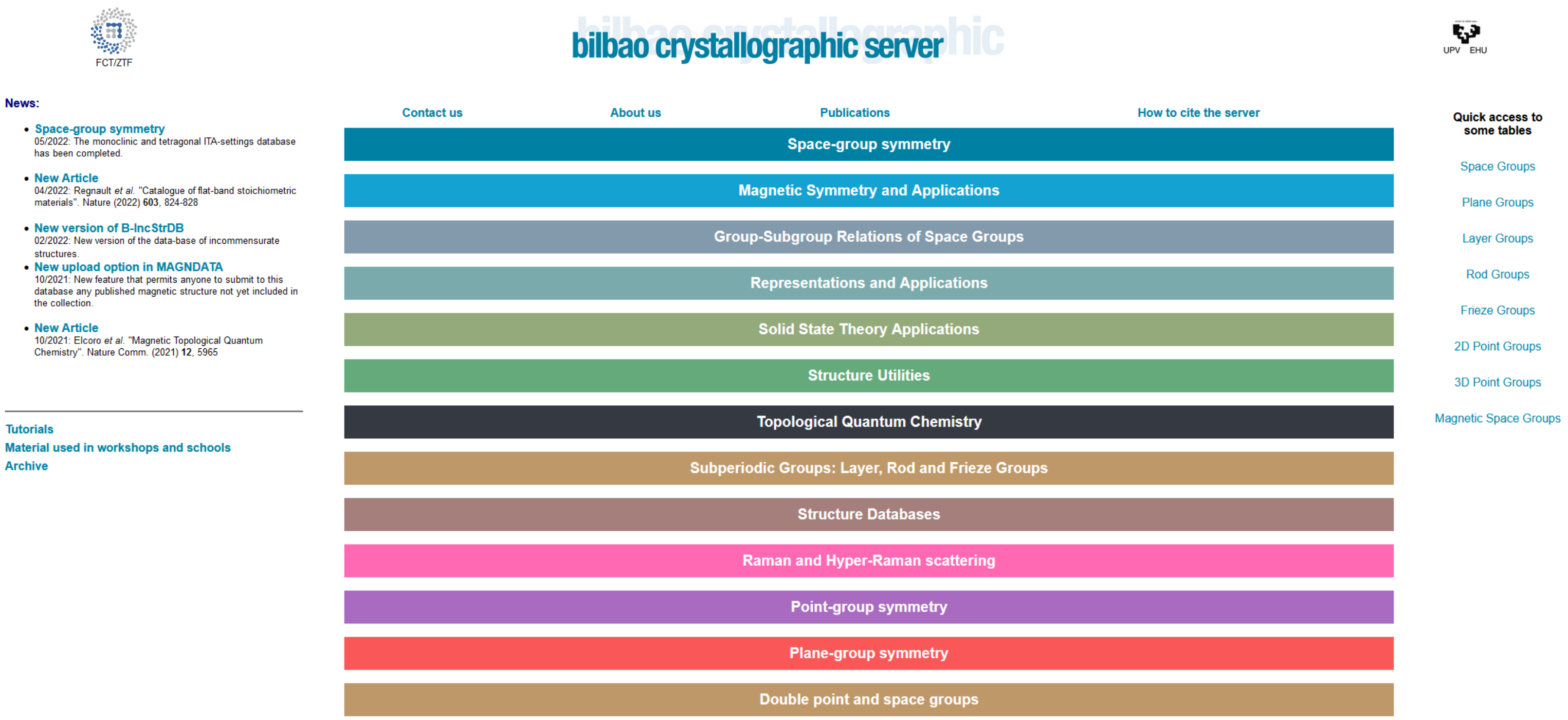
Example: Orthoferrites

$$\Gamma_{V_i} = m\Gamma_1^+ + m\Gamma_2^+ + m\Gamma_3^+ + m\Gamma_4^+$$

	$m\Gamma_1^+$ *Pbnm*	$m\Gamma_2^+$ *Pbn'm'*	$m\Gamma_3^+$ *Pb'nm'*	$m\Gamma_4^+$ *Pb'n'm*
V_c	C_c	G_c	A_c	F_c
V_a	A_a	F_a	C_a	G_a
V_b	G_b	C_b	F_b	A_b

Bilbao crystallographic server

https://www.cryst.ehu.es/



Isotropy suite

https://stokes.byu.edu/iso/isotropy.php

ISOTROPY Software Suite

Harold T. Stokes, Dorian M. Hatch, and Branton J. Campbell, Department of Physics and Astronomy, Brigham Young University, Provo, Utah 84606, USA, branton_campbell@byu.edu

Description: The ISOTROPY software suite is a collection of software which applies group theoretical methods to the analysis of phase transitions in crystalline solids.

How to cite: To cite a tool from the ISOTROPY Software Suite, see the citation instructions on the tool's individual home page. To cite the entire suite, use the following:
H. T. Stokes, D. M. Hatch, and B. J. Campbell, ISOTROPY Software Suite, iso.byu.edu.

References and Resources

Isotropy subgroups and distortions

- ISODISTORT: Explore and visualize distortions of crystalline structures. Possible distortions include atomic displacements, atomic ordering, strain, and magnetic moments.
- ISOSUBGROUP: Interactive program using user-friendly interface to list isotropy subgroups.
- ISOTROPY: Interactive program using command lines to explore isotropy subgroups and their associated distortions.
- ISOTILT: NEW! Interactive program for detecting cooperative rigid-unit modes (RUMs) in framework materials.
- SMODES: Find the displacement modes in a crystal which brings the dynamical matrix to block-diagonal form, with the smallest possible blocks.
- FROZSL: Calculate phonon frequencies and displacement modes using the method of frozen phonons.
- ISOVIZ: Stand-alone utility for viewing interactive distortions created by ISODISTORT (installers only, alpha version).

Space groups and irreducible representations

- ISOCIF: Create or modify CIF files.
- FINDSYM: Identify the space group of a crystal, given the positions of the atoms in a unit cell.
- ISOSPACEGROUP: NEW! Tables of crystallographic space groups: nonmagnetic and magnetic 3-dimensional space groups and (3+d)-dimensional superspace groups.
- ISO-IR: Tables of Irreducible Representations. The 2011 version of IR matrices.
- ISO-KOV: NEW! Mapping of the irreducible representations of Kovalev onto those of Cracknell, Davies, Miller and Love.
- ISO-MAG: Tables of magnetic space groups, both in human-readable and computer-readable forms.

Superspace Groups

- ISO(3+d)D: (3+d)-Dimensional Superspace Groups for d=1,2,3
- ISO(3+1)D: Isotropy Subgroups for Incommensurately Modulated Distortions in Crystalline Solids: A Complete List for One-Dimensional Modulations
- FINDSSG: Identify the superspace group symmetry given a list of symmetry operators.
- TRANSFORMSSG: Transform a superspace group to a new setting.

Phase Transitions

- COPL: Find a complete list of order parameters for a phase transition, given the space-group symmetries of the parent and subgroup phases.
- INVARIANTS: Generate invariant polynomials of the components of order parameters.
- COMSUBS: Find common subgroups of two structures in a reconstructive phase transition

Linux

- **ISOTROPY Software Suite for Linux**: includes ISOTROPY, FINDSYM, SMODES, COMSUBS.

Isodistort

https://stokes.byu.edu/iso/isodistort.php