



Introduction to Symmetry-Mode Analysis and the ISOTROPY Software Suite

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Argonne National Laboratory, USA



Parameterization of a distorted crystal

The ISOTROPY Software Suite supports the use of representational analysis to parameterize the symmetry-breaking distortions of a crystal, such as might arise in a phase transition.

The undistorted structure is called the parent, while the distorted structure is called the child. The space group of the child is a subgroup of the space group of the parent.

Each distortion parameter (*symmetry mode*) is a global pattern of structural changes (e.g. atomic displacements, site occupancies, magnetic moments, rigid-unit rotations, or lattice strains).

Each symmetry mode active in the child belongs to an irreducible representation of the parent space group.



Representational analysis: child vs parent

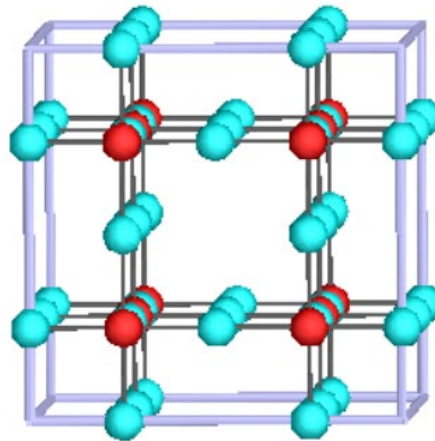
Define child by how it differs from parent.

High-symmetry
parent structure

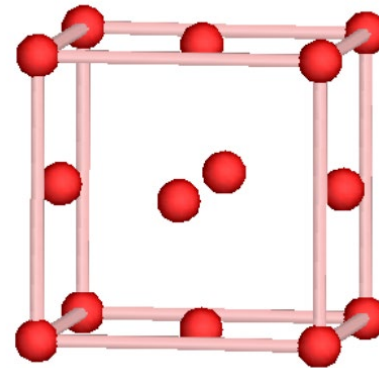
distortion
↓

Low-symmetry
child structure

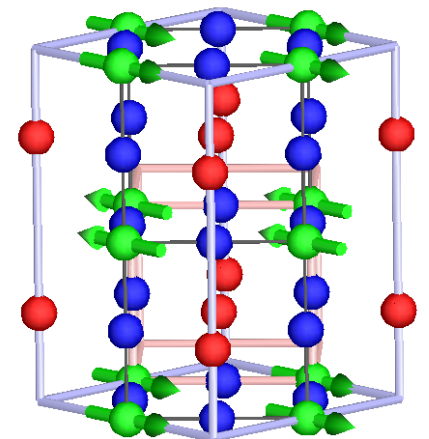
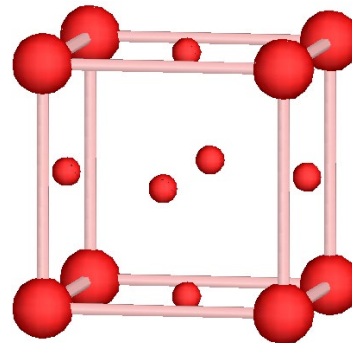
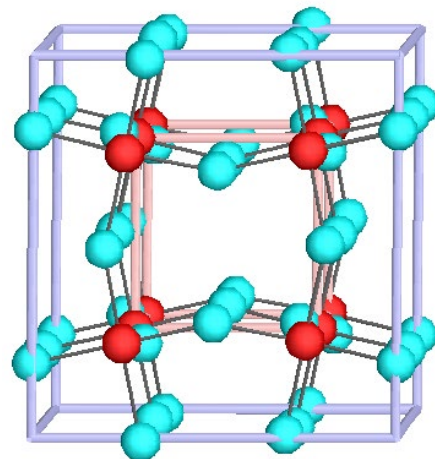
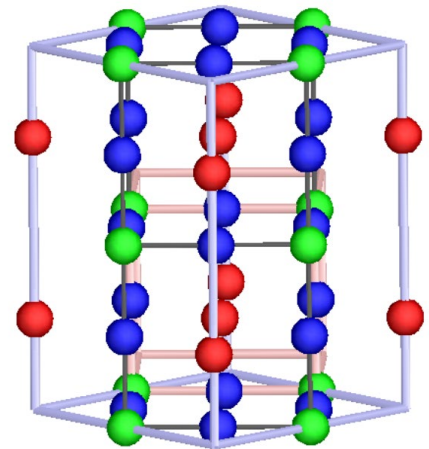
displacive



occupational



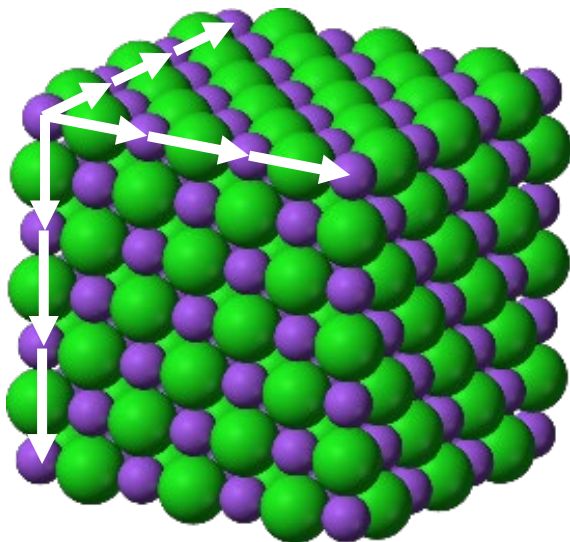
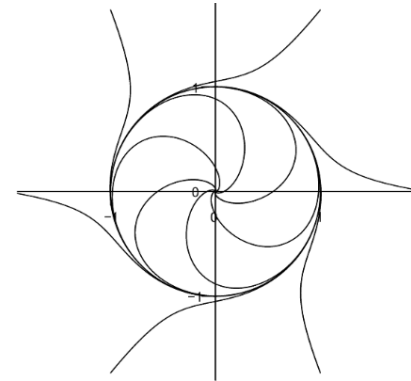
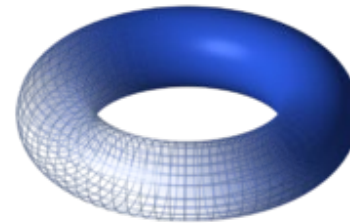
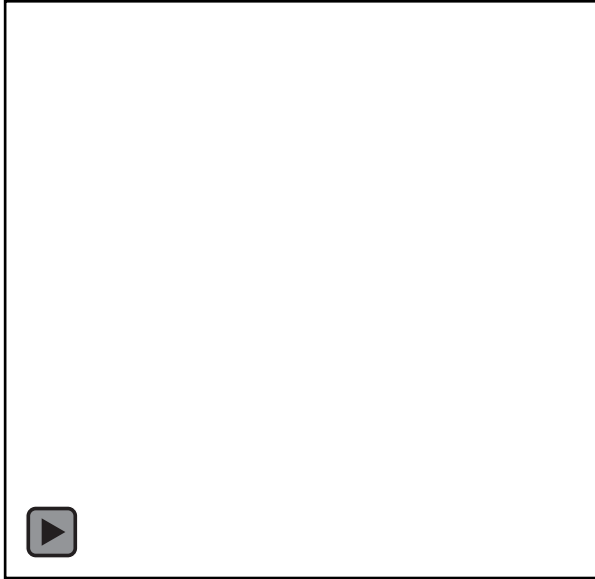
magnetic





Symmetry groups: crystals etc.

The **symmetries** of any system form a group!





Symmetry groups

A set with a binary operation (e.g. addition or multiplication)

Closure:

$$2_x 2_y = 2_z$$

Identity:

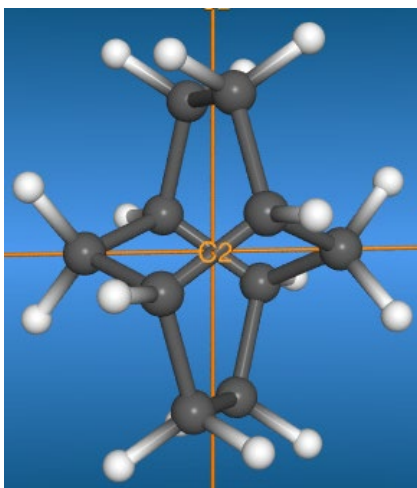
$$2_z 1 = 2_z$$

Inverses:

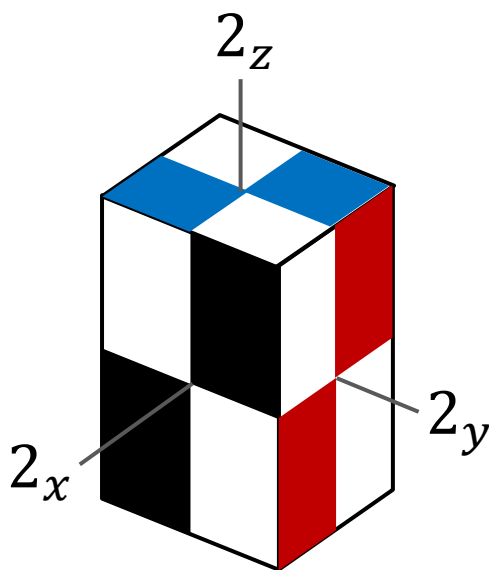
$$2_z (2_z)^{-1} = 1$$

Associativity:

$$(2_x 2_y) 2_z = 2_x (2_y 2_z)$$



Twistane ($C_{10}H_{16}$)



Point group: $222(D_2)$

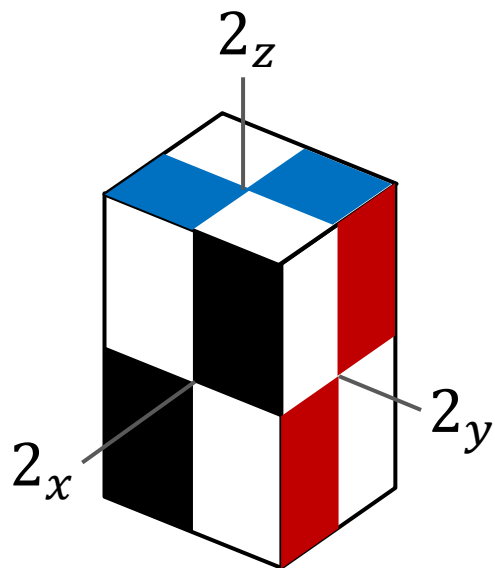
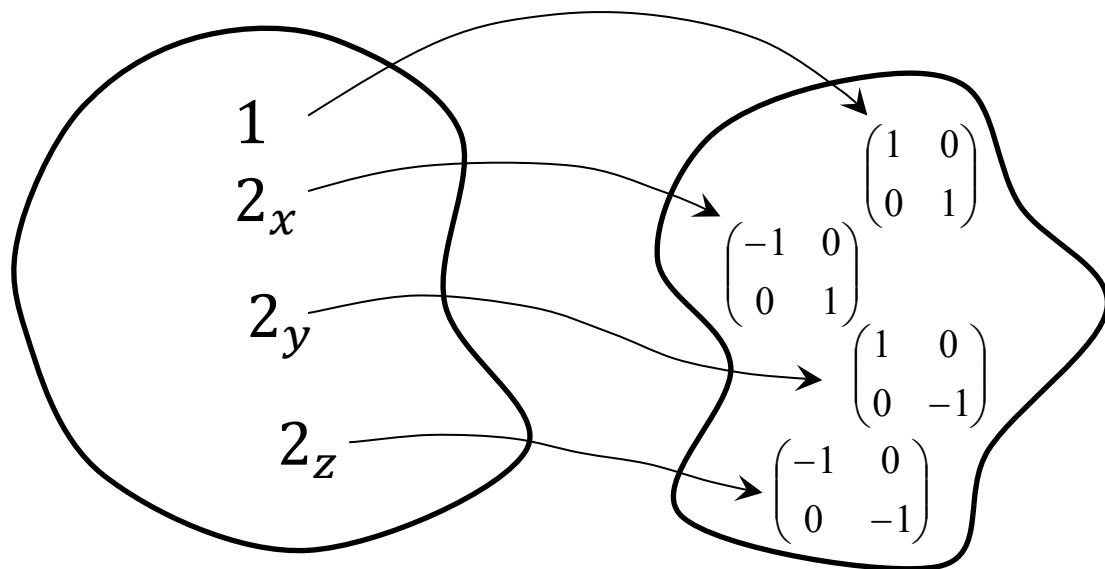
	1	2_x	2_y	2_z
1	1	2_x	2_y	2_z
2_x	2_x	1	2_z	2_y
2_y	2_y	2_z	1	2_x
2_z	2_z	2_y	2_x	1



Group representations

Point group: 222

	1	2_x	2_y	2_z
1	1	2_x	2_y	2_z
2_x	2_x	1	2_z	2_y
2_y	2_y	2_z	1	2_x
2_z	2_z	2_y	2_x	1



Representations map group elements onto matrices obeying the same multiplication table.

$$2_x 2_y = 2_z \rightarrow \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$$



Irreducible representations (irreps)

$$R1: \quad 1 \rightarrow (1) \quad 2_x \rightarrow (\bar{1}) \quad 2_y \rightarrow (1) \quad 2_z \rightarrow (\bar{1})$$

$$R2: \quad 1 \rightarrow (1) \quad 2_x \rightarrow (1) \quad 2_y \rightarrow (\bar{1}) \quad 2_z \rightarrow (\bar{1})$$

$$R3: \quad 1 \rightarrow \begin{pmatrix} \boxed{1} & 0 \\ 0 & \boxed{1} \end{pmatrix} \quad 2_x \rightarrow \begin{pmatrix} \boxed{\bar{1}} & 0 \\ 0 & \boxed{1} \end{pmatrix} \quad 2_y \rightarrow \begin{pmatrix} \boxed{1} & 0 \\ 0 & \boxed{\bar{1}} \end{pmatrix} \quad 2_z \rightarrow \begin{pmatrix} \boxed{\bar{1}} & 0 \\ 0 & \boxed{\bar{1}} \end{pmatrix}$$

$$\text{Reducible representation: } R3 = R1 \oplus R2 = \begin{pmatrix} R1 & 0 \\ 0 & R2 \end{pmatrix}$$

Irreducible representations (irreps) can't be separated into smaller pieces!

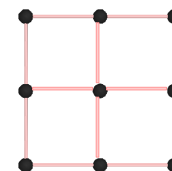
Irreps recipes for symmetry breaking!





Irrep/OPD recipe for symmetry-breaking

Example: Γ_5 irrep of space group $P4mm$



$$G = \begin{array}{cccccccc} \textcolor{red}{1} & \textcolor{red}{m_y} & \textcolor{red}{m_x} & \textcolor{red}{2_z} & \textcolor{red}{m_{\bar{x}z}} & \textcolor{red}{+4_z} & \textcolor{red}{-4_z} & \textcolor{red}{m_{xz}} \\ g_1 & g_2 & g_3 & g_4 & g_5 & g_6 & g_7 & g_8 \\ \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} & \begin{pmatrix} 1 & 0 \\ 0 & \bar{1} \end{pmatrix} & \begin{pmatrix} \bar{1} & 0 \\ 0 & 1 \end{pmatrix} & \begin{pmatrix} \bar{1} & 0 \\ 0 & \bar{1} \end{pmatrix} & \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} & \begin{pmatrix} 0 & \bar{1} \\ 1 & 0 \end{pmatrix} & \begin{pmatrix} 0 & 1 \\ \bar{1} & 0 \end{pmatrix} & \begin{pmatrix} 0 & \bar{1} \\ \bar{1} & 0 \end{pmatrix} \end{array}$$

Find the group elements whose matrices leave some vector invariant.

$$\begin{pmatrix} a \\ 0 \end{pmatrix} \Rightarrow \{g_1, g_2\}$$

$$\textcolor{red}{\{1, m_y\}}$$

$$\textcolor{red}{Pm}$$

$$\begin{pmatrix} a \\ a \end{pmatrix} \Rightarrow \{g_1, g_5\}$$

$$\textcolor{red}{\{1, m_{\bar{x}z}\}}$$

$$\textcolor{red}{Cm}$$

$$\begin{pmatrix} a \\ b \end{pmatrix} \Rightarrow \{g_1\}$$

$$\textcolor{red}{\{1\}}$$

$$\textcolor{red}{P1}$$

The vector used is called the *order parameter direction* or OPD.
The resulting symmetry is called an *isotropy subgroup* of the parent.



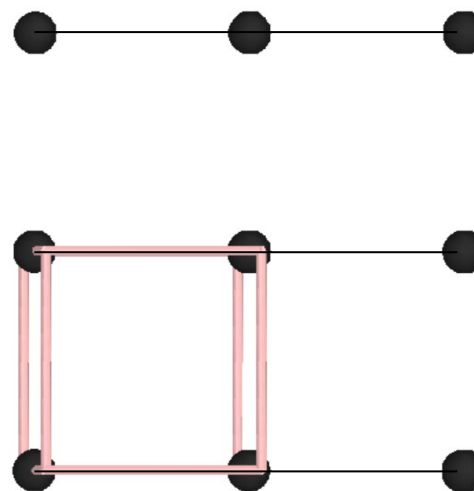
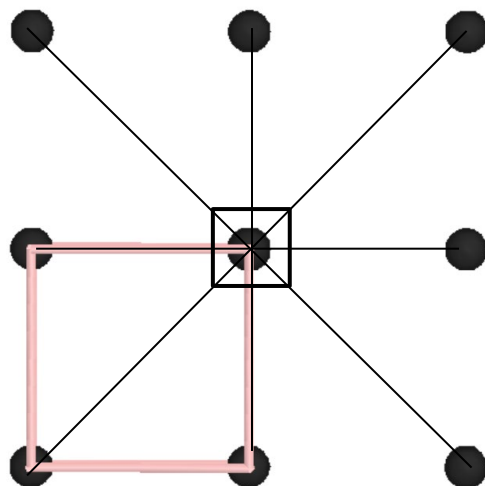
Irrep/OPD recipe for symmetry-breaking

$\Gamma_5(a, 0)$ of $P4mm$ induces vertical shear strain

1 m_y m_x 2_z $m_{\bar{x}z}$ $+4_z$ -4_z m_{xz}

$$G = \begin{matrix} g_1 & g_2 & g_3 & g_4 & g_5 & g_6 & g_7 & g_8 \\ \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} & \begin{pmatrix} 1 & 0 \\ 0 & \bar{1} \end{pmatrix} & \begin{pmatrix} \bar{1} & 0 \\ 0 & 1 \end{pmatrix} & \begin{pmatrix} \bar{1} & 0 \\ 0 & \bar{1} \end{pmatrix} & \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} & \begin{pmatrix} 0 & \bar{1} \\ 1 & 0 \end{pmatrix} & \begin{pmatrix} 0 & 1 \\ \bar{1} & 0 \end{pmatrix} & \begin{pmatrix} 0 & \bar{1} \\ \bar{1} & 0 \end{pmatrix} \end{matrix}$$

$$\begin{pmatrix} a \\ 0 \end{pmatrix} \Rightarrow \{g_1, g_2\} = \{1, m_y\} \rightarrow Pm$$



Symmetry element leaves child invariant iff irrep matrix leaves OPD invariant.



Magnetic representations

$[0, \frac{1}{4}, 0]m\Delta_2$ irrep of paramagnetic space-group $P222.1'$

(x, y, z)	(x, \bar{y}, \bar{z})	(\bar{x}, \bar{y}, z)	$(x, \bar{y} + 1, \bar{z})$	$(\bar{x}, y + 1, \bar{z})$	$(x, y + 1, z)$
$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$
↓	↓	↓	↓	↓	↓
$\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$
$(x, y, z)'$	$(x, \bar{y}, \bar{z})'$	$(\bar{x}, \bar{y}, z)'$	$(x, \bar{y} + 1, \bar{z})'$	$(\bar{x}, y + 1, \bar{z})'$	$(x, y + 1, z)'$

Magnetic irreps have twice as many matrices as corresponding non-magnetic irreps – primed and unprimed versions of every non-magnetic operation.

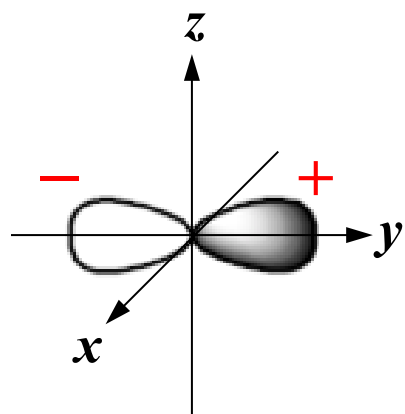
Let pure time reversal operation be the negative identity. Adding a prime to an operation just multiplies its matrix by -1 . This may not add unique matrices to the image. But it changes the isotropy subgroups.



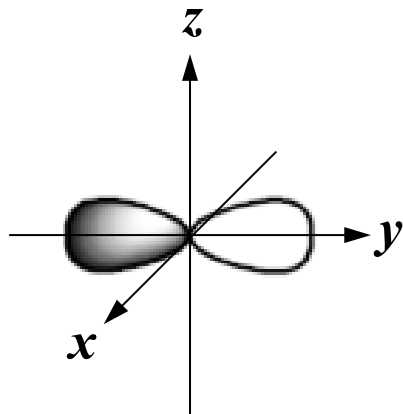
Irrep basis functions: the p_y orbital

Parent symmetry = 222

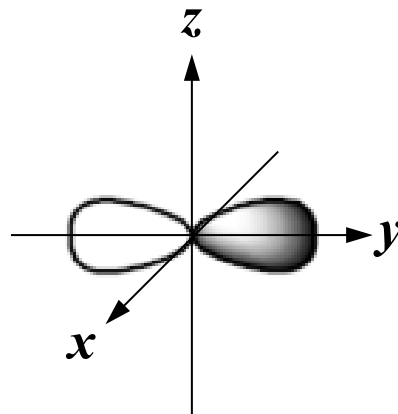
1



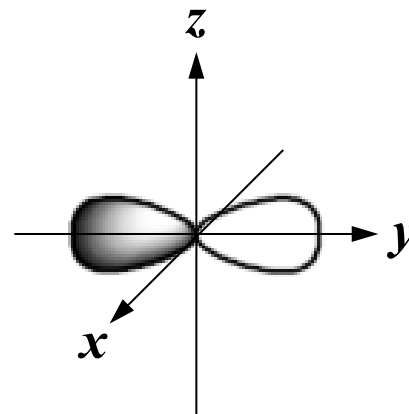
2_x



2_y



2_z



Under the symmetry operations of the group, a p_y orbital transforms the same way as which irrep?

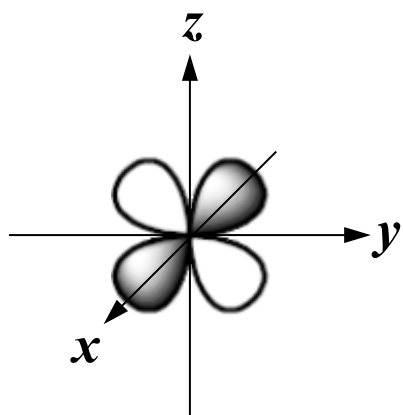
	1	2_x	2_y	2_z	
Γ_1	1	1	1	1	
Γ_2	1	-1	-1	1	p_z
Γ_3	1	1	-1	-1	p_x
Γ_4	1	-1	1	-1	p_y



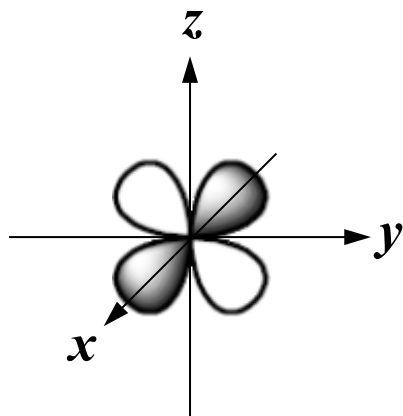
Irrep basis functions: the d_{yz} orbital

Parent symmetry = 222

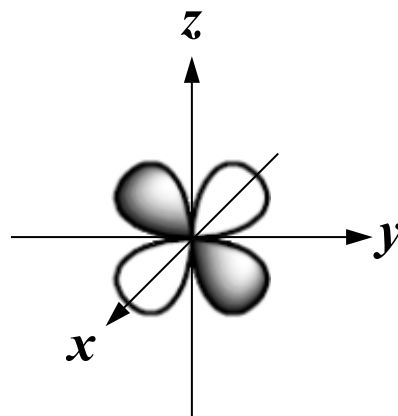
1



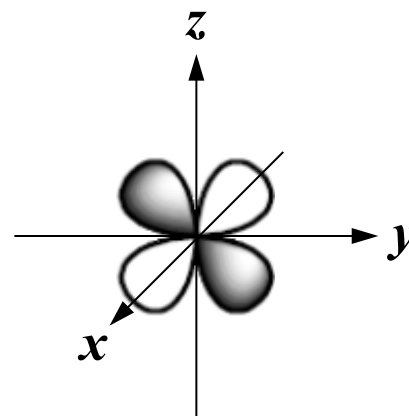
2_x



2_y



2_z



Under the symmetry operations of the group, a d_{yz} orbital transforms the same way as which irrep?

	1	2_x	2_y	2_z	
Γ_1	1	1	1	1	$d_{x^2-y^2}, d_{z^2}$
Γ_2	1	-1	-1	1	p_z, d_{xy}
Γ_3	1	1	-1	-1	p_x, d_{yz}
Γ_4	1	-1	1	-1	p_y, d_{xz}



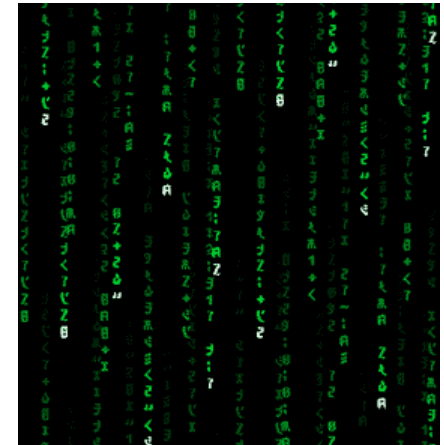
Wonderful orthogonality theorem (WOT)

Irreps



Beautiful

	1	2_x	2_y	2_z
Γ_1	1	1	1	1
Γ_2	1	-1	-1	1
Γ_3	1	1	-1	-1
Γ_4	1	-1	1	-1



Computable

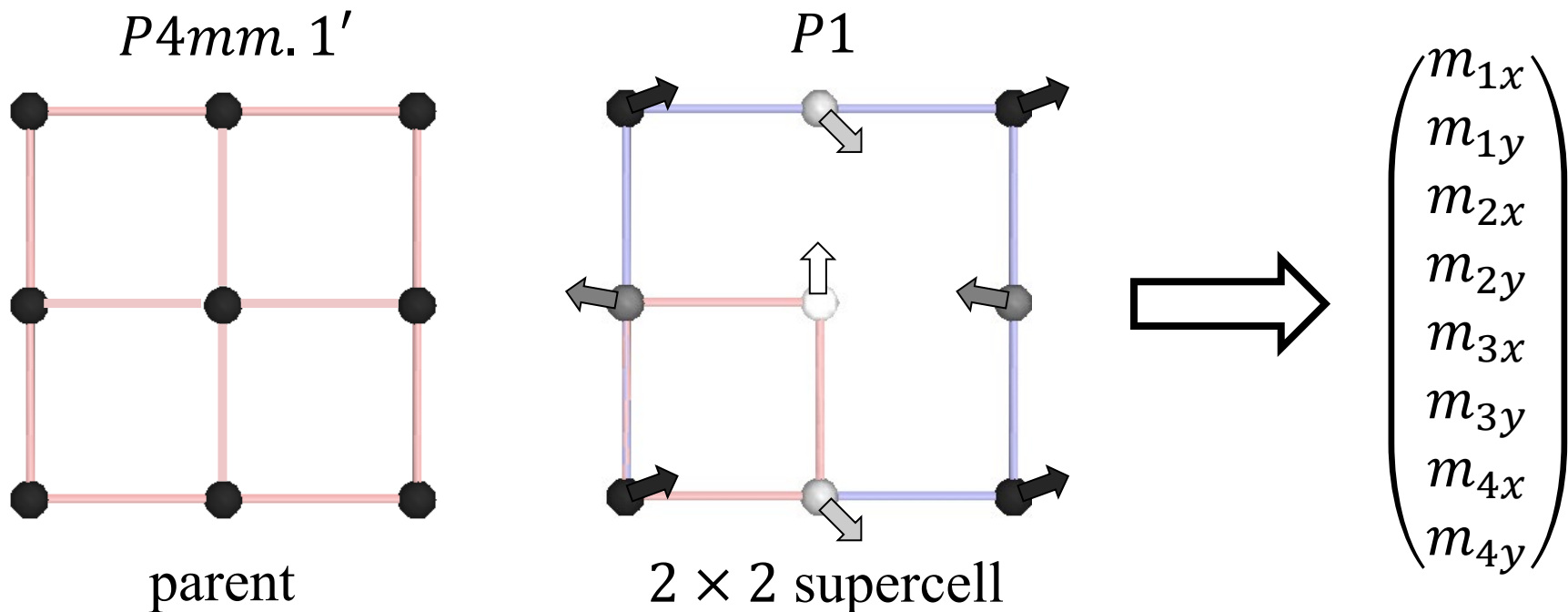
Irreps enjoy special orthogonality and completeness properties.

Irreps provide a symmetry-based coordinate system (parameter set) for describing any deviation from symmetry.



Distortion space

The collection of all structural variables define a vector space, which we can refer to as *distortion space*.

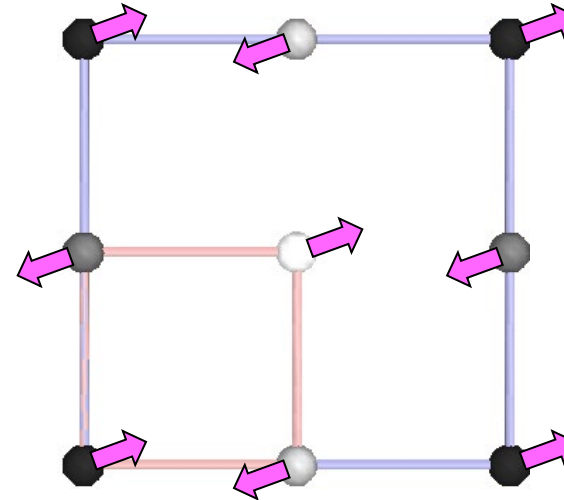
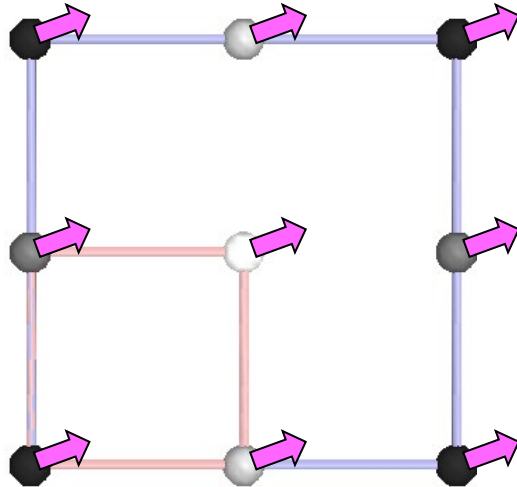


4 unique atoms in supercell \rightarrow 8 structural parameters



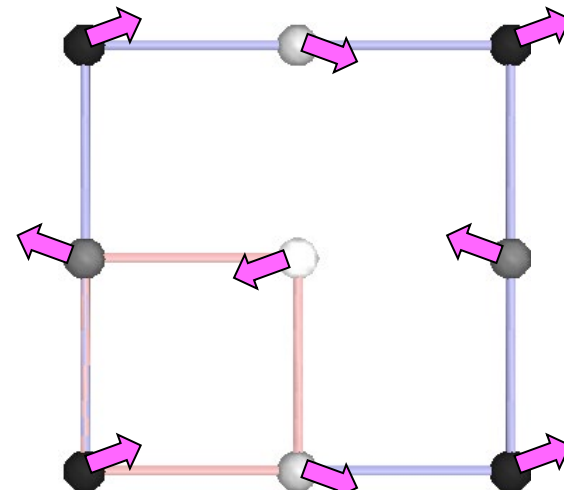
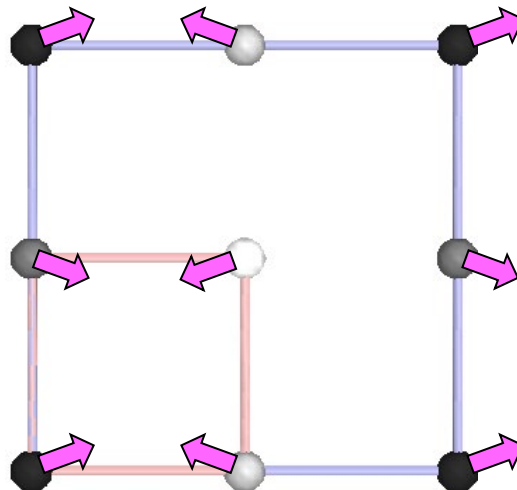
Symmetry modes: a new parameter set

$m\Gamma_5(a, b)$
 $P1$



$mM_5(a, b)$
 $P2.1'_a$

$mX_4(a, b)$
 $Pmm2.1'_c$



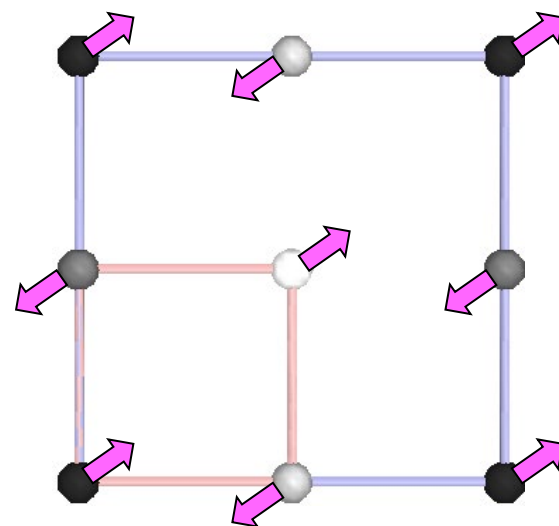
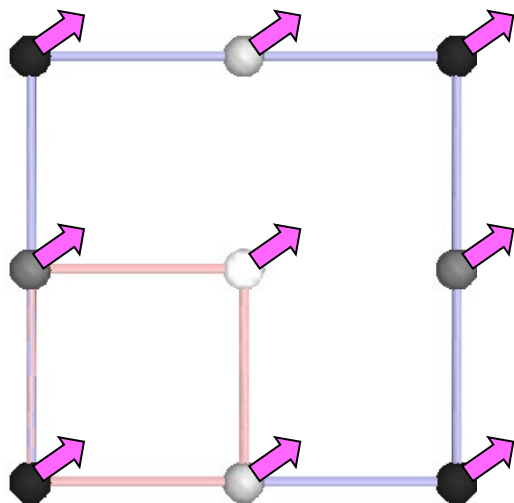
$mX_3(a, b)$
 $Pba2.1'_c$

Symmetry modes yield an orthogonal basis for distortion space.



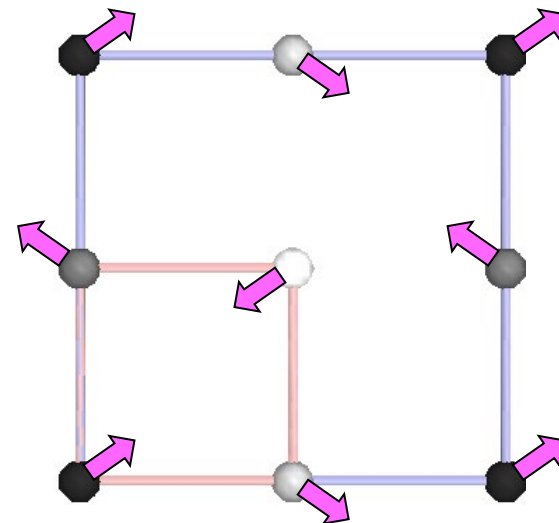
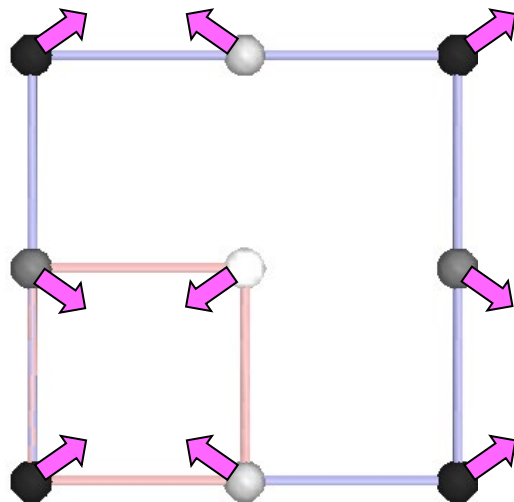
Symmetry modes: a new parameter set

$m\Gamma_5(a, b)$
 $P1$



$mM_5(a, b)$
 $P2.1'_a$

$mX_4(a, b)$
 $Pmm2.1'_c$



$mX_3(a, b)$
 $Pba2.1'_c$

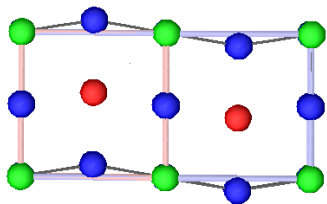
Symmetry modes yield an orthogonal basis for distortion space.



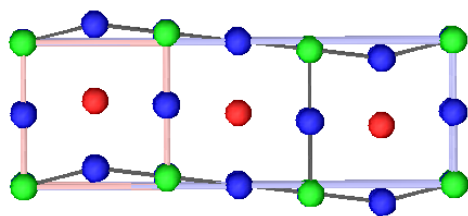
Modulation wavevector

A symmetry-breaking crystal distortion can be decomposed into modulation waves, each with a characteristic wavevector. Some modulations have a single k vector while other are multi- k .

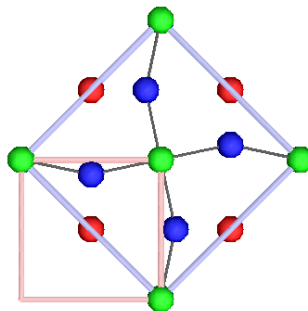
$$\mathbf{k} = (\frac{1}{2}, 0, 0)$$



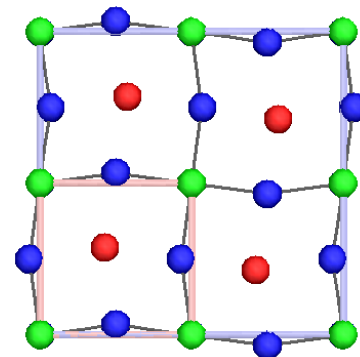
$$\mathbf{k} = (\frac{1}{3}, 0, 0)$$



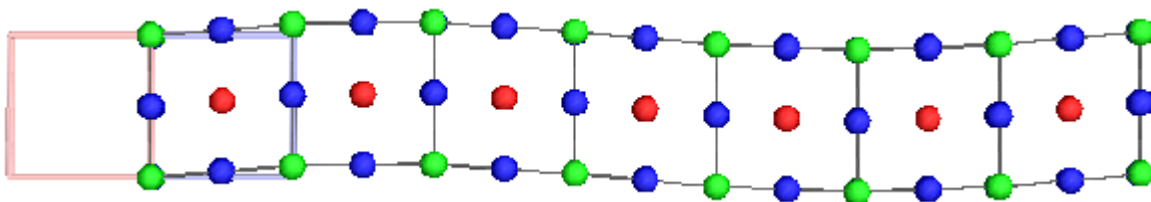
$$\mathbf{k} = (\frac{1}{2}, \frac{1}{2}, 0)$$



$$\mathbf{k} = \{(\frac{1}{2}, 0, 0), (0, \frac{1}{2}, 0)\}$$



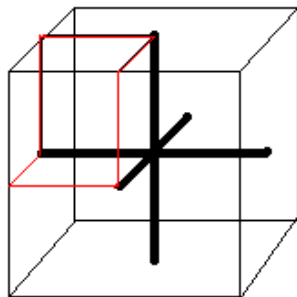
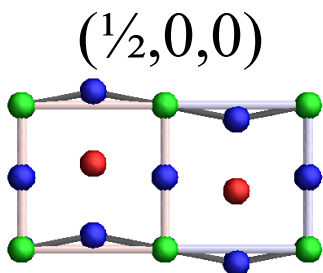
$$\text{incommensurate } \mathbf{k} = (0.1521, 0, 0)$$



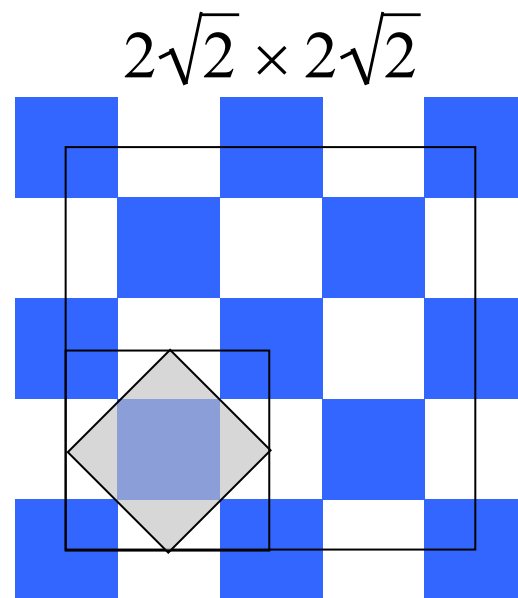
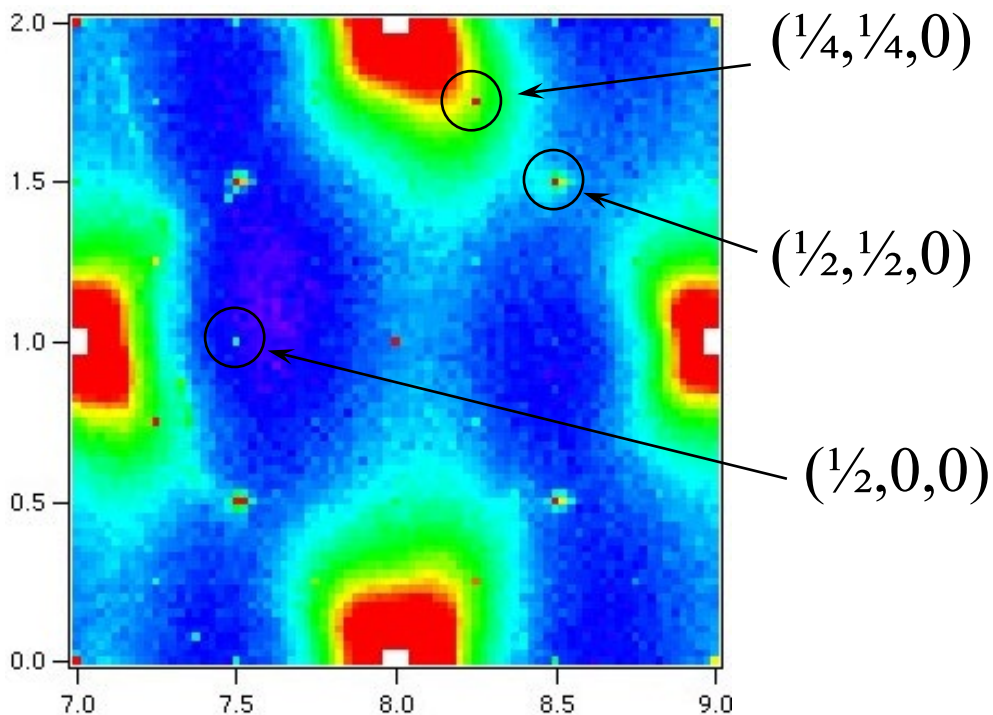
Incommensurate means the wavevector \mathbf{k} has irrational components.



Symmetry modes in crystals are waves

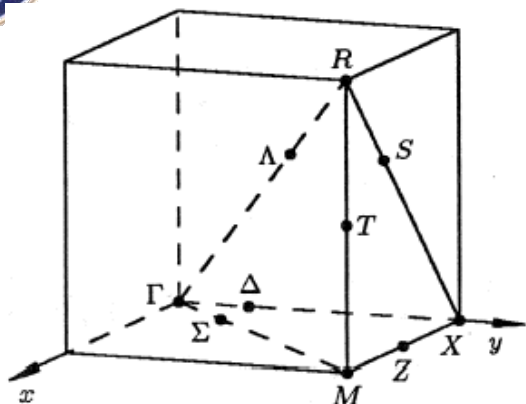


Crystallographic irreps are defined in reciprocal space. Distinct k vectors in the FBZ have distinct irreps.

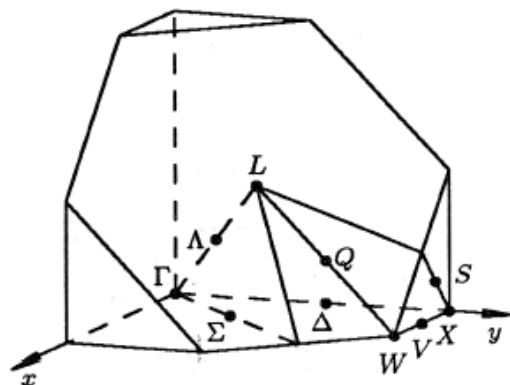




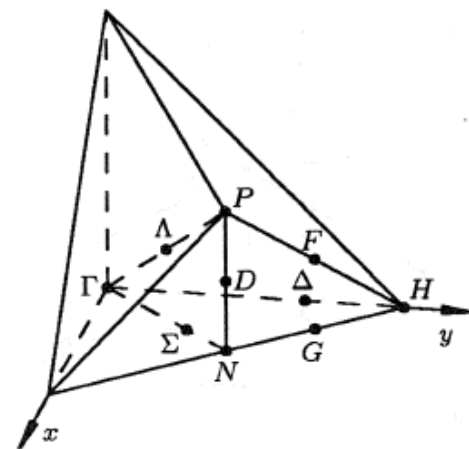
k -point labels and irrep labels



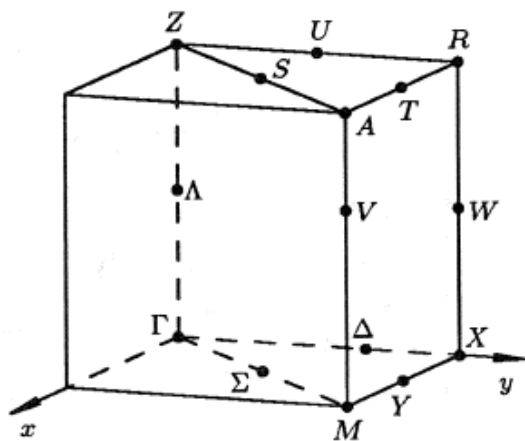
Primitive Cubic



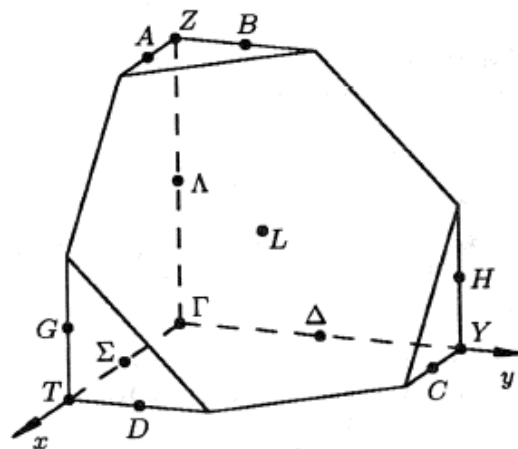
Face-Centered Cubic



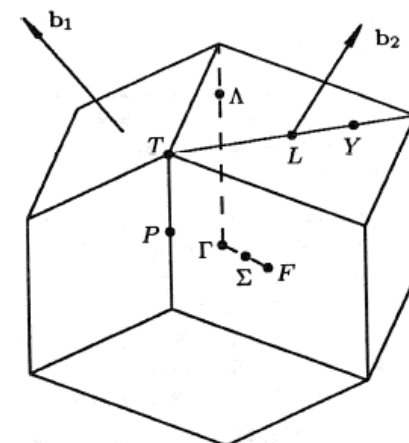
Body-Centered Cubic



Primitive Tetragonal



Face-Centered Ortho

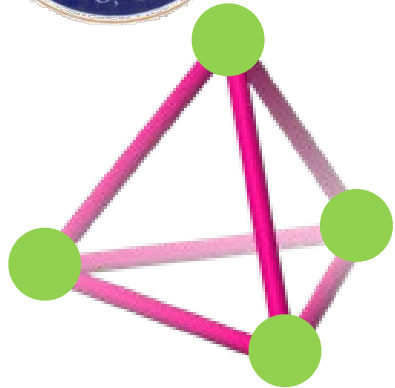


Rhombohedral

A. P. Cracknell, B. L. Davies, S. C. Miller, and W. F. Love, *Kronecker Product Tables, Vol. 1* (1979).
Based on work by S. C. Miller and W. F. Love (1967).



Symmetry modes and diffraction patterns



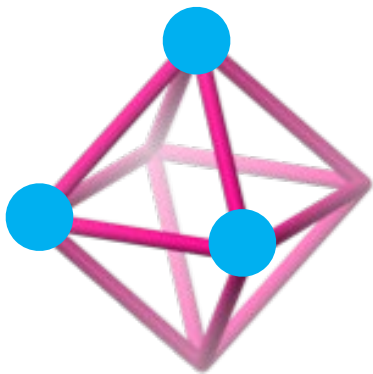
$$L_1^+(a;b;c;d)$$

$$\begin{pmatrix} 1/2, 1/2, 1/2 \end{pmatrix}$$

$$\begin{pmatrix} 1/2, -1/2, -1/2 \end{pmatrix}$$

$$\begin{pmatrix} -1/2, 1/2, -1/2 \end{pmatrix}$$

$$\begin{pmatrix} -1/2, -1/2, 1/2 \end{pmatrix}$$



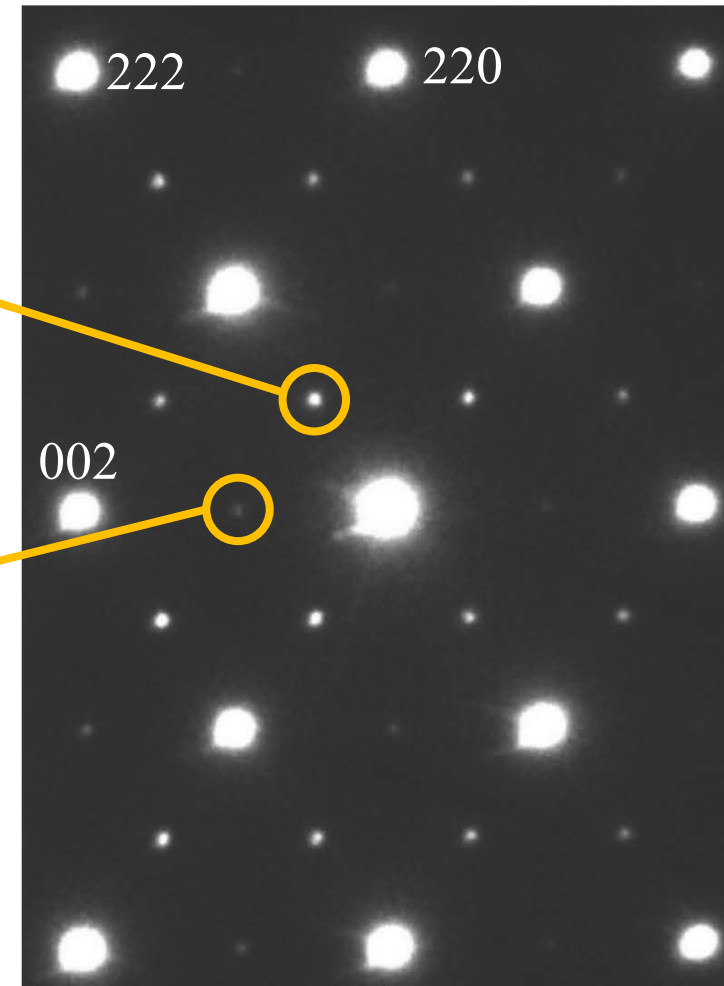
$$X_1^+(a;b;c)$$

$$\begin{pmatrix} 1, 0, 0 \end{pmatrix}$$

$$\begin{pmatrix} 0, 1, 0 \end{pmatrix}$$

$$\begin{pmatrix} 0, 0, 1 \end{pmatrix}$$

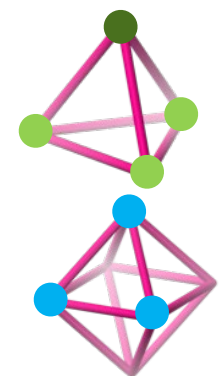
$[1\bar{1}0]_{\text{fcc}}$



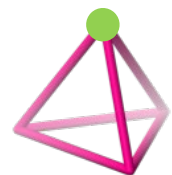
The “star” of a k-vector includes all symmetry-related peaks that are not related to one another via a reciprocal-lattice vector.



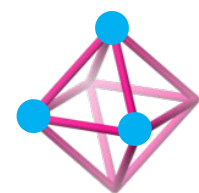
Cu_xPt_{3-x} phase diagram



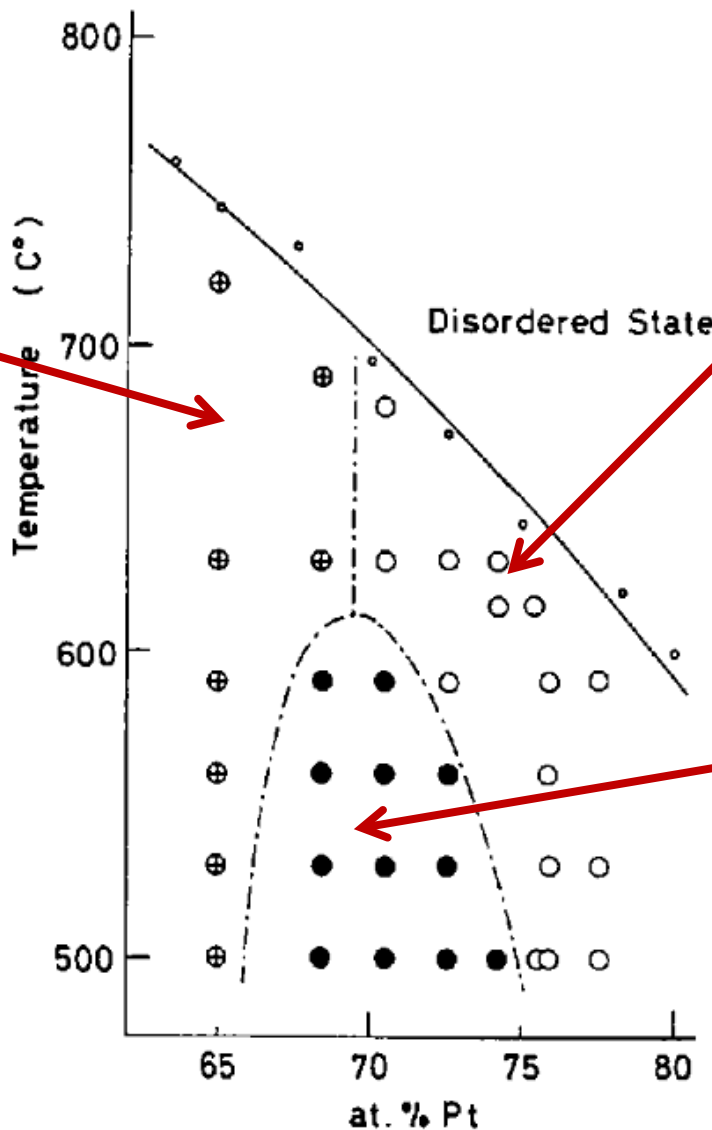
$L_1^+(a, b, b, b)$
 $X_1^+(a', a', a')$
 big rhomb



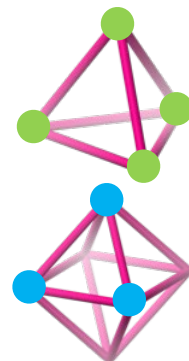
$L_1^+(a, 0, 0, 0)$
 small rhomb
 50% Pt



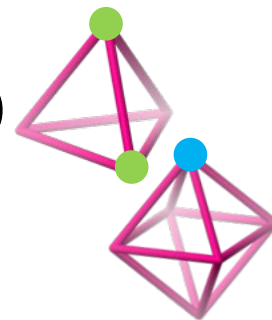
$X_1^+(a, a, a)$
 small cubic
 25% Pt



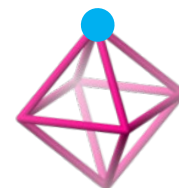
$L_1^+(a, a, a, a)$
 $X_1^+(a', a', a')$
 big cubic



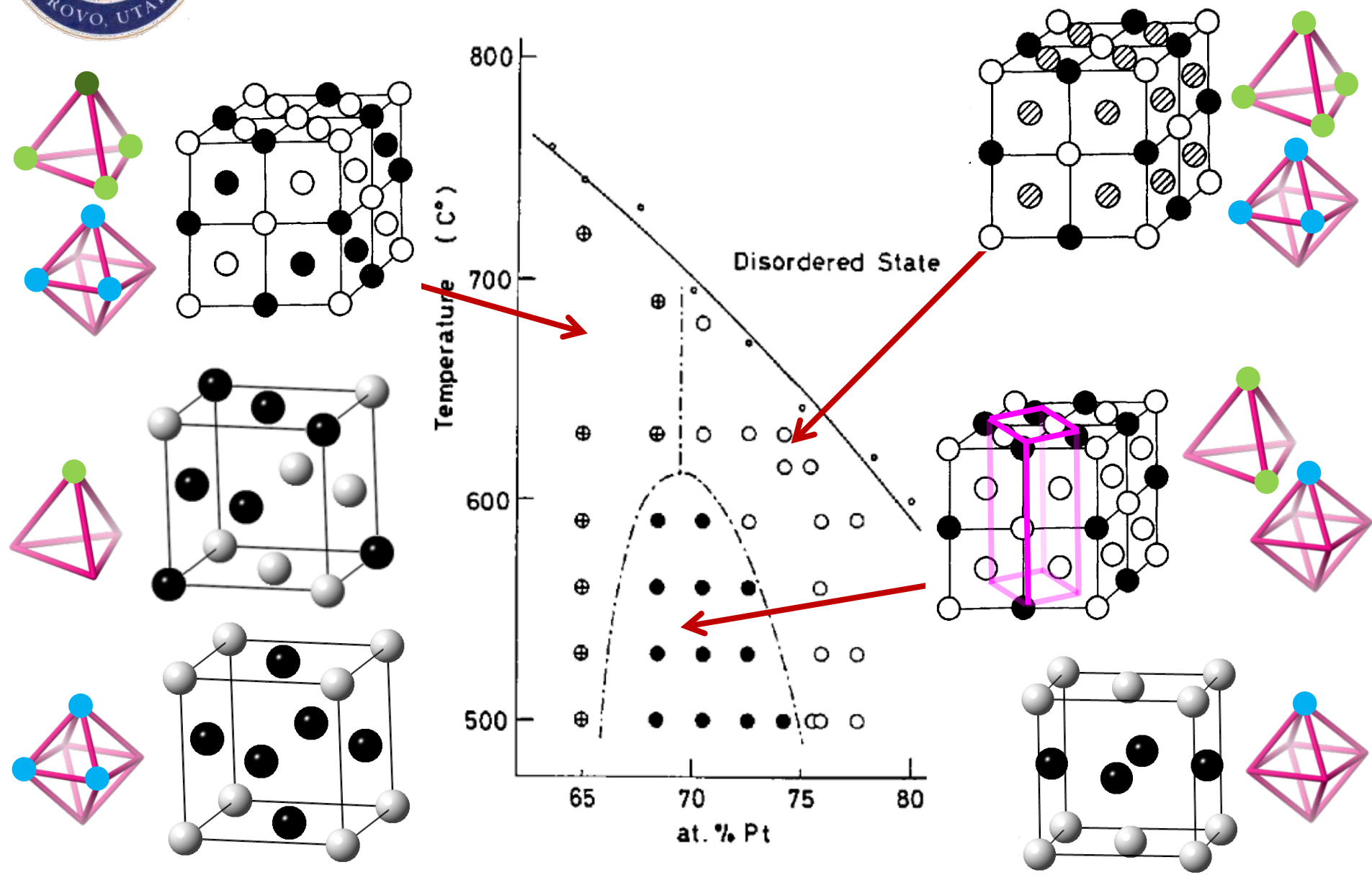
$L_1^+(a, a, 0, 0)$
 $X_1^+(a', 0, 0)$
 big ortho



$X_1^+(a, 0, 0)$
 common
 not in CuPt



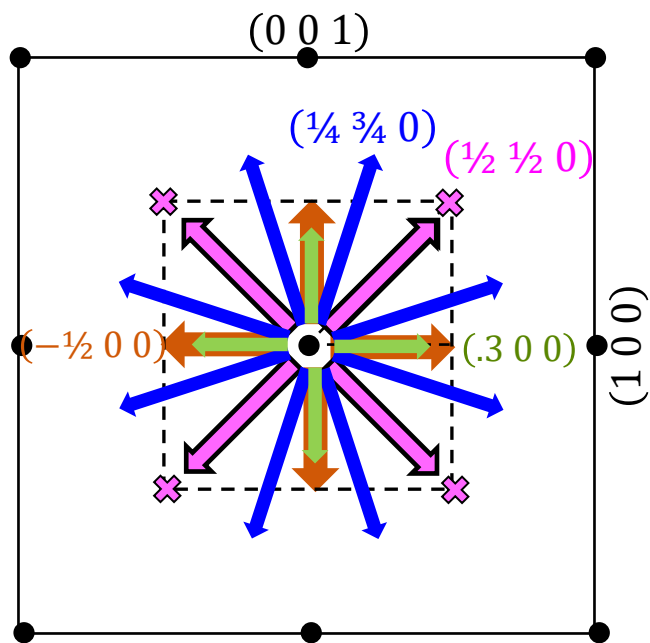
$\text{Cu}_x\text{Pt}_{3-x}$ phase diagram





Wavevector star

The *star* of a \mathbf{k} vector is the set of all symmetry-related \mathbf{k} vectors (relative to the reciprocal space group). Normally, we just identify a generating set of representative \mathbf{k} vectors, which are not related to each other by lattice translations.



$P4mm$ example:

$$\left(\frac{1}{2}, \frac{1}{2}, 0\right), \left(-\frac{1}{2}, \frac{1}{2}, 0\right), \left(\frac{1}{2}, -\frac{1}{2}, 0\right), \left(-\frac{1}{2}, -\frac{1}{2}, 0\right)$$

$$\left(\frac{1}{2}, 0, 0\right), \left(-\frac{1}{2}, 0, 0\right), \left(0, \frac{1}{2}, 0\right), \left(0, -\frac{1}{2}, 0\right)$$

$$\left(\frac{1}{4}, \frac{3}{4}, 0\right), \left(-\frac{1}{4}, \frac{3}{4}, 0\right), \left(\frac{1}{4}, -\frac{3}{4}, 0\right), \left(-\frac{1}{4}, -\frac{3}{4}, 0\right), \\ \left(\frac{3}{4}, \frac{1}{4}, 0\right), \left(-\frac{3}{4}, \frac{1}{4}, 0\right), \left(\frac{3}{4}, -\frac{1}{4}, 0\right), \left(-\frac{3}{4}, -\frac{1}{4}, 0\right)$$

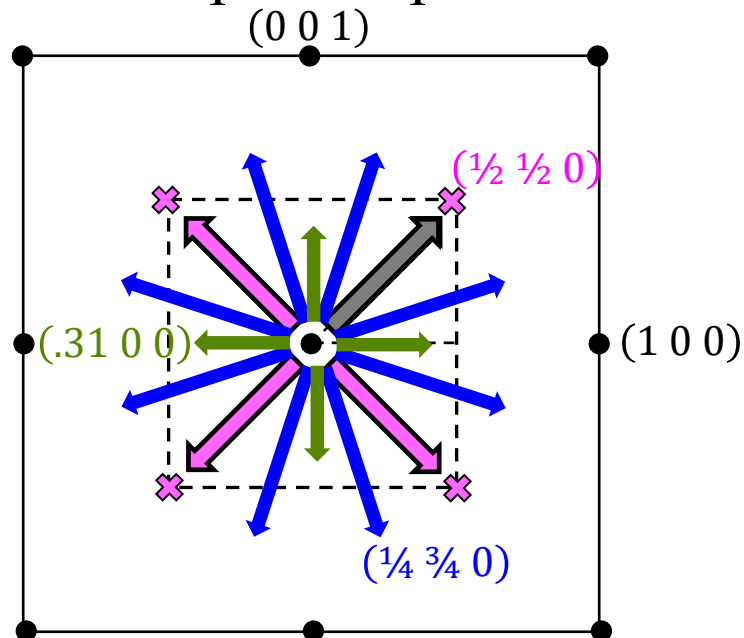
$$(0.3, 0, 0), (-0.3, 0, 0), (0, 0.3, 0), (0, -0.3, 0)$$

For each star, a set of representative \mathbf{k} vectors is colored **red**.



Space-group irrep calculations

reciprocal space



Complete space-group irreps
(any commensurate/incommensurate k)

ISO-IR, Stokes & Campbell (2014)
Tabulated – not real-time calculation!

Little- k group irreps

Faddeyev; Kovalev; Zak, Casher,
Glück & Gur; Bradley, Cracknell,
Davies, Miller, Love (1964-1979)

Complete space-group irreps
at special- k points

Simultaneous action of entire k star.
8 cases worked *manually* (1968-1984).

Tables of Stokes & Hatch (1984, 1987):
all 4777 space groups irreps at special k ;
15239 isotropy subgroups [green book].

Complete space-group irreps
at any commensurate k point

Karep (1992), ISOTROPY (1995).
Requires real-time calculations.



Irreps to $(3+d)$ D superspace

research papers *Acta Cryst.* A69, 75-90 (2013).



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Foundations of
Crystallography
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Tabulation of irreducible representations of the crystallographic space groups and their superspace extensions

Received 24 December 2012
Accepted 19 March 2013

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- New irreps matrices for all space groups at commensurate \mathbf{k} vectors. Similar to earlier matrices ($g' = AgA^{-1}$ for $g \in G$), modern form.
- Separated form makes tabulation possible for the first time!
- Irrep matrices tabulated for superspace extensions of all space groups for the first time. Their isotropy subgroups are superspace groups.



Selecting an isotropy subgroup

parent space-group symmetry

↓
 k -point

finite number of types (e.g. Γ , Δ , X),
but ∞ number of points

↓
irrep

finite number for each k -point (e.g. X_1^+ , X_3^+ , X_5^-)

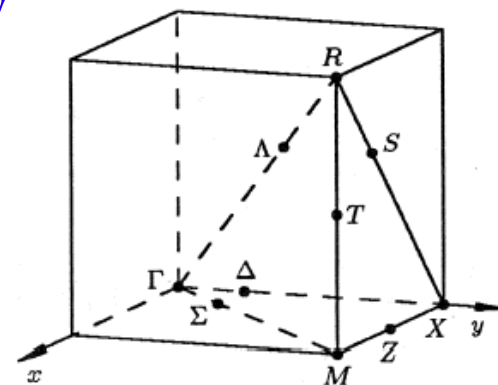
↓
order-parameter direction (OPD)

finite number for each IR; special points/lines/planes in abstract representations space



isotropy subgroup

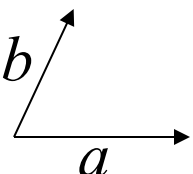
- [1] space-group type (230) or magnetic space group type (1651)
- [2] supercell basis (relative to parent)
- [3] origin of supercell (relative to parent)



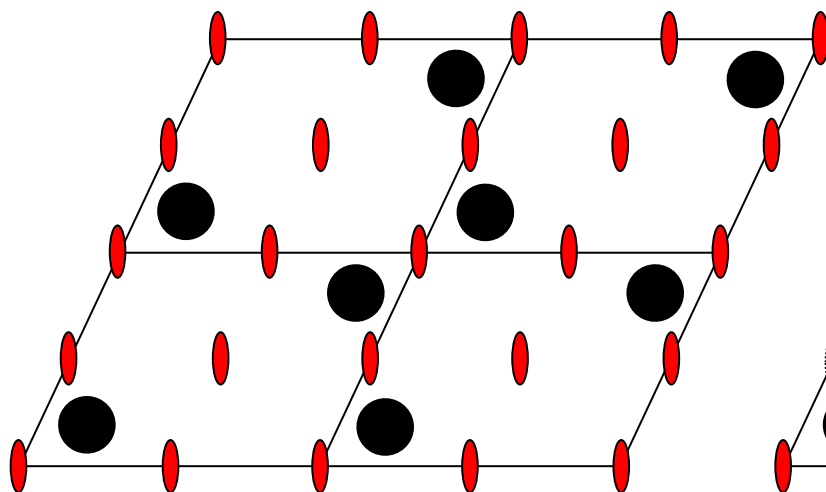


Distortion: (basis, SG-type)

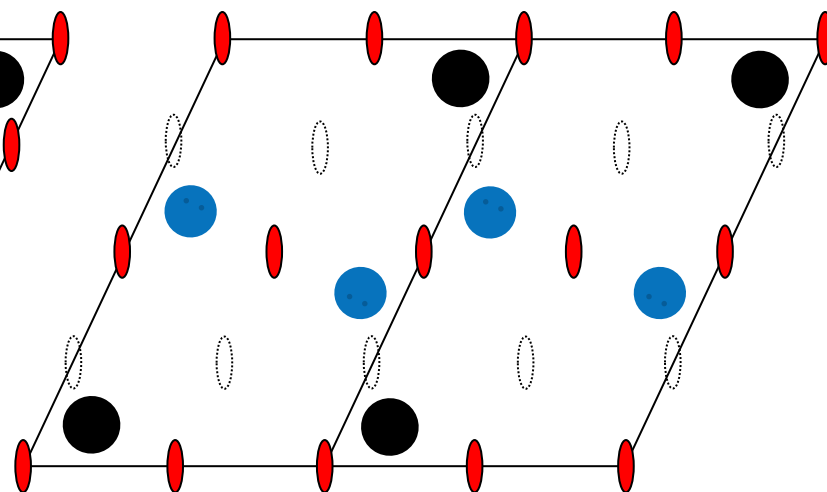
$P2$



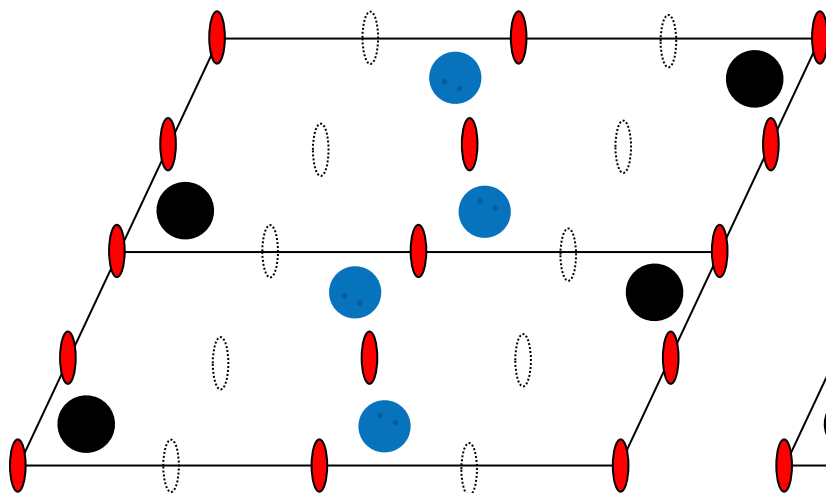
A diagram showing the coordinate axes for the P2 space group. The vertical axis is labeled b and the horizontal axis is labeled a .



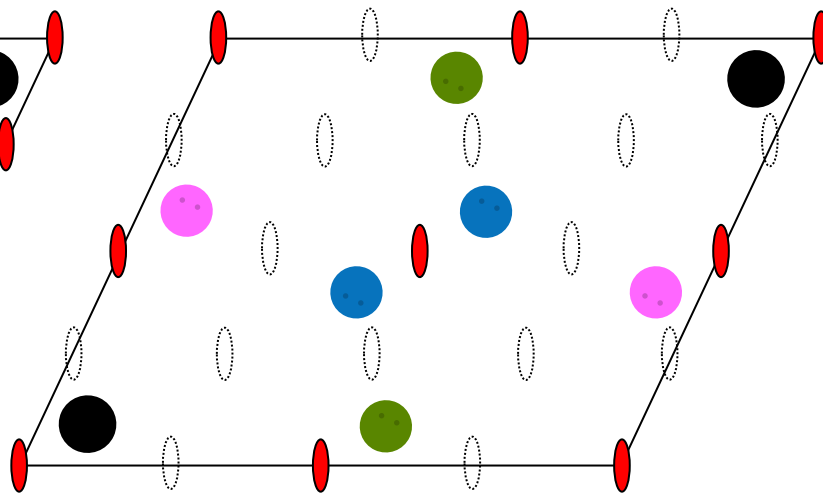
$\{(1,0,0), (0,1,0), (0,0,1)\}$



$\{(1,0,0), (0,2,0), (0,0,1)\}$



$\{(2,0,0), (0,1,0), (0,0,1)\}$



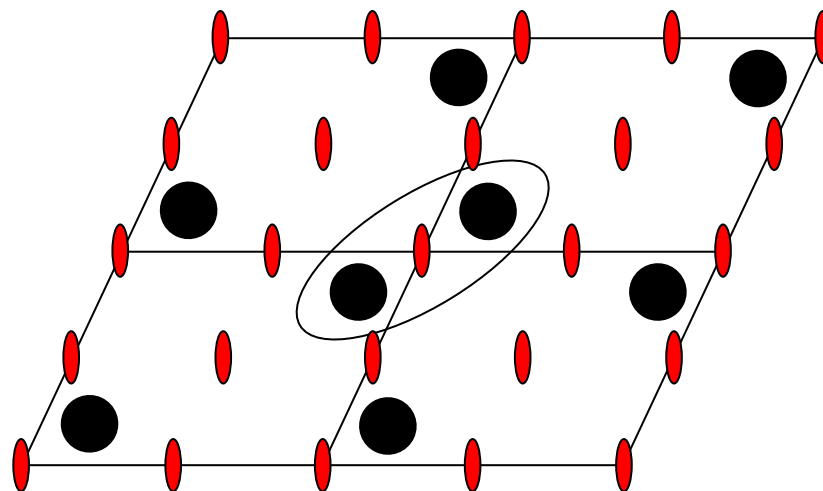
$\{(2,0,0), (0,2,0), (0,0,1)\}$

Distortion: (basis, origin, SG-type)

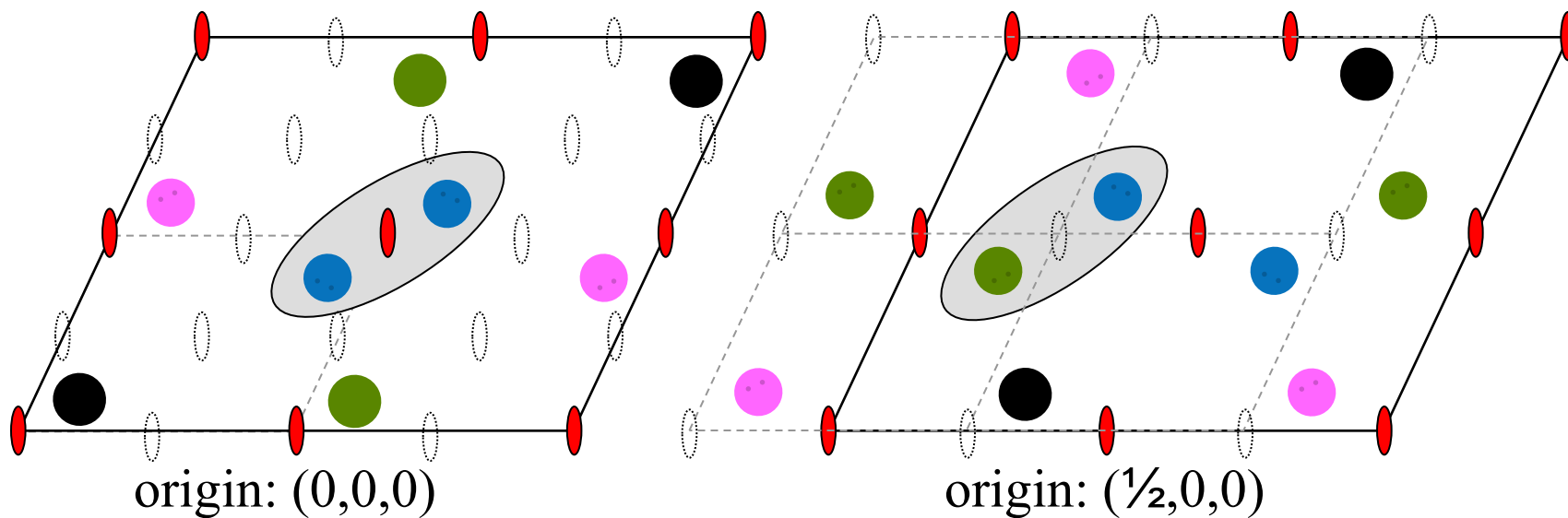
$P2$

b

a



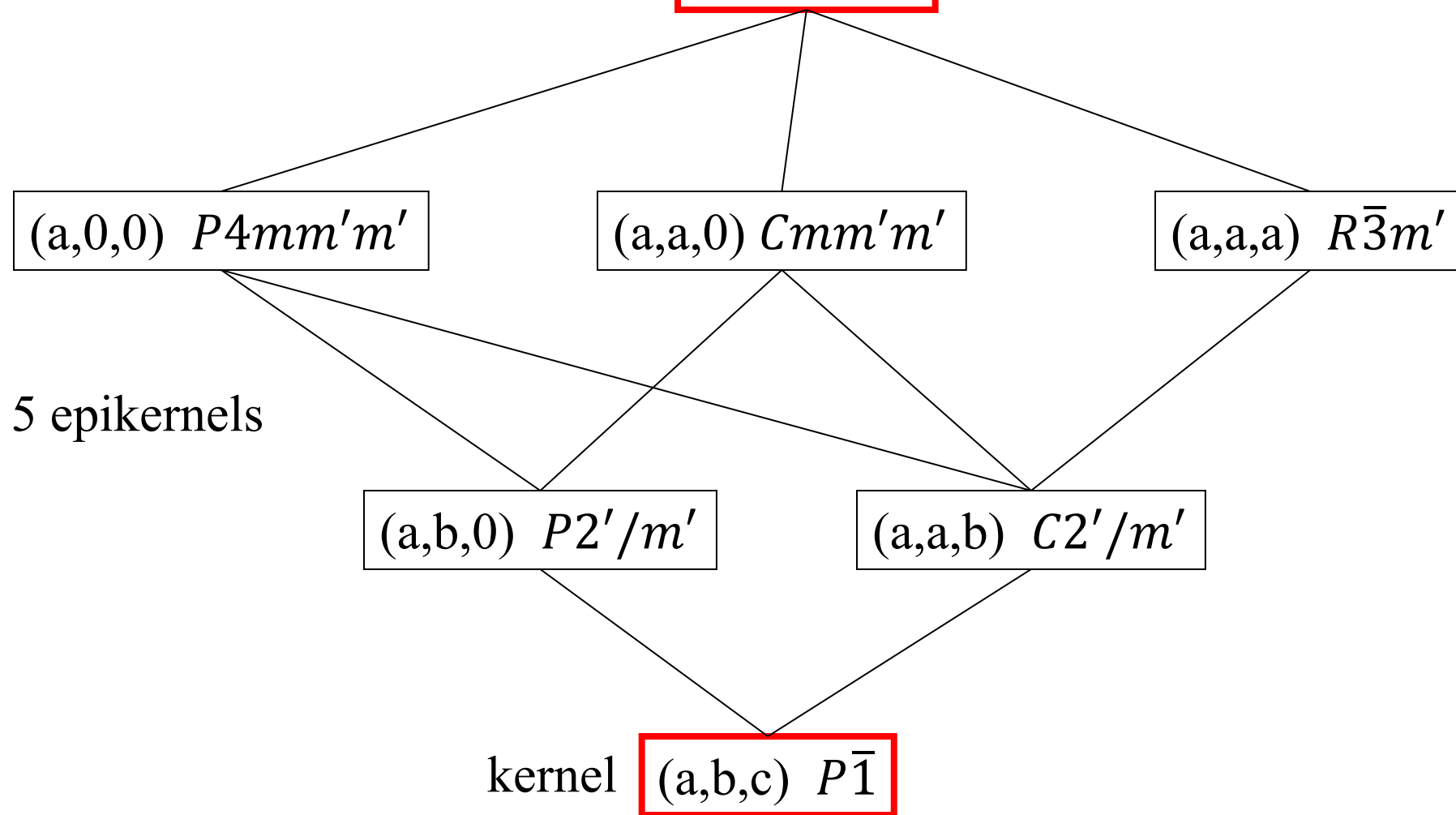
Two distinct cases with same basis = $\{(2,0,0), (0,2,0), (0,0,1)\}$





Single-k irrep \rightarrow many symmetry groups

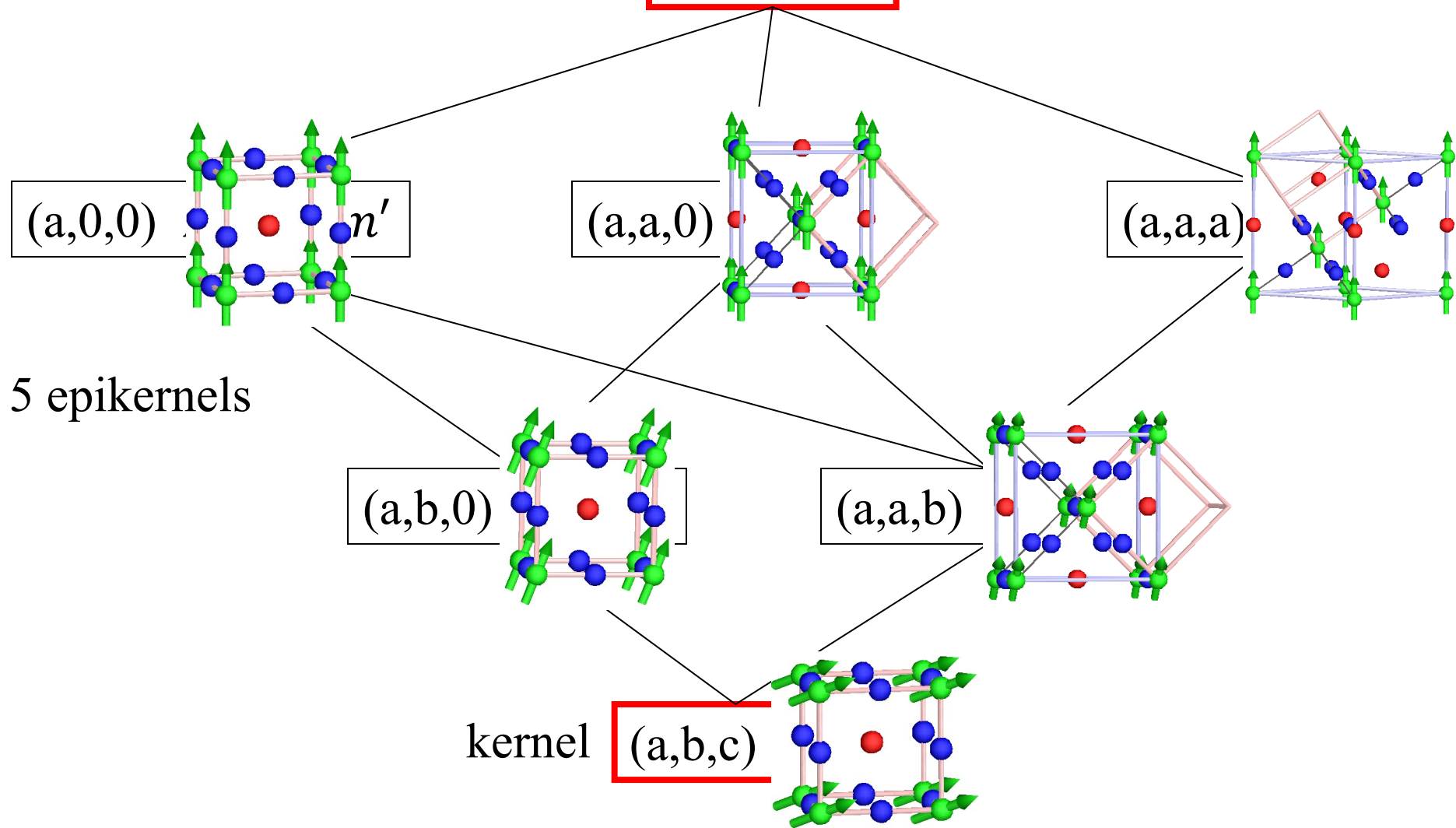
$m\Gamma_4^+$ irrep of $Pm\bar{3}m. 1'$ has 6 OPDs.





Single-k irrep \rightarrow many symmetry groups

$m\Gamma_4^+$ irrep of $Pm\bar{3}m. 1'$ has 6 OPDs.





One symmetry group, many irreps

Strain

$$[0,0,0]\Gamma_1^+, \Gamma_3^+, \Gamma_5^+$$

Displacive & rotational

$$[1/2, 1/2, 0]M_3^+$$

$$[1/2, 0, 0]X_5^+$$

$$[1/4, 1/4, 1/4]R_4^+$$

Site order (Co/Ru)

$$[1/2, 1/2, 1/2]R_4^+$$

Magnetic (Co)

$$[1/4, 1/4, 1/4]m\Lambda_3$$





Summary

- Symmetry modes can describe lattice strains, displacements, magnetic moments, occupancies, rigid-unit rotations, and thermal ellipsoids.
- Symmetry modes are classified by \mathbf{k} vector, irrep, and OPD. They provide a complete and orthogonal basis for the space of all distortions.
- Symmetry-modes span the same configurational space as traditional coordinates if all relevant k -points, irreps, and OPD components are considered simultaneously. Number of free variables is conserved!
- Symmetry modes are symmetry-adapted linear combinations of traditional parameters. One mode can affect many symmetry-distinct atoms. One atom can be affected by many modes.
- The linear transformation between traditional and symmetry-mode coordinate is accomplished with a numeric invertible square matrix.
- Symmetry modes very often provide the most natural/efficient basis. Nature tends to activate as few symmetry modes as possible. Even complicated magnetic structures are usually described by a single irrep!





Introduction to the ISOTROPY Software Suite

Branton J. Campbell

Department of Physics & Astronomy

Brigham Young University

2024 International Workshop on Magnetic Crystallography (IWMC2024)

Organized by the Chinese Spallation Neutron Source

Dongguan International Exhibition Hotel, Dongguan City, Guangdong, China

24-30 November 2024



ISOTROPY software suite (iso.byu.edu)

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:** 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:** 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:** 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.



ISOTROPY Software Suite

Tools for magnetic symmetry and magnetic structures

- **ISODISTORT**: parent structure file is required; treats any combination of order parameter types (displacive, magnetic, occupational, rotational, strain); accepts any combination of irreps/OPDs at commensurate and incommensurate k vectors.
- **ISOSUBGROUP**: no structural input required; for any space group, find magnetic and non-magnetic subgroups involving order parameters at any combination of commensurate and incommensurate k vectors.
- **FINDSYM**: Detect and enforce symmetry of a structure model to within user-specified tolerances on commensurate or incommensurate displacive, magnetic, rotational, and occupational parameters, as well as strains; the symmetry group can be a SG, SSG, MSG, or MSSG.
- **ISOCIF**: Build/modify structure files using a symmetry group and traditional parameters; employ FINDSYM to detect pseudo-symmetry; reduce symmetry to $P1$, apply arbitrary setting transformation; drop modulations or magnetic moments.



ISOTROPY Software Suite

Tools for magnetic symmetry and magnetic structures

- **ISO-MAG**: First computer readable table of MSG operations and Wyckoff sites (BNS and OG settings).
- **ISO-IR**: The only tabulation of complete space-group irreps for all special and non-special k -vectors of all crystallographic space groups (2011).
- **ISO(3+ d)D**: The only tabulation of all superspace groups and non-magnetic superspace groups and their operations, k vectors, and Wyckoff-site data.
- **ISOSPACEGROUP**: A tool for presenting the symmetry operations and Wyckoff positions of any SG, SSG, MSG, or MSSG in an arbitrary setting.
- **FINDSSG**: Identify an SSG or MSSG from a generating list of operations, together with the transformation to the standard group setting.
- **TRANSFORMSSG**: Tool for applying an arbitrary setting transforming to the operations and k vectors of an SSG or MSSG, starting from any setting.



ISODISTORT

- Generate child-structure models from a high-symmetry parent using either traditional or symmetry-mode parameters.
- Compare different child structures using common parent-centric parameter set.
- Export models for refinement, DFT analysis, and/or publication.

ISODISTORT

Version 6.12.1, Oct 2023

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.

[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](#).



The “search” for an isotropy subgroup

ISODISTORT has four search methods:

Method 1 (special): Filtered search of tabulated list of irreps/OPDs at special k points.

Method 2 (general): Arbitrary superposition of irreps/OPDs from multiple commensurate and incommensurate k stars.

Method 3 (supercell): Find all isotropy subgroups with a given point/space group and sublattice.

Method 4 (decomposition): Decompose a known child structure into symmetry modes of a known parent structure. Requires a group-subgroup relationship, with relative basis/origin.



Irrep basis function conventions

“basis vectors” (Fullprof/SARAh)

$$m_j = \sum_{k,v} \Psi_v^k e^{-2\pi i \mathbf{k} \cdot (\mathbf{t}_j - \mathbf{t}_0)} + \Psi_v^{k*} e^{-2\pi i (-\mathbf{k}) \cdot (\mathbf{t}_j - \mathbf{t}_0)}$$

$$= \sum_{k,v} 2\operatorname{Re}(\Psi_v^k) \cos(2\pi \mathbf{k} \cdot (\mathbf{t}_j - \mathbf{t}_0)) - 2\operatorname{Im}(\Psi_v^k) \sin(2\pi \mathbf{k} \cdot (\mathbf{t}_j - \mathbf{t}_0))$$

$$= \sum_{k,v} \boxed{|\Psi_v^k| \cos(2\pi \mathbf{k} \cdot (\mathbf{t}_j - \mathbf{t}_0) + \varphi_v^k)} \quad \begin{array}{l} \text{“basis function”} \\ \text{(ISOTROPY terminology)} \end{array}$$

SARAh and Fullprof use complex irreps and basis vectors, taking real part at the end. ISOTROPY uses physically-irreducible representations (pirreps), which have real matrices and basis vectors at every step. The end result is the same. ISOTROPY further uses $t_0 = 0$ (origin-referenced rather than atom-referenced) modulations.



Hands-on tutorials

The ISOTROPY Software Suite is web-based software. Our web servers have limited capacity for a large number of simultaneous calculations. Please work together in **teams of two people** to reduce server load. One team member opens the tutorial instructions, and one accesses the server.

During lunch, download tutorial materials from <https://iso.byu.edu/iso/isodistorttutorials.php> and **download/install the ISOVIZ/ISOVIZQ** programs from iso.byu.edu.

Any internet browser should work. I prefer Firefox because it gives the option to open isoviz files directly without a download step.

Work through the tutorial exercises at your own pace in any order you like. Inexperienced users may want to start with the first exercise.



LaMnO₃ (single k , 1D irrep, Γ point)

MSG: 62.448 $Pn'ma'$
colinear AF, $m = 3.87 \mu_B$

Parent: $Pnma$

$k = (0,0,0)$, IR/OPD = $m\Gamma_4^+(a)$

basis = $\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$, origin = (0,0,0)

volume index: $s = 1$

symmetry index: $i = 2$

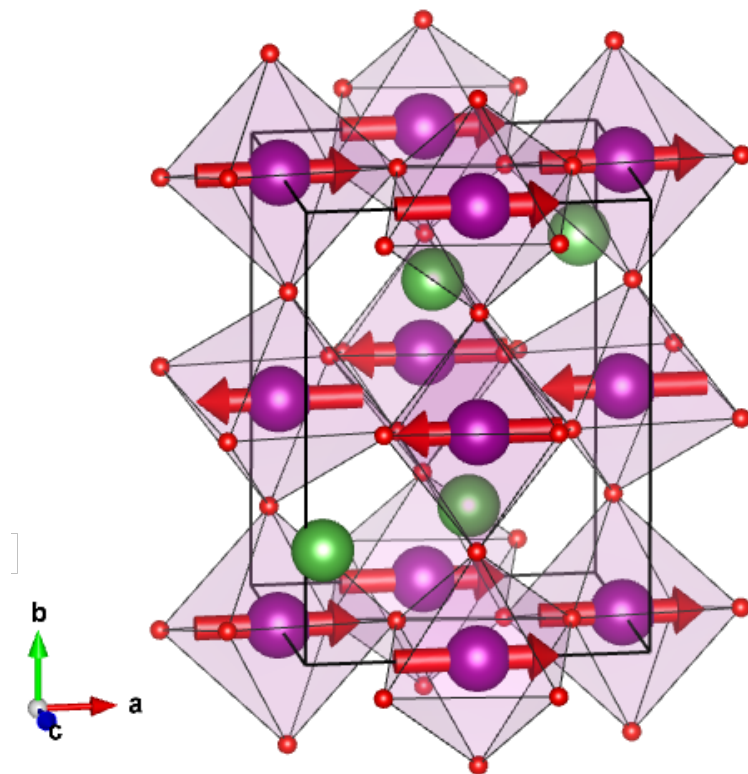
Parent: $Pm\bar{3}m$ (cubic perovskite)

$k = (\frac{1}{2}, 0, 0), (\frac{1}{2}, \frac{1}{2}, 0), (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$

Magnetic Irrep/OPD: $mX_5^+(a, -a; 0, 0; 0, 0)$

Other displacive IRs: $[\frac{1}{2}, \frac{1}{2}, 0]R_4^+(a, -a, 0)$, $[\frac{1}{2}, \frac{1}{2}, 0]M_{2,3}^+(0; a; 0)$

basis = $\begin{pmatrix} 1 & 1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}$, origin = (0,0,0), $s = 4, i = 48$





La_2CuO_4 (single k , 1D irrep)

MSG: 56.374 $Pbn\bar{b}.1'_C[Cmca]$
colinear AF, $m = 0.17 \mu_B$

Parent: $Cmca$ (#64)

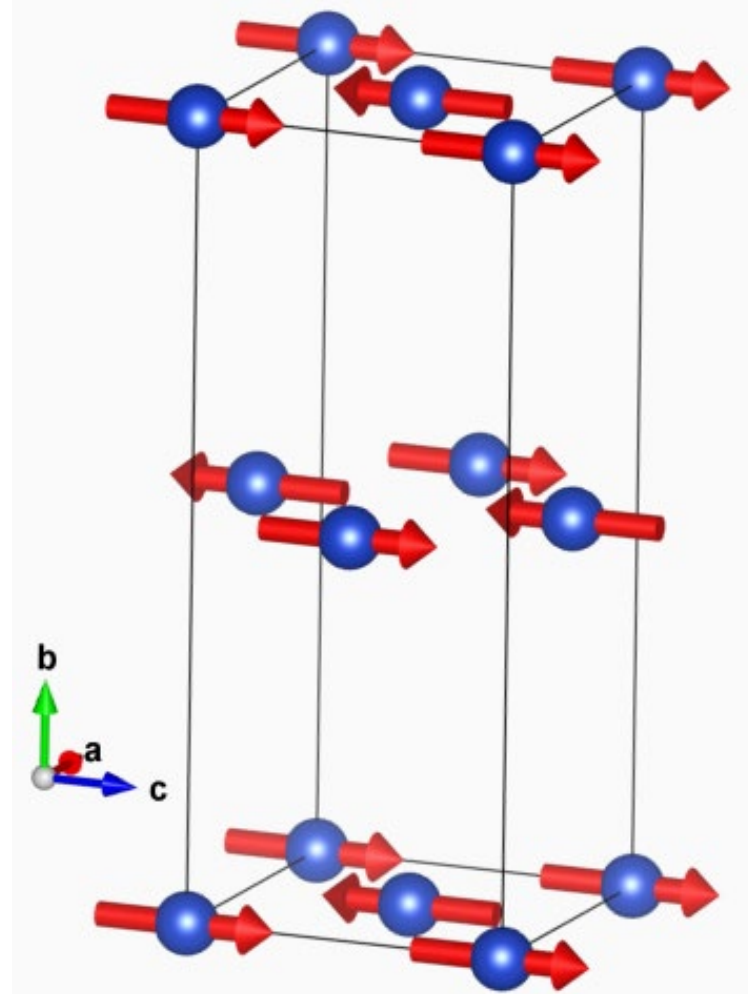
$k = (1,0,0)$

IR/OPD = $mY_4^+(a)$

basis = $\begin{pmatrix} 2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$, origin = $(0,0,0)$

volume index: $s = 2$

symmetry index: $i = 4$





HoMnO₃ (single k , 2D irrep)

MSG: 31.129 $Pmn2_1.1'_b[Pmn2_1]$

colinear AF, $m = 3.87 \mu_B$

Parent: $Pnma$

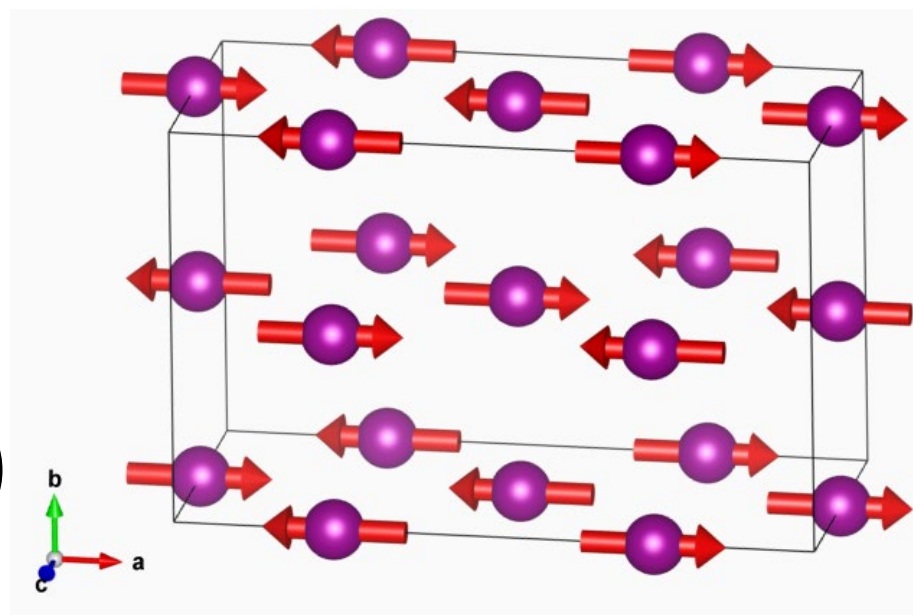
$k = (\frac{1}{2}, 0, 0)$

IR/OPD = $mX_1(a, a)$

basis = $\begin{pmatrix} 2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$, origin = $(-\frac{1}{4}, \frac{1}{4}, 0)$

volume index: $s = 2$

symmetry index: $i = 4$





$\text{Ba}_3\text{Nb}_2\text{NiO}_9$ (single k , 4D irrep)

MSG: 159.64 $P31c.1'_c[P31m]$

AF, $m = 3.87 \mu_B$

Parent: $P\bar{3}m1$ (#164)

Primary $k = (1/3, 1/3, 1/2)$

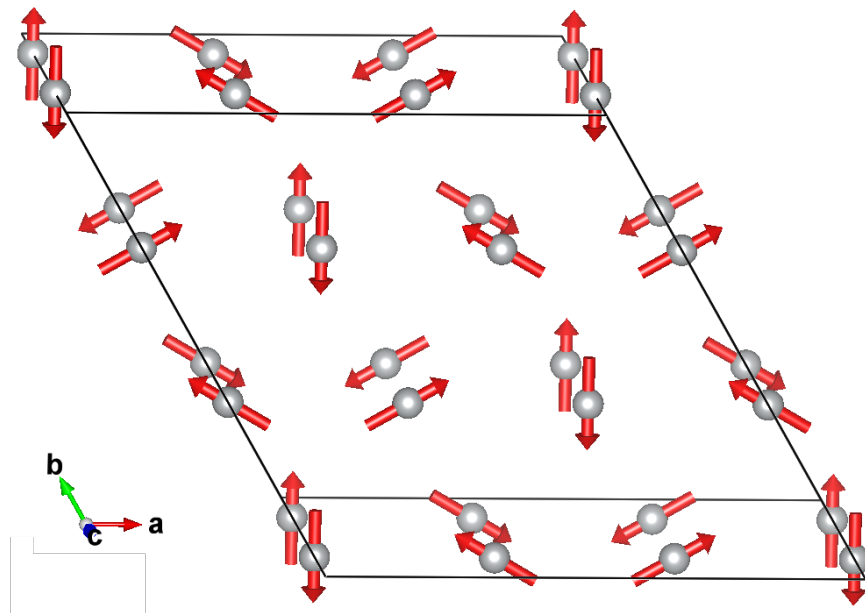
Primary IR/OPD: $mH_3(a, -a/\sqrt{3}, a/\sqrt{3}, a)$

basis = $\begin{pmatrix} -1 & 2 & 0 \\ -2 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}$, origin = $\left(-\frac{2}{3}, -\frac{4}{3}, 0\right)$

volume index: $s = 6$

symmetry index: $i = 12$

Secondary IR/OPD: $k = (0,0,1/2)$, $mA_1(a)$ -- not active.





Nd_2CuO_4 (multi k , (1+1)D irrep)

MSG: 134.481 $P4_2/nnm.1'_C[rP4_2/mmc]$
AF, $m = 1.0 \mu_B$

Parent: $I4/mmm$ (#139)

Multi- k structure

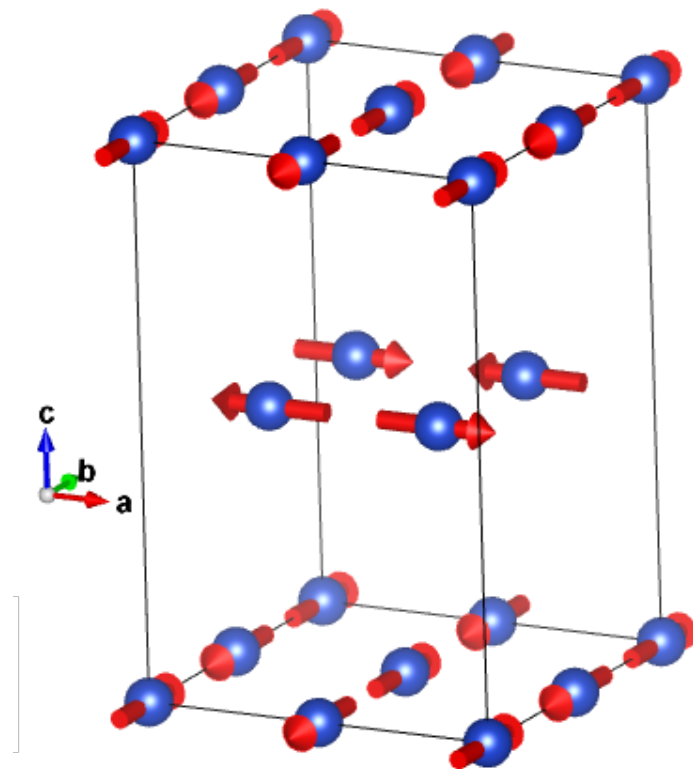
Primary $k = (\frac{1}{2}, \frac{1}{2}, 0), (-\frac{1}{2}, \frac{1}{2}, 0)$

Primary IR/OPD = $mX_4^+(a; a)$

basis = $\begin{pmatrix} 1 & 1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$, origin = $(0, 0, -\frac{1}{2})$

volume index: $s = 4$

symmetry index: $i = 8$





CE-type antiferromagnetic structure

$\text{La}_{0.5}\text{Ca}_{0.5}\text{MnO}_3$ ($Pnma$ at RT)

Mn(3+/4+) charge order and
electronic phase separation

CE-AF/CO structure

$2\sqrt{2} \times 2 \times 2\sqrt{2}$ supercell

Six k stars (Γ , X, M, R, Σ , S) of
cubic parent

48 params in $P1$, 9 in $P2_1m.1'_a$

