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Commission on Mathematical and Theoretical Crystallography

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Sixth MaThCryst school in Latin America
Workshop on the Applications of Group Theory in the Study of Phase Transitions

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CRYSTAL-STRUCTURE TOOLS-PSEUDO

BILBAO CRYSTALLOGRAPHIC SERVER

PRACTICAL EXERCISES

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Crystal-structure relationships

Phase transitions

STRUCTURAL PSEUDOSYMMETRY

Problem: PSEUDOSYMMETRY SEARCH

PSEUDO

Initial Structure $\mathcal{H}$ low symmetry	Structural Pseudosymmetry $\Leftrightarrow$ *Distortion*	Prototype Structure $\mathcal{G}$ high symmetry

Search for a structure of space-group symmetry G, supergroup of H, such that:

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

If the distortion is small enough, it can indicate a symmetry change at high temperature.

↓

phase transition

Applications: PSEUDO

Prediction of phase transitions

Search for ferroic materials
-new ferroelectrics
-new ferroelastics

Prediction of the symmetry and structure of some other phase of a material

Detection of false symmetry assignments (overlooked symmetry)

Space-group determination of theoretically determined structure (e.g. *ab initio* calculations)

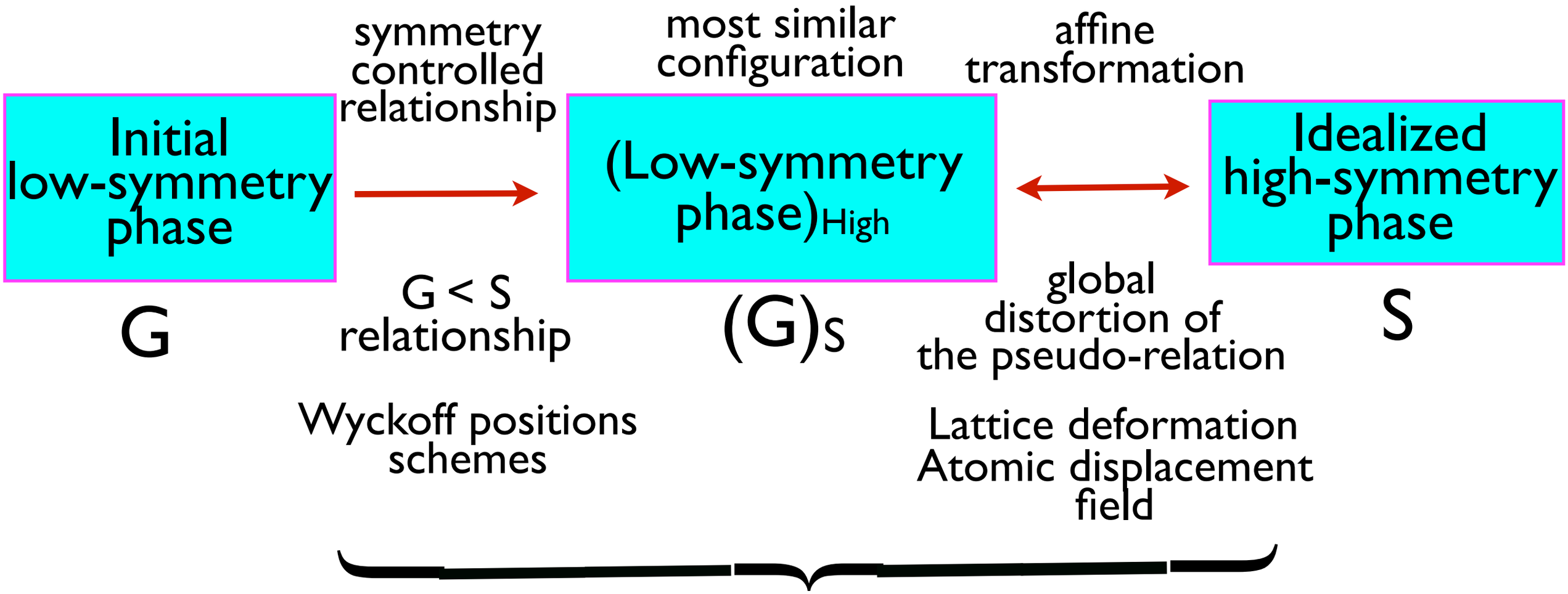
Determination of an optimised virtual parent structure (paraphase)

Structural Pseudosymmetry

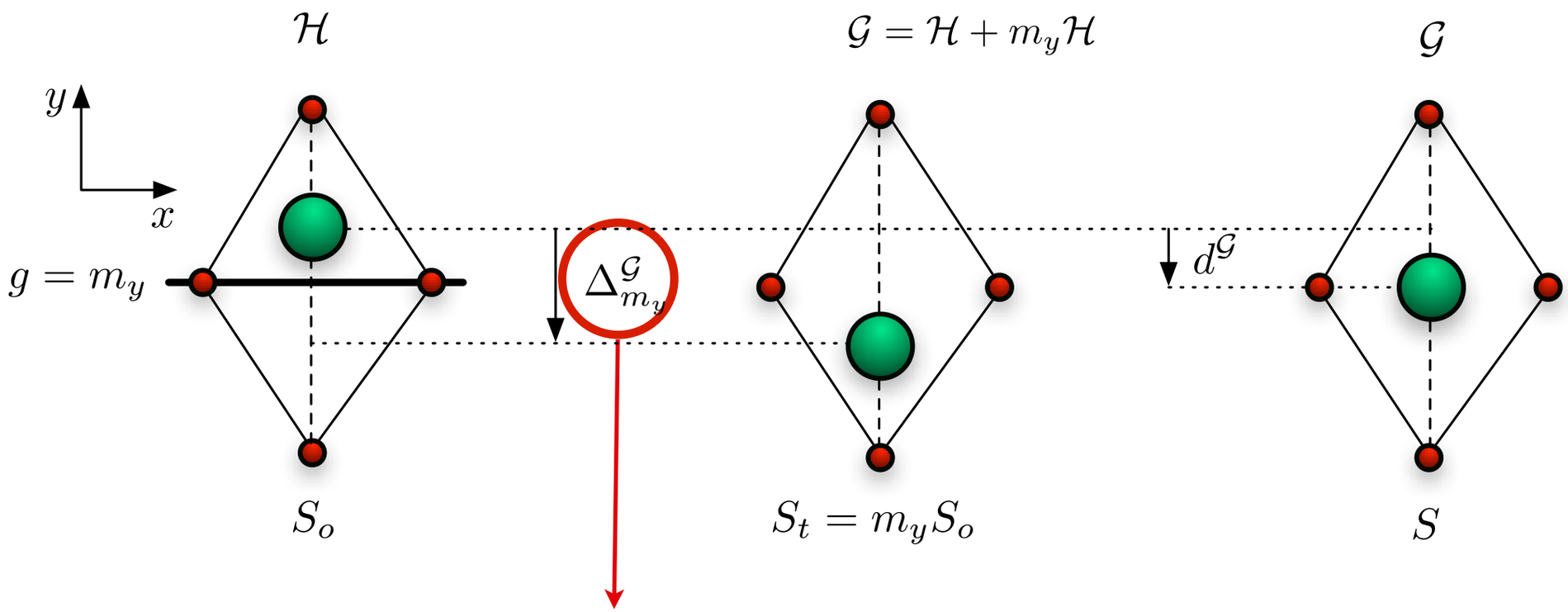
PROBLEM:

Given the initial structure specified by space-group symmetry G its unit-cell parameters and atomic coordinates

Search for a structure of space-group symmetry S>G such that the initial structure can be described by the high-symmetry structure with tolerably small distortion



PSEUDO: ATOMIC DISPLACEMENTS METHOD



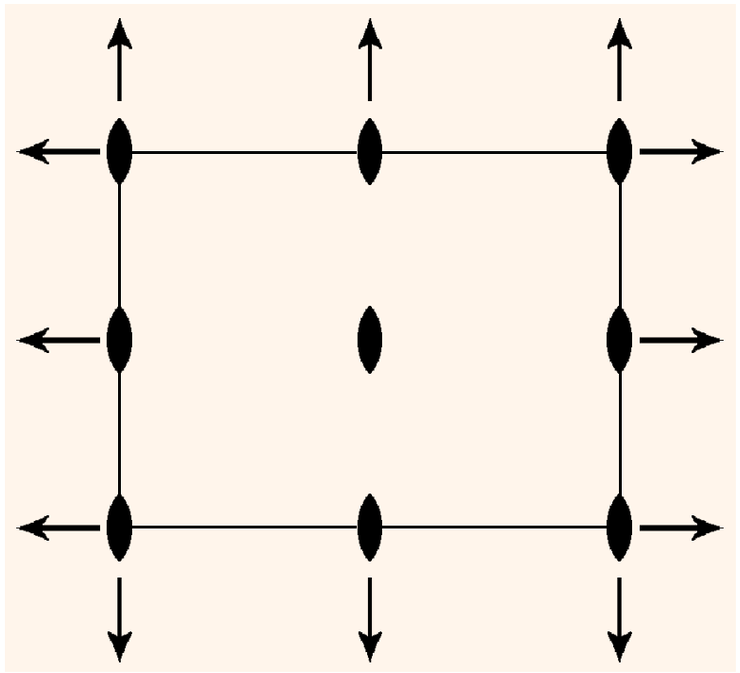
Maximal distance between all compatible atom pairings

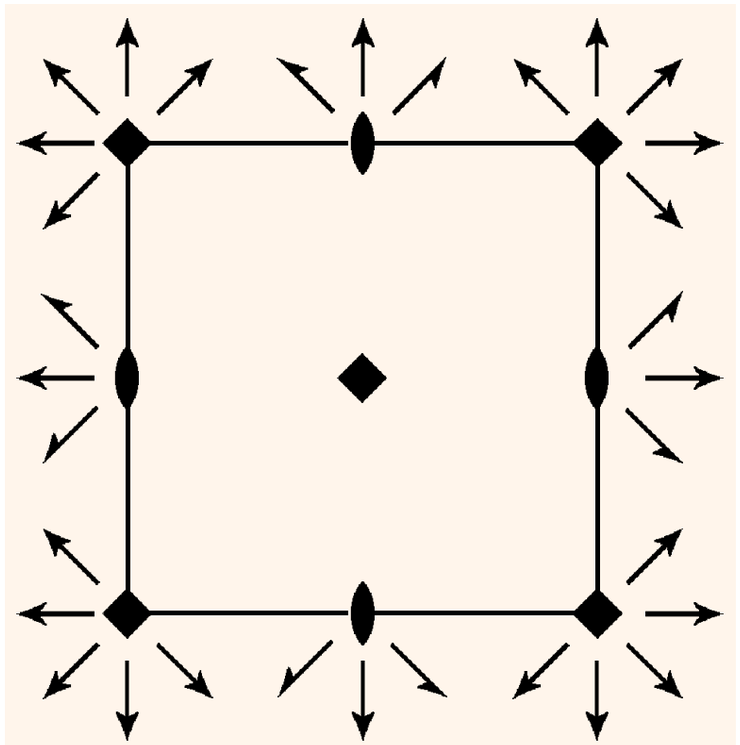
Asumption:
The high symmetry phase is described by a **supergroup** of the initial space group.

$$\mathcal{G} = \mathcal{H} + g_2\mathcal{H} + \cdots + g_m\mathcal{H}$$

SUPERGROUPS OF SPACE GROUPS

SUPERGROUPS MINSUP





$$\mathcal{H} = \mathrm{P}\mathbf{222}$$

$$\mathcal{G} = \mathrm{P}\mathbf{422}$$

$$\mathrm{P}\mathbf{422} = \mathrm{P}\mathbf{222} + (4|\omega)\mathrm{P}\mathbf{222}$$

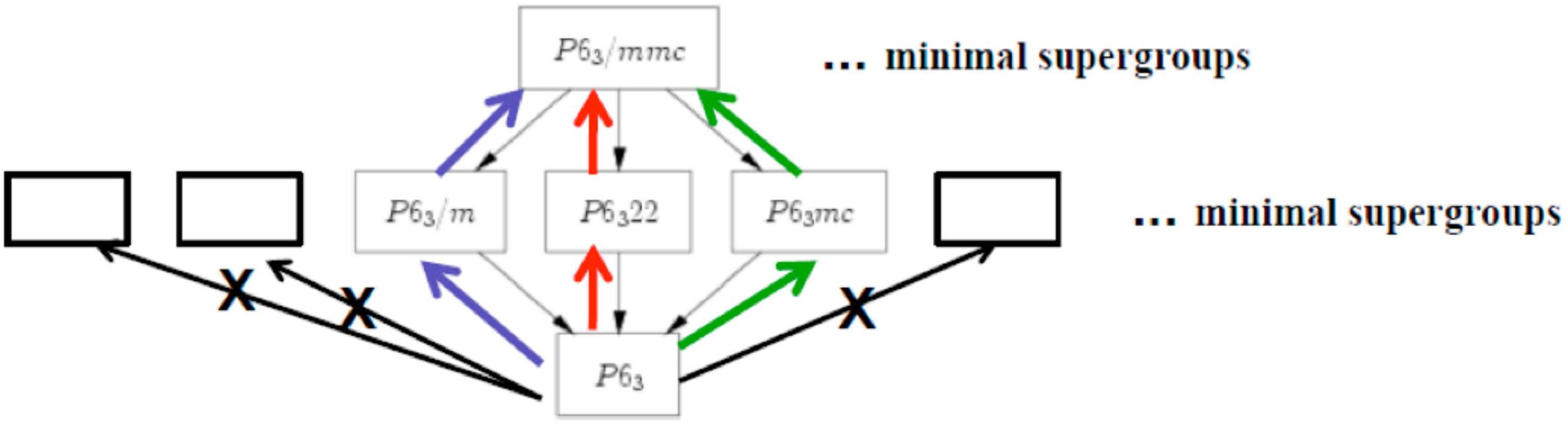
	4 en	ω	$\mathcal{G}$
4_z	$(0,0,0)$	$(0,0,0)$	$(P422)_1$
4_y	$(0,0,0)$	$(0,0,0)$	$(P422)_2$
4_x	$(0,0,0)$	$(0,0,0)$	$(P422)_3$
4_z	$(\frac{1}{2},0,0)$	$(\frac{1}{2},\frac{1}{2},0)$	$(P422)'_1$
4_y	$(\frac{1}{2},0,0)$	$(\frac{1}{2},0,\frac{1}{2})$	$(P422)'_2$
4_x	$(0,\frac{1}{2},0)$	$(0,\frac{1}{2},\frac{1}{2})$	$(P422)'_3$

Problem: PSEUDOSYMMETRY SEARCH

PSEUDO

Any group – supergroup relation can be represented by a chain of minimal supergroups.

$$\mathcal{G} > \mathcal{H} \rightarrow \mathcal{G} > \ldots > \mathcal{Z}_2 > \mathcal{Z}_1 > \mathcal{H}$$



If a structure of symmetry $\mathcal{H}$ is pseudosymmetric for a supergroup $\mathcal{G}$, it will be pseudosymmetric for all intermediate subgroups $\mathcal{Z}i$.

EXERCISES

Problem 3.11 (i)

Analyse the structural pseudosymmetry of Pb_2MgWO_6

Option 1: Search of maximal pseudosymmetry stepwise 'climbing' via minimal supergroups

```
#(Pb2MgWO6:Pseudo1)
# Space Group ITA number
62
# Lattice parameters
11.4059 7.9440 5.6866 90.00 90.00 90.00
# Number of independent atoms in the asymmetric unit
8
# [atom type] [number] [WP] [x] [y] [z]
Pb    1   8d    0.1422 0.0032 0.7804
Mg    1   4c    0.3772 0.25 0.7519
W     1   4c    0.1161 0.25 0.2577
O     1   8d    0.1314 0.4907 0.2365
O     2   4c    0.0027 0.25 0.0133
O     3   4c    0.0103 0.25 0.4991
O     4   4c    0.237 0.25 -0.0153
O     5   4c    0.2491 0.25 0.4745
```

Problem 3.11 (i)

SOLUTION

Option 1: Search of structural pseudosymmetry stepwise 'climbing' via minimal supergroups

1. Minimal supergroups ◉ ☐ [Show only indices in supergroups table]
2. Supergroups with k-index ○ ik: 1
3. Specify supergroup transformation ○ G: 221

	Rotational part			Origin Shift
Transf. Matrix (in option 3 only)	1	0	0	0
	0	1	0	0
	0	0	1	0

4. Lattice Pseudosymmetry with minimal supergroups ○ **Ang. Tol (in degrees)** 5 [*]

[*] Only for triclinics and monoclinics.

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

Maximum Δ: 2

tolerance [Å]

Select minimal supergroups of space group *Pnma* (62)

The next step is to select the supergroups which the pseudosymmetry should be searched for. Each supergroup in the table can be selected by marking the corresponding checkbox.

Select/Unselect all: ☐

No. #	Select	HM Symb.	IT Numb.	Index	Index i_k	Transformation (P,p)	Transformed Cell	Wyckoff Positions Splitting Consideration
1	☑	*Pbam*	055	2	2	**a,-2c,b** ; 0,0,0	11.4059 5.6866 3.9720 90.00 90.00 90.00	This transformation is **valid** under Wyckoff Splitting conditions. Details..
2	☐	*Pbcm*	057	2	2	**b,c,2a** ; 0,0,0	2.8433 11.4059 7.9440 90.00 90.00 90.00	This transformation is **invalid** under Wyckoff Splitting criteria. Details..
3	☑	*Pmmn*	059	2	2	**2c,b,-a** ; 0,0,0	5.6866 7.9440 5.7030 90.00 90.00 90.00	This transformation is **valid** under Wyckoff Splitting conditions. Details..
4	☐	*Pnma*	062	3	3	**3a,b,c** ; 0,0,0	3.8020 7.9440 5.6866 90.00 90.00 90.00	This transformation is **invalid** under Wyckoff Splitting criteria. Details..
5	☐	*Pnma*	062	3	3	**a,3b,c** ; 0,0,0	11.4059 2.6480 5.6866 90.00 90.00 90.00	This transformation is **invalid** under Wyckoff Splitting criteria. Details..
6	☐	*Pnma*	062	3	3	**a,b,3c** ; 0,0,0	11.4059 7.9440 1.8955 90.00 90.00 90.00 Lattice parameters don't comply [Threshold: 0.5Å for a,b,c ; 10° for α,β,γ & lengths must be >2.5Å]	This transformation is **invalid** under Wyckoff Splitting criteria. Details..
7	☐	*Pnma*	062	5	5	**5a,b,c** ; 0,0,0	2.2812 7.9440 5.6866 90.00 90.00 90.00 Lattice parameters don't comply [Threshold: 0.5Å for a,b,c ; 10° for α,β,γ & lengths must be >2.5Å]	This transformation is **invalid** under Wyckoff Splitting criteria. Details..
8	☐	*Pnma*	062	5	5	**a,5b,c** ; 0,0,0	11.4059 1.5888 5.6866 90.00 90.00 90.00 Lattice parameters don't comply [Threshold: 0.5Å for a,b,c ; 10° for α,β,γ & lengths must be >2.5Å]	This transformation is **invalid** under Wyckoff Splitting criteria. Details..
9	☐	*Pnma*	062	5	5	**a,b,5c** ; 0,0,0	11.4059 7.9440 1.1373 90.00 90.00 90.00 Lattice parameters don't comply [Threshold: 0.5Å for a,b,c ; 10° for α,β,γ & lengths must be >2.5Å]	This transformation is **invalid** under Wyckoff Splitting criteria. Details..
10	☐	*Pnma*	062	7	7	**7a,b,c** ; 0,0,0	1.6294 7.9440 5.6866 90.00 90.00 90.00 Lattice parameters don't comply [Threshold: 0.5Å for a,b,c ; 10° for α,β,γ & lengths must be >2.5Å]	This transformation is **invalid** under Wyckoff Splitting criteria. Details..
11	☐	*Pnma*	062	7	7	**a,7b,c** ; 0,0,0	11.4059 1.1349 5.6866 90.00 90.00 90.00 Lattice parameters don't comply [Threshold: 0.5Å for a,b,c ; 10° for α,β,γ & lengths must be >2.5Å]	This transformation is **invalid** under Wyckoff Splitting criteria. Details..
12	☐	*Pnma*	062	7	7	**a,b,7c** ; 0,0,0	11.4059 7.9440 0.8124 90.00 90.00 90.00 Lattice parameters don't comply [Threshold: 0.5Å for a,b,c ; 10° for α,β,γ & lengths must be >2.5Å]	This transformation is **invalid** under Wyckoff Splitting criteria. Details..
13	☑	*Cmcm*	063	2	2	**b,c,a** ; 0,0,0	5.6866 11.4059 7.9440 90.00 90.00 90.00	This transformation is **valid** under Wyckoff Splitting conditions. Details..
14	☑	*Cmcm*	063	2	2	**c,a,b** ; 1/4,1/4,0	7.9440 5.6866 11.4059 90.00 90.00 90.00	This transformation is **valid** under Wyckoff Splitting conditions. Details..
15	☑	*Cmce*	064	2	2	**-b,a,c** ; 1/4,1/4,0	7.9440 11.4059 5.6866 90.00 90.00 90.00	This transformation is **valid** under Wyckoff Splitting conditions. Details..

Wyckoff Positions Splitting Check Under Transformation

The Wyckoff Split Table for the transformation from *Pmmn* (#59) to *Pnma* (#62)

No	Wyckoff position(s)	
	Group	Subgroup
1	2a	4c
2	2b	4c
3	4c	4a 4b
4	4d	8d
5	4e	8d
6	4f	4c 4c
7	8g	8d 8d

This transformation is valid under the Wyckoff Splittings Criteria

Species : Mg Wyckoff Positions :c

WP(#59)		WP(#62)	# additional atoms
(1/2)f	=>	c	---
b	=>	c	---
a	=>	c	---
f	=>	c + *c*	(4) [1:1]

Species : Pb Wyckoff Positions :d

WP(#59)		WP(#62)	# additional atoms
(1/2)g	=>	d	---
e	=>	d	---
d	=>	d	---
g	=>	d + *d*	(8) [1:1]

Species : O Wyckoff Positions :d,c,c,c,c

WP(#59)		WP(#62)	# additional atoms
2f,(1/2)g	=>	d,c,c,c,c	---
4b,(1/2)g	=>	d,c,c,c,c	---
4a,(1/2)g	=>	d,c,c,c,c	---
e,2f	=>	d,c,c,c,c	---
d,2f	=>	d,c,c,c,c	---
4b,e	=>	d,c,c,c,c	---
4b,d	=>	d,c,c,c,c	---
4a,e	=>	d,c,c,c,c	---
4a,d	=>	d,c,c,c,c	---
2f,g	=>	d,c,c,c,c + *d*	(8) [3:1]
4b,g	=>	d,c,c,c,c + *d*	(8) [3:1]
4a,g	=>	d,c,c,c,c + *d*	(8) [3:1]

Flagged pseudosymmetry of Pb_2MgWO_6 with respect to the space group Pmmn (59)

Summary search results

Pseudosymmetry search among minimal supergroups.

Case #	Supergroup G	Index i	Index i_k	(P,p)	Tr. Matrix	Δ_{max}	u_{max}
1	*Pbam* (055)	2	2	**a,-2c,b** ; 0,0,0	[1 0 0] [0] [0 0 1] [0] [0 −2 0] [0]	>tol	-
2	*Pmmn* (059)	2	2	**2c,b,-a** ; 0,0,0	[0 0 −1] [0] [0 1 0] [0] [2 0 0] [0]	0.3457	0.1729
3	*Cmcm* (063)	2	2	**b,c,a** ; 0,0,0	[0 0 1] [0] [1 0 0] [0] [0 1 0] [0]	>tol	-
4	*Cmcm* (063)	2	2	**c,a,b** ; 1/4,1/4,0	[0 1 0] [1/4] [0 0 1] [1/4] [1 0 0] [0]	>tol	-
5	*Cmce* (064)	2	2	**-b,a,c** ; 1/4,1/4,0	[0 1 0] [1/4] [−1 0 0] [1/4] [0 0 1] [0]	>tol	-
6	*Imma* (074)	2	2	**a,b,c** ; 0,0,0	[1 0 0] [0] [0 1 0] [0] [0 0 1] [0]	>tol	-

Structural pseudosymmetry:

Pmmn(59)> Pnma(62)

[i]=2 (P,p)=2c,b,-a

Displacements:

Atom	Idealized Coordinates	u_x	u_y	u_z	|u|
Pb1	(0.1422, 0.0032, 0.7500)	0.000000	0.000000	0.030400	0.1729
Mg1	(0.3772, 0.2500, 0.7500)	0.000000	0.000000	0.001900	0.0108
W1	(0.1161, 0.2500, 0.2500)	0.000000	0.000000	0.007700	0.0438
O1	(0.1314, 0.4907, 0.2500)	0.000000	0.000000	-0.013500	0.0768
O2	(0.0065, 0.2500, 0.0071)	-0.003800	0.000000	0.006200	0.0559
O3	(0.0065, 0.2500, 0.4929)	0.003800	0.000000	0.006200	0.0559
O4	(0.2430, 0.2500, 0.0051)	-0.006050	0.000000	-0.020400	0.1350
O5	(0.2430, 0.2500, 0.4949)	0.006050	0.000000	-0.020400	0.1350

u_{max}=0.1729Å

Idealized structure data

Idealized structure (supergroup setting):

```
59
5.6866 7.9440 5.7030 90.00 90.00 90.00
6
Pb      1       4e      0.250000        0.003200        0.284400
Mg      1       2a      0.250000        0.250000        0.754400
W       1       2b      0.750000        0.250000        0.232200
O       1       4e      0.750000        0.490700        0.262800
O       2       4f      0.992900        0.250000        0.013000
O       4       4f      0.994900        0.250000        0.486100
```

-lattice parameters:

-atomic coordinates:
WPASSIGN

-redundant atoms

Continue to search for pseudosymmetry with this structure (#059) | Visualize this structure | CIF File

Plot the progress so far
[Click here to see full report]

to ‘climb up’ further...

Step2. Immm (71) pseudosymmetry of idealized structure of Pb_2MgWO_6 of symmetry Pmmn (59)

Case #	Supergroup G	Index i	Index i_k	(P,p)	Tr. Matrix	Δ_{max}	u_{max}
1	*Cmmm* (065)	2	2	**a,b,c** ; 1/4,1/4,0	[1 0 0] [1/4] [0 1 0] [1/4] [0 0 1] [0]	>tol	-
2	*Immm* (071)	2	2	**a,b,c** ; 1/4,1/4,1/4	[1 0 0] [1/4] [0 1 0] [1/4] [0 0 1] [1/4]	0.3924	0.1962

5# Supergroup *Immm* (071): a,b,c ; 1/4,1/4,1/4 and index 2

Displacements:

Atom	Idealized Coordinates	u_x	u_y	u_z	|u|
Pb1	(0.2500, 0.0032, 0.2500)	0.000000	0.000000	0.034400	0.1962
Mg1	(0.2500, 0.2500, 0.7500)	0.000000	0.000000	0.004400	0.0251
W1	(0.7500, 0.2500, 0.2500)	0.000000	0.000000	-0.017800	0.1015
O1	(0.7500, 0.4907, 0.2500)	0.000000	0.000000	0.012800	0.0730
O2	(0.9939, 0.2500, 0.0135)	-0.001000	0.000000	-0.000450	0.0062
O4	(0.9939, 0.2500, 0.4865)	0.001000	0.000000	-0.000450	0.0062

Idealized structure (supergroup setting):

```
071
5.6866 7.9440 5.7030 90.00 90.00 90.00
5
Pb     1    -   0.5000   0.2532   0.5000
Mg     1    -   0.5000   0.5000   0.0000
W      1    -   0.0000   0.5000   0.5000
O      1    -   0.0000   0.7407   0.5000
O      2    -   0.2439   0.5000   0.2635
#O      4    -   0.2439   0.5000   0.7366
```

NOTE: u_x, u_y and u_z are given in relative units. |u| is the absolute displacement given in Å

Step3. Pseudosymmetry of idealised structure of Pb_2MgWO_6 of symmetry Immn (71)

Idealized structures

7# Supergroup *I4/mmm* (139): b,c,a ; 0,1/2,0 and index 2

Displacements:

Atom	Idealized Coordinates	u_x	u_y	u_z	|u|
Pb1	(0.5000, 0.2500, 0.5000)	0.000000	0.003200	0.000000	0.0254
Mg1	(0.5000, 0.5000, 0.0000)	0.000000	0.000000	0.000000	0.0000
W1	(0.0000, 0.5000, 0.5000)	0.000000	0.000000	0.000000	0.0000
O1	(0.0000, 0.7407, 0.5000)	0.000000	0.000000	0.000000	0.0000
O2	(0.2402, 0.5000, 0.2598)	0.003700	0.000000	0.003700	0.0298

Idealized structure (supergroup setting):

```
139
5.7030 5.6866 7.9440 90.00 90.00 90.00
5
Pb     1    -   0.5000   0.0000   0.2500
Mg     1    -   0.0000   0.0000   0.5000
W      1    -   0.5000   0.5000   0.5000
O      1    -   0.5000   0.5000   0.7407
O      2    -   0.2598   0.7402   0.5000
```

lattice parameters:
not symmetrized

Step4. Pseudosymmetry of idealised structure of Pb_2MgWO_6 of symmetry I4/mmm (139)

2# Supergroup *Fm*-3*m* (225): 1/2a-1/2b,1/2a+1/2b,c ; 0,0,0 and index 3

Displacements:

Atom	Idealized Coordinates	u_x	u_y	u_z	|u|
Pb1	(0.5000, 0.0000, 0.2500)	0.000000	0.000000	0.000000	0.0000
Mg1	(0.0000, 0.0000, 0.5000)	0.000000	0.000000	0.000000	0.0000
W1	(0.5000, 0.5000, 0.5000)	0.000000	0.000000	0.000000	0.0000
O1	(0.5000, 0.5000, 0.7404)	0.000000	0.000000	0.000333	0.0026
O2	(0.2596, 0.7404, 0.5000)	0.000167	-0.000167	0.000000	0.0013

```
225
8.0537 8.0537 7.9440 90.00 90.00 90.17
4
Pb     1    -   0.2500   0.7500   0.2500
Mg     1    -   0.0000   0.0000   0.5000
W      1    -   0.5000   0.0000   0.5000
O      1    -   0.5000   0.0000   0.7404
#O      2    -   0.5000   0.2404   0.5000
```

WPASSIGN:

Pb 8c
Mg 4b
W 4a
O 24e

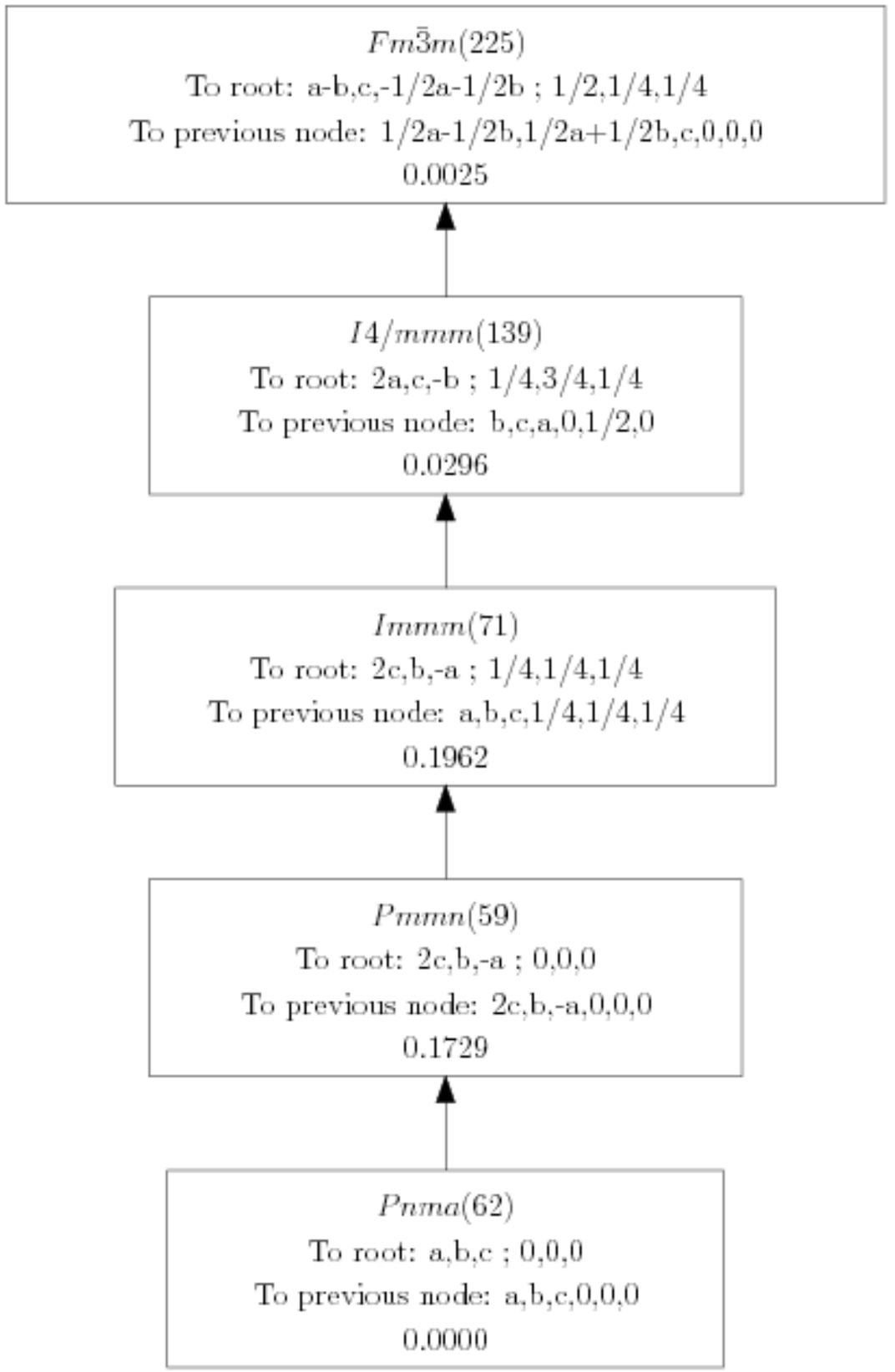
Structural pseudosymmetry of Pb_2MgWO_6

Graph of minimal supergroups

each step is characterized by:

-transformation matrices $(P,p)_i$

-maximal displacements

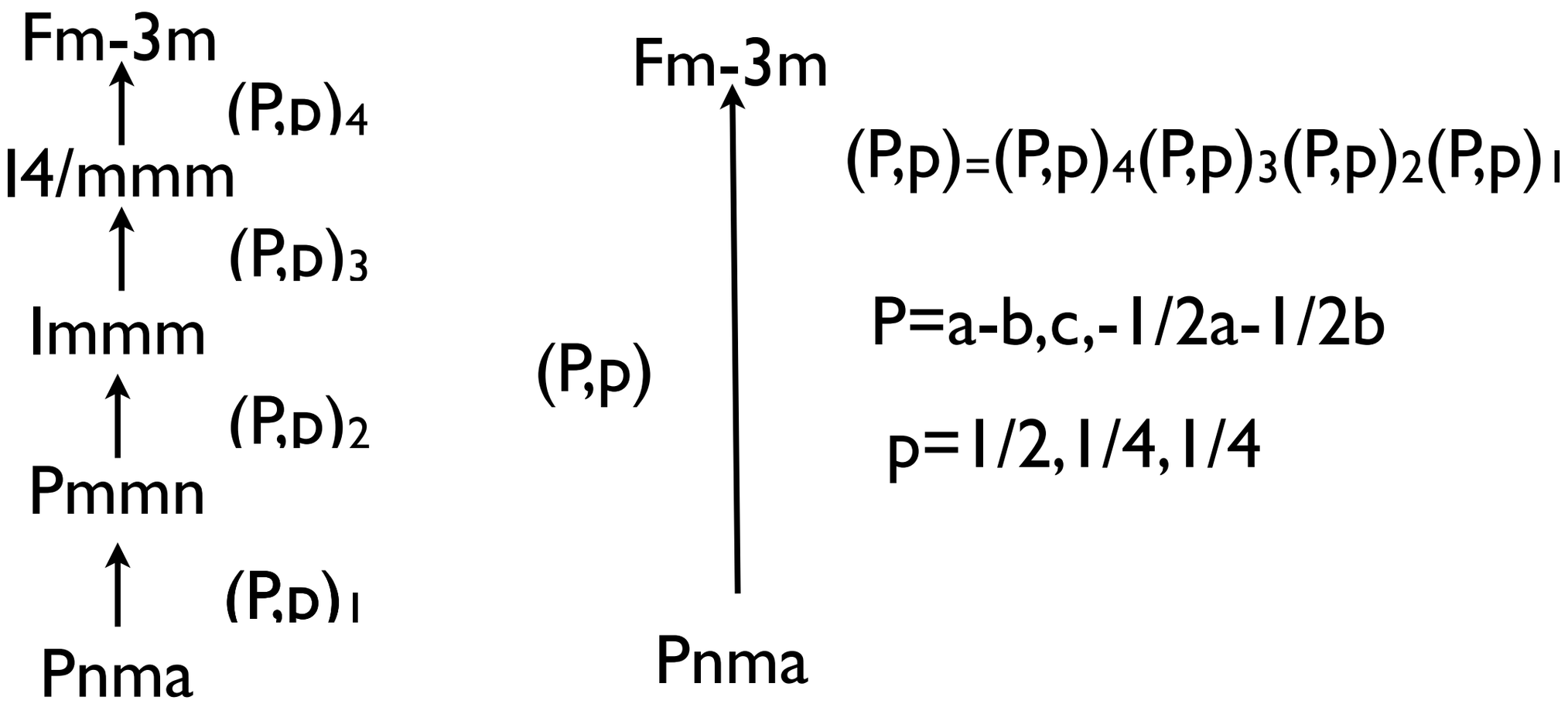


EXERCISES

Problem 3.11 (ii)

Analyse the structural pseudosymmetry of Pb_2MgWO_6

Option 3: Search of structural pseudosymmetry with respect to specific supergroup



Problem 3.11 (ii)

SOLUTION

Option 3: Search of structural pseudosymmetry with respect to a specific supergroup

1. Minimal supergroups ○ ☐ [Show only indices in supergroups table]
2. Supergroups with k-index ○ **ik:** 1
3. Specify supergroup transformation ○ **G:** 221

	Rotational part			Origin Shift
Transf. Matrix (in option 3 only)	1	0	0	0
	0	1	0	0
	0	0	1	0

4. Lattice Pseudosymmetry with minimal supergroups ○ **Ang. Tol (in degrees)** 5 [*]

[*] Only for triclinics and monoclinics.

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

Maximum Δ: 2

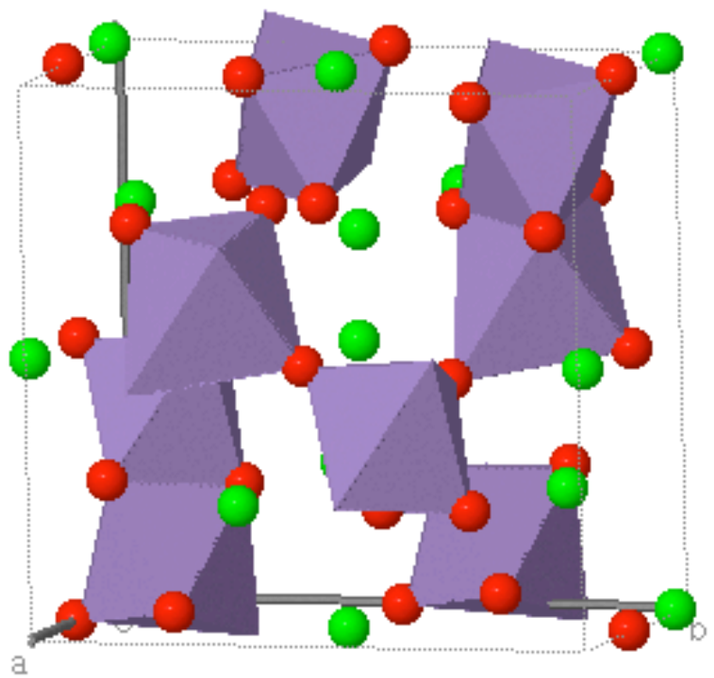
tolerance [Å]

EXERCISES

Problem 3.12

Analyse the structural pseudosymmetry of the virtual structure of $C222_1$ symmetry stepwise, i.e. via the minimal supergroup Option 1 of PSEUDO. Compare the results if different minimal-supergroup paths are followed.

C222 1
a=5,444Å
b=9,412Å
c=9,063Å
α=90,0°
β=90,0°
γ=90,0°



Problem 3.13

(combined application of Option 3 and Option 1 of PSEUDO)

Analyse the structural pseudosymmetry of the orthorhombic phase Ga-II of Ga under pressure. (For the structure data, see the Structure Data file.)

Hint: As a first step check the structural pseudosymmetry with respect to an isomorphic supergroup of index 13 (can you guess why?), specified by the transformation matrix: **a**,**b**, 13**c**, i.e. first apply Option 3 of PSEUDO.

Problem 3.14

GeF_2, having the $P2_12_12_1$ (N. 19) structure given below, is reported to have a high temperatures an unknown tetragonal phase, with the primitive unit cell volume being essentially maintained. Using PSEUDO, with the option 2, which allows to check supergroups with a fixed k-index (multiplication of the primitive unit cell) postulate a probable space group or groups and a starting structural model for this high-temperature phase.

```
19
4.682 5.158 8.312 90 90 90
3
Ge 1   4a 0.2340 0.0083 0.1311
F  1   4a 0.029  0.083  -0.018
F  2   4a 0.067  0.246  0.279
```

Problem 3.14

SOLUTION

Option 2: Search of structural pseudosymmetry with respect to supergroups of specific [i_L] index

1. Minimal supergroups ◉ ☐ [Show only indices in supergroups table]
2. Supergroups with k-index ○ **i_k:** 1
3. Specify supergroup transformation ○ **G:** 221

	Rotational part			Origin Shift
Transf. Matrix (in option 3 only)	1	0	0	0
	0	1	0	0
	0	0	1	0

4. Lattice Pseudosymmetry with minimal supergroups ○ **Ang. Tol (in degrees)** 5 [*]

[*] Only for triclinics and monoclinics.

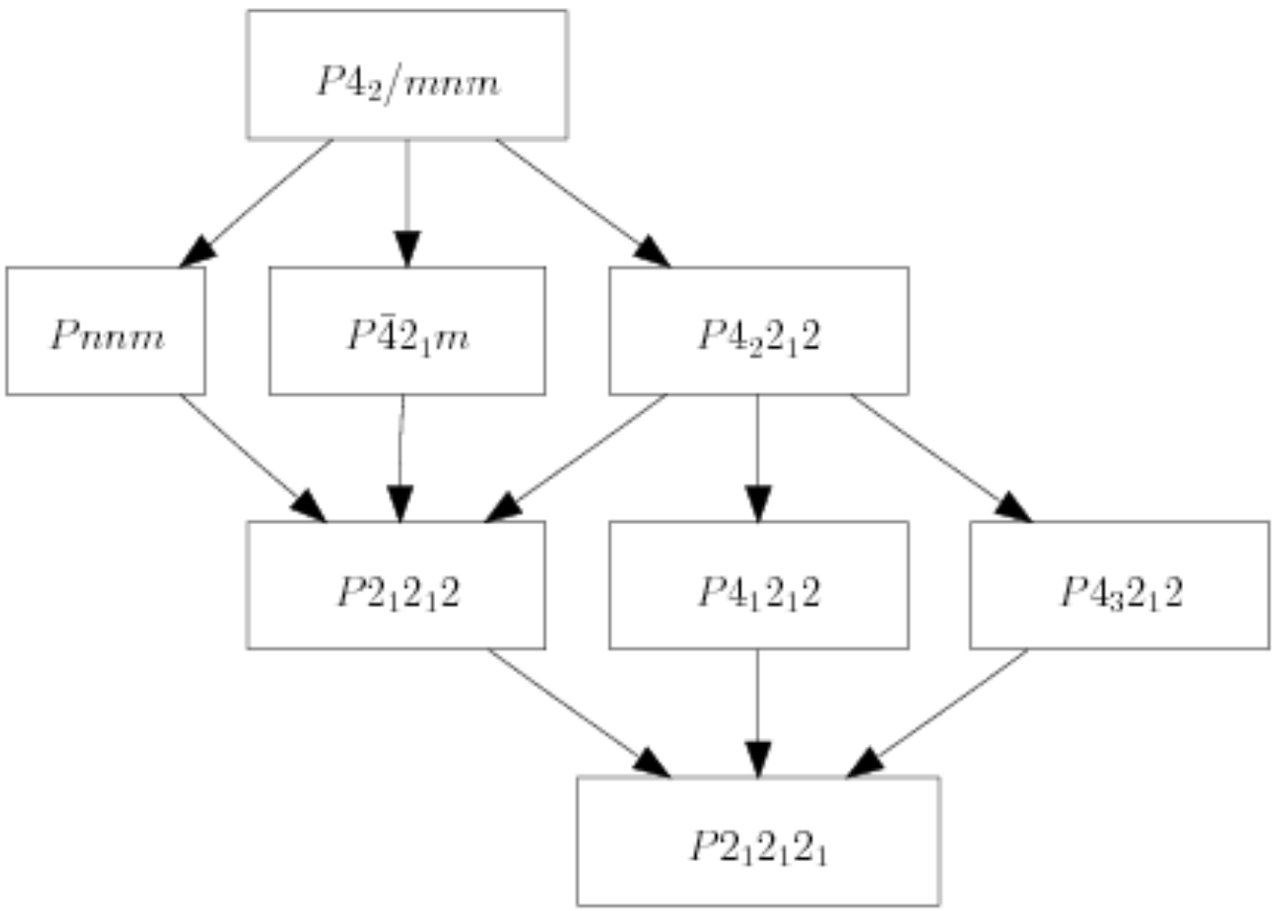
Enter the tolerance (maximum allowed distance) for pseudosymmetry search.

Maximum Δ: 2

tolerance [Å]

SUBGROUPGRAPH
for the pair $P4_2/mnm$ > $P2_12_12_1$, [i]=8

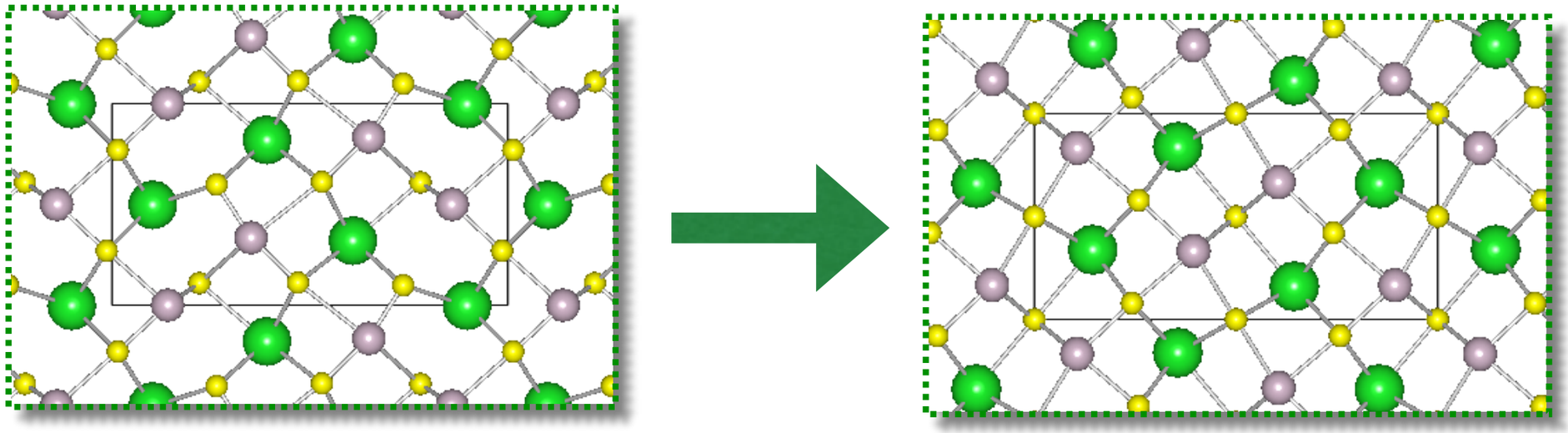
Group-Subgroup Lattice



Problem: Search for ferroelectrics (as pseudosymmetric structures)

Two necessary conditions for a structure to be ferroelectric:

- Polar symmetry group (it should allow non-zero polarization)
- Pseudosymmetry with respect to a non-polar symmetry group (the polar distortion should be small and “multistable”)

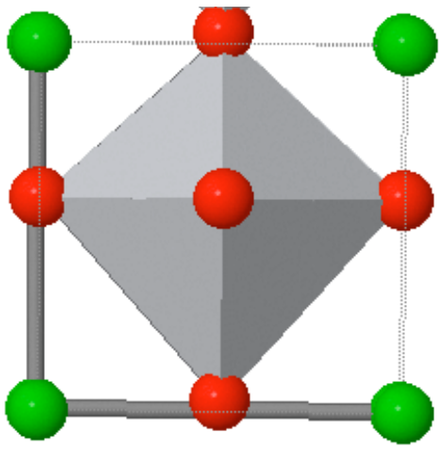


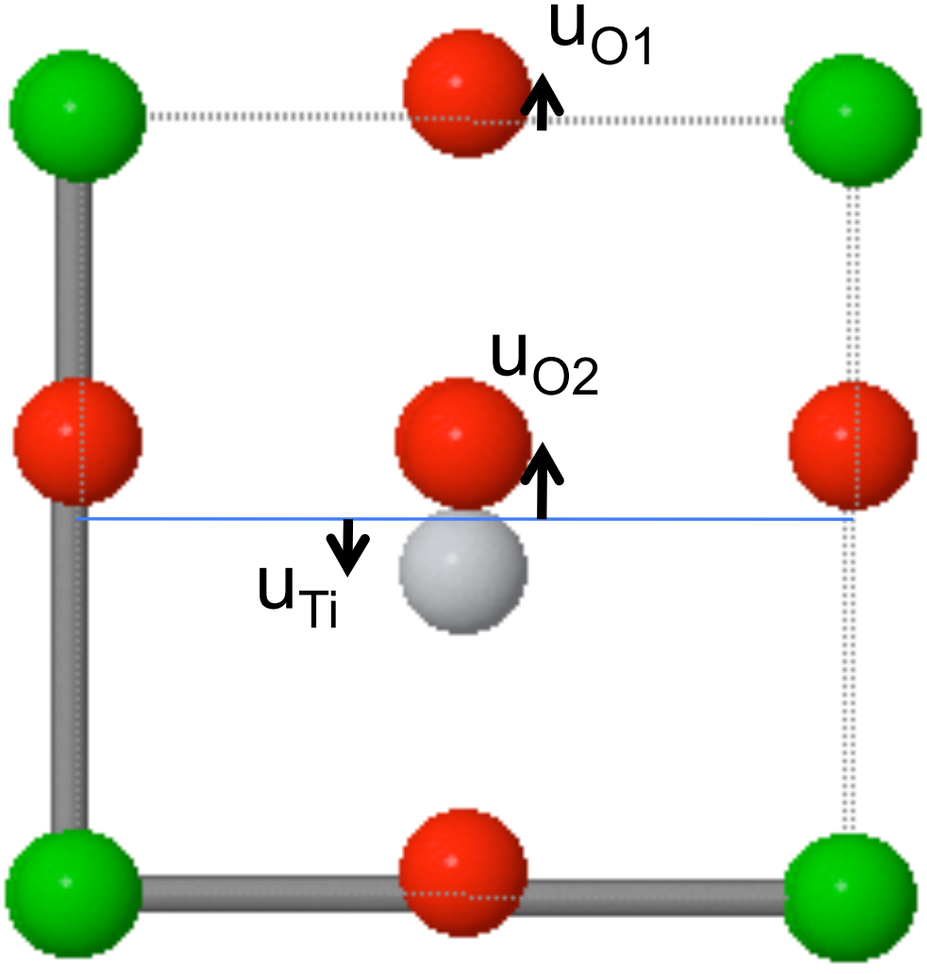
$Pna2_1$ $BaHgS_2$ Pbam

(max. displacement 0.49 A)

Problem: Search for ferroelectrics (as pseudosymmetric structures)

Polar groups… some additional care





$u_{Ba} = 0$

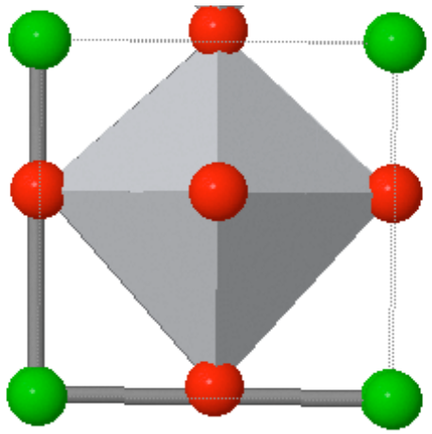
u_{Ti}

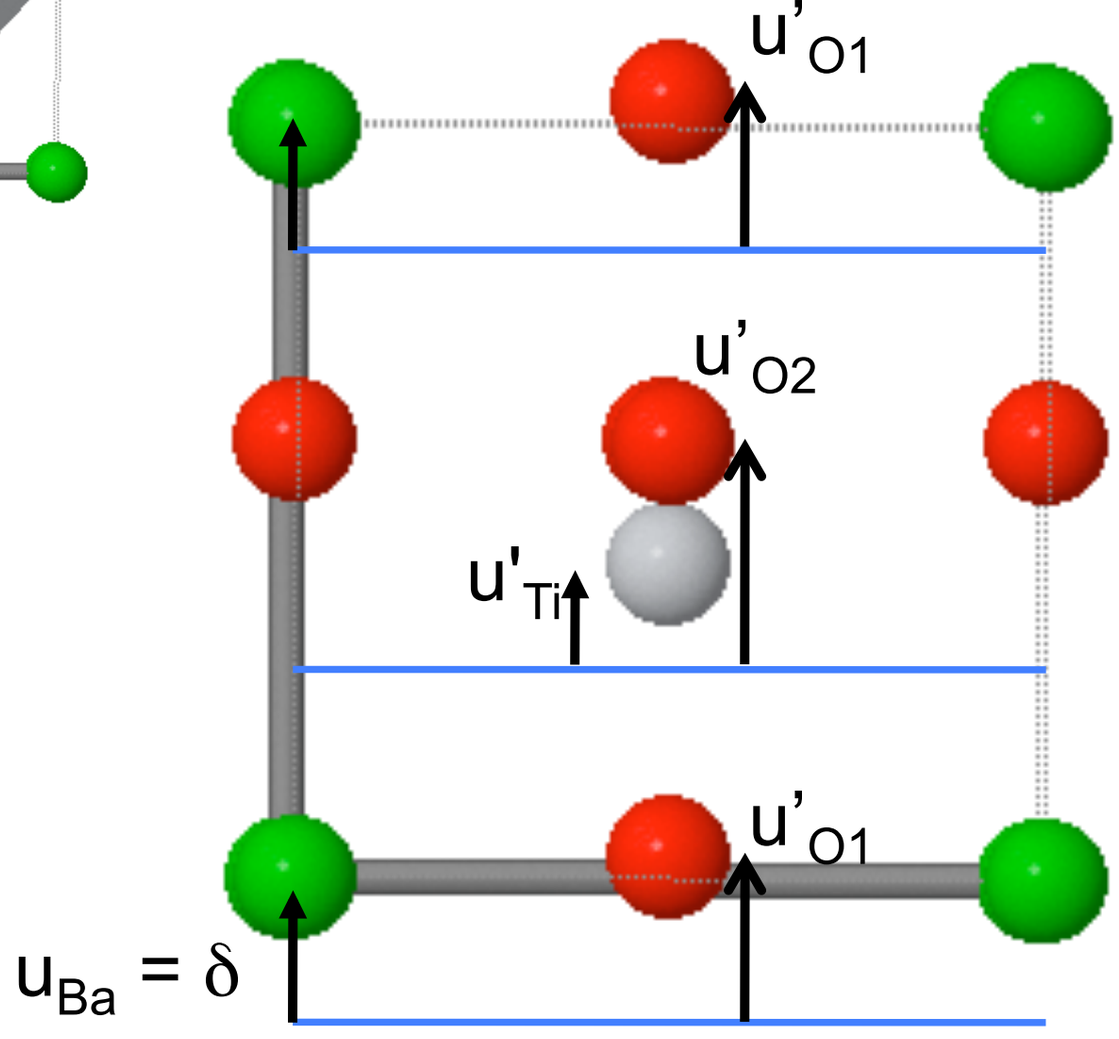
u_{O1}

u_{O2}

Problem: Search for ferroelectrics (as pseudosymmetric structures)

Polar groups… some additional care





$u'_{Ba} = \delta$

$u'_{Ti} = u_{Ti} + \delta$

$u'_{O1} = u_{O1} + \delta$

$u'_{O2} = u_{O2} + \delta$

Default example: $BaTiO_3$

Problem: Search for ferroelectrics

Select minimal supergroups of space group *P4mm* (99)

The next step is to select the supergroups which the pseudosymmetry should be searched for. Each supergroup in the table can be selected by marking the corresponding checkbox.

Select/Unselect all: ☐

No. #	Select	HM Symb.	IT Numb.	Index	Index i_k	Transformation (P,p)	Transformed Cell	Wyckoff Positions Splitting Consideration
1	☐	*P4mm*	099	2	2	**a,b,2c** ; 0,0,2t	3.9990 3.9990 2.0100 90.00 90.00 90.00 Lattice parameters don't comply [Threshold: 0.5Å for a,b,c ; 10° for α,β,γ & lengths must be >2.5Å]	This transformation is **invalid** under Wyckoff Splitting criteria. Details..
2	☐	*P4mm*	099	2	2	**a-b,a+b,c** ; 0,0,t	2.8277 2.8277 4.0200 90.00 90.00 90.00	This transformation is **invalid** under Wyckoff Splitting criteria. Details..
3	☐	*P4mm*	099	3	3	**a,b,3c** ; 0,0,3t	3.9990 3.9990 1.3400 90.00 90.00 90.00 Lattice parameters don't comply [Threshold: 0.5Å for a,b,c ; 10° for α,β,γ & lengths must be >2.5Å]	This transformation is **invalid** under Wyckoff Splitting criteria. Details..
4	☐	*P4mm*	099	5	5	**a,b,5c** ; 0,0,5t	3.9990 3.9990 0.8040 90.00 90.00 90.00 Lattice parameters don't comply [Threshold: 0.5Å for a,b,c ; 10° for α,β,γ & lengths must be >2.5Å]	This transformation is **invalid** under Wyckoff Splitting criteria. Details..
5	☐	*P4mm*	099	7	7	**a,b,7c** ; 0,0,7t	3.9990 3.9990 0.5743 90.00 90.00 90.00 Lattice parameters don't comply [Threshold: 0.5Å for a,b,c ; 10° for α,β,γ & lengths must be >2.5Å]	This transformation is **invalid** under Wyckoff Splitting criteria. Details..
6	☐	*P4mm*	099	9	9	**3a,3b,c** ; 0,0,t	1.3330 1.3330 4.0200 90.00 90.00 90.00 Lattice parameters don't comply [Threshold: 0.5Å for a,b,c ; 10° for α,β,γ & lengths must be >2.5Å]	This transformation is **invalid** under Wyckoff Splitting criteria. Details..
7	☐	*P4mm*	099	9	9	**a,b,9c** ; 0,0,9t	3.9990 3.9990 0.4467 90.00 90.00 90.00 Lattice parameters don't comply [Threshold: 0.5Å for a,b,c ; 10° for α,β,γ & lengths must be >2.5Å]	This transformation is **invalid** under Wyckoff Splitting criteria. Details..
8	☐	*I4mm*	107	2	2	**a,b,c** ; 0,0,t	3.9990 3.9990 4.0200 90.00 90.00 90.00	This transformation is **invalid** under Wyckoff Splitting criteria. Details..
9	☑	*P4/mmm*	123	2	1	**a,b,c** ; 0,0,t	3.9990 3.9990 4.0200 90.00 90.00 90.00	This transformation is **valid** under Wyckoff Splitting conditions. Details..
10	☐	*P4/nmm*	129	2	1	**a,b,c** ; 1/4,1/4,t	3.9990 3.9990 4.0200 90.00 90.00 90.00	This transformation is **invalid** under Wyckoff Splitting criteria. Details..

HINT: The initial structure is polar, which means that, in general, an origin shift will be necessary to minimize the displacements between the initial polar structure and the hypothetical idealized parent one. insert a minimum grid for the optimization (in Angstroms)

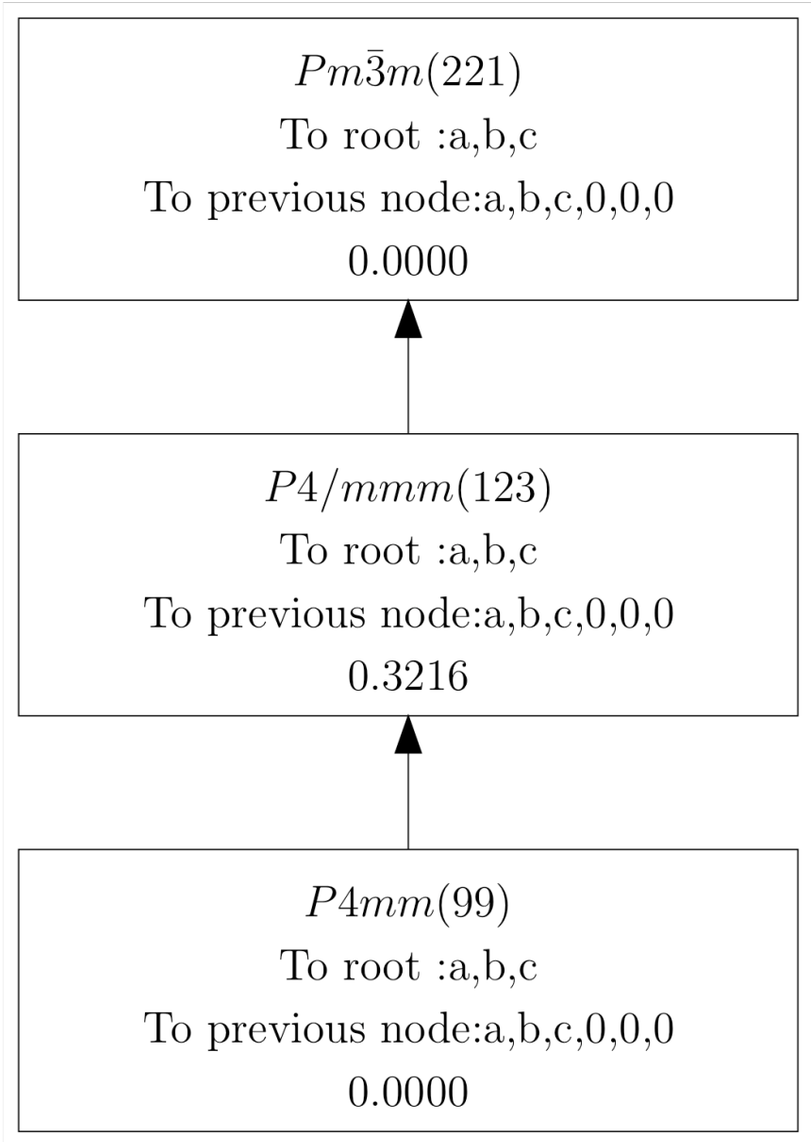
Grid: 0.5

grid for optimization

Default example: $BaTiO_3$

Problem: Search for ferroelectrics

Pseudosymmetry



$BaTiO_3$

Problem: Prediction of *Pna2$_1$* ferroelectrics

PSEUDO

ICSD (Inorganic Crystal Structure Database)

	Binary	Ternary	Quaternary	Total
Entries	39	202	223	464
Compounds	26	125	161	312
Pseudo. Entries	20	100	40	160
Pseudo. Compounds	12	66	36	114
Overlooked Sym.	7	30	9	46
Known Ferro.	1	14	4	19
Candidates?	1	13	4	18

Known Ferroelectrics

pseudosymmetry search

Compound	$\mathcal{G}$	$[i]$	$\Delta_{\max}$(Å)	η_g	γ	$T_c(K)$
Nb_6I_{11}	$Pccn$	2	0.547	0.623	0.189	274
$D_{0.45}Nb_6I_{11}$	$Pccn$	2	0.745	0.626	0.187	?
$NaTaO_3$	$Pnma$	2	0.232	0.988	0.006	753
$LaYbO_3$	$Pnma$	2	0.347	0.968	0.016	?
$RbGeBr_3$	$Pnma$	2	0.536	0.519	0.240	366
K_2SeO_4	$Pnma$	2	0.539	0.833	0.084	93
Cs_2BeF_4	$Pnma$	2	0.174	0.663	0.168	?
Rb_2BeF_4	$Pnma$	2	0.171	0.992	0.004	921
K_2BeF_4	$Pnma$	2	0.338	0.772	0.114	968
Rb_2ZnBr_4	$Pnma$	2	0.131	0.961	0.020	200
Rb_2ZnCl_4	$Pnma$	2	0.463	0.849	0.076	189
K_2ZnCl_4	$Pnma$	2	0.177	0.898	0.051	130
SbSI	$Pnma$	2	0.103	0.766	0.117	293
SbSBr	$Pnma$	2	0.109	0.821	0.089	23
$SbNbO_4$	$Pnna$	2	0.421	0.455	0.272	678
$(BiO)_4(NbO_4)Cl$	$Pbcn$	2	0.623	0.733	0.133	640
$CsTiO(AsO_4)$	$Pnna$	2	0.447	0.622	0.189	?
$KTiO(AsO_4)$	$Pnna$	2	0.610	0.997	0.002	?
$TlTiO(PO_4)$	$Pnna$	2	0.408	0.792	0.104	856

pseudosymmetry search

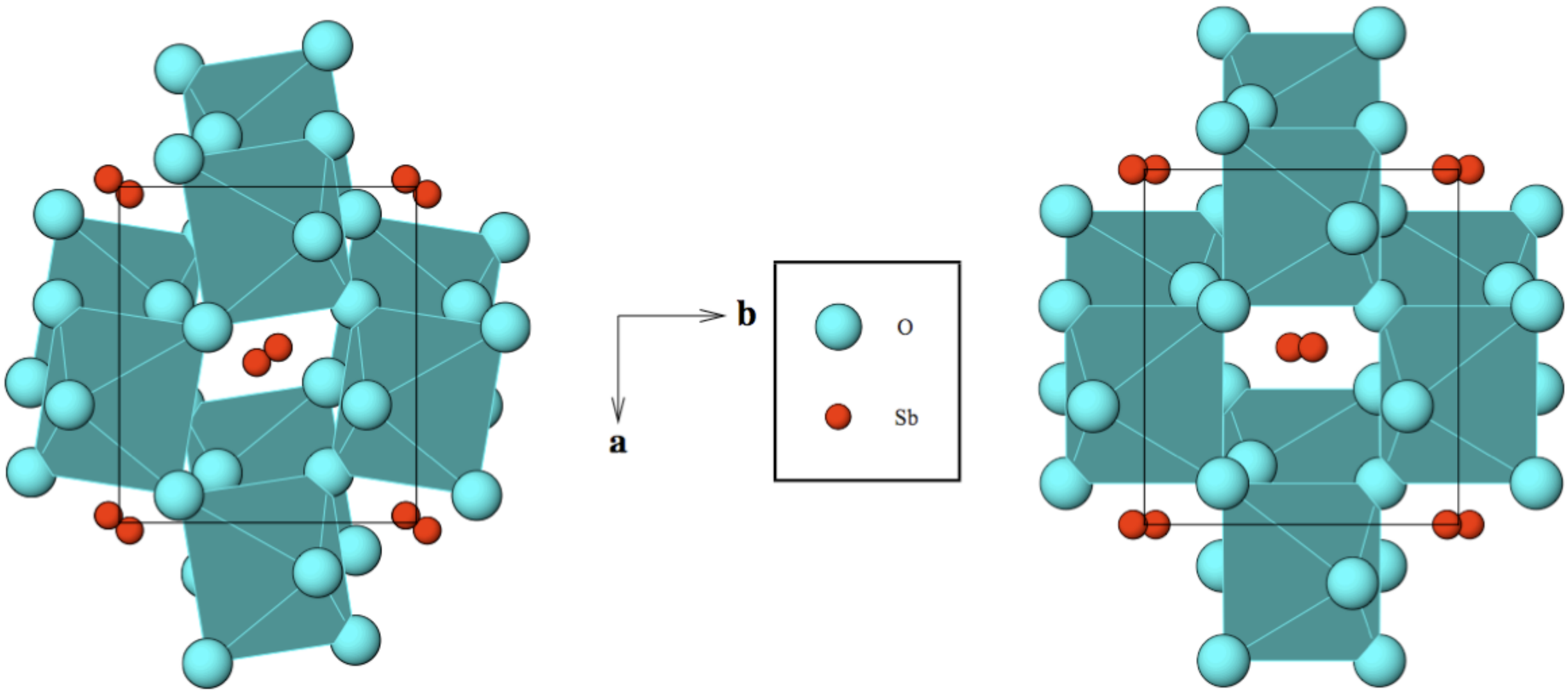
CANDIDATES FOR FERROELECTRICS

Compound	$\mathcal{G}$	$[i]$	$\Delta_{\max}$(Å)	η_g	γ
Sb_2O_4	$Pnna$	2	0.581	0.641	0.179
PbNCN	$Pnma$	2	0.193	0.996	0.002
$NaIO_3$	$Pnma$	2	0.194	0.977	0.012
$YScS_3$	$Pnma$	2	0.179	0.865	0.068
$CeSiP_3$	$Pnma$	2	0.648	0.935	0.032
$SmBeF_4$	$Pnma$	2	0.325	0.979	0.010
K_3AsS_4	$Pnma$	2	0.227	0.847	0.077
WPO_5	$Pnma$	2	0.457	0.986	0.007
$Sr_3Sb_4S_9$	$Pnma$	2	0.230	0.822	0.089
$Be_4Pr_9O_{20}$	$Pnma$	2	0.246	0.904	0.048
$Ca_{0.84}Sr_{1.16}SiO_4$	$Pnma$	2	0.580	0.747	0.127
$Tl_{1.1}AlSiO_4$	$Pnma$	2	0.590	0.953	0.024
$Na_2UO_2P_2O_7$	$Pnma$	2	0.559	0.991	0.040
$TlSnPS_4$	$Pnma$	2	0.488	0.734	0.133

pseudosymmetry search

Example: Sb_2O_4 ($Pna2_1 \xrightarrow{(2)} Pnna$)

$$\Delta = 0.581\text{Å y } \eta_g = 0.641\text{Å}$$



Problem 3.15

The compound $NaSb_3F_{10}$ whose room-temperature phase is polar, space group $P6_3$, has been predicted to be ferroelectric. (For the structure data, see the Structure Data file.) The symmetries $P6_322$ and $P6_3/mmc$ had been proposed for two successive non-polar phases at high temperature.

Applying the pseudosymmetry approach confirm the predictions for the non-polar phases of $NaSb_3F_{10}$. Show that apart from $P6_322$, there are two more appropriate candidates for the intermediate phases between the polar phase $P6_3$ and the non-polar one of maximal symmetry, $P6_3/mmc$.

Problem 3.15

SOLUTION

Pseudosymmetry search

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 tridinic and monodinic 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 of the atoms from their high symmetry position in Angstroms. Normally a default value between 0.75-1Å 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.

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)**, 186-195 DOI:10.1524/zkri.2011.1321.

If you are interested in other publications related to Bilbao Crystallographic Server, click here.

Please, enter structure data in the text area (or load CIF file).

We are developing a new version of PSEUDO. It is currently in beta version and it will be available soon. Please, let us know if you experience any problem with the program or you find errors. The e-mail for contact is cryst@wm.ic.ehu.es. Any comments and/or critics are welcome, too!.

Formulae: Na5b3F10

Structure data [in CIF format]: Browse...

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

Initial Structure (LS):

```
173
8.285 8.285 7.600 90. 90. 120.
6
Sb 1 6c 0.8837 0.2243 0.25
Na 1 2b 0.3333 0.6667 0.167
F 1 6c 0.204 0.393 0.994
F 2 6c 0.111 0.229 0.340
F 3 6c 0.035 0.491 0.281
F 4 2b 0.6667 0.3333 0.245
```

Select supergroups type for pseudosymmetry search.

1. Minimal supergroups [Show only indices in supergroups table]
2. Supergroups with k-index — k: 1
3. Specify supergroup transformation — g: 221

Transf. Matrix (in option 3 only)

	Rotational part			Origin Shift
	1	0	0	0
	0	1	0	0
	0	0	1	0

4. Lattice Pseudosymmetry with minimal supergroups — **Ang. Tol (in degrees)** 5 [*]

[*] Only for triclinics and monoclinics.

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

Maximum Δ: 2

Show

Example: $NaSb_3F_{10}$

Structural Data

Search options

Tolerance

Problem 3.15

SOLUTION

Example: $NaSb_3F_{10}$

1	☐	*P*6	168	2	2	**a,b,2c** ; 0,0,2t	8.2850 8.2850 3.8000 90.00 90.00 120.00	This transformation is invalid under Wyckoff Splitting criteria. Details..
2	☐	$P6_3$	173	3	3	**a,b,3c** ; 0,0,3t	8.2850 8.2850 2.5333 90.00 90.00 120.00	This transformation is invalid under Wyckoff Splitting criteria. Details..
3	☐	$P6_3$	173	3	3	**a-b,a+2b,c** ; 0,0,t	4.7833 4.7833 7.6000 90.00 90.00 120.00	This transformation is invalid under Wyckoff Splitting criteria. Details..
4	☐	$P6_3$	173	4	4	**2a,2b,c** ; 0,0,t	4.1425 4.1425 7.6000 90.00 90.00 120.00	This transformation is invalid under Wyckoff Splitting criteria. Details..
5	☐	$P6_3$	173	5	5	**a,b,5c** ; 0,0,5t	8.2850 8.2850 1.5200 90.00 90.00 120.00	This transformation is invalid under Wyckoff Splitting criteria. Details..
6	☐	$P6_3$	173	7	7	**a,b,7c** ; 0,0,7t	8.2850 8.2850 1.0857 90.00 90.00 120.00	This transformation is invalid under Wyckoff Splitting criteria. Details..
7	☐	$P6_3$	173	7	7	**a-2b,2a+3b,c** ; 0,0,t	3.1314 3.1314 7.6000 90.00 90.00 120.00	This transformation is invalid under Wyckoff Splitting criteria. Details..
8	☐	$P6_3$	173	7	7	**-2a-3b,-a+2b,-c** ; 0,0,-t	3.1314 3.1314 7.6000 90.00 90.00 120.00	This transformation is invalid under Wyckoff Splitting criteria. Details..
9	☑	$P6_3/m$	176	2	1	**a,b,c** ; 0,0,t	8.2850 8.2850 7.6000 90.00 90.00 120.00	This transformation is valid under Wyckoff Splitting conditions. Details..
10	☑	$P6_322$	182	2	1	**a,b,c** ; 0,0,t	8.2850 8.2850 7.6000 90.00 90.00 120.00	This transformation is valid under Wyckoff Splitting conditions. Details..
11	☐	$P6_3cm$	185	2	1	**a,b,c** ; 0,0,t	8.2850 8.2850 7.6000 90.00 90.00 120.00	This transformation is invalid under Wyckoff Splitting criteria. Details..
12	☑	$P6_3mc$	186	2	1	**a,b,c** ; 0,0,t	8.2850 8.2850 7.6000 90.00 90.00 120.00	This transformation is valid under Wyckoff Splitting conditions. Details..

HINT: The initial structure is polar, which means that, in general, an origin shift will be necessary to minimize the displacements between the initial polar structure and the hipothetical idealized parent one. Please, insert a minimum grid for the optimization (in Angstroms)

Grid: 0.5

Problem 3.15

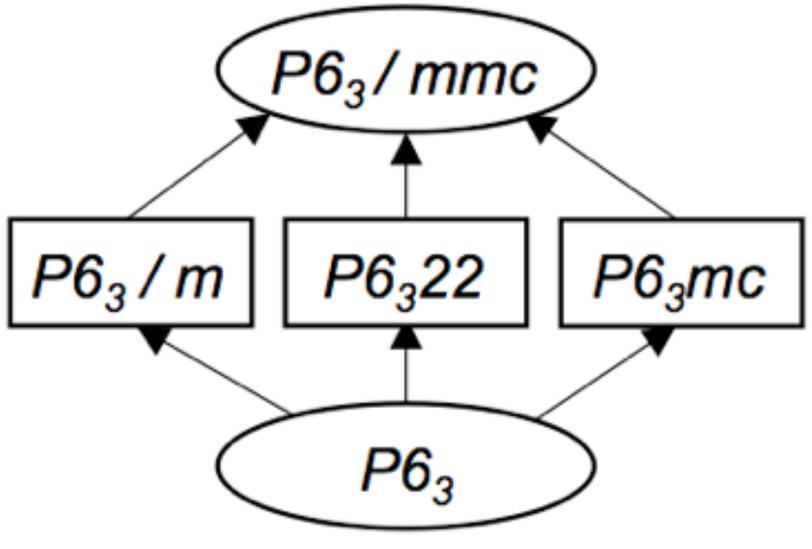
SOLUTION

Summary search results

Pseudosymmetry search among minimal supergroups.

Example: $NaSb_3F_{10}$

Case #	Supergroup G	Index i	Index i_k	(P,p)	Tr. Matrix	Δ_{max}	u_{max}
1	$P6_3/m$ (176)	2	1	**a,b,c** ; 0,0,0	[1 0 0] [0] [0 1 0] [0] [0 0 1] [0]	1.4010	0.7005
2	$P6_322$ (182)	2	1	**a,b,c** ; 0,0,0	[1 0 0] [0] [0 1 0] [0] [0 0 1] [0]	1.3984	0.6992
3	$P6_3mc$ (186)	2	1	**a,b,c** ; 0,0,0	[1 0 0] [0] [0 1 0] [0] [0 0 1] [0]	0.8948	0.4474



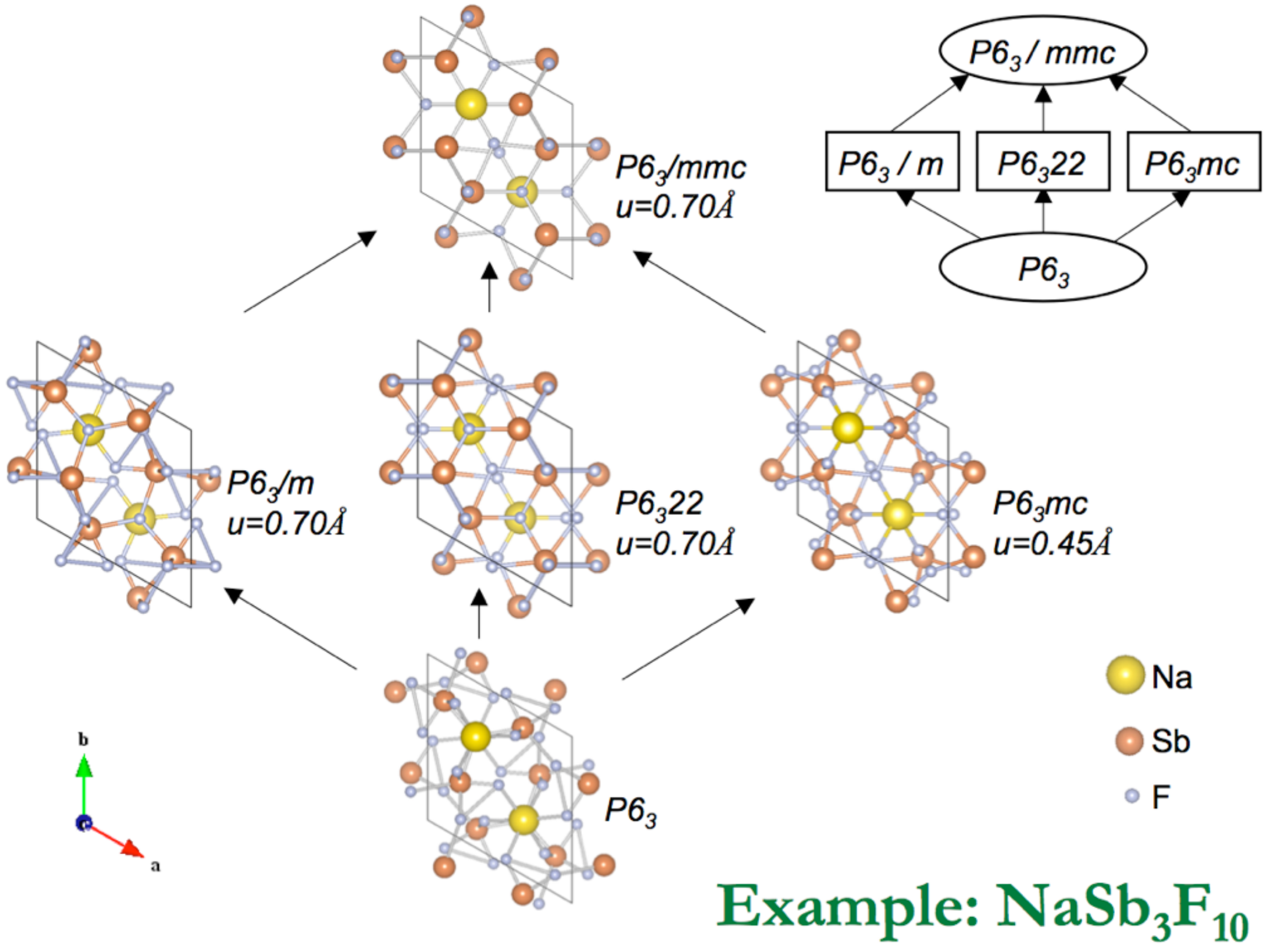
3# Supergroup $P6_3mc$ (186): a,b,c ; 0,0,0 and index 2

Displacements:

Atom	Idealized Coordinates	u_x	u_y	u_z	|u|
Sb1	(0.8297, 0.1703, 0.2500)	0.054000	0.054000	0.000000	0.4474
Na1	(0.3333, 0.6667, 0.1670)	0.000000	0.000000	0.000000	0.0000
F1	(0.1965, 0.3930, 0.9940)	0.007500	0.000000	0.000000	0.0621
F2	(0.1145, 0.2290, 0.3400)	-0.003500	0.000000	0.000000	0.0290
F3	(0.0350, 0.5175, 0.2810)	0.000000	-0.026500	0.000000	0.2196
F4	(0.6667, 0.3333, 0.2450)	0.000000	0.000000	0.000000	0.0000

Problem 3.15

SOLUTION



Example: $NaSb_3F_{10}$

Problem 3.16

The compound Nd_4GeO_8 is reported to have polar $Pmc2_1$ symmetry (Doklady Akademii Nauk SSSR (1978) 241, 353-356).

(i) Show using *PSEUDO* (option 1) that this structure can be considered a small distortion of a *Cmcm* structure.

(ii) Using *SUBGROUPGRAPH* show the graph of maximal subgroups connecting the two symmetries.

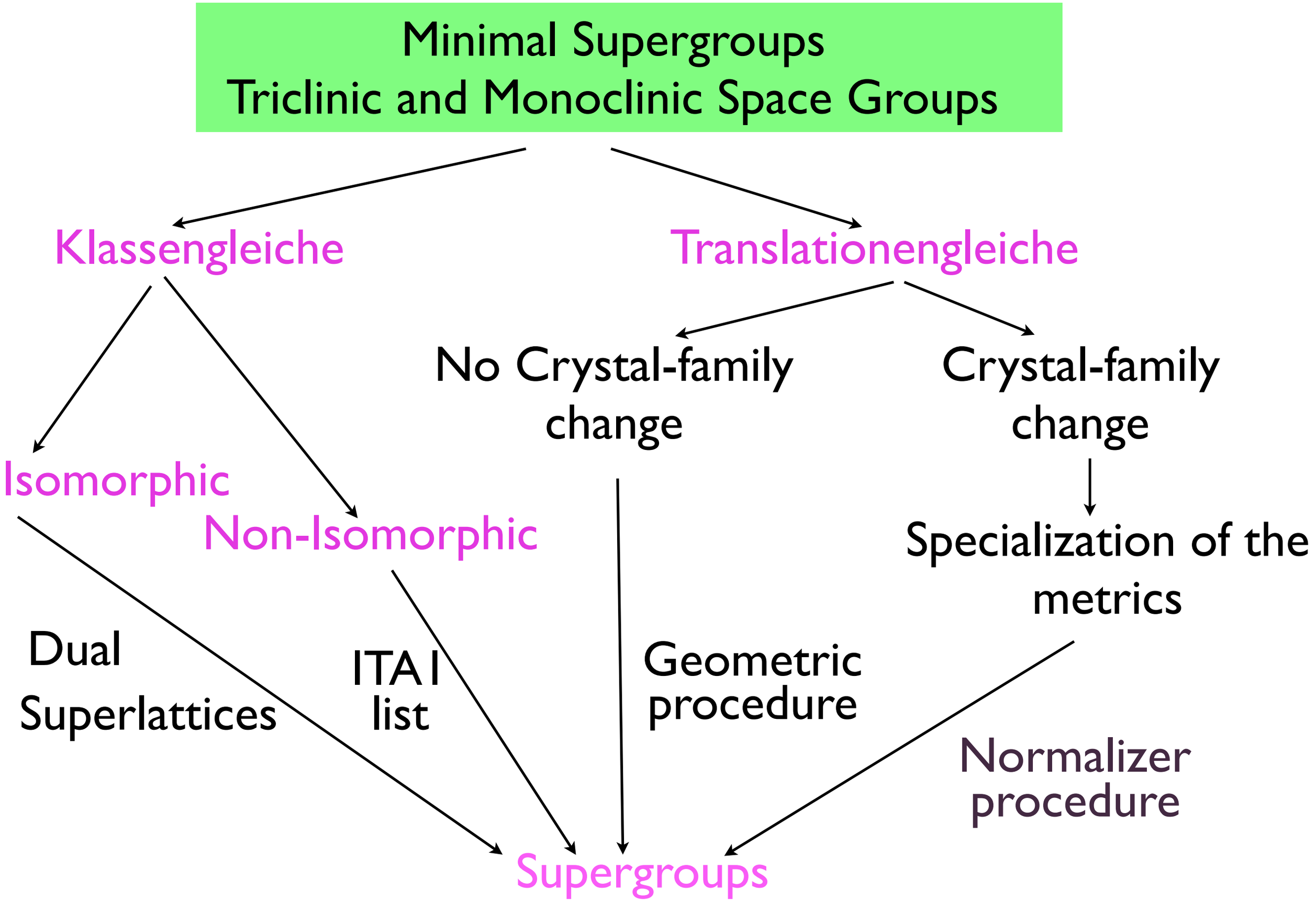
(iii) Using again *PSEUDO* (option 3) obtain the atomic displacements relating the two structures.

Problem 3.17

According to a structural model for $Ca_2Ge_7O_{16}$ published in Doklady Akademii Nauk SSSR (1979) 245, 110-113, the symmetry group of the compound is *Pba2*.

Using *PSEUDO*, demonstrate that this structure differs from a tetragonal one with space group *P-4b2*, by atomic displacements which are practically negligible or within experimental accuracy, so that in fact this structure file should be considered incorrect, being a case of "overlooked symmetry".

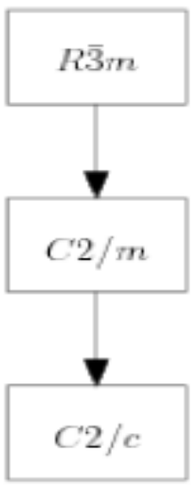
Problem: Minimal t-supergroups for monoclinic and triclinic groups



Problem 3.18(a) Lead phosphate phase transition

Lead phosphate $Pb_3(PO_4)_2$ shows a phase transition from a paraelastic high-temperature phase with symmetry R-3m (No.166) to a ferroelastic phase of symmetry C2/c (No.15).

Using the structure data of the low-symmetry monoclinic phase given in the *ExerciseData* file (Problem 6a) analyze its structural pseudosymmetry with respect to the symmetry group of the high-symmetry phase. Using the program COMPSTRU evaluate the difference between the experimentally determined R-3m structure and the idealized high-symmetry structure proposed by PSEUDO.



Hint:

For the analysis of the pseudosymmetry of the monoclinic structure, use a combination of Option 1 and Option 4 of PSEUDO

Problem 3.18

SOLUTION

Option 1: Search of structural pseudosymmetry stepwise 'climbing' via minimal supergroups

Formulae: Pb3(PO4)2

Structure data [in CIF format]

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

Initial Structure (LS):

```
15
13.80 5.691 9.42 90 102.3 90
7
O     1    8f    0.643 0.030 0.392
O     2    8f    0.634 0.464 0.374
O     3    8f    0.642 0.280 0.612
O     4    8f    0.491 0.222 0.420
P     1    8f    0.599 0.241 0.447
Pb    1    4e    0 0.291 0.25
Pb    2    8f    0.317 0.309 0.352
```

Select supergroups type for pseudosymmetry search.

1. Minimal supergroups — ☉ ☐ [Show only indices in supergroups table]
2. Supergroups with k-index — ○ **ik**: 1
3. Specify supergroup transformation — ○ **G**: 221

Flagged pseudosymmetry of $Pb_3(SO_4)_2$ with respect to C2/m (12)

Select minimal supergroups of space group *C2/c* (15)

The next step is to select the supergroups which the pseudosymmetry should be searched for. Each supergroup in the table can be selected by marking the corresponding checkbox.

Select/Unselect all: ☐

No. #	Select	HM Symb.	IT Numb.	Index	Index i_k	Transformation (P,p)	Transformed Cell	Wyckoff Positions Splitting Consid
1	☑	*C2/m*	012	2	2	**a,b,2c** ; 0,0,0	13.8000 5.6910 4.7100 90.00 102.30 90.00	This transformation is **valid** under Wycko conditions. Details..
2	☑	*C2/m*	012	2	2	**a,b,a+2c** ; 1/4,1/4,0	13.8000 5.6910 9.1455 90.00 149.79 90.00	This transformation is **valid** under Wycko conditions. Details..

Summary search results

Pseudosymmetry search among minimal supergroups.

Case #	Supergroup G	Index i	Index i_k	(P,p)	Tr. Matrix	Δ_{max}	u_{max}
1	*C2/m* (012)	2	2	**a,b,2c** ; 0,0,0	[1 0 0] [0] [0 1 0] [0] [0 0 2] [0]	>tol	-
	C2/m (012)	2	2	**a,b,a+2c** ; 1/4,1/4,0	[1 0 1] [1/4] [0 1 0] [1/4] [0 0 2] [0]	0.6715	0.3358

Option 3: Pseudosymmetry search for structures of monoclinic symmetry

Formulae: Pb3(PO4)2

Structure data [in CIF format]: Examinar…

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

```
12
13.8000 5.6910 9.1455 90.00 149.79 90.00
6
O       1       8j      0.271500        0.283000        0.766000
O       3       4i      0.504000        0.500000        0.224000
O       4       4i      0.161000        0.500000        0.840000
P       1       4i      0.296000        0.500000        0.894000
Pb      1       2c      0.500000        0.500000        0.500000
Pb      2       4i      0.919000        0.500000        0.704000
```

Select supergroups type for pseudosymmetry search.

1. Minimal supergroups ○ ☐ [Show only indices in supergroups table]
2. Supergroups with k-index ○ i_k: 1
3. Specify supergroup transformation ○ **G:** 221

Transf. Matrix (in option 3 only)

	Rotational part			Origin Shift
	1	0	0	0
	0	1	0	0
	0	0	1	0

4. [*] Lattice Pseudosymmetry with minimal supergroups ◉ **Ang. Tol (in degrees)** 10

Lattice pseudosymmetry

Please, select one the possible metrics:

No. #	Select	Latt.	Idealized/Transformed cell	Transformation matrix P	Strain	Tol.
1	⊙	hR	5.5662 5.5662 20.2270 90.00 90.00 120.00 5.5027 5.5027 20.2270 89.27 90.73 117.72	[1/3 1 −2/3] [−1/3 1 2/3] [2/3 0 −1/3]	0.01135	2.371

Note: $(a\ b\ c)_G = (a\ b\ c)_H\ P$

Possible minimal supergroups

Possible lattices: hR

No. #	Select	HM Symb.	IT Numb.	Latt.	Index
1	⊙	*P2/m*	10	mP	2
2	○	*Cmcm*	63	oC	2
3	○	*Cmce*	64	oC	2
4	○	*Cmmm*	65	oC	2
5	○	*Cmme*	67	oC	2
6	○	*Fmmm*	69	oF	2
7	○	*Immm*	71	oI	2
8	○	*Ibam*	72	oI	2
9	○	*Imma*	74	oI	2
10	○	*I4/m*	87	tI	2
11	○	*C2/m*	12	mC	2
12	○	*C2/m*	12	mC	3
13	○	*C2/m*	12	mC	5
14	○	*C2/m*	12	mC	7
15	○	*P*-31*m*	162	hP	3
16	○	*P*-3*m*1	164	hP	3
17	○	*R*-3*m*	166	hR	3

Show

Structural pseudosymmetry: R-3m(166)> C2/m(12)

[i]=3, u_{max}=0.064

Summary search results

Pseudosymmetry search among minimal supergroups within the specialized normalizer and compatible with possible high symmetry lattices

Case #	Supergroup G	Index i	Index i_k	(P,p)	Tr. Matrix	Δ_{max}	u_{max}
1	*R*-3*m* (166)	3	1	**1/3a-1/3b+2/3c,a+b,-2/3a+2/3b-1/3c** ; 0,0,0	[1/3 1 -2/3] [0] [-1/3 1 2/3] [0] [2/3 0 -1/3] [0]	0.1233	0.0640
2	*R*-3*m* (166)	3	1	**1/3a-1/3b+2/3c,a+b,-2/3a+2/3b-1/3c** ; 1/6,-1/6,1/3	[1/3 1 -2/3] [1/6] [-1/3 1 2/3] [-1/6] [2/3 0 -1/3] [1/3]	>tol	-

Idealized structure data

Idealized structure (supergroup setting):

```
166
5.5027 5.5027 20.2270 89.27 90.73 117.72
O       1       18h     0.851722        0.703444        0.926444
O       4       6c      0.000000        1.000000        0.827334
P       1       6c      0.000000        1.000000        0.899334
Pb      1       3b      0.333333        0.666667        0.166667
Pb      2       6c      0.333333        0.666666        0.378000
```

lattice parameters:
not symmetrized

Comparison between the idealized 'Pseudo' R-3m structure and the experimental one

Structure Data [in CIF format]

Examinar...

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

Structure 1

```
166
5.56 5.56 20.39 90 90 120
5
Pb 1   3a    0        0        0
Pb 2   6c    0        0        0.2126
P  1   6c    0        0        0.4021
O  1   6c    0        0        0.329
O  2   18h   0.181 -0.181   0.096
```

Structure Data [in CIF format]

Examinar...

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

Structure 2

```
166
5.5027 5.5027 20.2270 89.27 90.73 117.72
5
O        1        18h     0.851722        0.703444        0.926444
O        4        6c      0.000000        1.000000        0.827334
P        1        6c      0.000000        1.000000        0.899334
Pb       1        3b      0.333333        0.666667        0.166667
Pb       2        6c      0.333333        0.666666        0.378000
```

Enter the maximum distance allowed between the paired atoms: 1 Å

Enter the allowed tolerance (a b c α β γ): .5 .5 .5 5 5 5

Example COMPSTRU: $Pb_3(PO_4)_2$

Experimental data

```
166
5.56 5.56 20.39 90 90 120
5
Pb      1       3a      0.000000        0.000000        0.000000
Pb      2       6c      0.000000        0.000000        0.212600
P       1       6c      0.000000        0.000000        0.402100
O       1       6c      0.000000        0.000000        0.329000
O       2       18h     0.181000        0.819000        0.096000
```

Idealized 'Pseudo' data

```
166
5.5027 5.5027 20.2270 89.27 90.73 117.72
5
O       1       18h     0.851722        0.703444        0.926444
O       4       6c      0.000000        0.000000        0.827334
P       1       6c      0.000000        0.000000        0.899334
Pb      1       3b      0.333333        0.666667        0.166667
Pb      2       6c      0.333333        0.666666        0.378000
```

Evaluation of the structure similarity

S	$d_{max.}$ (Å)	$d_{av.}$ (Å)	Δ
0.0116	0.0707	0.0400	0.008

structural descriptor

$\Delta = 0.008$

affine normalizer

d_{max}=0.07 Å

maximal displacement

Most similar configuration

```
166
5.502700 5.502700 20.226999 89.269997 90.730003 117.720001
5
O       1       18h     0.185055        0.814945        0.093111
O       4       6c      0.000000        0.000000        0.327334
P       1       6c      0.000000        0.000000        0.399334
Pb      1       3a      0.000000        0.000000        0.000000
Pb      2       6c      0.000000        0.000000        0.211333
```

WP		Atom	Atomic Displacements			
			u_x	u_y	u_z	|u|
3a	(0,0,0)	Pb1	0.0000	0.0000	0.0000	0.0000
6c	(0,0,z)	Pb2	0.0000	0.0000	-0.0013	0.0258
6c	(0,0,z)	P1	0.0000	0.0000	-0.0028	0.0564
6c	(0,0,z)	O1	0.0000	0.0000	-0.0017	0.0340
18h	(x,-x,z)	O2	0.0041	-0.0041	-0.0029	0.0707

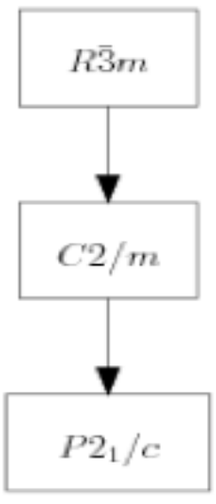
Atomic coordinates differences: along variable parameters

Problem 3.18(b)

Lead vanadate phase transition

Lead phosphate $Pb_3(VO_4)_2$ shows a phase transition from a paraelastic high-temperature phase with symmetry R-3m (No.166) to a ferroelastic phase of symmetry $P2_1/c$ (No.14).

Using the structure data of the low-symmetry monoclinic phase given in the *ExerciseData* file (Problem 6b) analyse its structural pseudosymmetry with respect to the symmetry group of the high-symmetry phase. Using the program COMPSTRU evaluate the difference between the experimentally determined R-3m structure and the idealized high-symmetry structure proposed by PSEUDO.



Hint:

For the analysis of the pseudosymmetry of the monoclinic structure, use a combination of Option 1 and Option 4 of PSEUDO