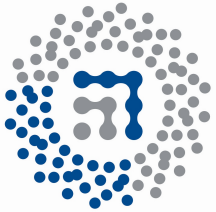


ZTF-FCT
Zientzia eta Teknologia Fakultatea
Facultad de Ciencia y Tecnología

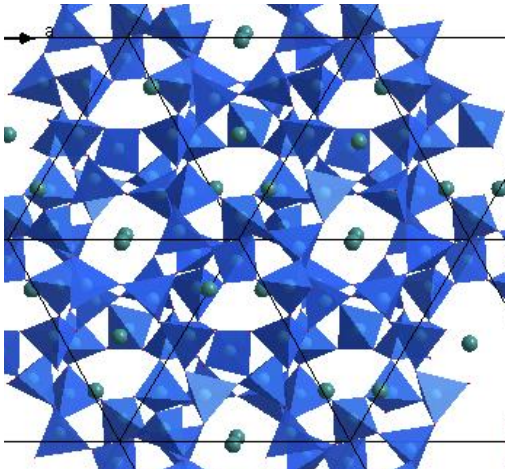
Universidad del País Vasco
Euskal Herriko Unibertsitatea

Analysis of distorted structures in the Bilbao Crystallographic Server.

Use of BCS programs: SUBGROUPS, PSEUDO, AMPLIMODES,…

J. Manuel Perez-Mato
Facultad de Ciencia y Tecnología
Universidad del País Vasco, UPV-EHU
BILBAO, SPAIN

Leucite $KAlSi_2O_6$



$I4_1/a$ (N. 88)

Palmer et. (Amer. Miner. 82 (1997) 16

T=(Al,Si)

88
12.99517 12.99517 13.76451 90 90 90
10

K	1	16f	0.366300	0.365400	0.117100
T	1	16f	0.058200	0.396700	0.165400
T	2	16f	0.168500	0.612400	0.128000
T	3	16f	0.393300	0.640600	0.086300
O	1	16f	0.130800	0.313600	0.111100
O	2	16f	0.092700	0.510500	0.131000
O	3	16f	0.145500	0.679000	0.226900
O	4	16f	0.134200	0.683900	0.035800
O	5	16f	0.289200	0.577300	0.121200
O	6	16f	0.484100	0.617500	0.166500

Problem 1: Is my structure with space group F a distorted structure?

? → F

Pseudosymmetry search

We should search for a structure with space group G (supergroup of F) such that:

Structure G = Structure F + small (symmetry-breaking) distortion

Program PSEUDO for displacive distorted structures

Solid State Theory Applications	
NEUTRON	Neutron Scattering Selection Rules
SYMMODES	Primary and Secondary Modes for a Group - Subgroup pair
AMPLIMODES	Symmetry Mode Analysis
PSEUDO	Pseudosymmetry Search in a Structure
DOPE	Degree of Pseudosymmetry Estimation
TRANPATH	Transition Paths (Group not subgroup relations)
TENSOR ⚠	Symmetry-adapted form of crystal tensors
Check Topological Mat ⚠	Check if a given material is topological or not

PSEUDO

Pseudosymmetry search

The program **PSEUDO** looks for a pseudosymmetry in a structure among the (minimal) supergroups of the structure's space group.

The first step in the program is the input of the structure's data. The data can be given using the form or it can be loaded from a CIF file. The necessary data for the structure consists in the number of its space group in the *International Tables for Crystallography*, Vol A, the lattice parameters (in A and degrees), the number of the atoms in the asymmetric unit and the corresponding atomic positions.

Then, it's necessary to select among what type of supergroups the search is performed. The available options are:

- Minimal supergroups
- Supergroups for a defined cell multiplication
- Supergroup for a well-known transformation matrix

Another option (only for triclinic and monoclinic groups) is to check first the pseudosymmetry of the given cell (obtaining the possible lattice transformations for a given angular tolerance and checking if they are compatible with a space supergroup transformation)

Finally, the program needs a maximum allowed tolerance for pseudosymmetry calculations, i.e., the maximal allowed displacement (in Angstroms) between the mapped atoms of the low symmetry structure obtained by applying the

Formulae

Structure data [in CIF format] Examinar... No se ha seleccionado ningún archivo.

HINT: [The option for a given filename is preferential]

Initial Structure (LS)

```
# Space Group ITA number
99
# Lattice parameters (lengths in angstroems and angles in degrees)
3.999 3.999 4.02 90 90 90
# Number of independent atoms in the asymmetric unit
4
# [atom type] [number] [WP] [x] [y] [z]
Ba 1 - 0.000000 0.000000 0.000000
Ti 2 - 0.500000 0.500000 0.420000
O  3 - 0.500000 0.500000 0.03
O  4 - 0.500000 0.000000 0.58
```

Select supergroups type for pseudosymmetry search.

- (•) Minimal supergroups [ ] [Show only indices in supergroups table]
- ( ) Supergroups with k-index i_k: 1
- ( ) Specify supergroup transformation G: 221

Transf. Matrix (in option 3 only)

	Linear part			Origin Shift
	1	0	0	0
	0	1	0	0
	0	0	1	0

PSEUDO

Finally, the program needs a maximum allowed tolerance for pseudosymmetry calculations, i.e., the maximal allowed displacement (in Angstroms) between the mapped atoms of the low symmetry structure obtained by applying the coset representatives of the supergroup with respect to the subgroup (for details, please refer to the article referenced below). Normally a default value of 2Å is a good choice.

When you have filled all of the data, click on the **[Show]** button to search for pseudosymmetry with respect to the chosen supergroups option.

NOTE: The program only accepts, as input data, structures described in a **standard/default setting** of the space group. If the original structure is described with respect to an **ITA setting**, the program **SETSTRU** can be used to transform it to the standard setting. In the case of more arbitrary non-conventional settings, the tool **TRANSTRU** can be of some help, if the **transformation** to the standard setting is known.

To get a tutorial about this program click here.

If you are using this program in the preparation of a paper, please cite it in the following form:

C. Capillas, E.S. Tasci, G. de la Flor, D. Orobengoa, J.M. Perez-Mato and M.I. Aroyo. "A new computer tool at the Bilbao Crystallographic Server to detect and characterize pseudosymmetry". *Z. Krist.* (2011), **226(2)**, 186-196 DOI:10.1524/zkri.2011.1321.

More articles

(in option 3 only)

0	1	0	0
0	0	1	0

For monoclinic and triclinic structures: previous check of lattice pseudosymmetry

Ang. Tol (in degrees) 5 [*]

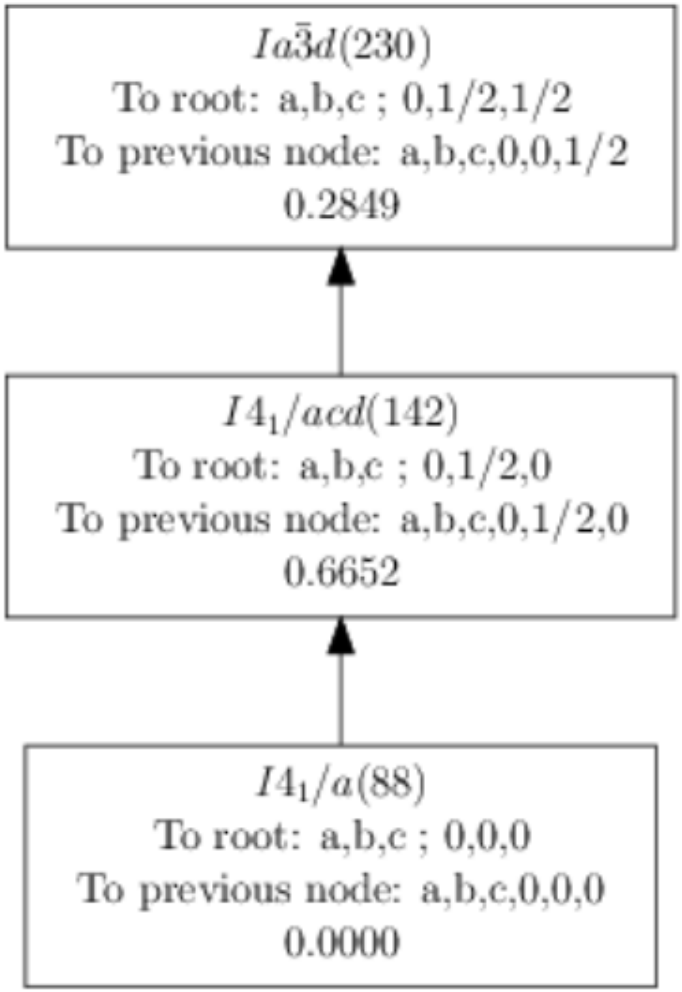
[*] Only for triclinics and monoclinics.

Enter the tolerance (maximum allowed distance) for pseudosymmetry search.

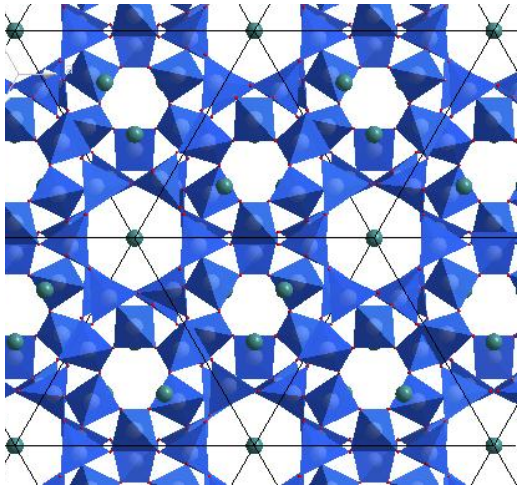
Maximum Δ: 2

Show

Tutorial with examples

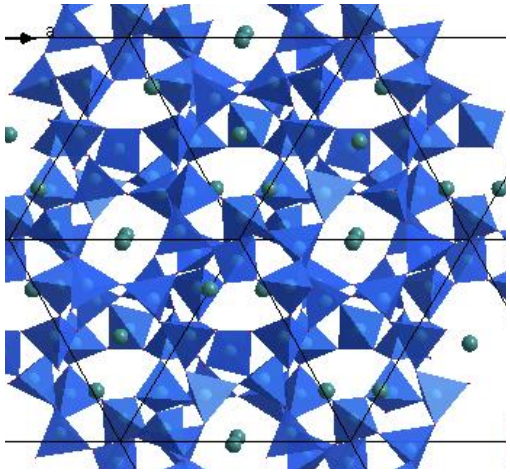

$Ia\bar{3}d(230)$
To root: a,b,c ; 0,1/2,1/2
To previous node: a,b,c,0,0,1/2
0.2849
$I4_1/acd(142)$
To root: a,b,c ; 0,1/2,0
To previous node: a,b,c,0,1/2,0
0.6652
$I4_1/a(88)$
To root: a,b,c ; 0,0,0
To previous node: a,b,c,0,0,0
0.0000

A distorted structure: Leucite $KAlSi_2O_6$



Ia-3d

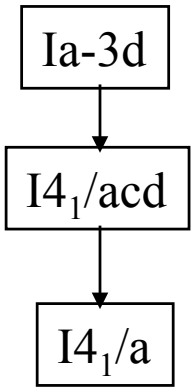
max. atomic displ. : 1.04Å



$I4_1/a$

G= Ia-3d → **F= $I4_1/a$** (a,b,c;0 ½, ½)

G: supergroup of **F**



A distorted structure is **pseudosymmetric** for a supergroup of its space group

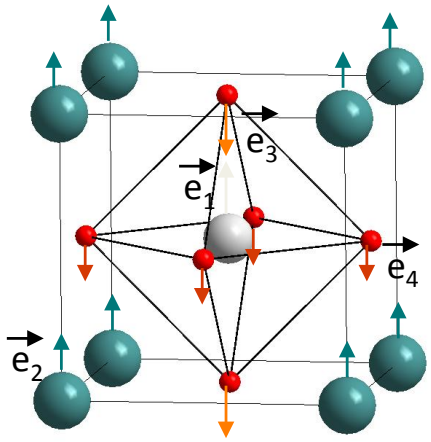
How do we describe a distorted structure?

The natural language to describe a symmetry break/phase transition or a distorted structure in general is the one of collective **symmetry-adapted** modes (Landau Theory)

IRREPS of G

Distorted Structure = High-symmetry Struct + "frozen" symmetry-breaking distortion modes

distortion mode = Amplitude * polarization vector



Description of a displacive "mode":

$\vec{u}(\text{atoms}) = Q\ \vec{e}$

amplitude | polarization vector

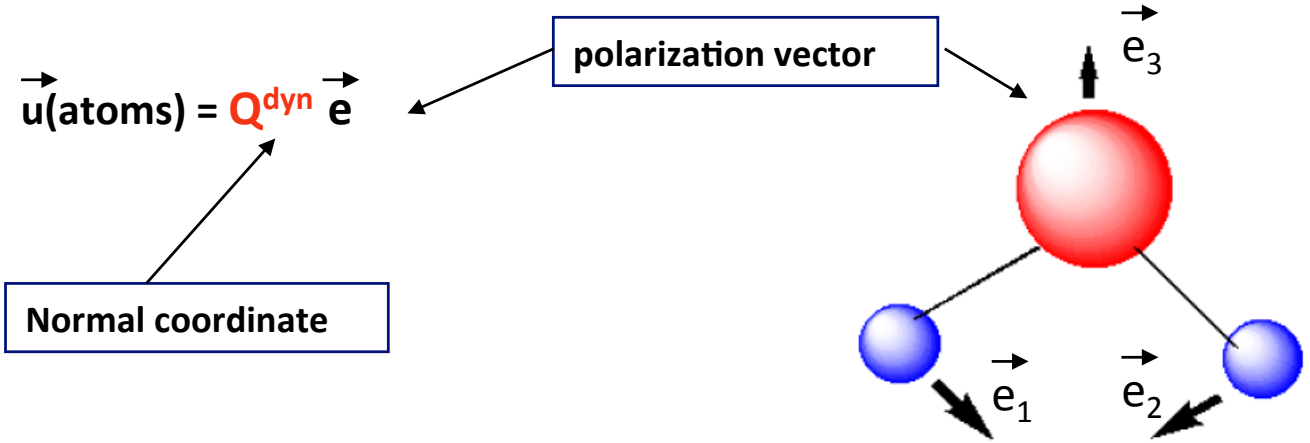
$e = (\ \vec{e}_1\ ,\vec{e}_2\ ,\vec{e}_3\ ,\vec{e}_4\ )$

normalization: $|\vec{e}_1|^2 + |\vec{e}_2|^2 + |\vec{e}_3|^2 + 2\,|\vec{e}_4|^2 = 1$
(within a unit cell)

distortion modes:

- displacive type: local variable =atomic displacements
- order-disorder type: local variable: site occupation probabilities
- magnetic type: local variable: atomic magnetic moments

Modes in the dynamics of molecules:



They transform according to irreps of the point group of the molecule

Mode frequency can be measured or calculated.

Mean value of mode normal coordinate zero: $< Q_i^{dyn} >=0$

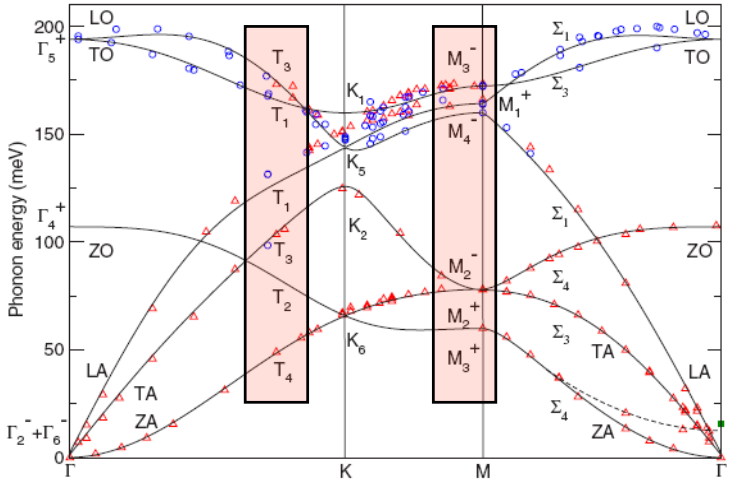
Energy as a function of the normal mode coordinate:

$$E = Eo + 1/2\ \omega^2\ Q^{dyn\,2} + \ldots$$

$$\omega^2(k) > 0$$

Modes in the dynamics of solids:

$\hbar\omega_j(k)$



Mohr et al. PRB 2007

Energy as a function of the normal (dynamic) coordinates:

$$E = Eo + 1/2 \sum \omega^2_j(k)\, Q_j^{dyn\,2}(k) + \ldots$$

$$\omega^2_j(k) > 0$$

Zero mean value of mode coordinates : $< Q_i^{dyn} >= 0$

Symmetry of vibrational modes: **irreducible representations** of the space group

irrep modes....

Modes in the description of the statics (STRUCTURE) of a distorted phase:

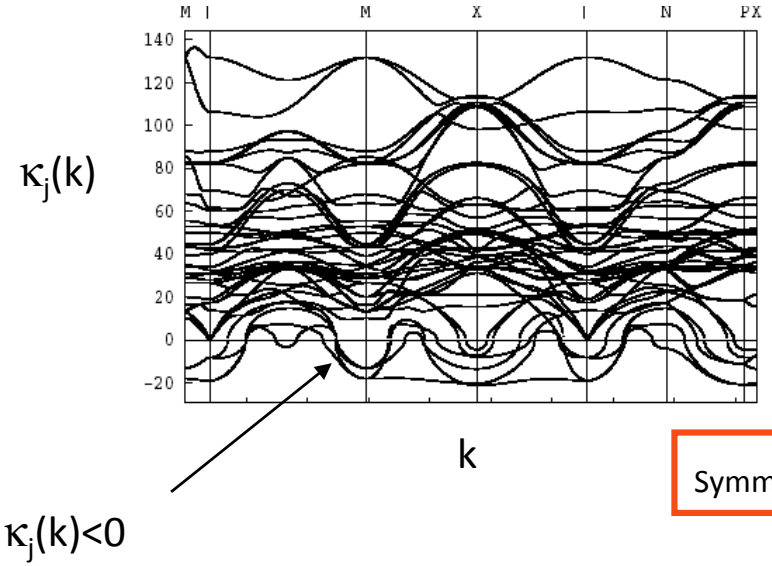
(Free) Energy around the high-symmetry non-distorted configuration:

$$E = E_o + 1/2 \sum \kappa_j(k)\, Q_j(k)^2 + \ldots$$

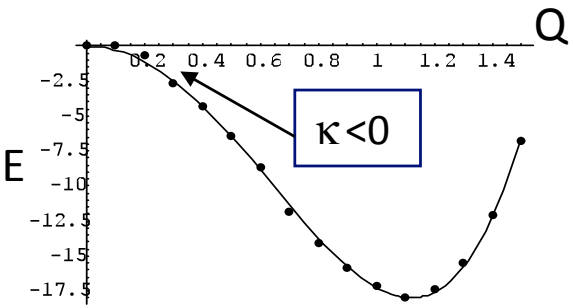
stiffness coefficients

Normal (static) coordinates

Ab-initio calculation of static normal modes in the high-symmetry configuration



Energy as a function of the amplitude Q of an unstable mode:



Symmetry of distortion modes: irreducible representations (group theory)

The mode description of a distortion is simply a change of basis:

Atomic displacements from positions in the parent structure :

u1x **e**x1

u1y **e**y1

u1z **e**z1

u2x **e**x2

u2y **e**y2 Atoms 1,...,N

u2z **e**z2

…

…

uNx **e**xN

uNy **e**yN

uNz **e**zN

Distortion:

U = (u1x, u1y, u1z, …..,uNx, uNy, uNz) – 3N parameters

Mode basis (orthonormal) :

$\varepsilon 1 = a_{11}\mathbf{e}x1 + a_{12}\mathbf{e}y1 + a_{13}\mathbf{e}x1 \ldots a_{13N}\mathbf{e}zN$

$\varepsilon 2 = a_{21}\mathbf{e}x1 + a_{22}\mathbf{e}y1 + a_{23}\mathbf{e}x1 \ldots a_{23}N\mathbf{e}zN$

$\varepsilon 3 = a_{31}\mathbf{e}x1 + a_{32}\mathbf{e}y1 + a_{33}\mathbf{e}x1 \ldots a_{33N}\mathbf{e}zN$

…

…

…

$\varepsilon 3N = a_{3N1}\mathbf{e}x1 + a_{3N2}\mathbf{e}y1 + a_{3N3}\mathbf{e}x1 \ldots a_{3N3N}\mathbf{e}zN$

(3N x 3N) matrix transformation

Distortion:

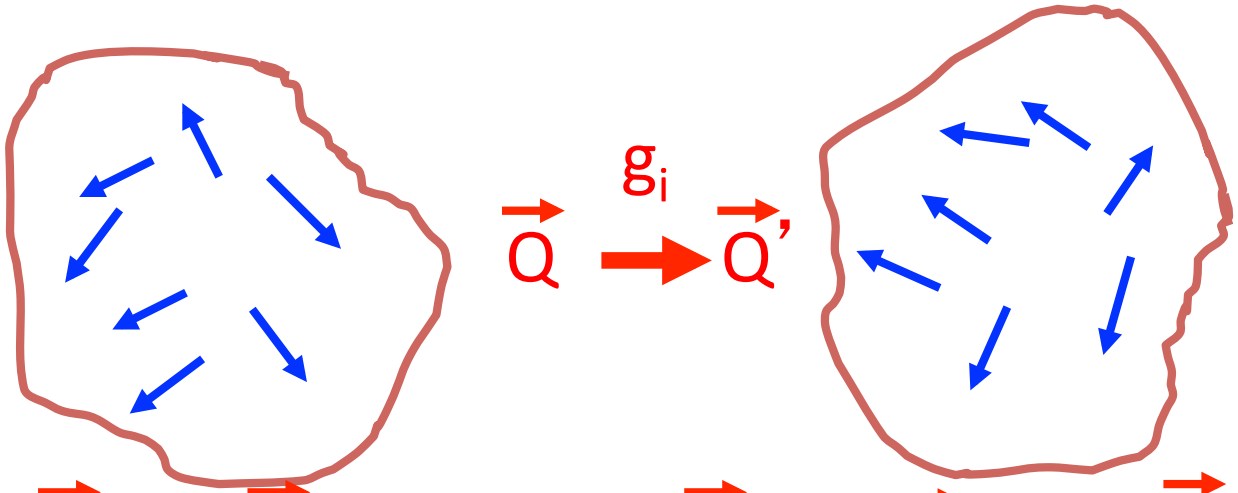
$\mathbf{U} = Q1\,\varepsilon 1 + Q2\,\varepsilon 2 + Q3\,\varepsilon 3 + \ldots + Q3N\,\varepsilon 3N$

U = (Q1, Q2, Q3, …, Q3N)

3N parameters (mode amplitudes)

(collective coordinates)

The Mechanical Representation: an arbitrary displacive distortion (set of atomic displacements) transforms according to a representation of the parent symmetry group



$\vec{Q} = Q_1\vec{d}_1 + \ldots + Q_n\vec{d}_n$

$\vec{Q}' = Q'_1\vec{d}_1 + \ldots + Q'_n\vec{d}_n$

$T(g)\,\vec{Q} = \vec{Q}'$

$n=3N$

representation of G (matrices)

$T(g)$: one nxn matrix for each operation g of G

$\{\vec{d}_1, \ldots\ldots, \vec{d}_n\}$ orthonormal basis of displacive modes

The Mechanical Representation is REDUCIBLE into irreps

Decomposition of the Mechanical Representation into IRREPS

MECHANICAL REP:

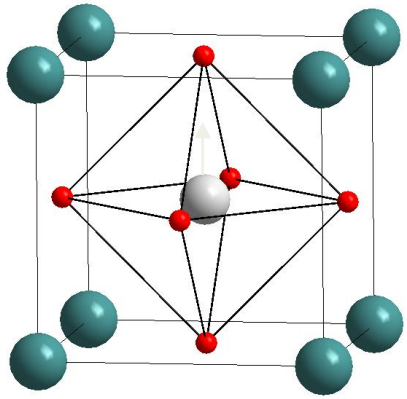
Representations and Applications	
	Point and Space Groups
REPRES	Space Groups Representations
Representations PG	Irreducible representations of the crystallographic Point Groups
Representations SG	Irreducible representations of the Space Groups
Get_irreps	Irreps and order parameters in a space group-subgroup phase transition
DIRPRO	Direct Products of Space Group Irreducible Representations
CORREL	Correlations relations between the irreducible representations of a group-subgroup pair
POINT	Point Group Tables
SITESYM	Site-symmetry induced representations of Space Groups
COMPATIBILITY RELATIONS	Compatibility relations between the irreducible representations of a space group
MECHANICAL REP.	Decomposition of the mechanical representation into irreps

Example: Perovkite structure (G=Pm-3m)

Wave-vectors of the star (1 vector):

GM:(0,0,0)

For modes with k=0



Wyckoff position	Decomposition into irreps
3c:(0,1/2,1/2)	2 GM4-(3) ⊕ GM5-(3)
1b:(1/2,1/2,1/2)	GM4-(3)
1a:(0,0,0)	GM4-(3)

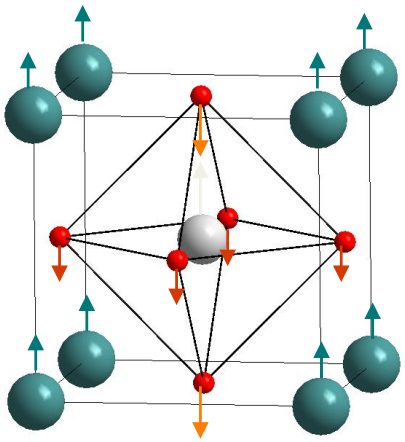
In parentheses the dimensions of the irreducible representations of the little group of k

$$Mech_{rep}\ (k=0) = 4\ \ GM4\text{-}(3) + GM5\text{-}(3)$$

15 degrees of freedom

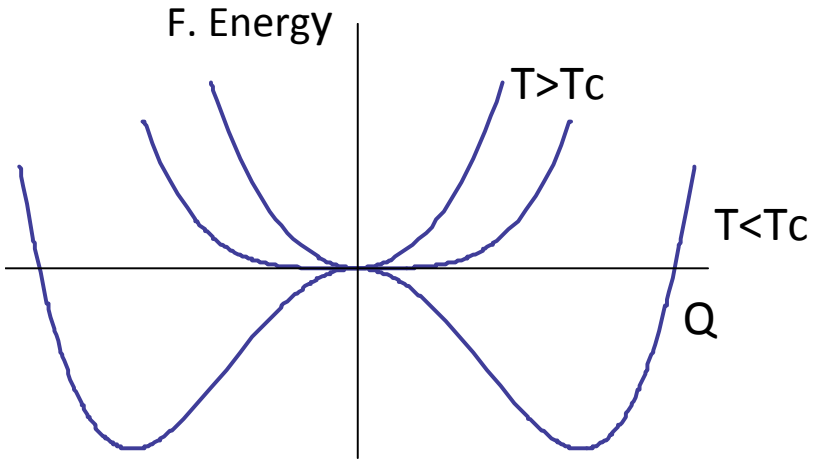
The natural language to describe a symmetry break/phase transition or a distorted structure in general is the one of collective **symmetry-adapted** modes (Landau Theory)

IRREPS of G



primary distortion mode : order parameter

Unstable collective degree of freedom:



$E = Eo + 1/2\ \kappa(T)\ Q^2 + \ldots$

$\kappa(T)<0 \quad T<Tc$

Collective irrep modes is the natural language to describe the structure of distorted phases:

Hierarchy of modes:

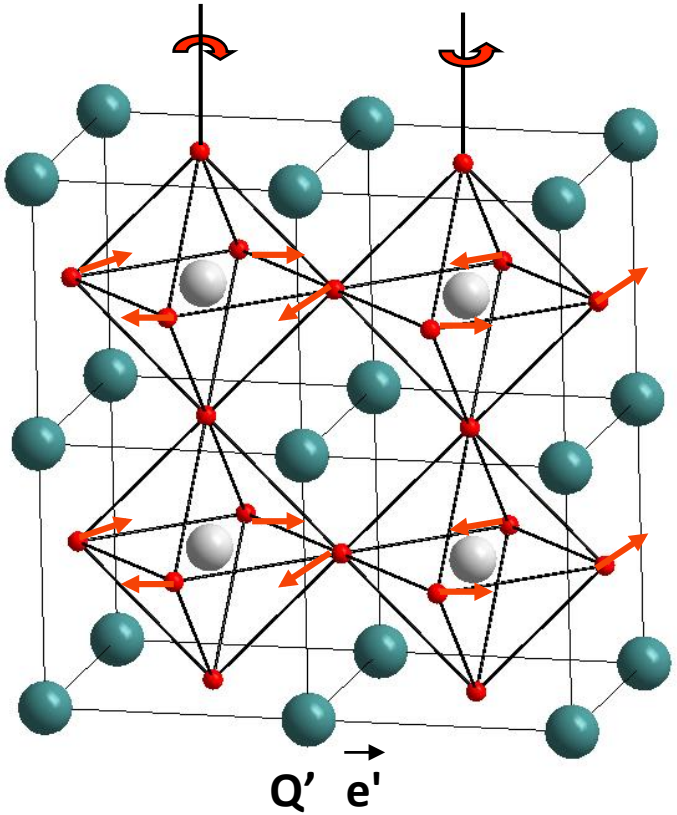
Von Neumann principle:
all modes compatible with the symmetry will be present in the total distortion ….

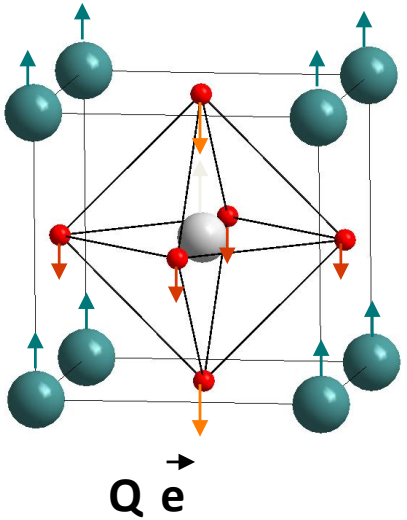
But not all with the same weight!:

primary mode(s): unstable ⟶ the origin of the distortion

secondary modes: induced by the presence of the primary one(s)

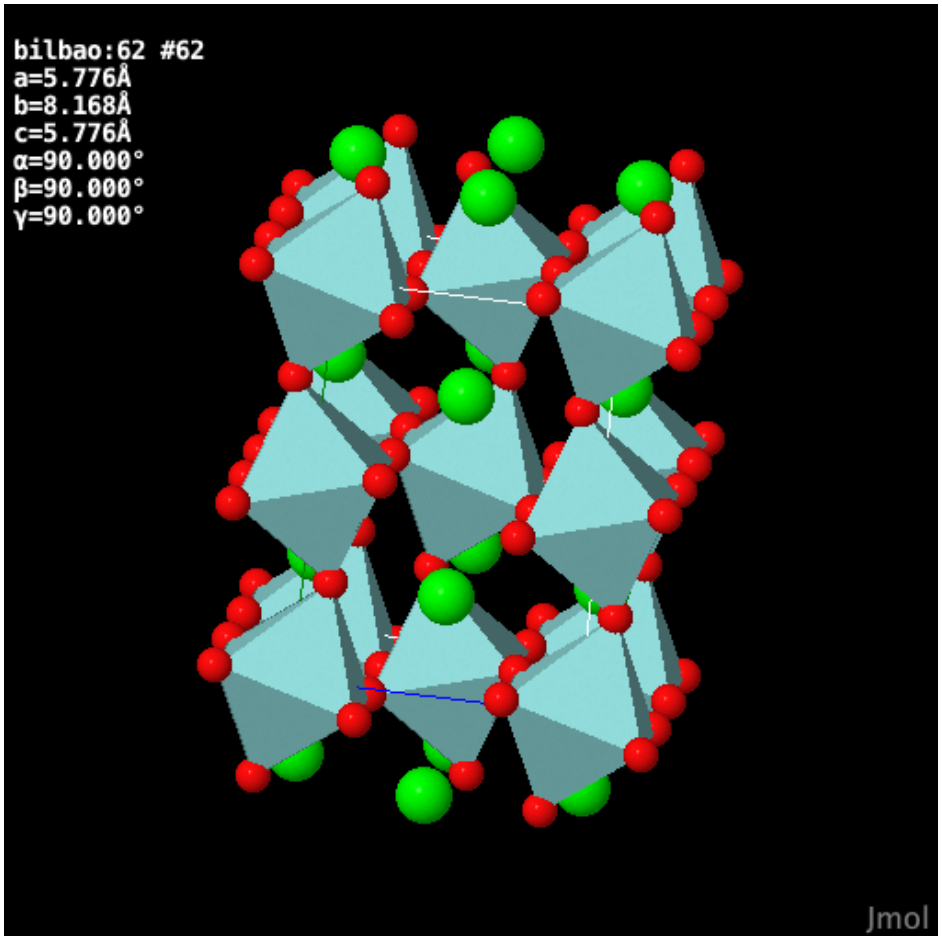
We can compare the amplitudes of different frozen distortion modes:





Q and Q' have the same dimensions and their values can be compared

Rigid Unit Modes in Perovskites ABX_3



R4+ modes

k=(½ , ½ , ½)

irrep R4+

Problem 2a: **We know the high symmetry and we want to know the possible symmetries of the distorted phase knowing primary irrep**

G ⟶ ?

possible space groups for the known primary irrep?

Group-Subgroup Relations of Space Groups	
SUBGROUPGRAPH	Lattice of Maximal Subgroups
HERMANN	Distribution of subgroups in conjugated classes
COSETS	Coset decomposition for a group-subgroup pair
WYCKSPLIT	The splitting of the Wyckoff Positions
MINSUP	Minimal Supergroups of Space Groups
SUPERGROUPS	Supergroups of Space Groups
CELLSUB	List of subgroups for a given k-index.
CELLSUPER	List of supergroups for a given k-index.
NONCHAR	Non Characteristic orbits.
COMMONSUBS	Common Subgroups of Space Groups
COMMONSUPER	Common Supergroups of Two Space Groups
INDEX	Index of a group subgroup pair
SUBGROUPS	Subgroups of a space group consistent with some given supercell, propagation vector(s) or irreducible representation(s)

Example: perovskite ABX_3

Parent space group: Pm-3m

k=(½ , ½ , ½)

Possible symmetries due to R4+ distortions?

Program SUBGROUPS

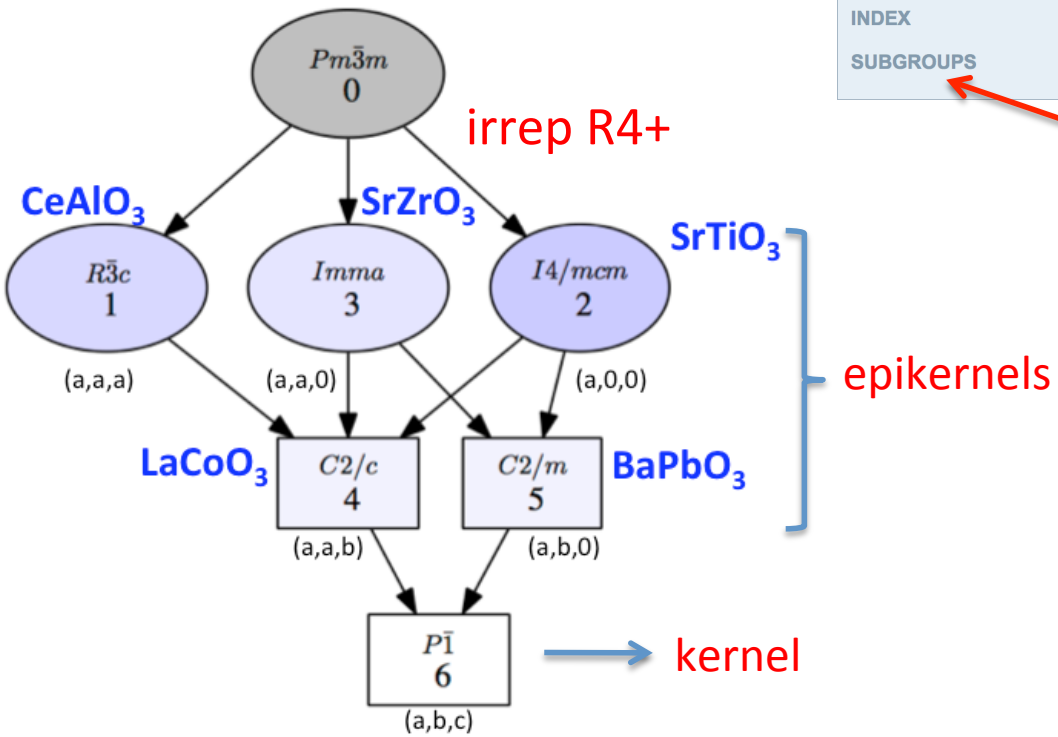
Problem 2a: **We know the high symmetry and we want to know the possible symmetries of the distorted phase knowing primary irrep**

G ⟶ ?

possible space groups for the known primary irrep?

k=(½ , ½ , ½)

Possible symmetries due to R4+ distortions



Group-Subgroup Relations of Space Groups	
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HERMANN	Distribution of subgroups in conjugated classes
COSETS	Coset decomposition for a group-subgroup pair
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SUPERGROUPS	Supergroups of Space Groups
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CELLSUPER	List of supergroups for a given k-index.
NONCHAR	Non Characteristic orbits.
COMMONSUBS	Common Subgroups of Space Groups
COMMONSUPER	Common Supergroups of Two Space Groups
INDEX	Index of a group subgroup pair
SUBGROUPS	Subgroups of a space group consistent with some given supercell, propagation vector(s) or irreducible representation(s)

Program SUBGROUPS

Problem 2b: We know the high symmetry and we want to know the possible symmetries of the distorted phase only knowing its unit cell

G ⟶ ?

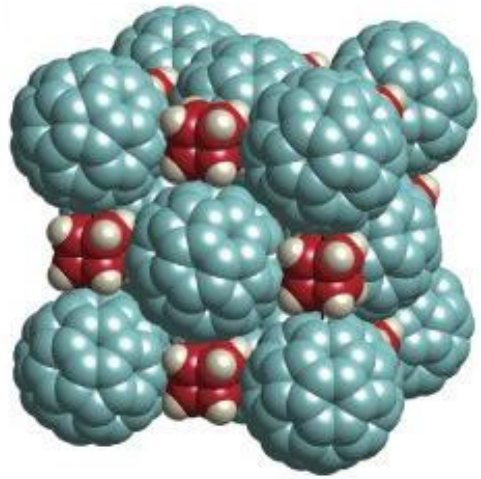
possible space groups for the known unit cell?

Group-Subgroup Relations of Space Groups	
SUBGROUPGRAPH	Lattice of Maximal Subgroups
HERMANN	Distribution of subgroups in conjugated classes
COSETS	Coset decomposition for a group-subgroup pair
WYCKSPLIT	The splitting of the Wyckoff Positions
MINSUP	Minimal Supergroups of Space Groups
SUPERGROUPS	Supergroups of Space Groups
CELLSUB	List of subgroups for a given k-index.
CELLSUPER	List of supergroups for a given k-index.
NONCHAR	Non Characteristic orbits.
COMMONSUBS	Common Subgroups of Space Groups
COMMONSUPER	Common Supergroups of Two Space Groups
INDEX	Index of a group subgroup pair
SUBGROUPS	Subgroups of a space group consistent with some given supercell, propagation vector(s) or irreducible representation(s)

Program SUBGROUPS

Orthorhombic subgroups of Fm-3m with a superlattice given by a unit cell P (**a**-**b**,**a**+**b**,2**c**) which are **most probable** :

Fullerene-cubane



?

Pnma or Pmma

Problem 3: **We know the structures and space group of both the parent and the distorted structure but we do not know the transformation identifying the low symmetry group as a subgroup of the parent space group**

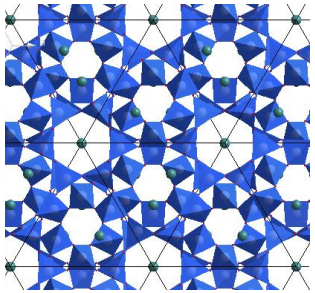
$$G \longrightarrow F\ (?)$$

transformation relating the unit cells and origin?

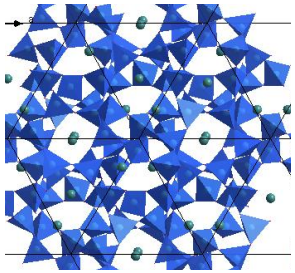
Program STRUCTURE RELATIONS:

Structure Utilities	
CELLTRAN	Transform Unit Cells
STRAIN	Strain Tensor Calculation
WPASSIGN	Assignment of Wyckoff Positions
TRANSTRU	Transform structures.
SETSTRU	Alternative Settings for a given Crystal Structure
EQUIVSTRU	Equivalent Descriptions for a given Crystal Structure
STRCONVERT	Convert & Edit Structure Data (supports the CIF, mCIF, VESTA, VASP formats -- with magnetic information where available)
VISUALIZE	Visualize structures using Jmol
COMPSTRU	Comparison of Crystal Structures with the same Symmetry
STRUCTURE RELATIONS	Evaluation of structure relationships [transformation matrix] between group-subgroup related phases
PSEUDOLATTICE	Pseudosymmetry of a lattice and compatible supergroups

A distorted structure: Leucite $KAlSi_2O_6$



Ia-3d



$I4_1/a$

G= Ia-3d

F= $I4_1/a$ (a,b,c;0,1/2,1/2)

this transformation is in general not unique!

From SRUCTURE RELATIONS:

```
230
13.55038 13.55038 13.55038 90 90 90
3
K      1    16b    0.875000 0.375000 0.125000
T      1    48g    0.588100 0.375000 0.161900
O      1    96h    0.633000 0.280900 0.103800
```

Low Symmetry Structure

```
88
12.99517 12.99517 13.76451 90 90 90
10
K      1    16f    0.366300 0.365400 0.117100
T      1    16f    0.058200 0.396700 0.165400
T      2    16f    0.168500 0.612400 0.128000
T      3    16f    0.393300 0.640600 0.086300
O      1    16f    0.130800 0.313600 0.111100
O      2    16f    0.092700 0.510500 0.131000
O      3    16f    0.145500 0.679000 0.226900
O      4    16f    0.134200 0.683900 0.035800
O      5    16f    0.289200 0.577300 0.121200
O      6    16f    0.484100 0.617500 0.166500
```

[Index: 6] *(Calculated formula units -- High Sym. Structure: 160; Low Sym. Structure: 160)*

Transformation Matrix (P,p): (a,b,c;0,1/2,1/2)

Matrix form:

$$(\mathbf{P},p)=\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1/2 \\ 0 & 0 & 1 & 1/2 \end{pmatrix}$$

Ferroic species: m-3mF4/m

Program TENSOR

Information about the selected tensor

- 3 rd rank Magneto-optical tensor (Faraday effect) F_{ijk}
- Axial tensor invariant under time-reversal symmetry operation
- Defining equation: $\Delta\beta_{ij}=F_{ijk}H_k$
- Relates Magnetic field **H** with the antisymmetric part of the Dielectric impermeability tensor variation $\Delta\beta_{ij}$.
- Pure imaginary in non-dissipative media.
- Intrinsic symmetry symbol: $e\{V^2\}V$
- Symmetrized indexes due to intrinsic symmetry:
  - $F_{ijk} = -F_{jik}$

Solid State Theory Applications

NEUTRON	Neutron Scattering Selection Rules
SYMMODES	Primary and Secondary Modes for a Group - Subgroup pair
AMPLIMODES	Symmetry Mode Analysis
PSEUDO	Pseudosymmetry Search in a Structure
DOPE	Degree of Pseudosymmetry Estimation
TRANPATH	Transition Paths (Group not subgroup relations)
TENSOR ⚠	Symmetry-adapted form of crystal tensors
Check Topological Mat ⚠	Check if a given material is topological or not

Faraday Effect:

m-3m

Table of tensor components

F_{ijk}	k		
ij	1	2	3
11	0	0	0
12	0	0	F_{123}
13	0	$-F_{123}$	0
21	0	0	$-F_{123}$
22	0	0	0
23	F_{123}	0	0
31	0	F_{123}	0
32	$-F_{123}$	0	0
33	0	0	0

Number of independent coefficients: 1

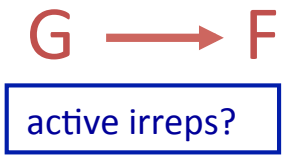
4/m

Table of tensor components

F_{ijk}	k		
ij	1	2	3
11	0	0	0
12	0	0	F_{123}
13	F_{131}	F_{132}	0
21	0	0	$-F_{123}$
22	0	0	0
23	$-F_{132}$	F_{131}	0
31	$-F_{131}$	$-F_{132}$	0
32	F_{132}	$-F_{131}$	0
33	0	0	0

Number of independent coefficients: 3

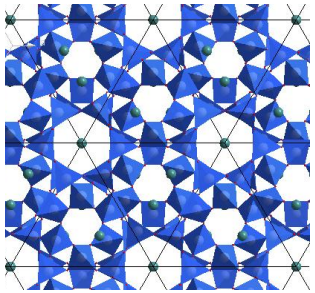
Problem 4: **We know the symmetry break (not necessarily the structures) and we want to identify the active irreps (primary and secondary ones)**



Program GET_irreps:

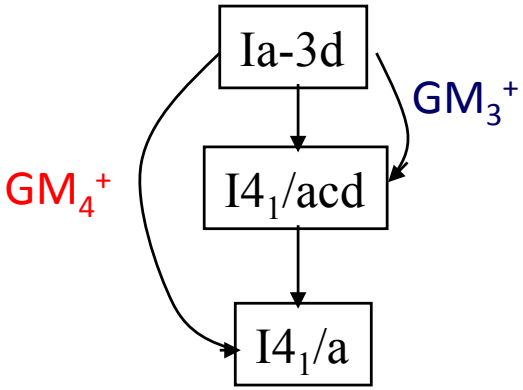
Representations and Applications	
	Point and Space Groups
REPRES	Space Groups Representations
Representations PG	Irreducible representations of the crystallographic Point Groups
Representations SG	Irreducible representations of the Space Groups
Get_irreps	Irreps and order parameters in a space group-subgroup phase transition
DIRPRO	Direct Products of Space Group Irreducible Representations
CORREL	Correlations relations between the irreducible representations of a group-subgroup pair
POINT	Point Group Tables
SITESYM	Site-symmetry induced representations of Space Groups
COMPATIBILITY RELATIONS	Compatibility relations between the irreducible representations of a space group
MECHANICAL REP.	Decomposition of the mechanical representation into irreps

A distorted structure: Leucite $KAlSi_2O_6$



Ia-3d ⟶ **F= $I4_1/a$ (a,b,c;0,1/2,1/2)**

From GET_irreps:



Input:

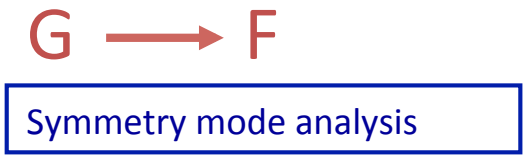
Group→subgroup	Transformation matrix
$Ia\bar{3}d$ (N. 230)→$I4_1/a$ (N. 88)	$\begin{pmatrix} 1 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$

Representations and order parameters

Show the graph of isotropy subgroups

k-vectors	irreps and order parameters	isotropy subgroup transformation matrix	link to the irreps
GM: **(0,0,0)**	GM_1^+: (a)	$Ia\bar{3}d$ (No. 230) a,b,c;0,0,0	matrices of the irreps
	GM_3^+: (a,0)	$I4_1/acd$ (No. 142) a,b,c;0,0,0	
	GM_4^+: (0,0,a)	$I4_1/a$ (No. 88) a,b,c;1/2,0,0	

Problem 5: **We know the symmetry break and we know the structures and we want to decompose the distortion into irrep distortion modes**



Program AMPLIMODES:

Solid State Theory Applications	
NEUTRON	Neutron Scattering Selection Rules
SYMMODES	Primary and Secondary Modes for a Group - Subgroup pair
AMPLIMODES	Symmetry Mode Analysis
PSEUDO	Pseudosymmetry Search in a Structure
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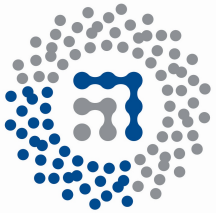
TRANPATH	Transition Paths (Group not subgroup relations)
TENSOR ⚠	Symmetry-adapted form of crystal tensors
Check Topological Mat ⚠	Check if a given material is topological or not

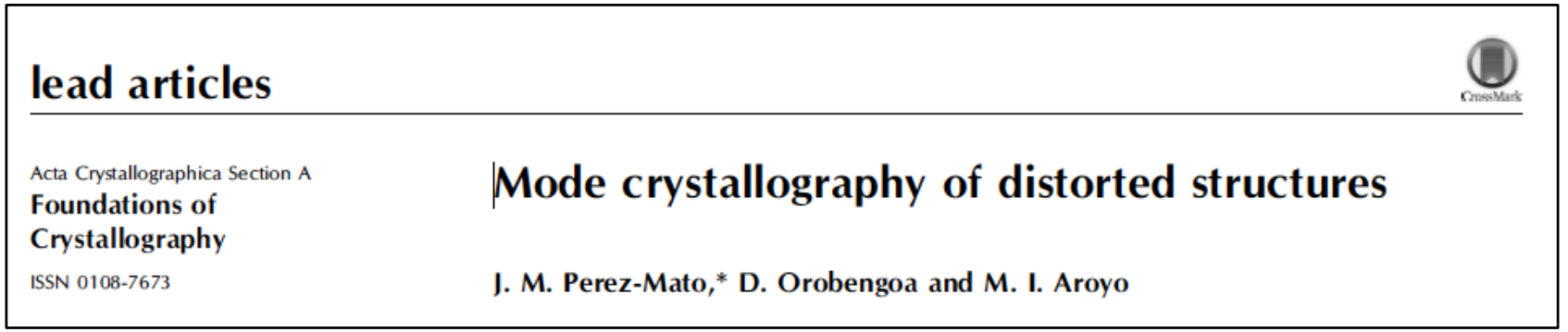


ZTF-FCT
Zientzia eta Teknologia Fakultatea
Facultad de Ciencia y Tecnología

Universidad del País Vasco
Euskal Herriko Unibertsitatea

Using AMPLIMODES

A detailed review of symmetry-mode analysis with many examples:
"Mode crystallography of distorted structure", Acta Cryst. (2010). A66, 558-590 (open access)



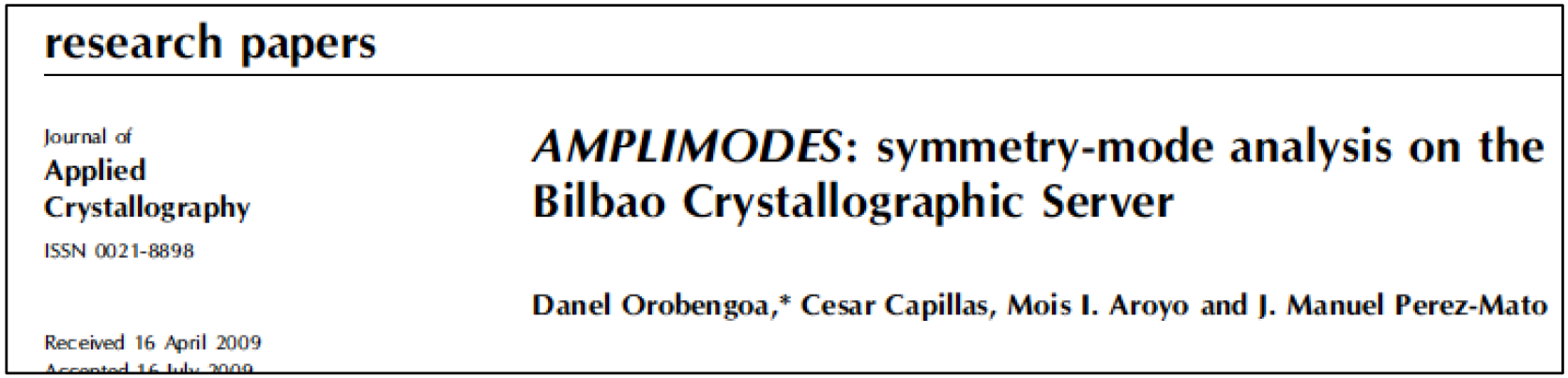
lead articles

Acta Crystallographica Section A
Foundations of Crystallography
ISSN 0108-7673

Mode crystallography of distorted structures

J. M. Perez-Mato,* D. Orobengoa and M. I. Aroyo

A detailed description of the program AMPLIMODES:
"AMPLIMODES: symmetry-mode analysis on the the Bilbao Crystallographic Server", J. Appl. Cryst. (2009). 42, 820-833



research papers

Journal of
Applied
Crystallography
ISSN 0021-8898

Received 16 April 2009

AMPLIMODES: symmetry-mode analysis on the Bilbao Crystallographic Server

Danel Orobengoa,* Cesar Capillas, Mois I. Aroyo and J. Manuel Perez-Mato

AMPLIMODES carries out a symmetry-mode analysis of a displacive phase transition. Starting from the experimental structures of the high- and low symmetry phases, the program determines the global structural distortion that relates the two phases. The symmetry modes compatible with the symmetry break are then calculated. Their orthogonality permits the decomposition of the global distortion, obtaining the amplitudes of the different symmetry-adapted distortions present in the structure, as well as their corresponding polarization vectors.

The input of the program consists of:

- The information about the structures of the high- and low symmetry phases: Space group number, lattice parameters and relative atomic coordinates of the asymmetric unit.
- The transformation matrix that relates the basis of the two space groups.

AMPLIMODES tutorial: download
FullProf tutorial: download
VISUALIZING_MODES tutorial: download

NEW: The output of AMPLIMODES (saved as an html file) can now be directly read by Jmol. This Java viewer allows to visualize in 3D in a straightforward manner all distortion modes of the output, with arrows and/or

Structure Data
[in CIF format]

Examinar... No se ha seleccionado ningún archivo.

HINT: [The option for a given filename is preferential]

High Symmetry Structure

```
# Space Group ITA number
221
# Lattice parameters
4.006 4.006 4.006 90 90 90
# Number of independent atoms in the asymmetric unit
3
# [atom type] [number] [WP] [x] [y] [z]
Ba   1 1a 0.0 0.0 0.0
Ti   1 1b 0.5 0.5 0.5
O    1 3c 0.5 0.0 0.5
```

Structure Data
[in CIF format]

Examinar... No se ha seleccionado ningún archivo.

HINT: [The option for a given filename is preferential]

Low Symmetry Structure

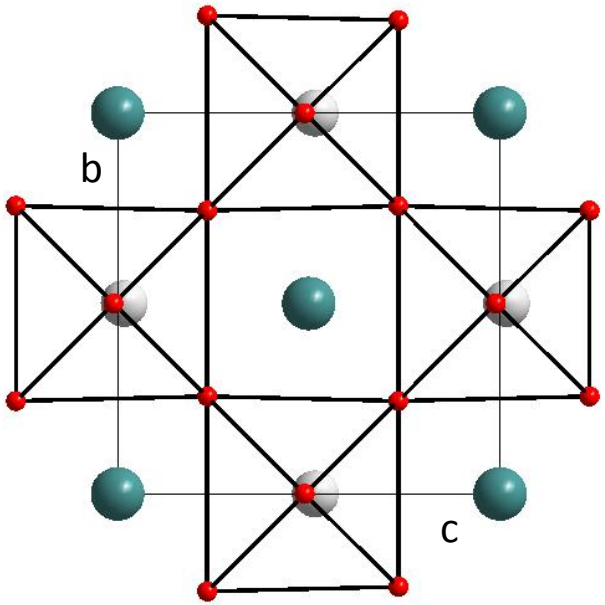
```
# Space Group ITA number
38
# Lattice parameters
3.9828 5.6745 5.6916 90 90 90
# Number of independent atoms in the asymmetric unit
4
# [atom type] [number] [WP] [x] [y] [z]
Ba   1 2a 0.0 0.0 0
Ti   1 2b 0.5 0.0 0.5170
O    1 2a 0.0 0.0 0.4890
O    2 4e 0.5 0.2561 0.2343
```

Tutorial-AMPLIMODES.pdf

Tutorial_VISUALIZING_MODES.pdf

Example of input of AMPLIMODES:

Amm2 phase of $BaTiO_3$



High symmetry structure

Pm-3m

```
221
4.006 4.006 4.006 90 90 90
3
Ba      1    1a      0.0 0.0 0
Ti      1    1b      0.5 0.5 0.5
O       1    3c      0.5 0.0 0.5
```

Low symmetry structure

Amm2

```
38
3.9828 5.6745 5.6916 90 90 90
4
Ba      1    2a      0.0 0.0 0.0
Ti      1    2b      0.5 0.0 0.5170
O       1    2a      0.0 0.0 0.4890
O       2    4e      0.5 0.2561 0.2343
```

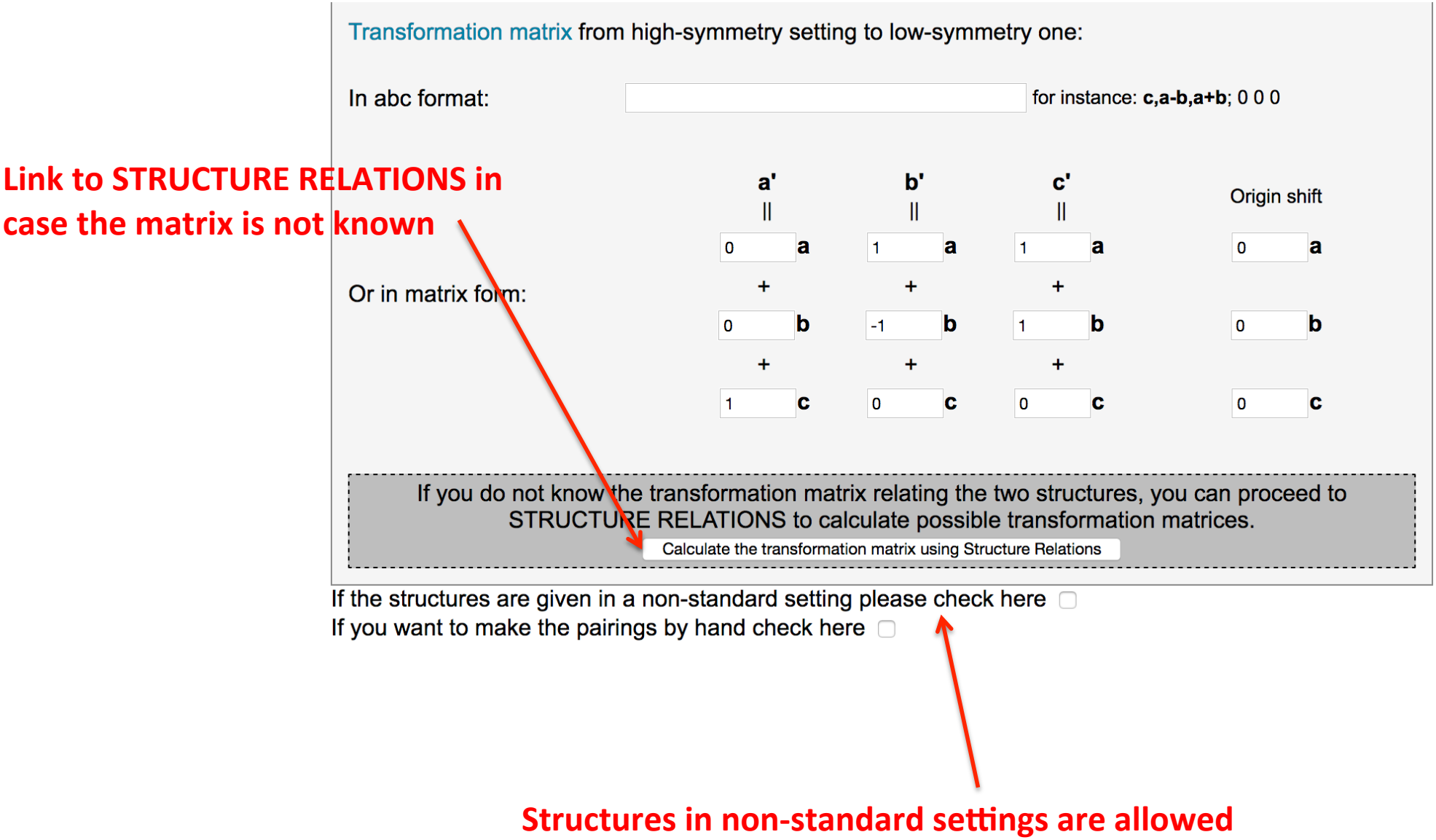
4 parameters

Transformation matrix

Transf.

necessary

```
[      0      1      1 ]  [      0]
[      0     -1      1 ]  [      0]
[      1      0      0 ]  [      0]
```


Transformation matrix from high-symmetry setting to low-symmetry one:
In abc format:
for instance: c,a-b,a+b; 0 0 0
Link to STRUCTURE RELATIONS in case the matrix is not known
Or in matrix form:
a' b' c' Origin shift
0 a 1 a 1 a 0 a
+ + + +
0 b -1 b 1 b 0 b
+ + + +
1 c 0 c 0 c 0 c
If you do not know the transformation matrix relating the two structures, you can proceed to STRUCTURE RELATIONS to calculate possible transformation matrices.
Calculate the transformation matrix using Structure Relations
If the structures are given in a non-standard setting please check here
If you want to make the pairings by hand check here
Structures in non-standard settings are allowed

Example of output of AMPLIMODES:

Transformed high symmetry structure in the subgroup basis

Reference Structure

```
038
4.006000 5.665339 5.665339 90.000000 90.000000 90.000000
4
Ba      1       2a      0.000000        0.000000        0.000000
Ti      1       2b      0.500000        0.000000        0.500000
O       1       4e      0.500000        0.250000        0.250000
O       1_2     2a      0.000000        0.000000        0.500000
```

Atom pairings and distances

Atom Mappings					
WP		Atom	Reference Struc.	Atom	Low Sym Struc.
2a	(0,0,z)	Ba1	(0.000000,0.000000,0.000000)	Ba1	(0.000000,0.000000,0.000000)
2b	(1/2,0,z)	Ti1	(0.500000,0.000000,0.500000)	Ti1	(0.500000,0.000000,0.517000)
4e	(1/2,y,z)	O1	(0.500000,0.250000,0.250000)	O2	(0.500000,0.256100,0.234300)
2a	(0,0,z)	O1_2	(0.000000,0.000000,0.500000)	O1	(0.000000,0.000000,0.489000)

WP		Atom	Atomic Displacements			
			u_x	u_y	u_z	|u|
2a	(0,0,z)	Ba1	0.0000	0.0000	0.0000	0.0000
2b	(1/2,0,z)	Ti1	0.0000	0.0000	0.0170	0.0963
4e	(1/2,y,z)	O1	0.0000	0.0061	-0.0157	0.0954
2a	(0,0,z)	O1_2	0.0000	0.0000	-0.0110	0.0623

NOTE: u_x, u_y and u_z are given in relative units. |u| is the absolute distance given in Å
Maximum atomic displacement in the distortion, Δ: 0.0963 Å
Total distortion amplitude: 0.1771 Å

After origin shift

Relative origin shift to eliminate a global displacement: (0.00000, 0.00000, -0.00508)

Atom Mappings					
WP		Atom	Coordinates in S_1	Atom	Coordinates in S_2
2a	(0,0,z)	Ba1	(0,0,0)	Ba1	(0,0,0.00508)
2b	(1/2,0,z)	Ti1	(1/2,0,1/2)	Ti1	(1/2,0,0.52208)
4e	(1/2,y,z)	O1	(1/2,1/4,1/4)	O2	(1/2,0.25610,0.23938)
2a	(0,0,z)	O1_2	(0,0,1/2)	O1	(0,0,0.49408)

WP		Atom	Atomic Distances			
			u_x	u_y	u_z	|d|
2a	(0,0,z)	Ba1	0.0000	0.0000	0.0051	0.0288
2b	(1/2,0,z)	Ti1	0.0000	0.0000	0.0221	0.1251
4e	(1/2,y,z)	O1	0.0000	0.0061	-0.0106	0.0694
2a	(0,0,z)	O1_2	0.0000	0.0000	-0.0059	0.0335

NOTE: d_x, d_y and d_z are given in relative units. |d| is the absolute distance given in Å
Maximum atomic displacement in the distortion, Δ: 0.1251 Å
Total distortion amplitude: 0.1650 Å

Symmetry Modes Summary

Atoms	WP	Modes
O1	3*c*	**GM4-(2) GM5-(1)**
Ti1	1*b*	**GM4-(1)**
Ba1	1*a*	**GM4-(1)**

Note: The primary mode is written in bold letters

Summary of Amplitudes

K-vector	Irrep	Direction	Isotropy Subgroup	Dimension	Amplitude (Å)
(0,0,0)	GM4-	(a,a,0)	Amm2 (38)	4	0.1649
(0,0,0)	GM5-	(0,a,-a)	Amm2 (38)	1	0.0056

Global distortion: 0.1650 Å

Example of output of AMPLIMODES:

atomic displacements

$$\mathbf{u}(i) = Q\, e(i)$$

Normalized Symmetry modes

The modes are normalized to the low symmetry unit c
cell and are given as relative displacements in this cell.

Irrep GM4-

GM4- Mode Ba1 1

Atom	δx	δy	δz
Ba1	0.000000	0.000000	0.176512

GM4- Mode Ti1 1

Atom	δx	δy	δz
Ti1	0.000000	0.000000	0.176512

GM4- Mode O1 1

Atom	δx	δy	δz
O1	0.000000	0.062406	0.062406
O1_2	0.000000	0.000000	0.124813

GM4- Mode O1 2

Atom	δx	δy	δz
O1	0.000000	-0.088256	0.088256
O1_2	0.000000	0.000000	0.000000

basis for this 4dim vector

Irrep GM5-

GM5- Mode O1 1

Atom	δx	δy	δz
O1	0.000000	-0.062406	-0.062406
O1_2	0.000000	0.000000	0.124813

K-vector: GM = (0,0,0)

Irrep: GM4-

Direction: (a,a,0)

Isotropy Subgroup: 38 Amm2 C2v-14

Transformation matrix:

```
[     0     1     1 ] [     0]
[     0    -1     1 ] [     0]
[     1     0     0 ] [     0]
```

amplitude of the GM4- distortion

The amplitude of this distortion is:
A_{GM4-} = 0.1649 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized)

Ba1 1	Ti1 1	O1 1	O1 2
0.1745	0.7585	-0.2536	-0.5744

as a vector (norm 1) with 4 components

NOTE: A second number next to the label counts the different symmetry modes that

Normalized polarization vector expressed as displacements (in cell relative un
Ångström)

Atom	δx	δy	δz
Ba1	0.0000	0.0000	0.0308
Ti1	0.0000	0.0000	0.1339
O1	0.0000	0.0349	-0.0665
O1_2	0.0000	0.0000	-0.0317

polarization vector in two forms

crystallographic form

Virtual structure with only this symmetry component of the distortion frozen.

Example of output of AMPLIMODES:

Normalized Symmetry modes

The modes are normalized to the low symmetry unit c
cell and are given as relative displacements in this cell.

Irrep GM4-

GM4- Mode Ba1 1

Atom	δx	δy	δz
Ba1	0.000000	0.000000	0.176512

GM4- Mode Ti1 1

Atom	δx	δy	δz
Ti1	0.000000	0.000000	0.176512

GM4- Mode O1 1

Atom	δx	δy	δz
O1	0.000000	0.062406	0.062406
O1_2	0.000000	0.000000	0.124813

GM4- Mode O1 2

Atom	δx	δy	δz
O1	0.000000	-0.088256	0.088256
O1_2	0.000000	0.000000	0.000000

Irrep GM5-

GM5- Mode O1 1

Atom	δx	δy	δz
O1	0.000000	-0.062406	-0.062406
O1_2	0.000000	0.000000	0.124813

c=5.665339 unit cell of reference structure
2a or 2b atomic site: 1 atom per PRIMITIVE unit cell
0.176512*5.665339 =1

basis modes
(normalized and orthogonal)

b=c=5.665339 unit cell of reference structure
O1 4e atomic site: 2 atoms per PRIMITIVE unit cell
O1_2 2a atomic site: 1 atom per PRIMITIVE unit cell
$[(0.124813*5.665339)^2 + 2*[(0.062406*5.665339)^2 + (0.062406*5.665339)^2]]^{1/2} = 0.999998$

Example of output of AMPLIMODES:

atomic displacements

$$\mathbf{u}(i) = Q\, e(i)$$

Normalized Symmetry modes

The modes are normalized to the low symmetry unit c
cell and are given as relative displacements in this cell.

Irrep GM4-

GM4- Mode Ba1 1

Atom	δx	δy	δz
Ba1	0.000000	0.000000	0.176512

GM4- Mode Ti1 1

Atom	δx	δy	δz
Ti1	0.000000	0.000000	0.176512

GM4- Mode O1 1

Atom	δx	δy	δz
O1	0.000000	0.062406	0.062406
O1_2	0.000000	0.000000	0.124813

GM4- Mode O1 2

Atom	δx	δy	δz
O1	0.000000	-0.088256	0.088256
O1_2	0.000000	0.000000	0.000000

basis for this 4dim vector

Irrep GM5-

GM5- Mode O1 1

Atom	δx	δy	δz
O1	0.000000	-0.062406	-0.062406
O1_2	0.000000	0.000000	0.124813

K-vector: GM = (0,0,0)

Irrep: GM4-

Direction: (a,a,0)

Isotropy Subgroup: 38 Amm2 C2v-14

Transformation matrix:

```
[     0     1     1 ] [     0]
[     0    -1     1 ] [     0]
[     1     0     0 ] [     0]
```

amplitude of the GM4- distortion

The amplitude of this distortion is:
A_{GM4-} = 0.1649 Å

Normalized polarization vector: (in terms of the amplitudes of the (normalized)

Ba1 1	Ti1 1	O1 1	O1 2
0.1745	0.7585	-0.2536	-0.5744

as a vector (norm 1) with 4 components

NOTE: A second number next to the label counts the different symmetry modes that

Normalized polarization vector expressed as displacements (in cell relative un
Ångström)

Atom	δx	δy	δz
Ba1	0.0000	0.0000	0.0308
Ti1	0.0000	0.0000	0.1339
O1	0.0000	0.0349	-0.0665
O1_2	0.0000	0.0000	-0.0317

polarization vector in two forms

crystallographic form

Virtual structure with only this symmetry component of the distortion frozen.

Example of output of AMPLIMODES:

O1	0.0000	0.0349	-0.0665
O1_2	0.0000	0.0000	-0.0317

= -0.2536 x

GM4- Mode O1 1

Atom	δx	δy	δz
O1	0.000000	0.062406	0.062406
O1_2	0.000000	0.000000	0.124813

+ (-0.5744)x

GM4- Mode O1 2

Atom	δx	δy	δz
O1	0.000000	-0.088256	0.088256
O1_2	0.000000	0.000000	0.000000

4dim vector

GM4- Mode O1 1

Atom	δx	δy	δz
O1	0.000000	0.062406	0.062406
O1_2	0.000000	0.000000	0.124813

GM4- Mode O1 2

Atom	δx	δy	δz
O1	0.000000	-0.088256	0.088256
O1_2	0.000000	0.000000	0.000000

Normalized polarization vector: (in terms of the amplitudes of the (normalized)

Ba1 1	Ti1 1	O1 1	O1 2
0.1745	0.7585	-0.2536	-0.5744

as a vector (norm 1) with 4 components

NOTE: A second number next to the label counts the different symmetry modes that

Normalized polarization vector expressed as displacements (in cell relative un
Ångström)

Atom	δx	δy	δz
Ba1	0.0000	0.0000	0.0308
Ti1	0.0000	0.0000	0.1339
O1	0.0000	0.0349	-0.0665
O1_2	0.0000	0.0000	-0.0317

polarization vector in two forms

crystallographic form

Irrep GM5-

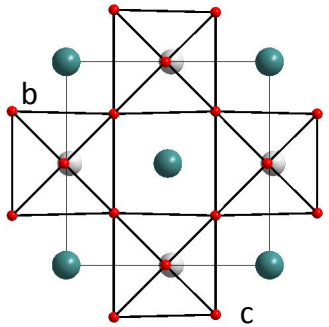
GM5- Mode O1 1

Atom	δx	δy	δz
O1	0.000000	-0.062406	-0.062406
O1_2	0.000000	0.000000	0.124813

Virtual structure with only this symmetry component of the distortion frozen.

The orthorhombic Amm2 structure of $BaTiO_3$

(Kwei et al. (1993) neutron-powder 190 K)



Perovskite in Amm2 setting

	δx	δy	δz
Ba1	0.0	0.0	0.0
Ti1	0.5	0.0	0.5
O1	0.5	0.25	0.25
O12	0.0	0.0	0.5

+

polarization vector GM4-

	δx	δy	δz
Ba1	0.0	0.0000	0.0308
Ti1	0.0	0.0000	0.1339
O1	0.0	0.0349	-0.0665
O12	0.0	0.0000	-0.0317

+ Q_{GM4-}

polarization vector GM5-

	δx	δy	δz
Ba1	0.0	0.0000	0.0000
Ti1	0.0	0.0000	0.0000
O1	0.0	0.0624	0.0624
O12	0.0	0.0000	-0.1248

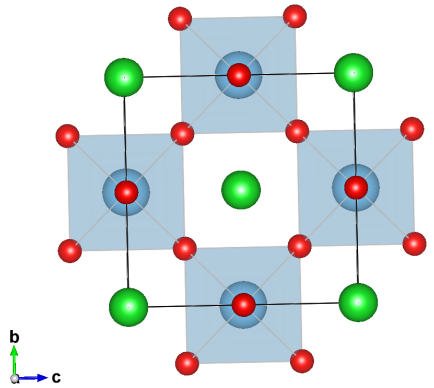
+ Q_{GM5-}

Q_{GM4-} = 0.165 Å

Q_{GM5-} = 0.006 Å

The orthorhombic Amm2 structure of $BaTiO_3$

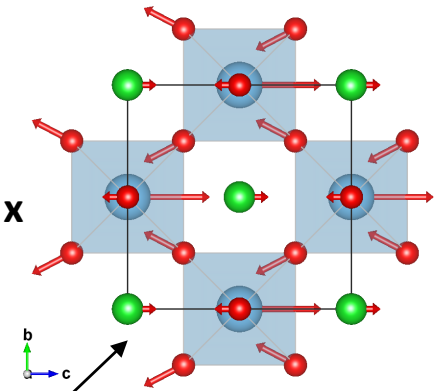
(Kwei et al. (1993) neutron-powder 190 K)



max. atomic displ. : 0.13 Å

Mode decomposition of distortion:

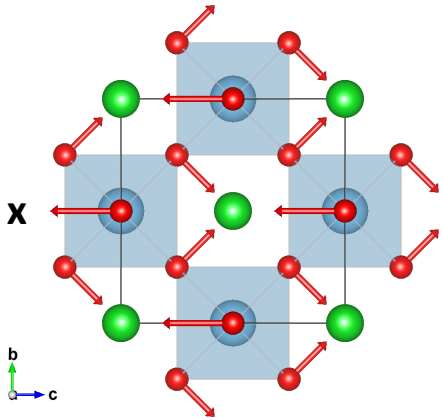
Q_{GM4-} x



GM4- mode

+

Q_{GM5-} x



GM5- mode

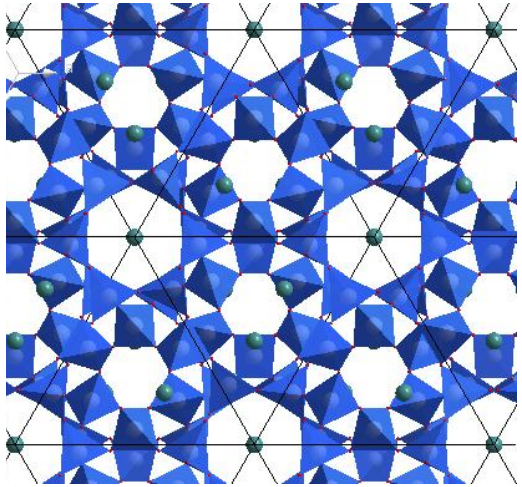
polar ferroelectric mode

$Q_{GM4-} >> Q_{GM5-}$

Applications of symmetry mode analysis of distorted structures:

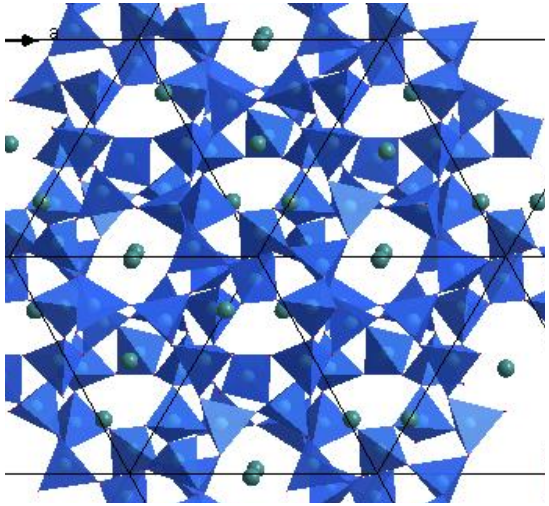
- identification of fundamental and marginal degrees of freedom
- reduction of the effective number of crystallographic parameters
- detection of false refinement minima
- quantitative comparison of structures with the same or different space group
- detection of hidden structural correlations (specially for low symmetry distortions)
- systematic characterization of variation of the structure with temperature
- rationalization of phase diagrams and various symmetries in families of compounds.

Leucite $KAlSi_2O_6$



Ia-3d

(N. 230)



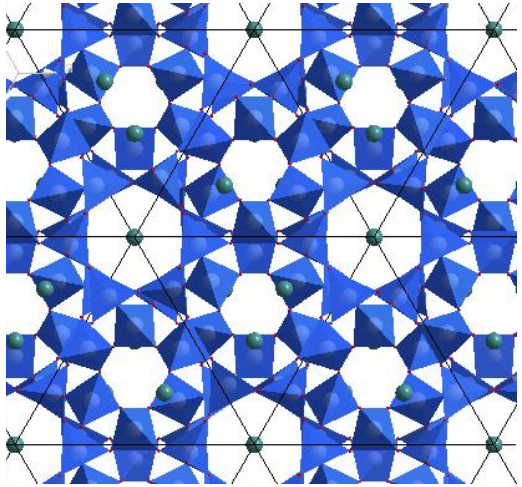
$I4_1/a$

(N. 88)

Ia-3d $\longrightarrow$ **$I4_1/a$** (a,b,c;0 ½, ½)

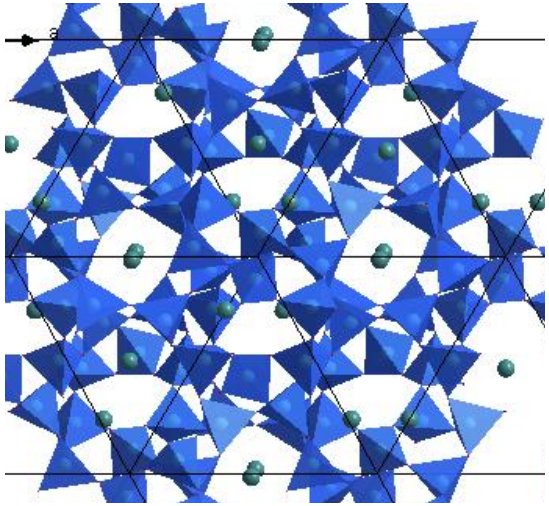
Symmetry mode decomposition with AMPLIMODES ?

Leucite $KAlSi_2O_6$



Ia-3d

(N. 230)



$I4_1/a$

(N. 88)

Symmetry Modes Summary

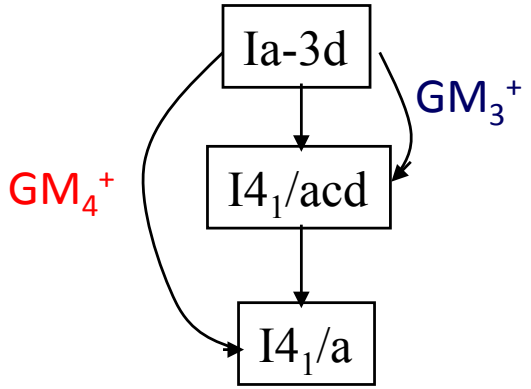
Atoms	WP	Modes
O1	96*h*	GM1+(3) GM3+(6) **GM4+(9)**
T1	48*g*	GM1+(1) GM3+(3) **GM4+(5)**
K1	16*b*	GM3+(1) **GM4+(2)**

Note: The primary mode is written in bold letters

Summary of Amplitudes

K-vector	Irrep	Direction	Isotropy Subgroup	Dimension	Amplitude (Å)
(0,0,0)	GM1+	(a)	Ia-3d (230)	4	0.4060
(0,0,0)	GM3+	(a,0)	I4_1/acd (142)	10	1.7219
(0,0,0)	GM4+	(0,0,a)	I4_1/a (88)	16	4.5374

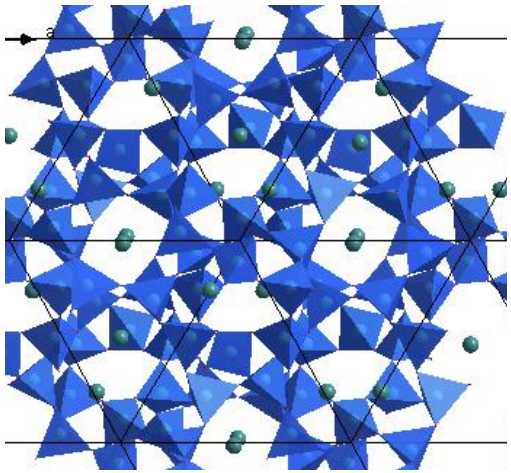
Global distortion: 4.8701 Å

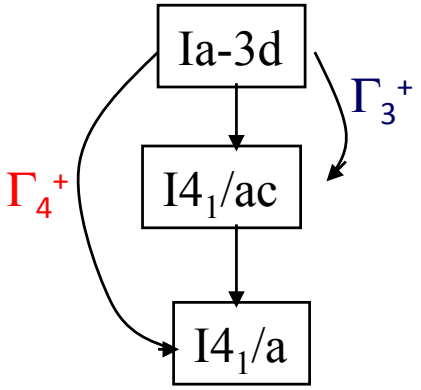


Polarization vectors in Leucite

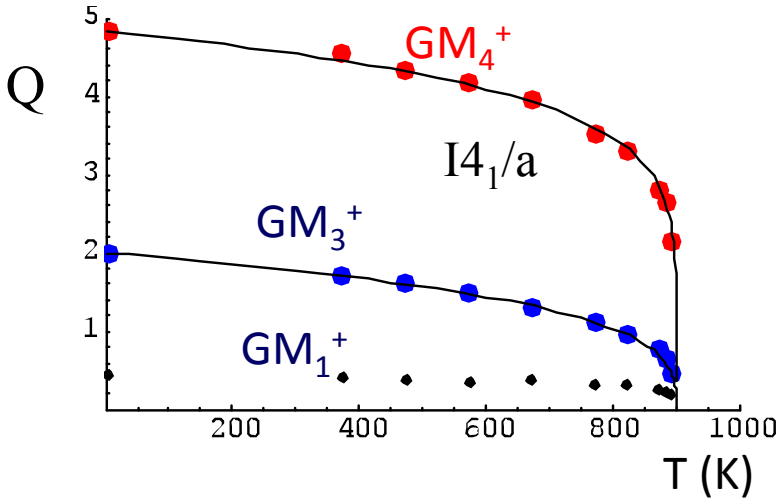
$I4_1/a$ Palmer et. (Amer. Miner. 82 (1997) 16

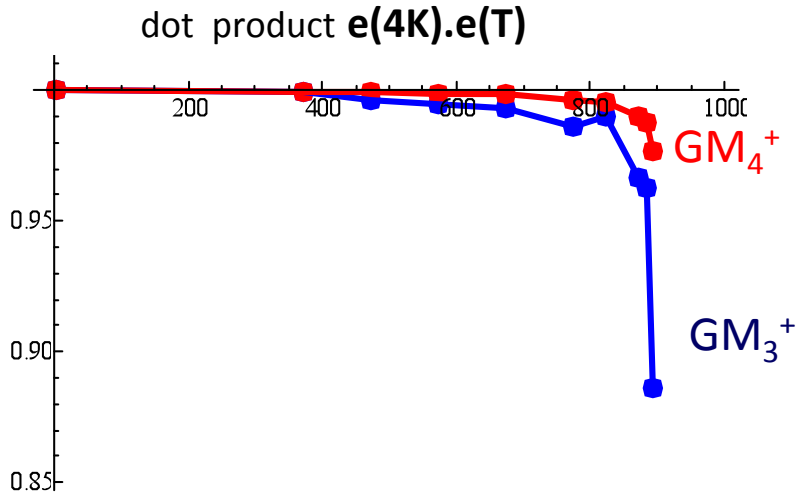
$KAlSi_2O_6$





DISTORTION MODES AMPLITUDES VS. TEMPERATURE:

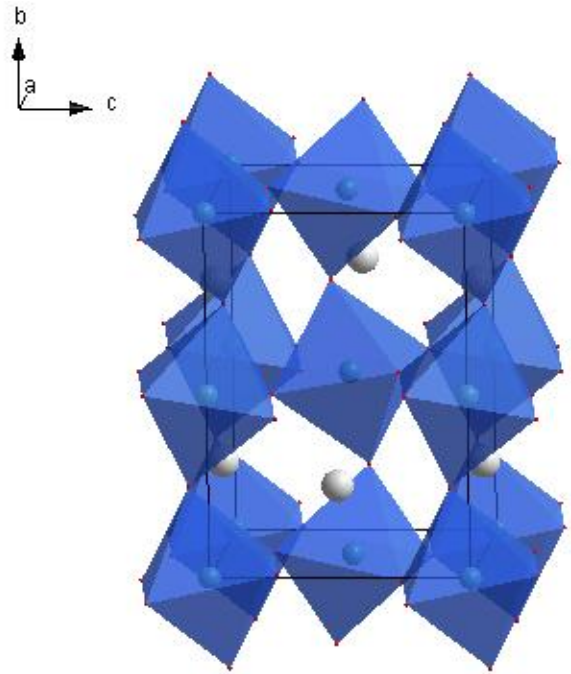




Induced effect : $Q_{\Gamma 3+} = \alpha\, Q^2_{\Gamma 4+}$

Symmetry-mode decomposition of $SrZrO_3$

20 C



Pnma

SrZrO3 parent
221
4.084 4.084 4.084 90 90 90
3
Sr 1 1a 0.000000 0.000000 0.000000
Zr 1 1b 0.500000 0.500000 0.500000
O 1 3c 0.500000 0.000000 0.500000

0 free atomic coordinates

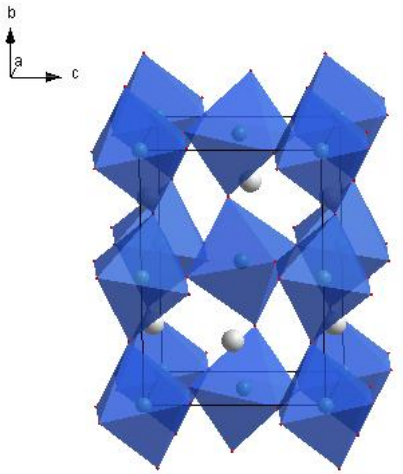
SrZrO3 Pnma phase
62
5.8206 8.1949 5.8045 90 90 90
4
Sr 1 4c 0.524000 0.250000 0.004000
Zr 1 4a 0.000000 0.000000 0.000000
O 1 4c -0.013000 0.250000 -0.069000
O 2 8d 0.284000 0.036000 0.215000

7 free atomic coordinates

Symmetry-mode decomposition of $SrZrO_3$ 20 C

(Howard et al. 2000 & data from B. Kennedy)

Pnma



WP		Atom	Atomic Displacements			
			u_x	u_y	u_z	|u|
4c	(x,1/4,z)	Sr1	0.0240	0.0000	0.0040	0.1405
4a	(0,0,0)	Zr1	0.0000	0.0000	0.0000	0.0000
8d	(x,y,z)	O1	0.0340	0.0360	-0.0350	0.4073
4c	(x,1/4,z)	O1_2	-0.0130	0.0000	-0.0690	0.4055

NOTE: u_x, u_y and u_z are given in relative units. |u| is the absolute distance given in Å
Maximum atomic displacement in the distortion, Δ: 0.4073 Å
Total distortion amplitude: 1.4366 Å

Symmetry Modes Summary

Atoms	WP	Modes
O1	3*d*	R4+(1) R5+(1) X5+(1) M2+(1) M3+(1)
Sr1	1*b*	R5+(1) X5+(1)

Summary of Amplitudes

Warning: Amplitudes are given for modes normalized within the primitive unit cell of the distorted structure. Under this normalization, mode amplitudes in distorted structures with different multiplication of their primitive unit cell are not directly comparable.

K-vector	Irrep	Direction	Isotropy Subgroup	Dimension	Amplitude (Å)
(1/2,1/2,1/2)	R4+	(0,a,a)	Imma (74)	1	1.1517
(1/2,1/2,1/2)	R5+	(0,a,-a)	Imma (74)	2	0.0523
(0,1/2,0)	X5+	(0,0,0,-a,0,0)	Cmcm (63)	2	0.3153
(1/2,1/2,0)	M2+	(a,0,0)	P4/mbm (127)	1	0.0116
(1/2,1/2,0)	M3+	(a,0,0)	P4/mbm (127)	1	0.7970

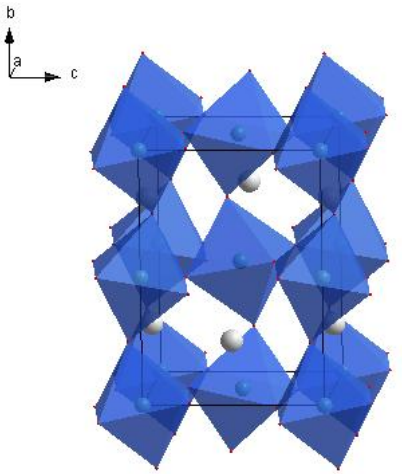
prevailing distortions

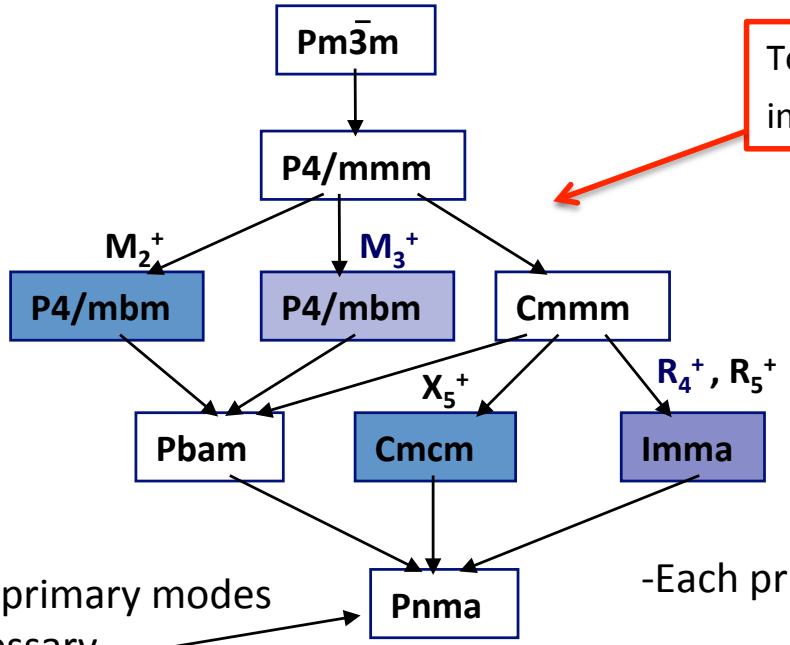
Sequence of transitions in $SrZrO_3$

20 C

Pnma

(Howard et al. 2000 & data from B. Kennedy)





To obtain this information: **Get_irreps**

two primary modes necessary

-Each primary mode is a different instability mechanism

- each primary mode condenses in general at different temperatures : two phase transitions

Q_{M2+} = 0.01 Å

Q_{M3+} = 0.80 Å

Q_{X5+} = 0.32 Å

Q_{R4+} = 1.15 Å

Q_{R5+} = 0.05 Å

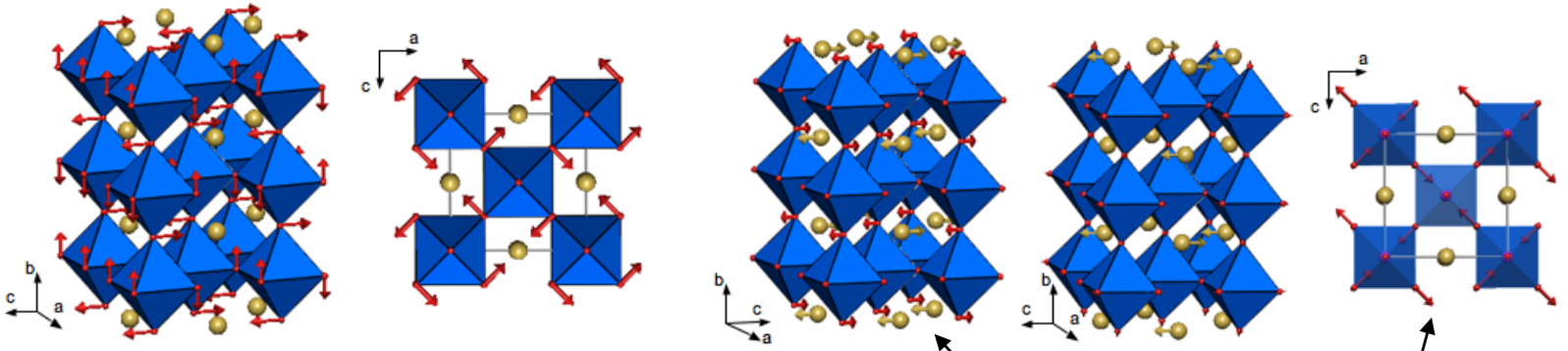
→ Pnma

Expected transition sequence:

T > →

Pnma (M_3^+, R_4^+) → Imma (R_4^+) → $Pm\bar{3}m$

Sequence of transitions in $SrZrO_3$



R_4^+
1.158 Å

M_3^+
0.80 Å

X_5^+
0.32 Å

R_5^+
0.05 Å

M_2^+
0.01 Å

They deform the octahedra.
X_5^+ has significant amplitude

AMPLIMODES carries out a symmetry-mode analysis of a displacive phase transition. Starting from the experimental structures of the high- and low symmetry phases, the program determines the global structural distortion that relates the two phases. The symmetry modes compatible with the symmetry break are then calculated. Their orthogonality permits the decomposition of the global distortion, obtaining the amplitudes of the different symmetry-adapted distortions present in the structure, as well as their corresponding polarization vectors.

The input of the program consists of:

- The information about the structures of the high- and low symmetry phases: Space group number, lattice parameters and relative atomic coordinates of the asymmetric unit.
- The transformation matrix that relates the basis of the two space groups.

AMPLIMODES tutorial: download
FullProf tutorial: download
VISUALIZING_MODES tutorial: download

NEW: The output of AMPLIMODES (saved as an html file) can now be directly read by Jmol. This Java viewer allows to visualize in 3D in a straightforward manner all distortion modes of the output, with arrows and/or

Structure Data
[in CIF format]

Examinar... No se ha seleccionado ningún archivo.

HINT: [The option for a given filename is preferential]

High Symmetry Structure

```
# Space Group ITA number
221
# Lattice parameters
4.006 4.006 4.006 90 90 90
# Number of independent atoms in the asymmetric unit
3
# [atom type] [number] [WP] [x] [y] [z]
Ba   1 1a 0.0 0.0 0.0
Ti   1 1b 0.5 0.5 0.5
O    1 3c 0.5 0.0 0.5
```

Structure Data
[in CIF format]

Examinar... No se ha seleccionado ningún archivo.

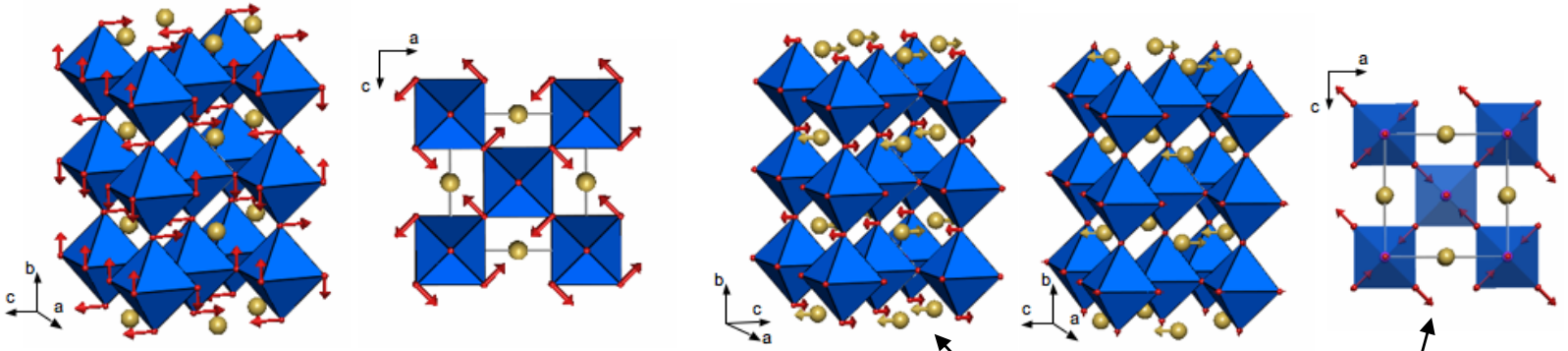
HINT: [The option for a given filename is preferential]

Low Symmetry Structure

```
# Space Group ITA number
38
# Lattice parameters
3.9828 5.6745 5.6916 90 90 90
# Number of independent atoms in the asymmetric unit
4
# [atom type] [number] [WP] [x] [y] [z]
Ba   1 2a 0.0 0.0 0
Ti   1 2b 0.5 0.0 0.5170
O    1 2a 0.0 0.0 0.4890
O    2 4e 0.5 0.2561 0.2343
```

Tutorial_VISUALIZING_MODES.pdf

Sequence of transitions in $SrZrO_3$



R_4^+
1.18 Å

M_3^+
0.79 Å

X_5^+
0.338 Å

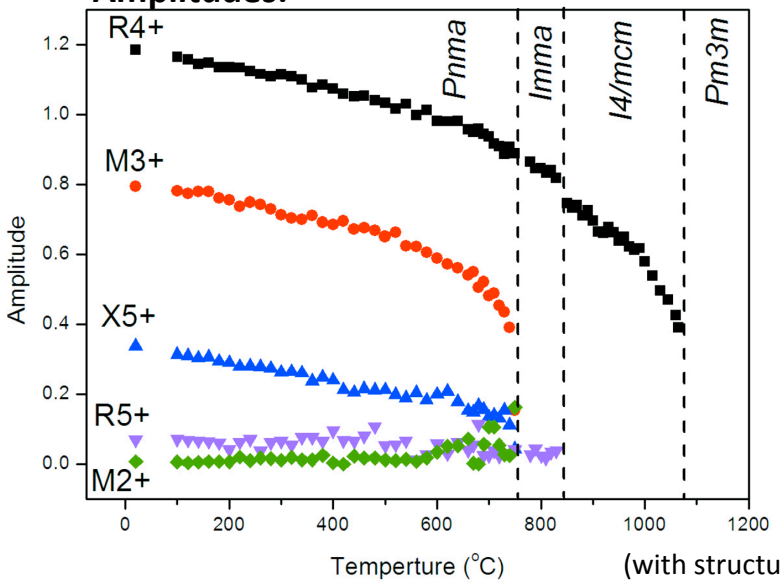
R_5^+
0.07 Å

M_2^+
0.007 Å

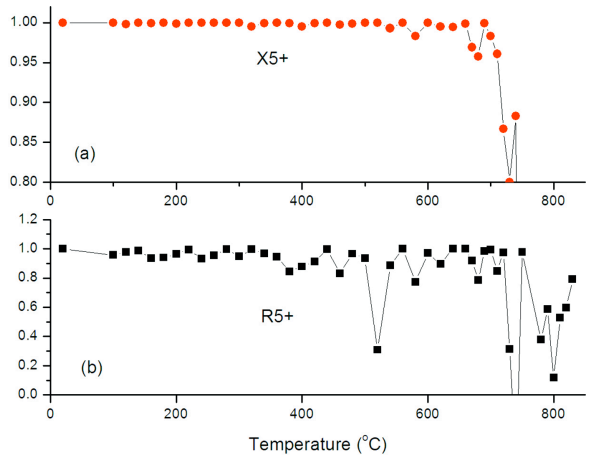
They deform the octahedra.
X_5^+ has significant amplitude

Temperature variation:

Amplitudes:



modes polarization vectors:



(with structural data from Kennedy, Howard and K.S. Knight, 2010)

Use of mode coordinates in the structure refinement, instead of the individual atomic coordinates?

One expects:

- a natural hierarchy of parameters
- less correlations with atomic (thermal) displacement parametes
- minimize correlations

AMPLIMODES for FullProf (and Jana)

Symmetry modes for FullProf

This version of AMPLIMODES produces a block of text to be inserted in the .pcr input file of FullProf to enable a direct refinement of the amplitudes of the basis symmetry-modes generated by AMPLIMODES, instead of performing a conventional refinement of individual atomic coordinates. The program can also generate a default starting .pcr file for simulation of a neutron powder diffraction diagram and for generating with FullProf Studio graphic representations of the different modes. The produced .pcr file can also be read by Jana2006.

In this version for FullProf (and Jana), the input of a low symmetry structure is optional; apart from the high-symmetry structure, only the input of the space group of the distorted structure and its transformation matrix is necessary. If a model for the low symmetry structure is also given, the program will return in the .pcr file the amplitudes of the basis modes corresponding to this starting model, instead of setting them to zero.

Fullprof tutorial: download
Extra data for the tutorial: download

Structure data: Examinar… SrZrO3_Pm-3m_parent.cif

HINT: [Upload the structure as a CIF file (default), or as a text in the window below]

High Symmetry Structure:

```
# Space Group ITA number
221
# Lattice parameters (lengths in angstroems and angles in degrees)
4.006 4.006 4.006 90 90 90
# Number of independent atoms in the asymmetric unit
3
# [atom type] [number] [WP] [x] [y] [z]
Ba   1 1a 0.0 0.0 0.0
Ti   1 1b 0.5 0.5 0.5
O    1 3c 0.5 0.0 0.5
```

For the low symmetry structure, only the space group (and transformation matrix) is necessary; the structure is optional. If given, the program will return the corresponding amplitudes of the modes instead of setting them to zero.

Examinar… No se ha seleccionado ningún archivo.

HINT: [Upload the structure as a CIF file (default), or as a text in the window below]

Low Symmetry Structure:

```
62
```

space group

Necessary: Only the subgroup defined by the space group type and the transformation to standard

transformation

Maximum Δ: 1 [Maximum distance allowed]

Summary of Decomposition

K-vector	Irrep	Direction	Isotropy Subgroup	Dimension
(1/2,1/2,1/2)	R4+	(0,a,a)	Imma (74)	1
(1/2,1/2,1/2)	R5+	(0,a,-a)	Imma (74)	2
(0,1/2,0)	X5+	(0,0,0,-a,0,0)	Cmcm (63)	2
(1/2,1/2,0)	M2+	(a,0,0)	P4/mbm (127)	1
(1/2,1/2,0)	M3+	(a,0,0)	P4/mbm (127)	1

You can copy and paste the following text on your .pcr file

```
062                    <--Space group symbol
!Atom   Typ       X         Y         Z      Biso      Occ     In Fin N_t Spc /Codes
Sr1     SR      0.500000  0.250000  0.000000 0.500000 0.500000  0   0   0     1
                  0.00      0.00      0.00      0.00      0.00
Zr1     ZR      0.000000  0.000000  0.000000 0.500000 0.500000  0   0   0     1
                  0.00      0.00      0.00      0.00      0.00
O1      O       0.250000  0.000000  0.250000 0.500000 1.000000  0   0   0     1
                  0.00      0.00      0.00      0.00      0.00
O1_2    O       0.000000  0.250000  0.000000 0.500000 0.500000  0   0   0     1
                  0.00      0.00      0.00      0.00      0.00
! Polarisation Vectors of Symmetry Modes for each atom
V_MODES    12
! Nm Atm      Irrep       Vx        Vy        Vz         Coeff
  1 O1       R4+      0.000000 -0.030607  0.000000 1.00
  1 O1_2     R4+      0.000000  0.000000  0.061214 1.00
  2 Sr1      R5+      0.000000  0.000000  0.086570 1.00
  3 O1       R5+      0.000000 -0.030607  0.000000 1.00
  3 O1_2     R5+      0.000000  0.000000 -0.061214 1.00
  4 Sr1      X5+      0.086570  0.000000  0.000000 1.00
  5 O1       X5+      0.000000  0.000000  0.000000 1.00
  5 O1_2     X5+     -0.086570  0.000000  0.000000 1.00
  6 O1       M2+      0.043285  0.000000  0.043285 1.00
  6 O1_2     M2+      0.000000  0.000000  0.000000 1.00
  7 O1       M3+      0.043285  0.000000 -0.043285 1.00
  7 O1_2     M3+      0.000000  0.000000  0.000000 1.00
!Amplitudes of Symmetry Modes
A_MODES     7    2
     A1_R4+     0.000000      1.00
     A2_R5+     0.000000      1.00
     A3_R5+     0.000000      1.00
     A4_X5+     0.000000      1.00
     A5_X5+     0.000000      1.00
     A6_M2+     0.000000      1.00
     A7_M3+     0.000000      1.00
```

All zero, because no distorted structure has been introduced.

All zero, because no distorted structure has been introduced.

You can download the full .pcr file for a default neutron simulation here

Important: The cell parameters in this .pcr file are those of the reference high symmetry structure in the low symmetry setting. For FullProf refinements