CRYSTALLOGRAPHY ONLINE Workshop

on the use and applications of the structural and magnetic tools of the

BILBAO CRYSTALLOGRAPHIC SERVER

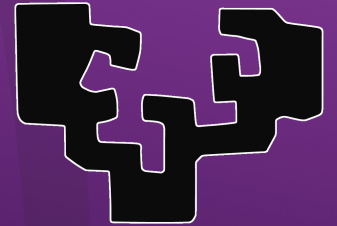**Leioa,   27 June -1 July 2022**

Pseudosymmetry

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UPV EHU

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DEFINITION OF THE PROBLEM

- Relation between two structures belonging to the same space group

  COMPSTRU

- Relation between two structures related by group-subgroup relations

  STRUCTURE RELATIONS

- But what if we have just the low symmetry (distorted) structure?..

DISTORTION

Initial (low symmetry) structure (distorted structure): H (Space Group: $\mathcal{H}$)

Prototype (high symmetry) structure: G (Space Group: $\mathcal{G}$)

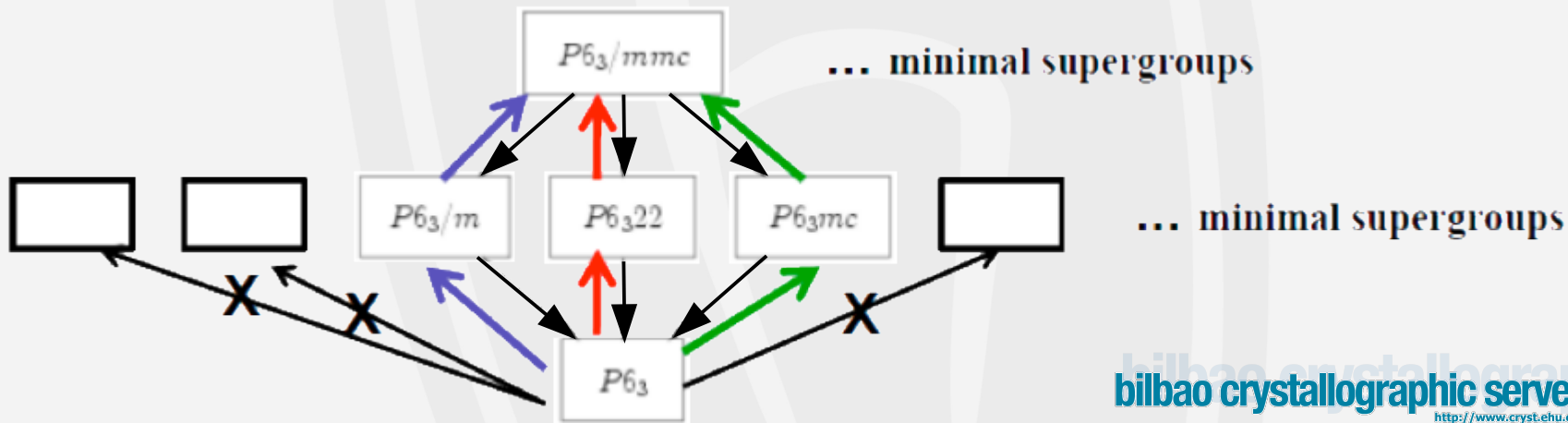$$H = G + \text{small (symmetry-breaking) distortion}$$

THE CHAIN RULE

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

A minimal supergroup is a supergroup of a given group such that there are no intermediate groups between them.

THE CHAIN RULE

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

$$\mathcal{H} < \mathcal{G} \rightarrow \mathcal{H} < \mathcal{Z}_1 < \mathcal{Z}_2 < \cdots < \mathcal{G}$$
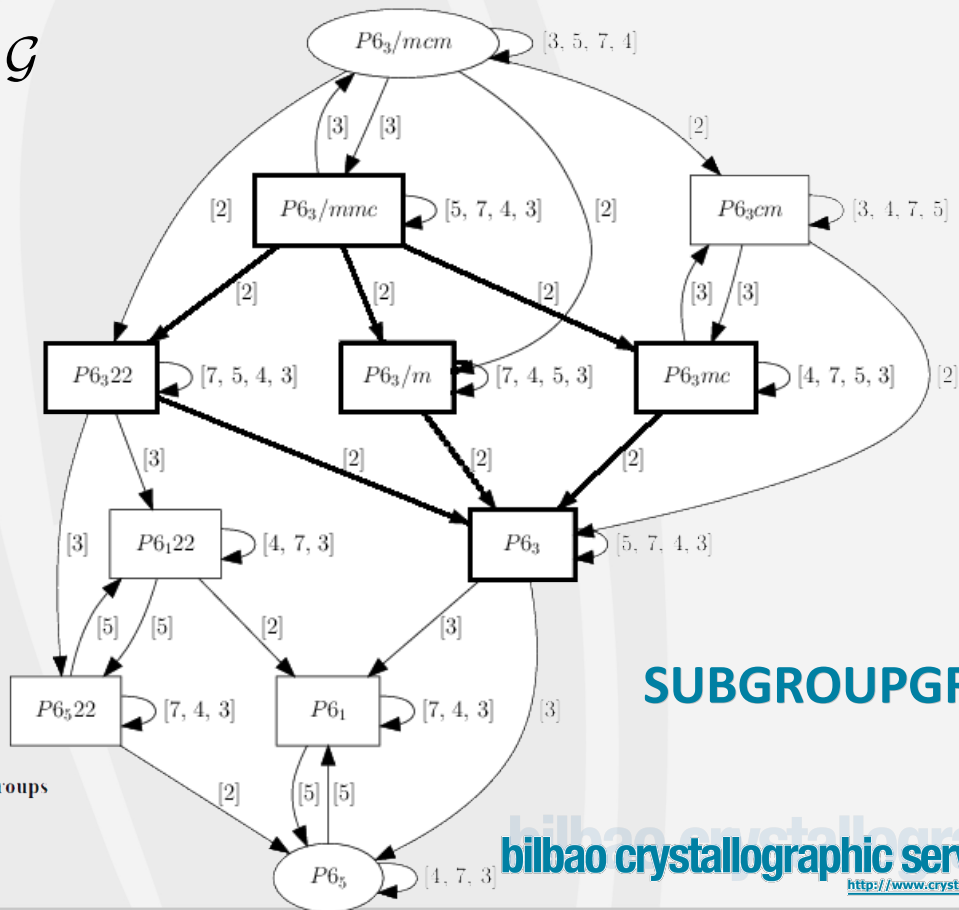
THE CHAIN RULE

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

A minimal supergroup is a supergroup of a given group such that there are no intermediate groups between them, in other words, the index relating the supergroup to the group must be a prime number
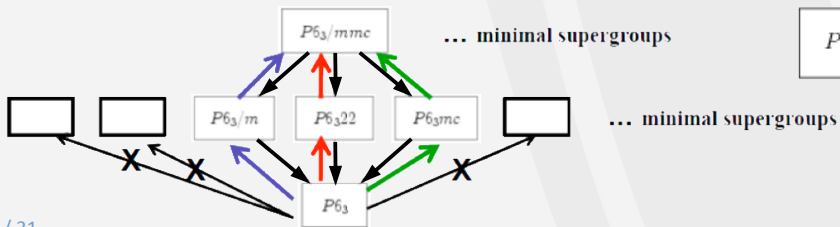
THE CHAIN RULE

$$\mathcal{H} < \mathcal{G} \rightarrow \mathcal{H} < \mathcal{Z}_1 < \mathcal{Z}_2 < \cdots < \mathcal{G}$$

P6₃/mcm (#193) – P6₅ (#170)
[without index specified]

SUBGROUPGRAPH

THE CHAIN RULE

$$\mathcal{H} < \mathcal{G} \rightarrow \mathcal{H} < \mathcal{Z}_1 < \mathcal{Z}_2 < \cdots < \mathcal{G}$$

P6$_3$/mcm (#193) – P6$_5$ (#170)
[without index specified]

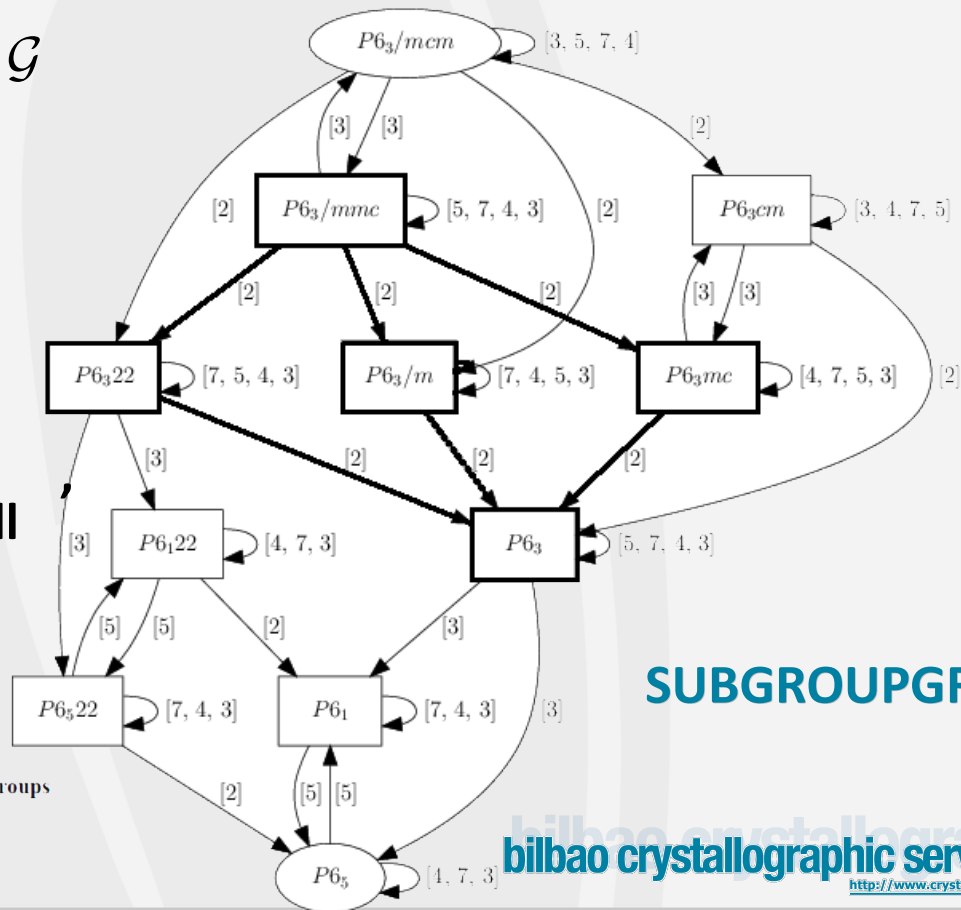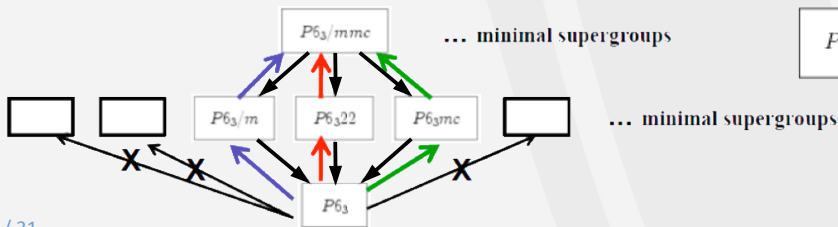**If a structure of symmetry $\mathcal{H}$ is pseudosymmetric for a supergroup $\mathcal{G}$, it will be pseudosymmetric for all intermediate subgroups $\mathcal{Z}_i$**

SUBGROUPGRAPH

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THE STRATEGY

- Obtain the list of minimal supergroups
  (along with transformation information)

  - <u>For each transformation related to the candidate supergroup:</u>

    - Check Wyckoff positions compatibility

    - Check lattice compatibility with the space group setting

    - Analyze the lattice deformation

    - Analyze the atomic displacement field

Initial low-symmetry phase	(Low-symmetry phase)$_{High}$	Idealized high-symmetry phase
H	$(H)_{\mathcal{G}}$	G

OBTAINING THE MINIMAL SUPERGROUPS

Please, enter the sequential number of group as given in *International Tables for Crystallography*, Vol. A or choose it :

$P4mm$

99

NOTE: the program uses the default choice for the group setting.

Show minimal supergroups

N	Transformation matrix	Coset representatives	Wyckoff Splitting	More...
1	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & t \end{pmatrix}$	(x, y, z) (x+1/2, y+1/2, z+1/2)	WP splitting	Full cosets

Wyckoff Positions Splitting for group - subgroup pair *I4mm*(107)>*P4mm*(99)

N		HM symbol	ITA number	Index	Type	Subgroup data
○	1	*P4/mmm*	123	2	t	transformation...
○	2	*P4/nmm*	129	2	t	transformation...
●	3	*I4mm*	107	2	k	transformation...
○	4	*P4mm*	99	3	k	transformation...
○	5	*P4mm*	99	2	k	transformation...

show

No	Wyckoff position(s)		
	Group	Subgroup	More...
1	16e	8g 8g	Relations
2	8d	4e 4f	Relations
3	8c	4d 4d	Relations
4	4b	2c 2c	Relations
5	2a	1a 1b	Relations

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THE RECOVERY OF THE "MISSING" SYMMETRIES

$$\mathcal{G} = \mathcal{H} + g_2\mathcal{H} + g_3\mathcal{H} + \cdots + g_m\mathcal{H}$$

Please, enter the sequential numbers of group and subgroup as given in International Tables for Crystallography, Vol. A:

Enter supergroup number (G) or choose it: 107

Enter subgroup number (H) or choose it: 99

Please, define the transformation that relates the group and the subgroup bases.

	Linear part			Origin Shift
Enter transformation matrix :	1	0	0	0
	0	1	0	0
	0	0	1	0

Decomposition: left ●   right ○   left (hermann) ○

Show Coset Decomposition

Left coset decomposition of the group *I4mm* (No. 107) with respect to the subgroup *P4mm* (No. 99)

G = H + g₁H + g₂H + ... + gₙH

The transformation matrix that relates the basis of the supergroup G=*I4mm* (No. 107) with that of the subgroup H=*P4mm* (No. 99) is:

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

The cosets in the decomposition of G with respect to H (in the basis of H) are given below:
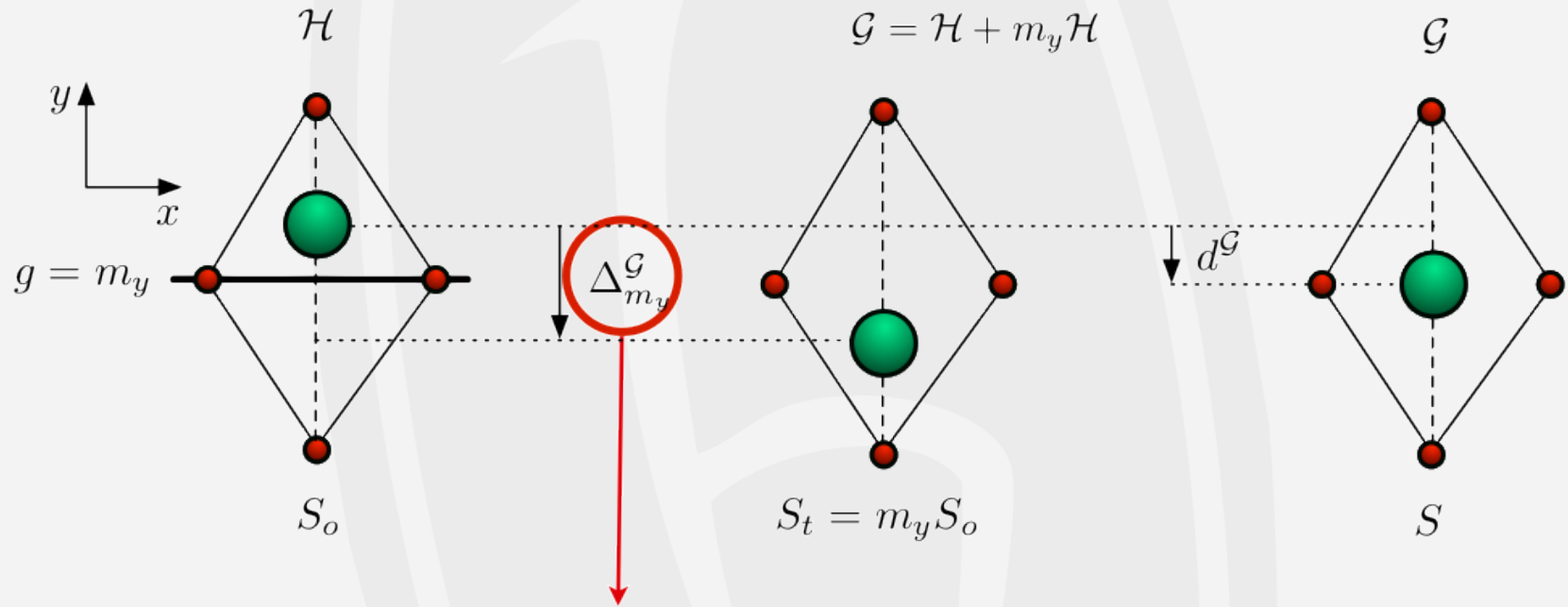
Coset 1:

```
(x,y,z)
(-x,-y,z)
(-y,x,z)
(y,-x,z)
(x,-y,z)
(-x,y,z)
(-y,-x,z)
(y,x,z)
```

Coset 2:

```
(x+1/2,y+1/2,z+1/2)
(-x+1/2,-y+1/2,z+1/2)
(-y+1/2,x+1/2,z+1/2)
(y+1/2,-x+1/2,z+1/2)
(x+1/2,-y+1/2,z+1/2)
(-x+1/2,y+1/2,z+1/2)
(-y+1/2,-x+1/2,z+1/2)
(y+1/2,x+1/2,z+1/2)
```
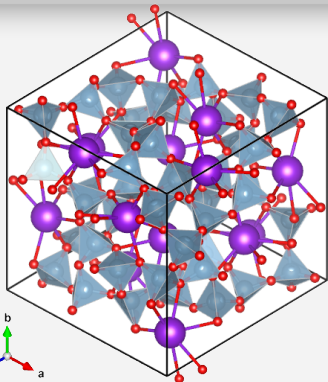
DETERMINATION OF THE "UNDISTORTED" POSITIONS

Maximal distance between all compatible atom pairings

KAlSi$_2$O$_6$

KAlSi$_2$O$_6$ (Leucite) | I4$_1$/a (#88)

```
88
13.05476 13.05476 13.75182 90. 90. 90.
13
K  1 16f 0.3659 0.3637 0.1169
Al 1 16f 0.0574 0.3969 0.1665
#Si 1 16f 0.0574 0.3969 0.1665
Al 2 16f 0.1675 0.6116 0.1287
#Si 2 16f 0.1675 0.6116 0.1287
Al 3 16f 0.3930 0.6420 0.0862
#Si 3 16f 0.3930 0.6420 0.0862
O 1 16f 0.1324 0.3141 0.1099
O 2 16f 0.0908 0.5112 0.1308
O 3 16f 0.1461 0.6808 0.2278
O 4 16f 0.1331 0.6851 0.0348
O 5 16f 0.2889 0.5756 0.1204
O 6 16f 0.4836 0.6172 0.1673
```

Palmer, D. C., Dove, M. T., Ibberson, R. M., & Powell, B. M. (1997). Structural behavior, crystal chemistry, and phase transitions in substituted leucite: High-resolution neutron powder diffraction studies. American Mineralogist, 82(1-2), 16-29.

PSEUDO

Formulae

Structure data
[in CIF format] **HINT:** [The option for a given filename is preferential]

Choose File No file chosen

```
88
13.05476 13.05476 13.75182 90. 90. 90.
10
K   1   16f   0.365900 0.363700 0.116900
Al  1   16f   0.057400 0.396900 0.166500
Al  2   16f   0.167500 0.611600 0.128700
Al  3   16f   0.393000 0.642000 0.086200
O   1   16f   0.132400 0.314100 0.109900
O   2   16f   0.090800 0.511200 0.130800
O   3   16f   0.146100 0.680800 0.227800
O   4   16f   0.133100 0.685100 0.034800
O   5   16f   0.288900 0.575600 0.120400
O   6   16f   0.483600 0.617200 0.167300
```

Initial Structure (LS)

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]

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

○ ⚠ For monoclinic and triclinic structures: previous check of lattice pseudosymmetry   Ang. Tol (in degrees) [5] [*]
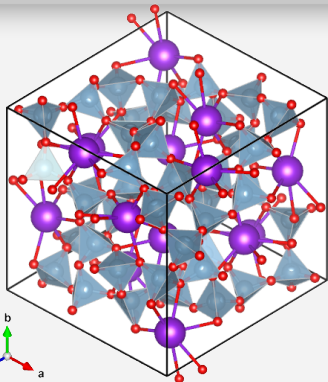
[*] Only for triclinics and monoclinics.

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

Maximum Δ: [2]

Show

PSEUDO

$KAlSi_2O_6$

$KAlSi_2O_6$ (Leucite) | $I4_1/a$ (#88)

```
88
13.05476 13.05476 13.75182 90. 90. 90.
13
K  1 16f 0.3659 0.3637 0.1169
Al 1 16f 0.0574 0.3969 0.1665
#Si 1 16f 0.0574 0.3969 0.1665
Al 2 16f 0.1675 0.6116 0.1287
#Si 2 16f 0.1675 0.6116 0.1287
Al 3 16f 0.3930 0.6420 0.0862
#Si 3 16f 0.3930 0.6420 0.0862
O 1 16f 0.1324 0.3141 0.1099
O 2 16f 0.0908 0.5112 0.1308
O 3 16f 0.1461 0.6808 0.2278
O 4 16f 0.1331 0.6851 0.0348
O 5 16f 0.2889 0.5756 0.1204
O 6 16f 0.4836 0.6172 0.1673
```

Palmer, D. C., Dove, M. T., Ibberson, R. M., & Powell, B. M. (1997). Structural behavior, crystal chemistry, and phase transitions in substituted leucite: High-resolution neutron powder diffraction studies. American Mineralogist, 82(1-2), 16-29.
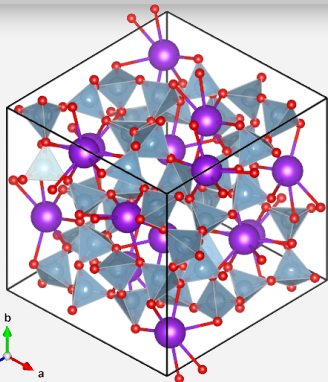
Select minimal supergroups of space group $I4_1/a$ (88)

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	☑	$P4_2/n$	086	2	2	a-b,a+b,2c ; 0,0,0	9.2311 9.2311 6.8759 90.00 90.00 90.00	This transformation is **valid** under Wyckoff Splitting conditions. Details..
2	☐	$I4_1/a$	088	3	3	a,b,3c ; 1/2,0,0	13.0548 13.0548 4.5839 90.00 90.00 90.00	This transformation is **invalid** under Wyckoff Splitting criteria. Details..
3	☐	$I4_1/a$	088	5	5	a,b,5c ; 0,0,0	13.0548 13.0548 2.7504 90.00 90.00 90.00	This transformation is **invalid** under Wyckoff Splitting criteria. Details..

7	☐	$I4_1/a$	088	9	9	3a,3b,c ; 1/2,0,0	4.3516 4.3516 13.7518 90.00 90.00 90.00	This transformation is **invalid** under Wyckoff Splitting criteria. Details..
8	☐	$I4_1/a$	088	9	9	a,b,9c ; 1,0,0	13.0548 13.0548 1.5280 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 >2.0Å]	This transformation is **invalid** under Wyckoff Splitting criteria. Details..
9	☑	$I4_1/amd$	141	2	1	a,b,c ; 0,1/2,0	13.0548 13.0548 13.7518 90.00 90.00 90.00	This transformation is **valid** under Wyckoff Splitting conditions. Details..
10	☑	$I4_1/acd$	142	2	1	a,b,c ; 0,1/2,0	13.0548 13.0548 13.7518 90.00 90.00 90.00	This transformation is **valid** under Wyckoff Splitting conditions. Details..

PSEUDO

KAlSi$_2$O$_6$

KAlSi$_2$O$_6$ (Leucite)| I4$_1$/a (#88)

```
88
13.05476 13.05476 13.75182 90. 90. 90.
13
K   1 16f 0.3659 0.3637 0.1169
Al 1 16f 0.0574 0.3969 0.1665
#Si 1 16f 0.0574 0.3969 0.1665
Al 2 16f 0.1675 0.6116 0.1287
#Si 2 16f 0.1675 0.6116 0.1287
Al 3 16f 0.3930 0.6420 0.0862
#Si 3 16f 0.3930 0.6420 0.0862
O 1 16f 0.1324 0.3141 0.1099
O 2 16f 0.0908 0.5112 0.1308
O 3 16f 0.1461 0.6808 0.2278
O 4 16f 0.1331 0.6851 0.0348
O 5 16f 0.2889 0.5756 0.1204
O 6 16f 0.4836 0.6172 0.1673
```

Palmer, D. C., Dove, M. T., Ibberson, R. M., & Powell, B. M. (1997). Structural behavior, crystal chemistry, and phase transitions in substituted leucite: High-resolution neutron powder diffraction studies. American Mineralogist, 82(1-2), 16-29.

Select minimal supergroups of space group I4$_1$/a (88)

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	☑	P4$_2$/n	086	2	2	a-b,a+b,2c ; 0,0,0	9.2321 9.2321 6.8758 90.00 90.00 90.00	This transformation is **valid** under Wyckoff Splitting conditions. Details..
2	☐	I4$_1$/a	088	3	3	a,b,3c ; 1/2,0,0	13.0548 13.0548 4.5839 90.00 90.00 90.00	This transformation is **invalid** under Wyckoff Splitting criteria. Details..
3	☐	I4$_1$/a	088	5	5	a,b,5c ; 0,0,0	13.0548 13.0548 2.7504 90.00 90.00 90.00	This transformation is **invalid** under Wyckoff Splitting criteria. Details..

PSEUDO

KAlSi$_2$O$_6$

Select minimal supergroups of space group $I4_1/a$ (88)

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	☑							
2	☐							
3	☐							

The Wyckoff Split Table for the transformation from $I4_1/a$ (#88) to $I4_1/a$ (#88)

No	Wyckoff position(s)	
	Group	**Subgroup**
1	4a	4a 8e
2	4b	4b 8e
3	8c	8d 16f
4	8d	8c 16f
5	8e	8e 8e 8e
6	16f	16f 16f 16f

with the transformation matrix:

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 3 \end{bmatrix} \begin{bmatrix} 1/2 \\ 0 \\ 0 \end{bmatrix}$$
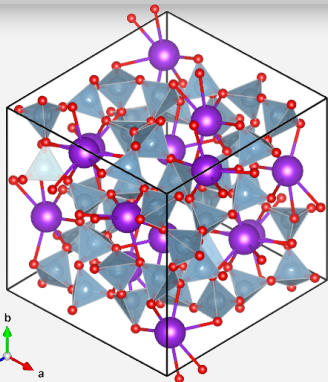
KAlSi$_2$O$_6$ (Leucite) | $I4_1/a$ (#88)

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88
13.05476 13.05476 13.75182 90. 90. 90.
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K   1 16f 0.3659 0.3637 0.1169
Al 1 16f 0.0574 0.3969 0.1665
#Si 1 16f 0.0574 0.3969 0.1665
Al 2 16f 0.1675 0.6116 0.1287
#Si 2 16f 0.1675 0.6116 0.1287
Al 3 16f 0.3930 0.6420 0.0862
#Si 3 16f 0.3930 0.6420 0.0862
O 1 16f 0.1324 0.3141 0.1099
O 2 16f 0.0908 0.5112 0.1308
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Palmer, D. C., Dove, M. T., Ibberson, R. M., & Powell, B. M. (1997). Structural behavior, crystal chemistry, and phase transitions in substituted leucite: High-resolution neutron powder diffraction studies. American Mineralogist, 82(1-2), 16-29.

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PSEUDO

KAlSi$_2$O$_6$

10	☑	I4$_1$/acd	142	2	1	a,b,c ; 0,1/2,0	13.0548 13.0548 13.7518 90.00 90.00 90.00	This transformation is **valid** under Wyckoff Splitting conditions. Details..

The Wyckoff Split Table for the transformation from I4$_1$/acd (#142) to I4$_1$/a (#88)

No	Wyckoff position(s)	
	Group	**Subgroup**
1	8a	4a 4b
2	8b	8e
3	16c	8c 8d
4	16d	8e 8e
5	16e	16f
6	16f	16f
7	32g	16f 16f

with the transformation matrix:

```
[    1     0     0 ] [     0]
[    0     1     0 ] [   1/2]
[    0     0     1 ] [     0]
```

KAlSi$_2$O$_6$ (Leucite) | I4$_1$/a (#88)

```
88
13.05476 13.05476 13.75182 90. 90. 90.
13
K  1 16f 0.3659 0.3637 0.1169
Al 1 16f 0.0574 0.3969 0.1665
#Si 1 16f 0.0574 0.3969 0.1665
Al 2 16f 0.1675 0.6116 0.1287
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Palmer, D. C., Dove, M. T., Ibberson, R. M., & Powell, B. M. (1997). Structural behavior, crystal chemistry, and phase transitions in substituted leucite: High-resolution neutron powder diffraction studies. American Mineralogist, 82(1-2), 16-29.

This transformation is valid under the Wyckoff Splittings Criteria

Species : Al Wyckoff Positions :f,f,f

WP(#142)		WP(#88)	# additional atoms	
g	=>	f,f,f + -1f	(-16) [-3:1]
(3/2)g	=>	f,f,f	---
3f	=>	f,f,f	---
3e	=>	f,f,f	---

Species : K Wyckoff Positions :f

WP(#142)		WP(#88)	# additional atoms	
(1/2)g	=>	f	---
f	=>	f	---
e	=>	f	---
g	=>	f + f	(16) [1:1]

Species : O Wyckoff Positions :f,f,f,f,f,f

WP(#142)		WP(#88)	# additional atoms	
3g	=>	f,f,f,f,f,f	---
6f	=>	f,f,f,f,f,f	---
6e	=>	f,f,f,f,f,f	---

PSEUDO

$KAlSi_2O_6$

$KAlSi_2O_6$ (Leucite) | $I4_1/a$ (#88)

```
88
13.05476 13.05476 13.75182 90. 90. 90.
13
K  1 16f 0.3659 0.3637 0.1169
Al 1 16f 0.0574 0.3969 0.1665
#Si 1 16f 0.0574 0.3969 0.1665
Al 2 16f 0.1675 0.6116 0.1287
#Si 2 16f 0.1675 0.6116 0.1287
Al 3 16f 0.3930 0.6420 0.0862
#Si 3 16f 0.3930 0.6420 0.0862
O 1 16f 0.1324 0.3141 0.1099
O 2 16f 0.0908 0.5112 0.1308
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O 4 16f 0.1331 0.6851 0.0348
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```

Palmer, D. C., Dove, M. T., Ibberson, R. M., & Powell, B. M. (1997). Structural behavior, crystal chemistry, and phase transitions in substituted leucite: High-resolution neutron powder diffraction studies. American Mineralogist, 82(1-2), 16-29.

Select minimal supergroups of space group $I4_1/a$ (88)

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	☑	$P4_2/n$	086	2	2	a-b,a+b,2c ; 0,0,0	9.2311 9.2311 6.8759 90.00 90.00 90.00	This transformation is **valid** under Wyckoff Splitting conditions. Details..
2	☐	$I4_1/a$	088	3	3	a,b,3c ; 1/2,0,0	13.0548 13.0548 4.5839 90.00 90.00 90.00	This transformation is **invalid** under Wyckoff Splitting criteria. Details..
3	☐	$I4_1/a$	088	5	5	a,b,5c ; 0,0,0	13.0548 13.0548 2.7504 90.00 90.00 90.00	This transformation is **invalid** under Wyckoff Splitting criteria. Details..

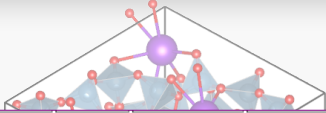| 7 | ☐ | $I4_1/a$ | 088 | 9 | 9 | 3a,3b,c ; 1/2,0,0 | 4.3516 4.3516 13.7518 90.00 90.00 90.00 | This transformation is **invalid** under Wyckoff Splitting criteria. Details.. |
8	☐	$I4_1/a$	088	9	9	a,b,9c ; 1,0,0	13.0548 13.0548 1.5280 90.00 90.00 90.00 **Lattice parameters don't comply** [Threshold: 0.5Å for a,b,c ; 10° for α,β,γ & lengths must be >2.0Å]	This transformation is **invalid** under Wyckoff Splitting criteria. Details..
9	☑	$I4_1/amd$	141	2	1	a,b,c ; 0,1/2,0	13.0548 13.0548 13.7518 90.00 90.00 90.00	This transformation is **valid** under Wyckoff Splitting conditions. Details..
10	☑	$I4_1/acd$	142	2	1	a,b,c ; 0,1/2,0	13.0548 13.0548 13.7518 90.00 90.00 90.00	This transformation is **valid** under Wyckoff Splitting conditions. Details..

KAlSi$_2$O$_6$

Case #	Supergroup G	Index i	Index i$_k$	(P,p)	Tr. Matrix	Δ$_{max}$	u$_{max}$
7	☐	*Fd-3c*	228	3	1	1/2a-1/2b,1/2a+1/2b,c ; 0,0,0		

18.4623 18.4623 13.7518 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 >2.0Å]

This transformation is **invalid** under Wyckoff Splitting criteria.
Details..

| 8 | ☑ | *Ia-3d* | 230 | 3 | 1 | a,b,c ; 0,0,0 |

13.0548 13.0548 13.7518 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 >2.0Å]

This transformation is **valid** under Wyckoff Splitting conditions.
Details..

| 9 | ☑ | *Ia-3d* | 230 | 3 | 1 | a,b,c ; 0,0,1/2 |

13.0548 13.0548 13.7518 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 >2.0Å]

This transformation is **valid** under Wyckoff Splitting conditions.
Details..

88
13.05476 13.05476 13.75
13
K 1 16f 0.3659 0.3637
Al 1 16f 0.0574 0.3969
#Si 1 16f 0.0574 0.3969
Al 2 16f 0.1675 0.6116
#Si 2 16f 0.1675 0.6116
Al 3 16f 0.3930 0.6420
#Si 3 16f 0.3930 0.6420
O 1 16f 0.1324 0.3141 0
O 2 16f 0.0908 0.5112 0
O 3 16f 0.1461 0.6808 0
O 4 16f 0.1331 0.6851 0
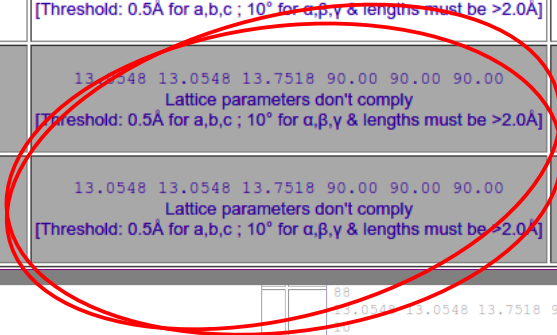O 5 16f 0.2889 0.5756 0
O 6 16f 0.4836 0.6172 0

Palmer, D. C., Dove, M. T., Ibberso
Structural behavior, crystal chemi
substituted leucite: High-resolutio
studies. American Mineralogist, 8

Displacements:

Atom	Idealized Coordinates	u$_x$	u$_y$	u$_z$	|u|
K1	(0.3761, 0.3739, 0.1250)	-0.010200	-0.010200	-0.008100	0.2188
Al1	(0.0827, 0.3769, 0.1652)	-0.025300	0.019950	0.001350	0.4210
Al2	(0.1530, 0.5971, 0.1250)	0.014550	0.014550	0.003700	0.2734
Al3	(0.3730, 0.6673, 0.0848)	0.019950	-0.025300	0.001350	0.4210
O1	(0.1326, 0.2903, 0.0963)	-0.000200	0.023850	0.013600	0.3632
O2	(0.1326, 0.4861, 0.1302)	-0.041800	0.025050	0.000600	0.6362
O3	(0.1055, 0.6488, 0.2215)	0.040600	0.031950	0.006300	0.6800
O4	(0.1011, 0.6445, 0.0285)	0.031950	0.040600	0.006300	0.6800
O5	(0.2638, 0.6174, 0.1198)	0.025050	-0.041800	0.000600	0.6362
O6	(0.4597, 0.6174, 0.1537)	0.023850	-0.000200	0.013600	0.3632

NOTE: u$_x$, u$_y$ and u$_z$ are given in relative units. |u| is the absolute displacement given in Å

88
13.0548 13.0548 13.7518 90.00 90.00 90.00
6
K   1   16f   0.376100   0.373900   0.125000
Al   1   16f   0.082700   0.376950   0.165150
Al   2   16f   0.152950   0.597050   0.125000
Al   3   16f   0.373050   0.667300   0.084850
O   1   16f   0.132600   0.290250   0.096300
O   2   16f   0.132600   0.486150   0.130200
O   3   16f   0.105500   0.648850   0.221500
O   4   16f   0.101150   0.644500   0.028500
O   5   16f   0.263850   0.617400   0.119800
O   6   16f   0.459750   0.617400   0.153700

Idealized structure (supergroup setting):

142
13.0548 13.0548 13.7518 90.00 90.00 90.00
6
K   1   16f   0.376100   0.873900   0.125000
Al   1   32g   0.082700   0.876950   0.165150
Al   2   16f   0.152950   0.097050   0.125000
O   1   32g   0.132600   0.790250   0.096300
O   2   32g   0.132600   0.986150   0.130200
O   3   32g   0.105500   0.148850   0.221500

Continue to search for pseudosymmetry with this structure (#142) | Visualize this structure | CIF File

KAlSi$_2$O$_6$

Case #	Supergroup G	Index i	Index i$_k$	(P,p)	Tr. Matrix			Δ_{max}	u$_{max}$
1	Ia-3d (230)	3	1	a,b,c ; 0,0,0	[1 0 0] [0] [0 1 0] [0] [0 0 1] [0]			>tol	-
2	Ia-3d (230)	3	1	a,b,c ; 0,0,1/2	[1 0 0] [0] [0 1 0] [0] [0 0 1] [1/2]			0.4805	0.2989

88
13.05476 13.05476 13.75
13
K 1 16f 0.3659 0.3637
Al 1 16f 0.0574 0.3969
#Si 1 16f 0.0574 0.3969
Al 2 16f 0.1675 0.6116
#Si 2 16f 0.1675 0.6116
Al 3 16f 0.3930 0.6420
#Si 3 16f 0.3930 0.6420
O 1 16f 0.1324 0.3141
O 2 16f 0.0908 0.5112
O 3 16f 0.1461 0.6808
O 4 16f 0.1331 0.6851
O 5 16f 0.2889 0.5756
O 6 16f 0.4836 0.6172

Palmer, D. C., Dove, M. T., Ibberso...
Structural behavior, crystal chemi...
substituted leucite: High-resoluti...
studies. American Mineralogist, 8...

NOTE: u$_x$,

Displacements:

Atom	Idealized
K1	(0.3761, 0
Al1	(0.0827, 0
Al2	(0.1530, 0
Al3	(0.3730, 0
O1	(0.1326, 0
O2	(0.1326, 0
O3	(0.1055, 0
O4	(0.1011, 0
O5	(0.2638, 0
O6	(0.4597, 0

Idealized structure (subgroup setting):

```
142
13.0548 13.0548 13.7518 90.00 90.00 90.00
6
K   1    16f    0.375000    0.875000    0.125000
Al  1    32g    0.088200    0.875000    0.161800
Al  2    16f    0.161800    0.088200    0.125000
O   1    32g    0.133750    0.777533    0.106400
O   2    32g    0.143600    0.972467    0.116250
O   3    32g    0.106400    0.133750    0.222467
```

Idealized structure (supergroup setting):

```
230
13.0548 13.0548 13.7518 90.00 90.00 90.00
3
K   1    16b    0.375000    0.875000    0.625000
Al  1    48g    0.088200    0.875000    0.661800
O   1    96h    0.133750    0.777533    0.606400
```

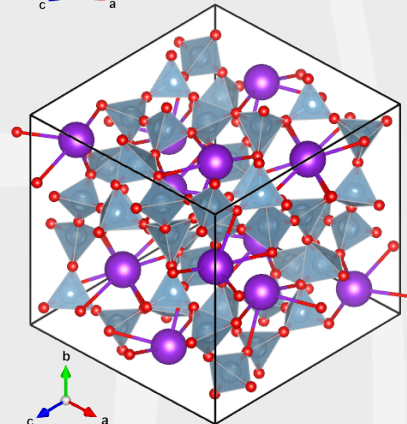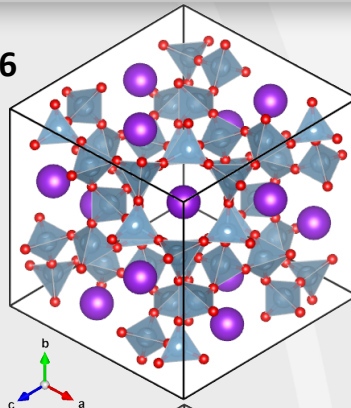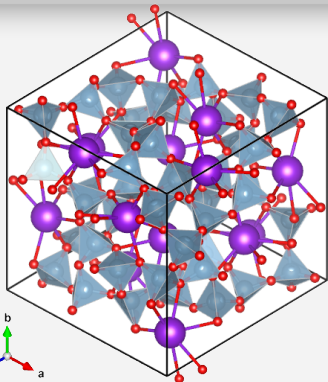[Continue to search for pseudosymmetry with this structure (#230)] [Visualize this structure] [CIF File]

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

structure (supergroup setting):

```
8.0548 13.7518 90.00 90.00 90.00
```

16f	0.376100	0.873900	0.125000
32g	0.082700	0.876950	0.165150
16f	0.152950	0.097050	0.125000
32g	0.132600	0.790250	0.096300
32g	0.132600	0.986150	0.130200
32g	0.105500	0.148850	0.221500

structure (supergroup setting):

```
13.0548 13.7518 90.00 90.00 90.00
```

16f	0.376100	0.373900	0.125000
16f	0.082700	0.376950	0.165150
16f	0.152950	0.597050	0.125000
16f	0.373050	0.667300	0.084850
16f	0.132600	0.290250	0.096300
16f	0.132600	0.486150	0.130200
16f	0.105500	0.648850	0.221500
16f	0.101150	0.644500	0.028500
16f	0.263850	0.617400	0.119800
16f	0.459750	0.617400	0.153700

[...o search for pseudosymmetry with this structure (#142)] [Visualize this structure] [CIF File]

KAlSi$_2$O$_6$

KAlSi$_2$O$_6$ (Leucite) | I4$_1$/a (#88)

```
88
13.05476 13.05476 13.75182 90. 90. 90.
13
K  1 16f 0.3659 0.3637 0.1169
Al 1 16f 0.0574 0.3969 0.1665
#Si 1 16f 0.0574 0.3969 0.1665
Al 2 16f 0.1675 0.6116 0.1287
#Si 2 16f 0.1675 0.6116 0.1287
Al 3 16f 0.3930 0.6420 0.0862
#Si 3 16f 0.3930 0.6420 0.0862
O 1 16f 0.1324 0.3141 0.1099
O 2 16f 0.0908 0.5112 0.1308
O 3 16f 0.1461 0.6808 0.2278
O 4 16f 0.1331 0.6851 0.0348
O 5 16f 0.2889 0.5756 0.1204
O 6 16f 0.4836 0.6172 0.1673
```

*Palmer, D. C., Dove, M. T., Ibberson, R. M., & Powell, B. M. (1997).
Structural behavior, crystal chemistry, and phase transitions in
substituted leucite: High-resolution neutron powder diffraction
studies. American Mineralogist, 82(1-2), 16-29.*

$Ia\bar{3}d(230)$
To root: a,b,c ; 0,1/2,1/2
To previous node: a,b,c,0,0,1/2
0.2989

$I4_1/acd(142)$
To root: a,b,c ; 0,1/2,0
To previous node: a,b,c,0,1/2,0
0.6800

$I4_1/a(88)$
To root: a,b,c ; 0,0,0
To previous node: a,b,c,0,0,0
0.0000

KAlSi$_2$O$_6$ | Ia$\bar{3}$d (#230)

```
230
13.0548 13.0548 13.7518 90.00 90.00
90.00
3
K  1 16b 0.375000 0.875000 0.625000
Al 1 48g 0.088200 0.875000 0.661800
O  1 96h 0.133750 0.777533 0.606400
```



```
142
13.0548 13.0548 13.7518 90.00 90.00
90.00
6
K  1 16f 0.376100 0.873900 0.125000
Al 1 32g 0.082700 0.876950 0.165150
Al 2 16f 0.152950 0.097050 0.125000
O  1 32g 0.132600 0.790250 0.096300
O  2 32g 0.132600 0.986150 0.130200
O  3 32g 0.105500 0.148850 0.221500
```
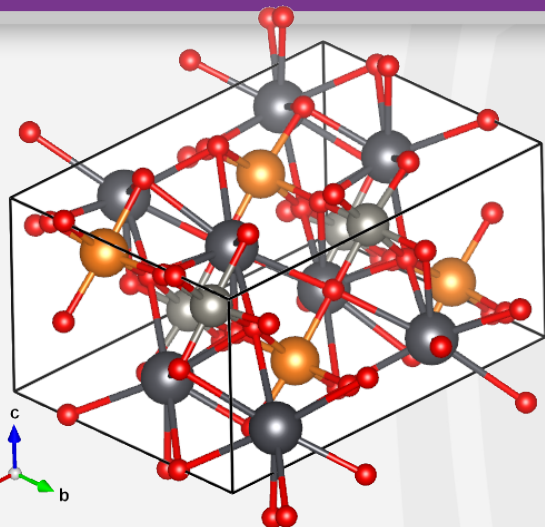
KAlSi$_2$O$_6$ | I4$_1$/acd (#142)

Pb_2MgWO_6

Analyze the structural pseudosymmetry of Pb_2MgWO_6 by searching of maximal pseudosymmetry stepwise 'climbing' via minimal supergroups

Pb_2MgWO_6 | Pnma (#62)

```
62
11.4059 7.9440 5.6866 90.00 90.00 90.00
8
Pb 1 8d 0.142200 0.003200 0.780400
Mg 1 4c 0.377200 0.250000 0.751900
W  1 4c 0.116100 0.250000 0.257700
O  1 8d 0.131400 0.490700 0.236500
O  2 4c 0.002700 0.250000 0.013300
O  3 4c 0.010300 0.250000 0.499100
O  4 4c 0.237000 0.250000 -0.015300
O  5 4c 0.249100 0.250000 0.474500
```

Baldinozzi, G., Sciau, P., Pinot, M., & Grebille, D. (1995). Crystal structure of the antiferroelectric perovskite Pb2MgWO6. Acta Crystallographica Section B: Structural Science, 51(5), 668-673.

bilbao crystallographic server
http://www.cryst.ehu.es

Pb_2MgWO_6

Analyze the structural pseudosymmetry of Pb_2MgWO_6 by searching of maximal pseudosymmetry stepwise 'climbing' via minimal supergroups
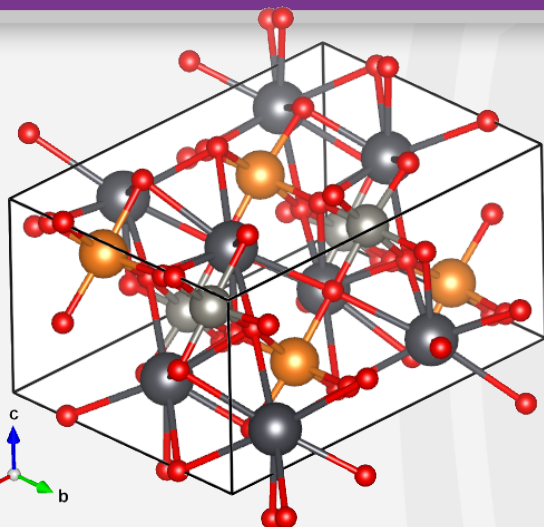

Pb_2MgWO_6| Pnma (#62)

```
62
11.4059 7.9440 5.6866 90.00 90.00 90.00
8
Pb 1 8d 0.142200 0.003200 0.780400
Mg 1 4c 0.377200 0.250000 0.751900
W  1 4c 0.116100 0.250000 0.257700
O  1 8d 0.131400 0.490700 0.236500
O  2 4c 0.002700 0.250000 0.013300
O  3 4c 0.010300 0.250000 0.499100
O  4 4c 0.237000 0.250000 -0.015300
O  5 4c 0.249100 0.250000 0.474500
```

Baldinozzi, G., Sciau, P., Pinot, M., & Grebille, D. (1995). Crystal structure of the antiferroelectric perovskite Pb2MgWO6. Acta Crystallographica Section B: Structural Science, 51(5), 668-673.

bilbao crystallographic server
http://www.cryst.ehu.es

Pb$_2$MgWO$_6$

Pb$_2$MgWO$_6$ | Pnma (#62)
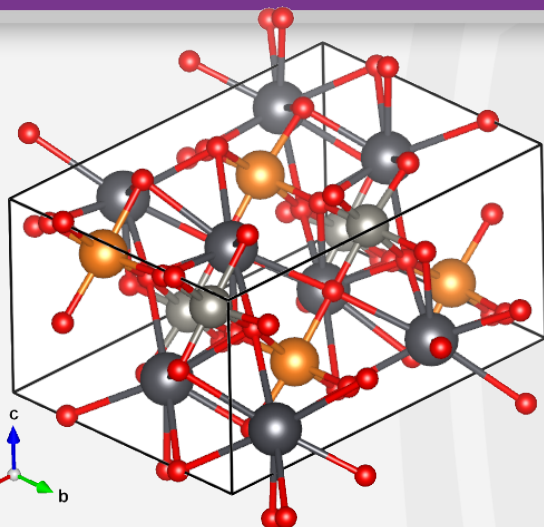
```
62
11.4059 7.9440 5.6866 90.00 90.00 90.00
8
Pb 1 8d 0.142200 0.003200 0.780400
Mg 1 4c 0.377200 0.250000 0.751900
W  1 4c 0.116100 0.250000 0.257700
O  1 8d 0.131400 0.490700 0.236500
O  2 4c 0.002700 0.250000 0.013300
O  3 4c 0.010300 0.250000 0.499100
O  4 4c 0.237000 0.250000 -0.015300
O  5 4c 0.249100 0.250000 0.474500
```

Baldinozzi, G., Sciau, P., Pinot, M., & Grebille, D. (1995). Crystal structure of the antiferroelectric perovskite Pb2MgWO6. Acta Crystallographica Section B: Structural Science, 51(5), 668-673.

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 >2.0Å]	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	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 >2.0Å]	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 >2.0Å]	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 >2.0Å]	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 >2.0Å]	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 >2.0Å]	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..
16	☑	Imma	074	2	2	a,b,c ; 0,0,0	11.4059 7.9440 5.6866 90.00 90.00 90.00	This transformation is **valid** under Wyckoff Splitting conditions. Details..

Pb₂MgWO₆

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

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

Pb₂MgWO₆ | Pnma (#62)

```
62
11.4059 7.9440 5.6866 90.00 90.00 90.00
8
Pb 1 8d 0.142200 0.003200 0.780400
Mg 1 4c 0.377200 0.250000 0.751900
W  1 4c 0.116100 0.250000 0.257700
O  1 8d 0.131400 0.490700 0.236500
O  2 4c 0.002700 0.250000 0.013300
O  3 4c 0.010300 0.250000 0.499100
O  4 4c 0.237000 0.250000 -0.015300
O  5 4c 0.249100 0.250000 0.474500
```

Baldinozzi, G., Sciau, P., Pinot, M., & Grebille, D. (1995). Crystal structure of the antiferroelectric perovskite Pb2MgWO6. Acta Crystallographica Section B: Structural Science, 51(5), 668-673.

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 : W   Wyckoff Positions :c

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

Pb$_2$MgWO$_6$

Pb$_2$MgWO$_6$ | Pnma (#62)

```
62
7.1940009576946601 5.6650 90.00090900 90.00
8
Pb 1 8d 0.003200 0.0803200402780400
Mg 1 4c 0.257000 0.09200000 0.751900
W  1 4c 0.002510 0.050000 0.257700
O  1 8d 0.191400 0.0369000303 4236500
O  2 4c 0.002700 0.0326000070 0.013300
O  3 4c 0.050000 0.090120000300 0.499100
O  4 4c 0.257000 0.0332600000 -0.015300
O  5 4c 0.239000 0.0752600000 0.474500
```
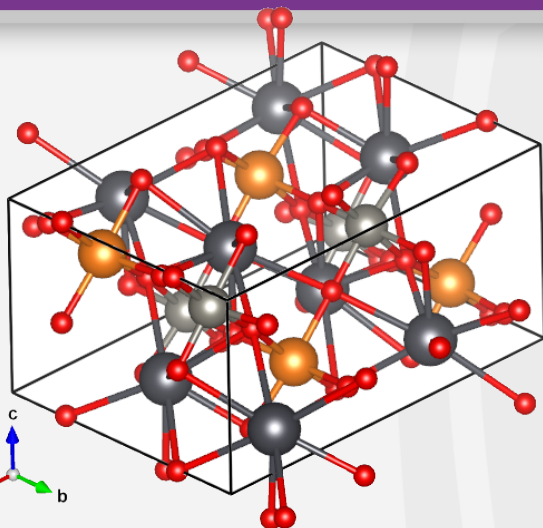
Baldinozzi, G., Sciau, P., Pinot, M., & Grebille, D. (1995). Crystal structure of the antiferroelectric perovskite Pb2MgWO6. Acta Crystallographica Section B: Structural Science, 51(5), 668-673.

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	-

Pb$_2$MgWO$_6$

Pb$_2$MgWO$_6$ | Pmmn (#69)

```
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
```

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

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

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
```

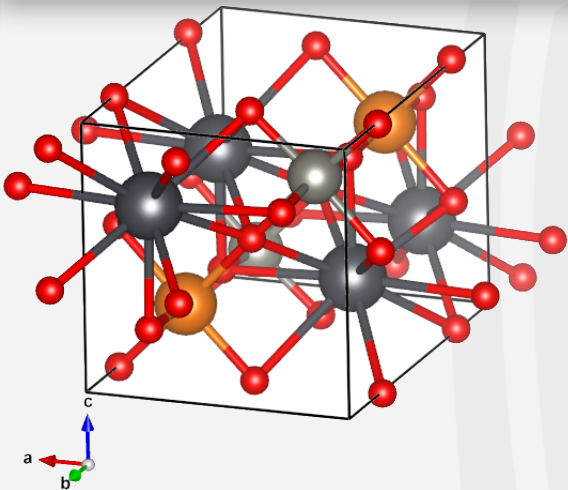[Continue to search for pseudosymmetry with this structure (#059)] [Visualize this structure] [CIF File]

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

Pb_2MgWO_6

Pb_2MgWO_6 | Pmmn (#69)

```
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
```

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

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):
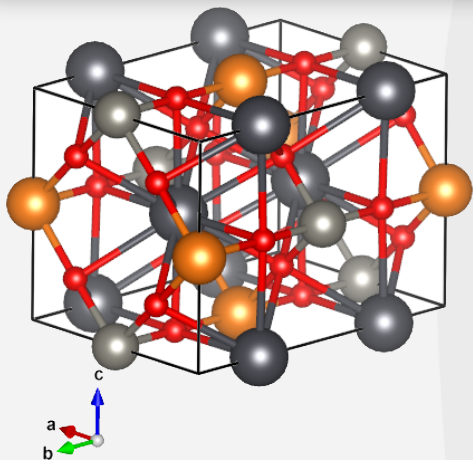
```
71
5.6866 7.9440 5.7030 90.00 90.00 90.00
5
Pb  1    4g     0.500000     0.253200    0.500000
Mg  1    2c     0.500000     0.500000    0.000000
W   1    2b     0.000000     0.500000    0.500000
O   1    4h     0.000000     0.740700    0.500000
O   2    8m     0.243900     0.500000    0.263450
```

Pb$_2$MgWO$_6$

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

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):

```
71
5.6866 7.9440 5.7030 90.00 90.00 90.00
5
Pb    1    4g    0.500000    0.253200    0.500000
Mg    1    2c    0.500000    0.500000    0.000000
W     1    2b    0.000000    0.500000    0.500000
O     1    4h    0.000000    0.740700    0.500000
O     2    8m    0.243900    0.500000    0.263450
```
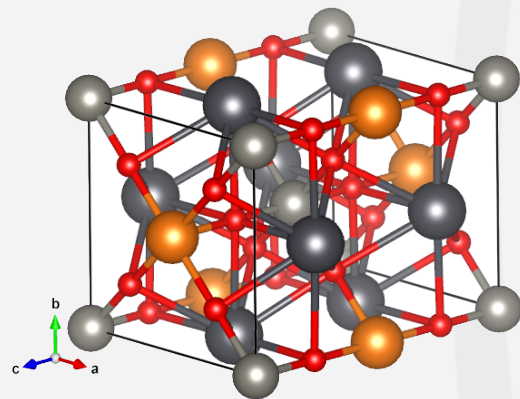
Pb$_2$MgWO$_6$ | Immm (#71)

```
71
5.6866 7.9440 5.7030 90.00 90.00 90.00
5
Pb 1 4g 0.500000 0.253200 0.500000
Mg 1 2c 0.500000 0.500000 0.000000
W  1 2b 0.000000 0.500000 0.500000
O  1 4h 0.000000 0.740700 0.500000
O  2 8m 0.243900 0.500000 0.263450
```

Pb$_2$MgWO$_6$

Case #	Supergroup G	Index i	Index i$_k$	(P,p)	Tr. Matrix		Δ$_{max}$	u$_{max}$
1	I4/mmm (139)	2	1	b,c,a ; 0,1/2,0	[0 0 1] [0] [1 0 0] [1/2] [0 1 0] [0]		0.0592	0.0296

Idealized structures

1# 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)	0.003675	0.000000	0.003675	0.0296

Idealized structure (supergroup setting):

```
139
5.7030 5.6866 7.9440 90.00 90.00 90.00
5
Pb      1      4d      0.500000      0.000000      0.250000
Mg      1      2b      0.000000      0.000000      0.500000
W       1      2a      0.500000      0.500000      0.500000
O       1      4e      0.500000      0.500000      0.740700
O       2      8h      0.259775      0.740225      0.500000
```
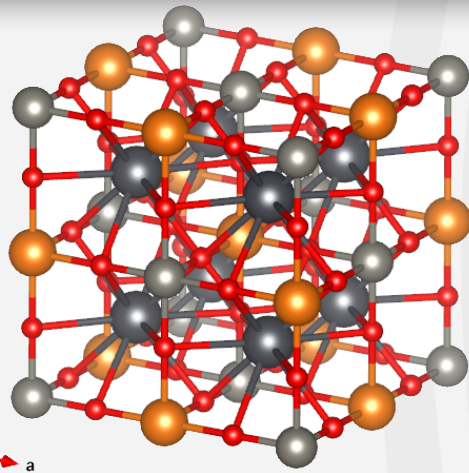
Pb$_2$MgWO$_6$ | I4/mmm (#139)

```
139
5.7030 5.6866 7.9440 90.00 90.00 90.00
5
Pb 1 4d 0.500000 0.000000 0.250000
Mg 1 2b 0.000000 0.000000 0.500000
W  1 2a 0.500000 0.500000 0.500000
O  1 4e 0.500000 0.500000 0.740700
O  2 8h 0.259775 0.740225 0.500000
```

Pb$_2$MgWO$_6$

Case #	Supergroup G	Index i	Index i$_k$	(P,p)	Tr. Matrix		Δ$_{max}$	u$_{max}$
1	Fm-3m (225)	3	1	1/2a-1/2b,1/2a+1/2b,c ; 0,0,0	[1/2 1/2 0] [0] [-1/2 1/2 0] [0] [0 0 1] [0]		0.0038	0.0025

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	0.000313	0.0025
O2	(0.2596, 0.7404, 0.5000)	0.000157	-0.000157	0.000000	0.0013

NOTE: u$_x$, u$_y$ and u$_z$ are given in relative units. |u| is the absolute displacement given in Å

Pb$_2$MgWO$_6$ | Fm-3m (#225)

```
225
8.0537 8.0537 7.9440 90.00 90.00 90.17
4
Pb 1  8c 0.250000 0.750000 0.250000
Mg 1  4b 0.000000 0.000000 0.500000
W  1  4a 0.500000 0.000000 0.500000
O  1 24e 0.500000 0.000000 0.740387
```

Idealized structure (supergroup setting):

```
225
8.0537 8.0537 7.9440 90.00 90.00 90.17
4
Pb     1      8c      0.250000      0.750000      0.250000
Mg     1      4b      0.000000      0.000000      0.500000
W      1      4a      0.500000      0.000000      0.500000
O      1      24e     0.500000      0.000000      0.740387
```
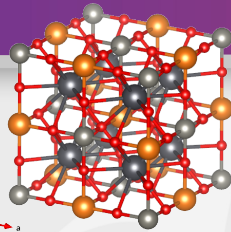
Pb$_2$MgWO$_6$

$$Fm\bar{3}m\,(225) \rightarrow Pnma\,(62)$$

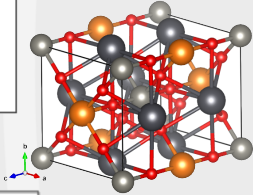$$P = a - b, c, -\frac{1}{2}a - \frac{1}{2}b;\ \frac{1}{2}, \frac{1}{4}, \frac{1}{4}$$

Fm$\bar{3}$m(225)
To root: a-b,c,-1/2a-1/2b ; 1/2,1/4,1/4
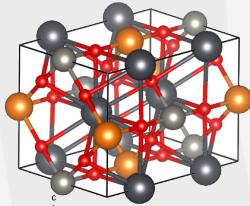To previous node: 1/2a-1/2b,1/2a+1/2b,c,0,0,0
0.0025

I4/mmm(139)
To root: 2a,c,-b ; 1/4,3/4,1/4
To previous node: b,c,a,0,1/2,0
0.0296

Immm(71)
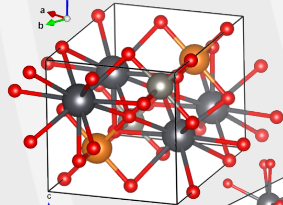To root: 2c,b,-a ; 1/4,1/4,1/4
To previous node: a,b,c,1/4,1/4,1/4
0.1962

Pmmn(59)
To root: 2c,b,-a ; 0,0,0
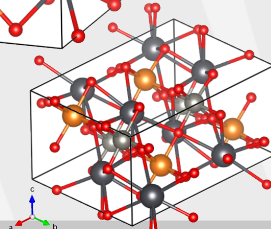To previous node: 2c,b,-a,0,0,0
0.1729

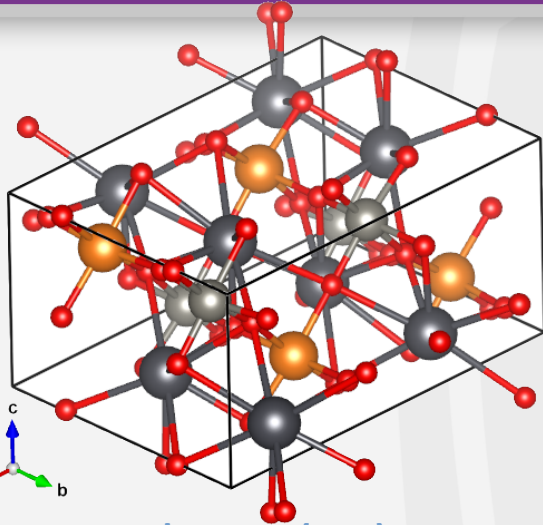Pnma(62)
To root: a,b,c ; 0,0,0
To previous node: a,b,c,0,0,0
0.0000

Pb₂MgWO₆

Analyze the structural pseudosymmetry of Pb₂MgWO₆ by searching of structural pseudosymmetry with respect to specific supergroup

Pb₂MgWO₆ | Pnma (#62)

```
62
11.4059 7.9440 5.6866 90.00 90.00 90.00
8
Pb 1 8d 0.142200 0.003200 0.780400
Mg 1 4c 0.377200 0.250000 0.751900
W  1 4c 0.116100 0.250000 0.257700
O  1 8d 0.131400 0.490700 0.236500
O  2 4c 0.002700 0.250000 0.013300
O  3 4c 0.010300 0.250000 0.499100
O  4 4c 0.237000 0.250000 -0.015300
O  5 4c 0.249100 0.250000 0.474500
```

Baldinozzi, G., Sciau, P., Pinot, M., & Grebille, D. (1995). Crystal structure of the antiferroelectric perovskite Pb2MgWO6. Acta Crystallographica Section B: Structural Science, 51(5), 668-673.

Pb$_2$MgWO$_6$

Analyze the structural pseudosymmetry of Pb$_2$MgWO$_6$ by searching of structural pseudosymmetry with respect to specific supergroup

Case #	Supergroup G	Index i	Index i$_k$	(P,p)	Tr. Matrix		Δ_{max}	u$_{max}$
1	Fm-3m (225)	24	4	a-b,c,-1/2a-1/2b ; 1/2,1/4,1/4	[1 0 -1/2] [-1 0 -1/2] [0 1 0]	[1/2] [1/4] [1/4]	0.5243	0.2627

Idealized structures

1# Supergroup Fm-3m (225): a-b,c,-1/2a-1/2b ; 1/2,1/4,1/4 and index 24

Displacements:

Atom	Idealized Coordinates	u$_x$	u$_y$	u$_z$	|u|
Pb1	(0.1250, 0.0000, 0.7500)	0.017200	0.003200	0.030400	0.2627
Mg1	(0.3750, 0.2500, 0.7500)	0.002200	0.000000	0.001900	0.0273
W1	(0.1250, 0.2500, 0.2500)	-0.008900	-0.000000	0.007700	0.1106
O1	(0.1250, 0.4904, 0.2500)	0.006400	0.000317	-0.013500	0.1060
O2	(0.0048, 0.2500, 0.0096)	-0.002108	0.000000	0.003683	0.0319
O3	(0.0048, 0.2500, 0.4904)	0.005492	0.000000	0.008717	0.0799
O4	(0.2452, 0.2500, 0.0096)	-0.008192	0.000000	-0.024917	0.1697
O5	(0.2452, 0.2500, 0.4904)	0.003908	0.000000	-0.015883	0.1007

NOTE: u$_x$, u$_y$ and u$_z$ are given in relative units. |u| is the absolute displacement

Pb$_2$MgWO$_6$| Pnma (#62)

```
62
11.4059 7.9440 5.6866 90.00 90.00 90.00
8
Pb 1 8d 0.142200 0.003200 0.780400
Mg 1 4c 0.377200 0.250000 0.751900
W  1 4c 0.116100 0.250000 0.257700
O  1 8d 0.131400 0.490700 0.236500
O  2 4c 0.002700 0.250000 0.013300
O  3 4c 0.010300 0.250000 0.499100
O  4 4c 0.237000 0.250000 -0.015300
O  5 4c 0.249100 0.250000 0.474500
```

Baldinozzi, G., Sciau, P., Pinot, M., & Grebille, D. (1995). Crystal structure of the antiferroelectric perovskite Pb2MgWO6. Acta Crystallographica Section B: Structural Science, 51(5), 668-673.

Pb$_2$MgWO$_6$| Fm-3m (#225)

```
225
8.0537 8.0537 7.9440 90.00 90.00 90.17
4
Pb 1  8c 0.250000 0.750000 0.250000
Mg 1  4b 0.000000 0.000000 0.500000
W  1  4a 0.500000 0.000000 0.500000
O  1 24e 0.500000 0.000000 0.740387
```

Idealized structure (supergroup setting):

```
225
8.0536 8.0536 7.9440 90.00 90.00 90.16
4
Pb     1     8c      0.250000      0.750000      0.250000
Mg     1     4b      0.500000      0.500000      0.500000
W      1     4a      0.500000      0.000000      0.500000
O      1    24e      0.500000      0.000000      0.740383
```
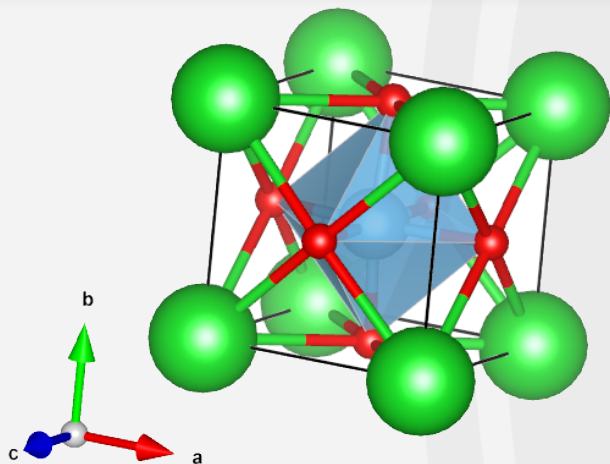
Baldinozzi, G., Sciau, P., & Buffat, P. A. (1993). Investigation of the orthorhombic structures of Pb2MgWO6 and Pb2CoWO6. Solid state communications, 86(9), 541-544.

BaTiO$_3$

General Position of the Group P4mm (No. 99)

BaTiO$_3$ | Pnma (#99)

```
99
3.999 3.999 4.02 90 90 90
4
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
```

No.	(x,y,z) form	Matrix form	Symmetry operation	
			ITA	Seitz $\mathbf{i}$
1	x,y,z	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	1	{ 1 | 0 }
2	-x,-y,z	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	2 0,0,z	{ 2$_{001}$ | 0 }
3	-y,x,z	$\begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	4$^+$ 0,0,z	{ 4$^+_{001}$ | 0 }
4	y,-x,z	$\begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	4$^-$ 0,0,z	{ 4$^-_{001}$ | 0 }
5	x,-y,z	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	m x,0,z	{ m$_{010}$ | 0 }
6	-x,y,z	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	m 0,y,z	{ m$_{100}$ | 0 }
7	-y,-x,z	$\begin{pmatrix} 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	m x,-x,z	{ m$_{110}$ | 0 }
8	y,x,z	$\begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	m x,x,z	{ m$_{1-10}$ | 0 }

bilbao crystallographic server

http://www.cryst.ehu.es

BaTiO$_3$

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	$P4/mmm$ (123)	2	1	a,b,c ; 0,0,0	[1 0 0] [0] [0 1 0] [0] [0 0 1] [0]			0.6432	0.3216

Idealized structures

1# Supergroup $P4/mmm$ (123): a,b,c ; 0,0,0 and index 2

Displacements:

Atom	Idealized Coordinates	u$_x$	u$_y$	u$_z$	|u|
Ba1	(0.0000, 0.0000, 0.0000)	0.000000	0.000000	0.000000	0.0000
Ti2	(0.5000, 0.5000, 0.5000)	0.000000	0.000000	-0.080000	0.3216
O3	(0.5000, 0.5000, 0.0000)	0.000000	0.000000	0.030000	0.1206
O4	(0.5000, 0.0000, 0.5000)	0.000000	0.000000	0.080000	0.3216

NOTE: u$_x$, u$_y$ and u$_z$ are given in relative units. |u| is the absolute displacement given in Å

Idealized structure (supergroup setting):

```
123
3.9990 3.9990 4.0200 90.00 90.00 90.00
4
Ba    1    1a    0.000000    0.000000    0.000000
Ti    2    1d    0.500000    0.500000    0.500000
O     3    1c    0.500000    0.500000    0.000000
O     4    2e    0.500000    0.000000    0.500000
```

BaTiO$_3$ | P4/mmm (#123)

```
123
3.9990 3.9990 4.0200 90.00 90.00 90.00
4
Ba 1 1a 0.000000 0.000000 0.000000
Ti 2 1d 0.500000 0.500000 0.500000
O  3 1c 0.500000 0.500000 0.000000
O  4 2e 0.500000 0.000000 0.500000
```

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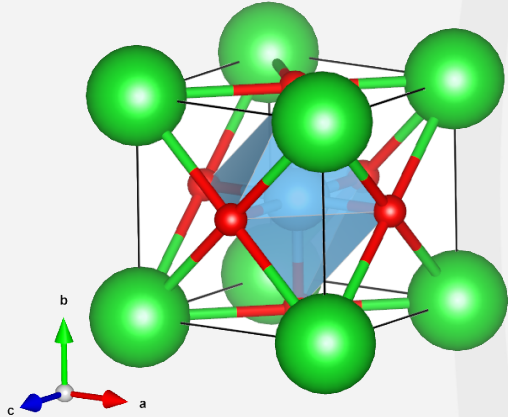
BaTiO$_3$ | P4/mmm (#123)

```
123
3.9990 3.9990 4.0200 90.00 90.00 90.00
4
Ba 1 1a 0.000000 0.000000 0.000000
Ti 2 1d 0.500000 0.500000 0.500000
O  3 1c 0.500000 0.500000 0.000000
O  4 2e 0.500000 0.000000 0.500000
```
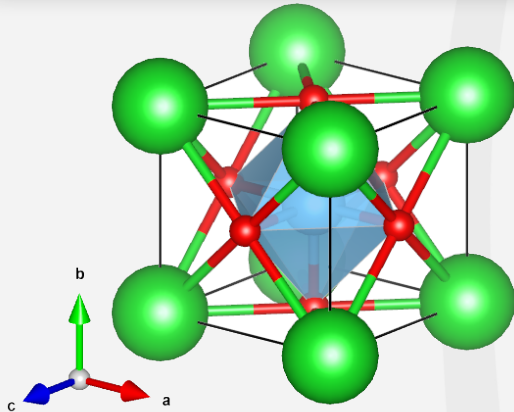
General Position of the Group P4/mmm (No. 123)

Click here to get the general position in text format

No.	(x,y,z) form	Matrix form	Symmetry operation ITA	Symmetry operation Seitz
1	x,y,z	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	1	{ 1 | 0 }
2	-x,-y,z	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	2 0,0,z	{ 2$_{001}$ | 0 }
3	-y,x,z	$\begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	4$^+$ 0,0,z	{ 4$^+_{001}$ | 0 }
4	y,-x,z	$\begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	4$^-$ 0,0,z	{ 4$^-_{001}$ | 0 }
5	-x,y,-z	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{pmatrix}$	2 0,y,0	{ 2$_{010}$ | 0 }
6	x,-y,-z	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{pmatrix}$	2 x,0,0	{ 2$_{100}$ | 0 }
7	y,x,-z	$\begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{pmatrix}$	2 x,x,0	{ 2$_{110}$ | 0 }
8	-y,-x,-z	$\begin{pmatrix} 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{pmatrix}$	2 x,-x,0	{ 2$_{1-10}$ | 0 }
9	-x,-y,-z	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{pmatrix}$	-1 0,0,0	{ -1 | 0 }
10	x,y,-z	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{pmatrix}$	m x,y,0	{ m$_{001}$ | 0 }
11	y,-x,-z	$\begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{pmatrix}$	-4$^+$ 0,0,z; 0,0,0	{ -4$^+_{001}$ | 0 }
12	-y,x,-z	$\begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{pmatrix}$	-4$^-$ 0,0,z; 0,0,0	{ -4$^-_{001}$ | 0 }
13	x,-y,z	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	m x,0,z	{ m$_{010}$ | 0 }
14	-x,y,z	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	m 0,y,z	{ m$_{100}$ | 0 }
15	-y,-x,z	$\begin{pmatrix} 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	m x,-x,z	{ m$_{110}$ | 0 }
16	y,x,z	$\begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	m x,x,z	{ m$_{1-10}$ | 0 }

BaTiO₃

BaTiO$_3$ | Pm$\overline{3}$m (#221)

```
221
3.9990 3.9990 4.0200 90.00 90.00 90.00
3
Ba 1 1a 0.000000 0.000000 0.000000
Ti 2 1b 0.500000 0.500000 0.500000
O  3 3c 0.500000 0.500000 0.000000
```

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	Pm-3m (221)	3	1	a,b,c ; 0,0,0	[1 0 0] [0] [0 1 0] [0] [0 0 1] [0]			0	0.0000

Idealized structures

1# Supergroup Pm-3m (221): a,b,c ; 0,0,0 and index 3

Displacements:

Atom	Idealized Coordinates	u$_x$	u$_y$	u$_z$	|u|
Ba1	(0.0000, 0.0000, 0.0000)	0.000000	0.000000	0.000000	0.0000
Ti2	(0.5000, 0.5000, 0.5000)	0.000000	0.000000	0.000000	0.0000
O3	(0.5000, 0.5000, 0.0000)	0.000000	0.000000	0.000000	0.0000
O4	(0.5000, 0.0000, 0.5000)	0.000000	0.000000	0.000000	0.0000

NOTE: u$_x$, u$_y$ and u$_z$ are given in relative units. |u| is the absolute displacement given in Å

Idealized structure (supergroup setting):

```
221
3.9990 3.9990 4.0200 90.00 90.00 90.00
3
Ba    1        1a      0.000000      0.000000      0.000000
Ti    2        1b      0.500000      0.500000      0.500000
O     3        3c      0.500000      0.500000      0.000000
```

BaTiO$_3$

(48 Symmetry Operations)

BaTiO$_3$ | Pm$\bar{3}$m (#221)

```
221
3.9990 3.9990 4.0200 90.00 90.00 90.00
3
Ba 1 1a 0.000000 0.000000 0.000000
Ti 2 1b 0.500000 0.500000 0.500000
O  3 3c 0.500000 0.500000 0.000000
```
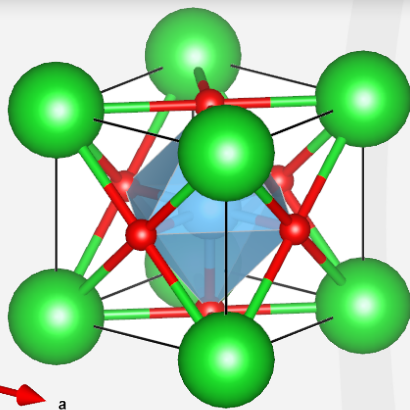
General Position of the Group Pm-3m (No. 221)

Click here to get the general position in text format

No.	(x,y,z) form	Matrix form	Symmetry operation	
			ITA	**Seitz**
1	x,y,z	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	1	{ 1 | 0 }
2	-x,-y,z	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	2 0,0,z	{ 2$_{001}$ | 0 }
3	-x,y,-z	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{pmatrix}$	2 0,y,0	{ 2$_{010}$ | 0 }
4	x,-y,-z	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{pmatrix}$	2 x,0,0	{ 2$_{100}$ | 0 }
5	z,x,y	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$	3$^+$ x,x,x	{ 3$^+_{111}$ | 0 }
6	z,-x,-y	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}$	3$^+$ -x,x,-x	{ 3$^+_{-11-1}$ | 0 }

22	z,-y,x	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$	2 x,0,x	{ 2$_{101}$ | 0 }
23	-z,y,x	$\begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$	4$^-$ 0,y,0	{ 4$^-_{010}$ | 0 }
24	-z,-y,-x	$\begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$	2 -x,0,x	{ 2$_{-101}$ | 0 }
25	-x,-y,-z	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{pmatrix}$	-1 0,0,0	{ -1 | 0 }
26	x,y,-z	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{pmatrix}$	m x,y,0	{ m$_{001}$ | 0 }
27	x,-y,z	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	m x,0,z	{ m$_{010}$ | 0 }
28	-x,y,z	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	m 0,y,z	{ m$_{100}$ | 0 }

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FERROELECTRICS (KNOWN)

Compound	$\mathcal{G}$	$[i]$	Δ_{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

FERROELECTRICS (POSSIBLE)

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

MYSQL + ICSD

SELECT *

FROM (

SELECT CONCAT(SGR," (#",sgrnumm,")") as SG, sgrnumm, STRUCT_FORM

FROM icsd

WHERE sgrnumm IN (1,3,4,5,6,7,8,9,25,26,27,28,29,30,31,32,33,34,35,36,37,38,39,40,41,42,43,44,45,46,75,76,77,78,79,80,99,100,101,102,103,104,105,106,107,108,109,110,143,144,145,146,156,157,158,159,160,161,168,169,170,171,172,173,183,184,185,186)

GROUP BY STRUCT_FORM

) AS A

INNER JOIN (

SELECT CONCAT(SGR," (#",sgrnumm,")") as SG, sgrnumm, STRUCT_FORM

FROM icsd

WHERE sgrnumm NOT IN (1,3,4,5,6,7,8,9,25,26,27,28,29,30,31,32,33,34,35,36,37,38,39,40,41,42,43,44,45,46,75,76,77,78,79,80,99,100,101,102,103,104,105,106,107,108,109,110,143,144,145,146,156,157,158,159,160,161,168,169,170,171,172,173,183,184,185,186)

GROUP BY STRUCT_FORM

) AS B

USING (STRUCT_FORM)

Acknowledgment

Most of this presentation is composed of adapting, rewriting & rearranging Mois Aroyo's and J. Manuel Perez Mato's past presentations & tutorials.

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Related BCS Tools

COSETS, MINSUP, SUBGROUPGRAPH

CELLTRAN, COMPSTRU, EQUIVSTRU, GENPOS, HERMANN,INDEX, MAXSUB, NORMALIZER, PSEUDO, STRAIN, STRCONVERT, STRUCTURE RELATIONS, SUBGROUPGRAPH, TRANSTRU, WPASSIGN, WYCKPOS, WYCKSETS, WYCKSPLIT