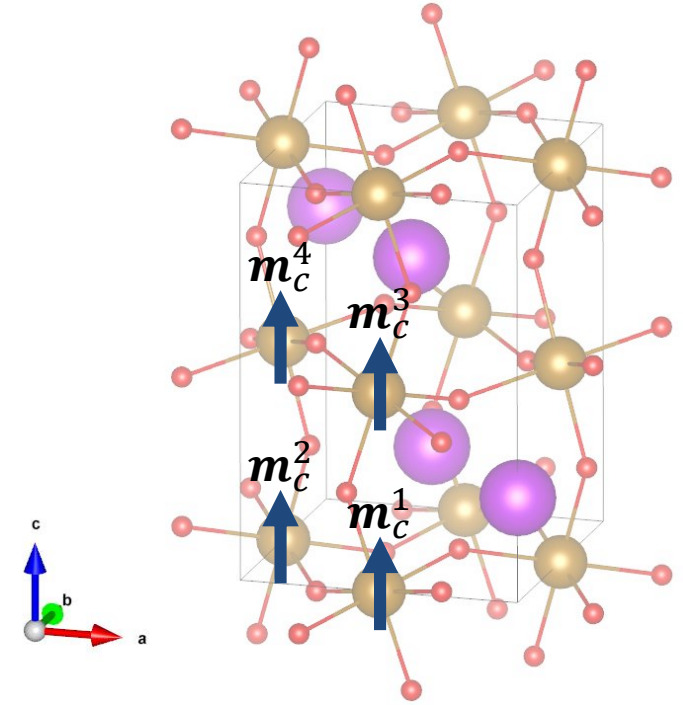

Magnetic Refinement: Tutorial (Symmetry)

Roger Johnson

Example: Orthoferrites

- Space group $Pbnm$
- Consider a vector space $V_c = \{\mathbf{m}_c^1, \mathbf{m}_c^2, \mathbf{m}_c^3, \mathbf{m}_c^4\}$
- Assume $\mathbf{k}=(0,0,0)$



Example: Orthoferrites

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

$$1: \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad \bar{1}: \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad 2_{100}: \begin{pmatrix} 0 & \bar{1} & 0 & 0 \\ \bar{1} & 0 & 0 & 0 \\ 0 & 0 & 0 & \bar{1} \\ 0 & 0 & \bar{1} & 0 \end{pmatrix}$$

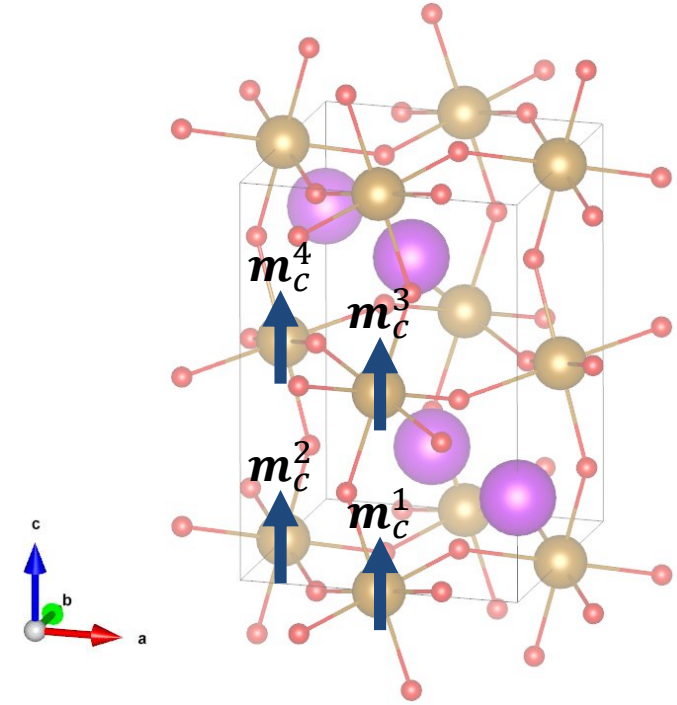
[0.5,0,0]

$$2_{010}: \begin{pmatrix} 0 & 0 & 0 & \bar{1} \\ 0 & 0 & \bar{1} & 0 \\ 0 & \bar{1} & 0 & 0 \\ \bar{1} & 0 & 0 & 0 \end{pmatrix} \quad 2_{001}: \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \quad m_{100}: \begin{pmatrix} 0 & \bar{1} & 0 & 0 \\ \bar{1} & 0 & 0 & 0 \\ 0 & 0 & 0 & \bar{1} \\ 0 & 0 & \bar{1} & 0 \end{pmatrix}$$

[0.5,0.5,0]

$$m_{010}: \begin{pmatrix} 0 & 0 & 0 & \bar{1} \\ 0 & 0 & \bar{1} & 0 \\ 0 & \bar{1} & 0 & 0 \\ \bar{1} & 0 & 0 & 0 \end{pmatrix} \quad m_{001}: \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$$

[0.5,0,0.5]



Example: Orthoferrites

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

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

	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
$m\Gamma_1^-$	1	1	1	1	-1	-1	-1	-1
$m\Gamma_2^+$	1	1	-1	-1	1	1	-1	-1
$m\Gamma_2^-$	1	1	-1	-1	-1	-1	1	1
$m\Gamma_3^+$	1	-1	-1	1	1	-1	-1	1
$m\Gamma_3^-$	1	-1	-1	1	-1	1	1	-1
$m\Gamma_4^+$	1	-1	1	-1	1	-1	1	-1
$m\Gamma_4^-$	1	-1	1	-1	-1	1	-1	1

Pbnm

Pb'n'm'

Pbn'm'

Pb'nm

Pb'nm'

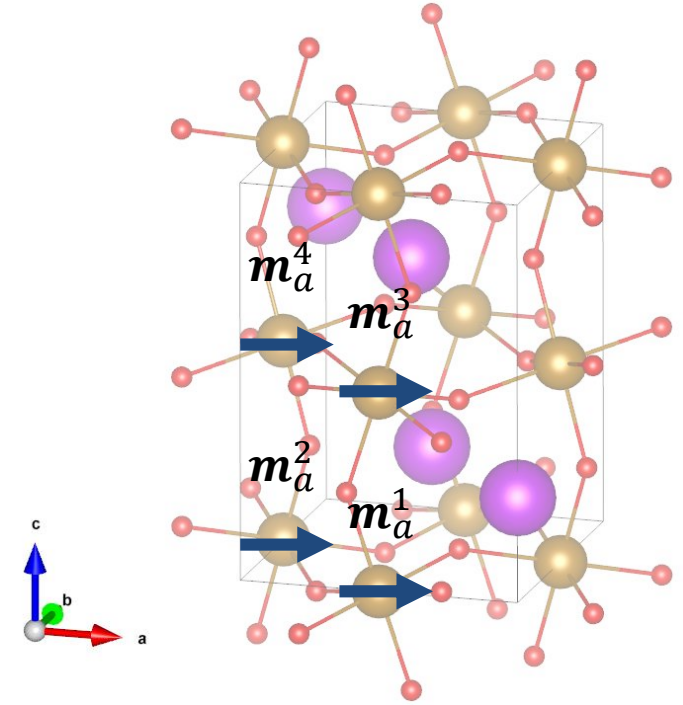
Pbn'm

Pb'n'm

Pbnm'

Example: Orthoferrites

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



Example: Orthoferrites

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

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

	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
$m\Gamma_1^-$	1	1	1	1	-1	-1	-1	-1
$m\Gamma_2^+$	1	1	-1	-1	1	1	-1	-1
$m\Gamma_2^-$	1	1	-1	-1	-1	-1	1	1
$m\Gamma_3^+$	1	-1	-1	1	1	-1	-1	1
$m\Gamma_3^-$	1	-1	-1	1	-1	1	1	-1
$m\Gamma_4^+$	1	-1	1	-1	1	-1	1	-1
$m\Gamma_4^-$	1	-1	1	-1	-1	1	-1	1

Pbnm

Pb'n'm'

Pbn'm'

Pb'nrm

Pb'nrm'

Pbn'm

Pb'n'm

Pbnm'

Example: Orthoferrites

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

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

	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
$m\Gamma_1^-$	1	1	1	1	-1	-1	-1	-1
$m\Gamma_2^+$	1	1	-1	-1	1	1	-1	-1
$m\Gamma_2^-$	1	1	-1	-1	-1	-1	1	1
$m\Gamma_3^+$	1	-1	-1	1	1	-1	-1	1
$m\Gamma_3^-$	1	-1	-1	1	-1	1	1	-1
$m\Gamma_4^+$	1	-1	1	-1	1	-1	1	-1
$m\Gamma_4^-$	1	-1	1	-1	-1	1	-1	1

Pbnm

Pb'n'm'

Pbn'm'

Pb'nrm

Pb'nrm'

Pbn'm

Pb'n'm

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 :

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

$$\phi = (m_c^1, -m_c^2, m_c^3, -m_c^4)$$

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

$$\phi = (m_c^1, -m_c^2, -m_c^3, m_c^4)$$

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

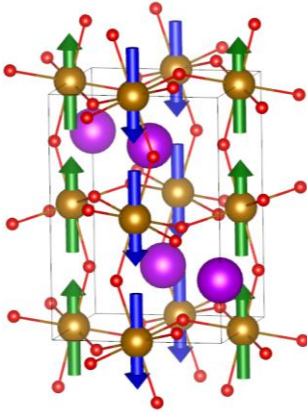
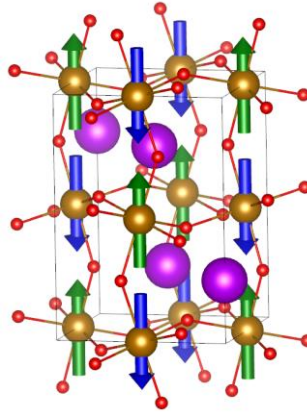
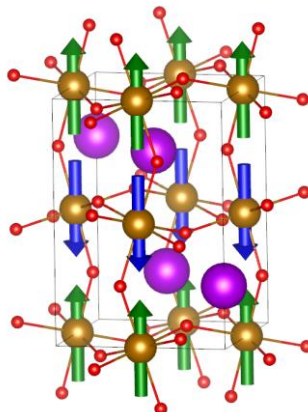
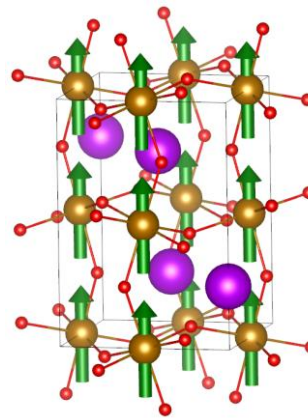
$$\phi = (m_c^1, m_c^2, -m_c^3, -m_c^4)$$

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

$$\phi = (m_c^1, m_c^2, m_c^3, m_c^4)$$

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 $(m_c^1, -m_c^2, m_c^3, -m_c^4)$ 	G_c $(m_c^1, -m_c^2, -m_c^3, m_c^4)$ 	A_c $(m_c^1, m_c^2, -m_c^3, -m_c^4)$ 	F_c $(m_c^1, m_c^2, m_c^3, m_c^4)$ 

Example: Orthoferrites

V_a :

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

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

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/>



bilbao crystallographic server



News:

- **Space-group symmetry**
05/2022: The monoclinic and tetragonal ITA-settings database has been completed.
- **New Article**
04/2022: Regnault *et al.* "Catalogue of flat-band stoichiometric materials". Nature (2022) 603, 824-828
- **New version of B-IncStrDB**
02/2022: New version of the data-base of incommensurate structures.
- **New upload option in MAGNDATA**
10/2021: New feature that permits anyone to submit to this database any published magnetic structure not yet included in the collection.
- **New Article**
10/2021: Elcoro *et al.* "Magnetic Topological Quantum Chemistry". Nature Comm. (2021) 12, 5965

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Space-group symmetry

Magnetic Symmetry and Applications

Group-Subgroup Relations of Space Groups

Representations and Applications

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Subperiodic Groups: Layer, Rod and Frieze Groups

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Double point and space groups

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>

ISODISTORT SUITE HELP

ISODISTORT

Version 6.11.1, Jan 2022

Harold T. Stokes, Branton J. Campbell, and Dorian M. Hatch, Department of Physics and Astronomy, Brigham Young University, Provo, Utah, 84602, USA, branton_campbell@byu.edu

Description: ISODISTORT is a user-friendly internet-based tool for exploring the structural distortion modes of crystalline materials induced by irreducible representations of the parent space-group symmetry. The stand-alone ISOVIZ application further allows one to visualize and interactively manipulate the modes generated in ISODISTORT.

NOTE: Interactive visualizations must now be saved to disk and opened with the standalone ISOVIZ application.

[Help](#), [Tutorials](#), [Version History](#)

[Legacy copy of ISODISTORT version 5.6.1, August 2013](#)

Begin by entering the structure of parent phase: ?

[Get started quickly with a cubic perovskite parent.](#)

Import parent structure from a CIF structure file: No file selected.

If you don't have a parent CIF, create one using [ISOCIF](#).

Alternatively, you can begin with a previously-saved distortion: ?

[Get started quickly with a distorted perovskite example.](#) (Select this link and click "OK" on the next page to test your Java installation.)

Import an ISODISTORT distortion file: No file selected.

How to cite ISODISTORT (cite both of the following):

H. T. Stokes, D. M. Hatch, and B. J. Campbell, ISODISTORT, ISOTROPY Software Suite, iso.byu.edu.

B. J. Campbell, H. T. Stokes, D. E. Tanner, and D. M. Hatch, "ISODISPLACE: An Internet Tool for Exploring Structural Distortions." *J. Appl. Cryst.* **39**, 607-614 (2006).