

***Comparison of crystal structures connected via group-subgroup relations***

Dr. Emre S. Tasci

Dept. Eng. Physics  
Hacettepe University, Ankara,  
Turkey

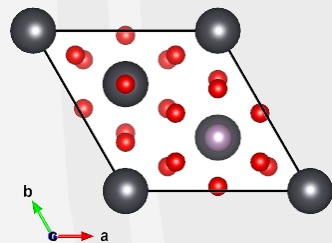
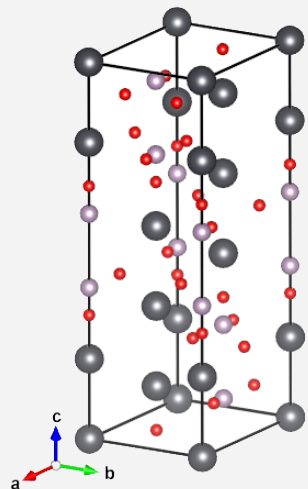


Mathematics and Computer Science for Materials  
Innovation: Crystal Lattice Classifications  
*Satellite of the 33<sup>rd</sup> European Crystallography Meeting  
5-9 September 2022, Liverpool Materials Innovation Factory, UK*



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<http://www.cryst.ehu.es>

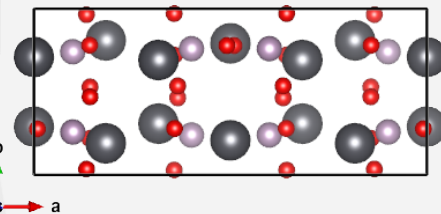
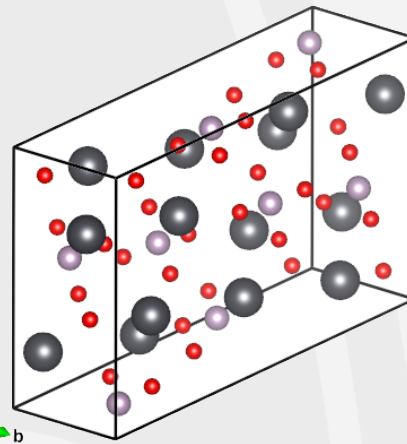
# SPOT THE DIFFERENCES SIMILARITIES



$\text{Pb}_3(\text{PO}_4)_2$  | R-3m (#166)

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 -0.181000 0.096000

Ng, H. N., & Calvo, C. (1975). Electron paramagnetic resonance and X-ray studies of the phase transformation in  $\text{Pb}_3\text{P}_2\text{O}_8$ . *Canadian Journal of Physics*, 53(1), 42-51.

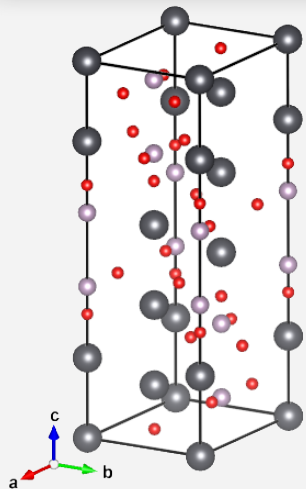


$\text{Pb}_3(\text{PO}_4)_2$  | C2/c (#15)

15  
 13.8 5.691 9.42 90. 102.3 90.  
 7  
 Pb 1 4e 0 0.291 0.25  
 Pb 2 8f 0.317 0.309 0.352  
 P 1 8f 0.599 0.241 0.447  
 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

Guimaraes, D. M. C. (1979). Ferroelastic transformations in lead orthophosphate and its structure as a function of temperature. *Acta Crystallographica Section A: Crystal Physics, Diffraction, Theoretical and General Crystallography*, 35(1), 108-114.

# PLAN OF ATTACK

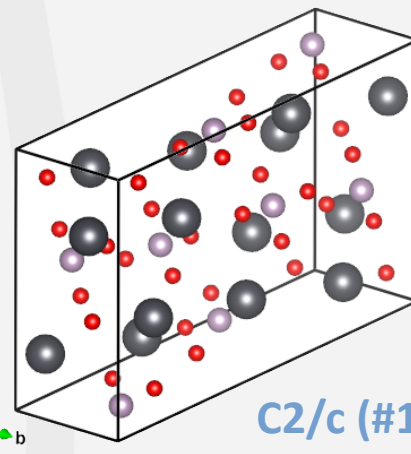


R-3m (#166)

*symmetry reduction*



*affine transformation*



C2/c (#15)

**bilbao crystallographic server**

<http://www.cryst.ehu.es>

# INDEX

$$\left. \begin{array}{l} f_{R\bar{3}m} = 3, \quad Z_{R\bar{3}m} = 3 \\ f_{C2/c} = 2, \quad Z_{C2/c} = 4 \end{array} \right\} i_L = \frac{f_{R\bar{3}m} \times Z_{C2/c}}{f_{C2/c} \times Z_{R\bar{3}m}} = 2 \quad \text{klassengleiche index}$$

$$\left. \begin{array}{l} |\text{PG}_{R\bar{3}m}| = |\bar{3}m| = 12 \\ |\text{PG}_{C2/c}| = |2/m| = 4 \end{array} \right\} i_P = \frac{|\text{PG}_{R\bar{3}m}|}{|\text{PG}_{C2/c}|} = 3 \quad \text{translationengleiche index}$$

$$i = i_L \times i_P = 2 \times 3 = 6$$

INDEX

INDEX

$$\left. \begin{array}{l} f_{R\bar{3}m} = 3, \quad Z_{R\bar{3}m} = 3 \\ f_{C2/c} = 2, \quad Z_{C2/c} = 4 \end{array} \right\} i_L = \frac{f_{R\bar{3}m} \times Z_{C2/c}}{f_{C2/c} \times Z_{R\bar{3}m}} = 2 \quad \text{klassengleiche index}$$

$$\left. \begin{array}{l} |PG_{R\bar{3}m}| = |\bar{3}m| = 12 \\ |PG_{C2/c}| = |2/m| = 4 \end{array} \right\} i_P = \frac{|PG_{R\bar{3}m}|}{|PG_{C2/c}|} = 3 \quad \text{translationengleiche index}$$

$$i = i_L \times i_P = 2 \times 3 = 6$$

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

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

• Option A: Introduce the formula units (conventional of the high and low symmetry structure.

The formula units (conventional) on the high symmetry structure:

The formula units (conventional) on the low symmetry structure:



**Index of a group-subgroup pair**

High symmetry Space Group:	$R\bar{3}m$ (No. 166) [hexagonal axes]
Low symmetry Space Group:	$C2/c$ (No. 15) [unique axis b]
$i_L$	2
$i_P$	3
Total index	6

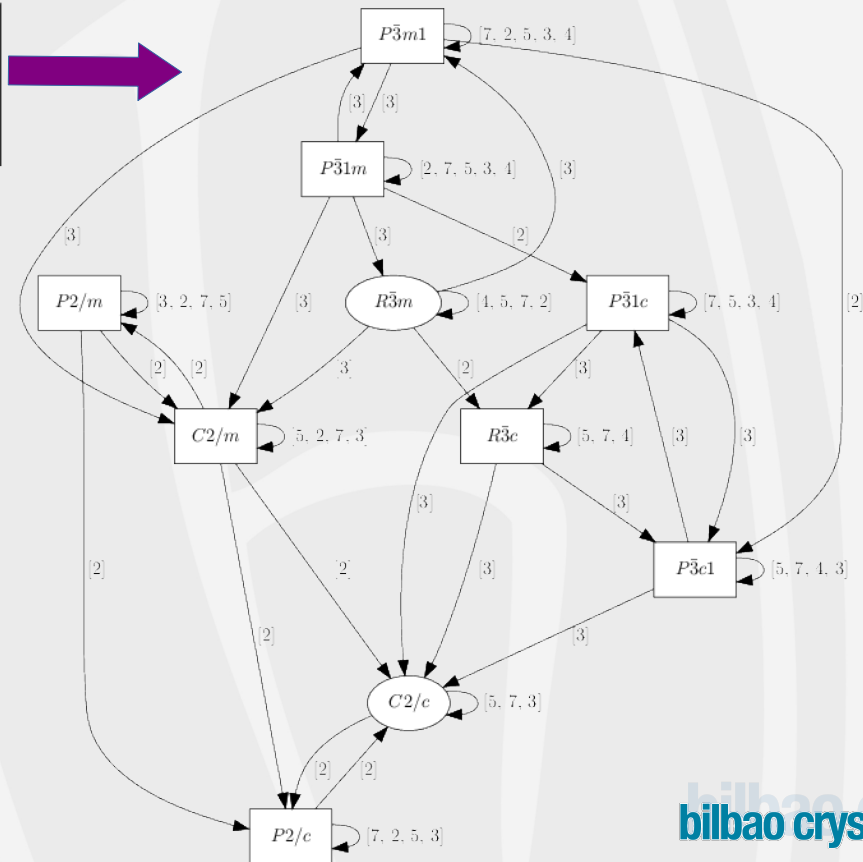
Please, enter the sequential numbers of group and subgroup as given in International Tables for Crystallography, Vol. A:

Enter supergroup number (G) or choose it:

Enter subgroup number (H) or choose it:

Enter the index [G:H] (optional):

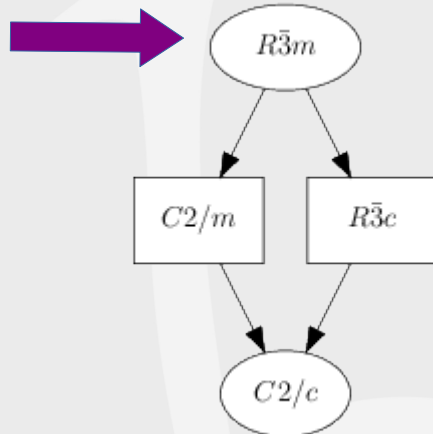
Construct the lattice



## POSSIBLE PATHS (WITH INDEX)

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:	<input type="text" value="166"/>
Enter subgroup number (H) or choose it:	<input type="text" value="15"/>
Enter the index [G:H] (optional):	<input type="text" value="6"/>



Classification of the subgroups of type  $C2/c$  (No. 15) [unique axis b] of group  $R-3m$  (No. 166) [hexagonal axes] with index 6

Note: The group-subgroup relation is type *general*

Hermann Group:  $C2/m$  (12) with  $i_t = 3$  and  $i_k = 2$

Classes representatives

Class #	Transformation Matrix	Matrix Representation	WP Splitting	Symmetry Modes	All subgroups
1	$-1/3a+1/3b-2/3c, -a, b, 2c$	$\begin{pmatrix} -1/3 & -1 & 0 & 0 \\ 1/3 & -1 & 0 & 0 \\ -2/3 & 0 & 2 & 0 \end{pmatrix}$	go to Splitting..	go to Symmodes..	<input type="button" value="Show"/>
2	$-1/3a+1/3b-8/3c, -a, b, 2c$	$\begin{pmatrix} -1/3 & -1 & 0 & 0 \\ 1/3 & -1 & 0 & 0 \\ -8/3 & 0 & 2 & 0 \end{pmatrix}$	go to Splitting..	go to Symmodes..	<input type="button" value="Show"/>
3	$-1/3a+1/3b-8/3c, -a, b, 2c+1/2$	$\begin{pmatrix} -1/3 & -1 & 0 & 0 \\ 1/3 & -1 & 0 & 0 \\ -8/3 & 0 & 2 & 1/2 \end{pmatrix}$	go to Splitting..	go to Symmodes..	<input type="button" value="Show"/>
4	$-1/3a+1/3b-2/3c, -a, b, 2c+1/2$	$\begin{pmatrix} -1/3 & -1 & 0 & 0 \\ 1/3 & -1 & 0 & 0 \\ -2/3 & 0 & 2 & 1/2 \end{pmatrix}$	go to Splitting..	go to Symmodes..	<input type="button" value="Show"/>

HERMANN

# WYCKOFF POSITIONS SPLITTING COMPATIBILITY

## $\text{Pb}_3(\text{PO}_4)_2$ | R-3m (#166)

```

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 -0.181000 0.096000
    
```

## $\text{Pb}_3(\text{PO}_4)_2$ | C2/c (#15)

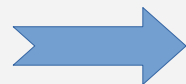
```

15
13.8 5.691 9.42 90. 102.3 90.
7
Pb 1 4e 0 0.291 0.25
Pb 2 8f 0.317 0.309 0.352
P  1 8f 0.599 0.241 0.447
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
    
```

### R-3m

```

Pb  3a
    6c
P   6c
O   6c
    18h
    
```



### C2/c

```

4e  Pb
8f
8f  P
8f  O
8f
8f
8f
    
```

WPASSIGN



# WYCKOFF POSITIONS SPLITTING COMPATIBILITY

## $Pb_3(PO_4)_2$ | R-3m (#166)

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 -0.181000 0.096000

## $Pb_3(PO_4)_2$ | C2/c (#15)

15  
 13.8 5.691 9.42 90. 102.3 90.  
 7  
 Pb 1 4e 0 0.291 0.25  
 Pb 2 8f 0.317 0.309 0.352  
 P 1 8f 0.599 0.241 0.447  
 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

Class #	Transformation Matrix	Matrix Representation
1	$-1/3a+1/3b-2/3c,-a-b,2c$	$\begin{pmatrix} -1/3 & -1 & 0 & 0 \\ 1/3 & -1 & 0 & 0 \\ -2/3 & 0 & 2 & 0 \end{pmatrix}$
2	$-1/3a+1/3b-8/3c,-a-b,2c$	$\begin{pmatrix} -1/3 & -1 & 0 & 0 \\ 1/3 & -1 & 0 & 0 \\ -8/3 & 0 & 2 & 0 \end{pmatrix}$
3	$-1/3a+1/3b-8/3c,-a-b,2c+1/2$	$\begin{pmatrix} -1/3 & -1 & 0 & 0 \\ 1/3 & -1 & 0 & 0 \\ -8/3 & 0 & 2 & 1/2 \end{pmatrix}$
4	$-1/3a+1/3b-2/3c,-a-b,2c+1/2$	$\begin{pmatrix} -1/3 & -1 & 0 & 0 \\ 1/3 & -1 & 0 & 0 \\ -2/3 & 0 & 2 & 1/2 \end{pmatrix}$

**R-3m**

Pb 3a

6c

P 6c

O 6c

18h

**C2/c**

4e Pb

8f

8f P

8f O

8f

8f

8f

# WYCKOFF POSITIONS SPLITTING COMPATIBILITY

## Pb<sub>3</sub>(PO<sub>4</sub>)<sub>2</sub> | R-3m (#166)

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 -0.181000 0.096000

## Pb<sub>3</sub>(PO<sub>4</sub>)<sub>2</sub> | C2/c (#15)

15  
 13.8 5.691 9.42 90. 102.3 90.  
 7  
 Pb 1 4e 0 0.291 0.25  
 Pb 2 8f 0.317 0.309 0.352  
 P 1 8f 0.599 0.241 0.447  
 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

## WYCKSPLIT

Class #	Transformation Matrix	Matrix Representation
1	$-1/3a+1/3b-2/3c,-a,b,2c$	$\begin{pmatrix} -1/3 & -1 & 0 & 0 \\ 1/3 & -1 & 0 & 0 \\ -2/3 & 0 & 2 & 0 \end{pmatrix}$
2	$-1/3a+1/3b-8/3c,-a,b,2c$	$\begin{pmatrix} -1/3 & -1 & 0 & 0 \\ 1/3 & -1 & 0 & 0 \\ -8/3 & 0 & 2 & 0 \end{pmatrix}$
3	$-1/3a+1/3b-8/3c,-a-b,2c+1/2$	$\begin{pmatrix} -1/3 & -1 & 0 & 0 \\ 1/3 & -1 & 0 & 0 \\ -8/3 & 0 & 2 & 1/2 \end{pmatrix}$
4	$-1/3a+1/3b-2/3c,-a-b,2c+1/2$	$\begin{pmatrix} -1/3 & -1 & 0 & 0 \\ 1/3 & -1 & 0 & 0 \\ -2/3 & 0 & 2 & 1/2 \end{pmatrix}$

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

Enter supergroup  OR

Enter subgroup or

Please, define the [transformation](#) relating the group and the subgroup bases.  
 (NOTE: If you don't know the transformation click [here](#) for possible workarounds)

Linear part:

Origin shift:

### R-3m

Pb 3a  
 6c  
 P 6c  
 O 6c  
 18h

### C2/c

4e Pb  
 8f  
 8f P  
 8f O  
 8f  
 8f

# WYCKOFF POSITIONS SPLITTING COMPATIBILITY

## $\text{Pb}_3(\text{PO}_4)_2$ | R-3m (#166)

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 -0.181000 0.096000

## $\text{Pb}_3(\text{PO}_4)_2$ | C2/c (#15)

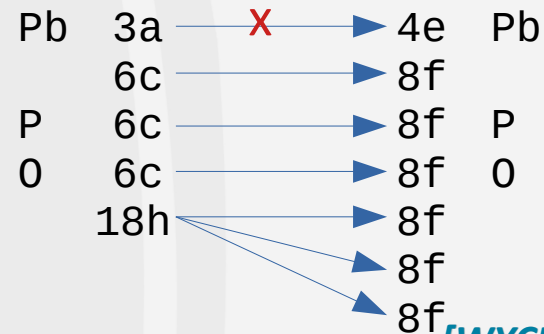
15  
13.8 5.691 9.42 90. 102.3 90.  
7  
Pb 1 4e 0 0.291 0.25  
Pb 2 8f 0.317 0.309 0.352  
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O 2 8f 0.634 0.464 0.374  
O 3 8f 0.642 0.280 0.612  
O 4 8f 0.491 0.222 0.420

## WYCKSPLIT

Class #	Transformation Matrix	Matrix Representation
1	$-1/3a+1/3b-2/3c, -a-b, 2c$	$\begin{pmatrix} -1/3 & -1 & 0 & 0 \\ 1/3 & -1 & 0 & 0 \\ -2/3 & 0 & 2 & 0 \end{pmatrix}$
2	$-1/3a+1/3b-8/3c, -a-b, 2c$	$\begin{pmatrix} -1/3 & -1 & 0 & 0 \\ 1/3 & -1 & 0 & 0 \\ -8/3 & 0 & 2 & 0 \end{pmatrix}$
3	$-1/3a+1/3b-8/3c, -a-b, 2c+1/2$	$\begin{pmatrix} -1/3 & -1 & 0 & 0 \\ 1/3 & -1 & 0 & 0 \\ -8/3 & 0 & 2 & 1/2 \end{pmatrix}$
4	$-1/3a+1/3b-2/3c, -a-b, 2c+1/2$	$\begin{pmatrix} -1/3 & -1 & 0 & 0 \\ 1/3 & -1 & 0 & 0 \\ -2/3 & 0 & 2 & 1/2 \end{pmatrix}$

No	Wyckoff position(s)		
	Group	Subgroup	More...
1	36i	8f 8f 8f 8f 8f 8f	Relations
2	18h	8f 8f 8f	Relations
3	18g	8f 8f 4e 4e	Relations
4	18f	8f 8f 8f	Relations
5	9e	8f 4b	Relations
6	9d	4d 4c 4e	Relations
7	6c	8f	Relations
8	3b	4e	Relations
9	3a	4a	Relations

R-3m



# WYCKOFF POSITIONS SPLITTING COMPATIBILITY

$\text{Pb}_3(\text{PO}_4)_2$  | R-3m (#166)

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 -0.181000 0.096000

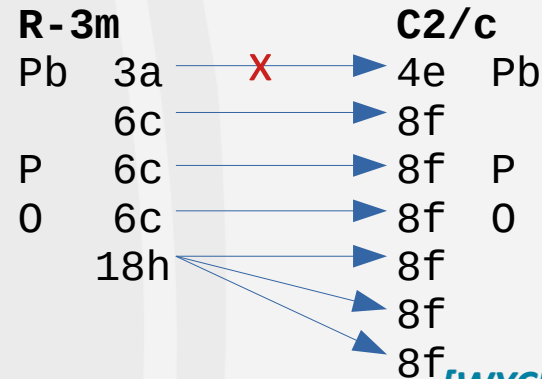
$\text{Pb}_3(\text{PO}_4)_2$  | C2/c (#15)

15  
 13.8 5.691 9.42 90. 102.3 90.  
 7  
 Pb 1 4e 0 0.291 0.25  
 Pb 2 8f 0.317 0.309 0.352  
 P 1 8f 0.599 0.241 0.447  
 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

## WYCKSPLIT

Class #	Transformation Matrix	Matrix Representation
1	$\begin{matrix} -1/3a+1/3b- \\ 2/3c,-a-b,2c \end{matrix}$	$\begin{pmatrix} -1/3 & -1 & 0 & 0 \\ 1/3 & -1 & 0 & 0 \\ -2/3 & 0 & 2 & 0 \end{pmatrix}$
2	$\begin{matrix} -1/3a+1/3b- \\ 8/3c,-a-b,2c \end{matrix}$	$\begin{pmatrix} -1/3 & -1 & 0 & 0 \\ 1/3 & -1 & 0 & 0 \\ -8/3 & 0 & 2 & 0 \end{pmatrix}$
3	$\begin{matrix} -1/3a+1/3b- \\ 8/3c,-a-b,2c+1/2 \end{matrix}$	$\begin{pmatrix} -1/3 & -1 & 0 & 0 \\ 1/3 & -1 & 0 & 0 \\ -8/3 & 0 & 2 & 1/2 \end{pmatrix}$
4	$\begin{matrix} -1/3a+1/3b- \\ 2/3c,-a-b,2c+1/2 \end{matrix}$	$\begin{pmatrix} -1/3 & -1 & 0 & 0 \\ 1/3 & -1 & 0 & 0 \\ -2/3 & 0 & 2 & 1/2 \end{pmatrix}$

No	Wyckoff position(s)		
	Group	Subgroup	More...
1	36i	8f 8f 8f 8f 8f 8f	Relations
2	18h	8f 8f 8f	Relations
3	18g	8f 8f 4e 4e	Relations
4	18f	8f 8f 8f	Relations
5	9e	4d 4c 4b	Relations
6	9d	8f 4e	Relations
7	6c	8f	Relations
8	3b	4e	Relations
9	3a	4a	Relations



# WYCKOFF POSITIONS SPLITTING COMPATIBILITY

$Pb_3(PO_4)_2$  | R-3m (#166)

166  
5.56 5.56 20.39 90. 90. 120.  
5  
Pb 1 3a 0.000000 0.000000 0.000000  
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Pb 1 4e 0 0.291 0.25  
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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

$$2 \quad \begin{matrix} -1/3a+1/3b- \\ 8/3c,-a-b,2c \end{matrix} \quad \begin{pmatrix} -1/3 & -1 & 0 & 0 \\ 1/3 & -1 & 0 & 0 \\ -8/3 & 0 & 2 & 0 \end{pmatrix}$$



No	Wyckoff position(s)		
	Group	Subgroup	More...
1	36i	8f 8f 8f 8f 8f	Relations
2	18h	8f 8f 8f	Relations
3	18g	8f 8f 4e 4e	Relations
4	18f	8f 8f 8f	Relations
5	9e	4d 4c 4b	Relations
6	9d	8f 4e	Relations
7	6c	8f	Relations
8	3b	4e	Relations
9	3a	4a	Relations

## [WYCKSETS]

### Wyckoff Sets of Space Group C2/c (No. 15) [unique axis b]

NOTE: The program uses the default choice for the group settings.

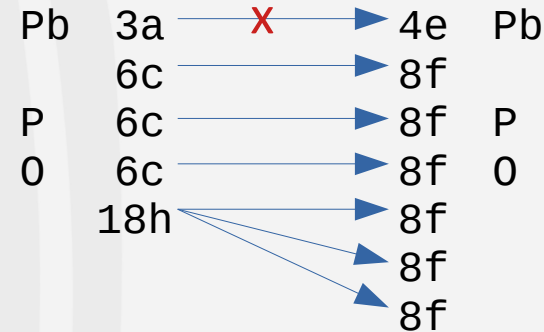
Letter	Mult	SS	Rep.	Equivalent WP under Euclidean normalizer	Equivalent WP under affine normalizer
f	8	1	(x, y, z)	f	f
e	4	2	(0, y, 1/4)	e	e
d	4	-1	(1/4, 1/4, 1/2)	cd	abcd
c	4	-1	(1/4, 1/4, 0)	cd	abcd
b	4	-1	(0, 1/2, 0)	ab	abcd
a	4	-1	(0, 0, 0)	ab	abcd

### Transformation of the Wyckoff Positions of C2/c (015) [unique axis b] under the coset representatives of its Euclidean normalizer

Index: 4

No. #	Coset Representative	Geometrical Interpretation	Transformed WP
1	x,y,z $\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	1	a b c d e f
2	x+1/2,y,z $\begin{pmatrix} 1 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	t (1/2,0,0)	b a d c e f
3	x,y,z+1/2 $\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1/2 \end{pmatrix}$	t (0,0,1/2)	a b d c e f
4	x+1/2,y,z+1/2 $\begin{pmatrix} 1 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1/2 \end{pmatrix}$	t (1/2,0,1/2)	b a c d e f

R-3m



C2/c

# WYCKOFF POSITIONS SPLITTING COMPATIBILITY

## Pb<sub>3</sub>(PO<sub>4</sub>)<sub>2</sub> | R-3m (#166)

166  
 5.56 5.56 20.39 90. 90. 120.  
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 Pb 1 3a 0.000000 0.000000 0.000000  
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 P 1 6c 0.000000 0.000000 0.402100  
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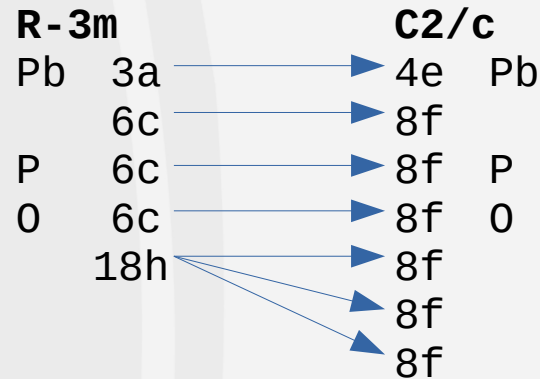
## Pb<sub>3</sub>(PO<sub>4</sub>)<sub>2</sub> | C2/c (#15)

15  
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 Pb 1 4e 0 0.291 0.25  
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 P 1 8f 0.599 0.241 0.447  
 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

## WYCKSPLIT

Class #	Transformation Matrix	Matrix Representation
1	$-1/3a+1/3b-2/3c,-a-b,2c$	$\begin{pmatrix} -1/3 & -1 & 0 & 0 \\ 1/3 & -1 & 0 & 0 \\ -2/3 & 0 & 2 & 0 \end{pmatrix}$
2	$-1/3a+1/3b-8/3c,-a-b,2c$	$\begin{pmatrix} -1/3 & -1 & 0 & 0 \\ 1/3 & -1 & 0 & 0 \\ -8/3 & 0 & 2 & 0 \end{pmatrix}$
3	$-1/3a+1/3b-8/3c,-a-b,2c+1/2$	$\begin{pmatrix} -1/3 & -1 & 0 & 0 \\ 1/3 & -1 & 0 & 0 \\ -8/3 & 0 & 2 & 1/2 \end{pmatrix}$
4	$-1/3a+1/3b-2/3c,-a-b,2c+1/2$	$\begin{pmatrix} -1/3 & -1 & 0 & 0 \\ 1/3 & -1 & 0 & 0 \\ -2/3 & 0 & 2 & 1/2 \end{pmatrix}$

No	Wyckoff position(s)		
	Group	Subgroup	More...
1	36i	8f 8f 8f 8f 8f 8f	Relations
2	18h	8f 8f 8f	Relations
3	18g	8f 8f 8f	Relations
4	18f	8f 8f 4e 4e	Relations
5	9e	8f 4e	Relations
6	9d	4d 4c 4b	Relations
7	6c	8f	Relations
8	3b	4a	Relations
9	3a	4e	Relations



# WYCKOFF POSITIONS SPLITTING COMPATIBILITY

## Pb<sub>3</sub>(PO<sub>4</sub>)<sub>2</sub> | R-3m (#166)

```
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 -0.181000 0.096000
```

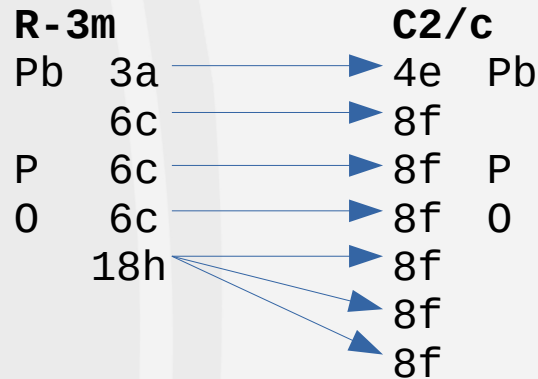
## Pb<sub>3</sub>(PO<sub>4</sub>)<sub>2</sub> | C2/c (#15)

```
15
13.8 5.691 9.42 90. 102.3 90.
7
Pb 1 4e 0 0.291 0.25
Pb 2 8f 0.317 0.309 0.352
P 1 8f 0.599 0.241 0.447
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
```

## WYCKSPLIT

Class #	Transformation Matrix	Matrix Representation
1	-1/3a+1/3b-2/3c,-a-b,2c	$\begin{pmatrix} -1/3 & -1 & 0 & 0 \\ 1/3 & -1 & 0 & 0 \\ -2/3 & 0 & 2 & 0 \end{pmatrix}$
2	-1/3a+1/3b-8/3c,-a-b,2c	$\begin{pmatrix} -1/3 & -1 & 0 & 0 \\ 1/3 & -1 & 0 & 0 \\ -8/3 & 0 & 2 & 0 \end{pmatrix}$
3	-1/3a+1/3b-8/3c,-a-b,2c+1/2	$\begin{pmatrix} -1/3 & -1 & 0 & 0 \\ 1/3 & -1 & 0 & 0 \\ -8/3 & 0 & 2 & 1/2 \end{pmatrix}$
4	-1/3a+1/3b-2/3c,-a-b,2c+1/2	$\begin{pmatrix} -1/3 & -1 & 0 & 0 \\ 1/3 & -1 & 0 & 0 \\ -2/3 & 0 & 2 & 1/2 \end{pmatrix}$

No	Wyckoff position(s)		
	Group	Subgroup	More...
1	36i	8f 8f 8f 8f 8f 8f	Relations
2	18h	8f 8f 8f	Relations
3	18g	8f 8f 8f	Relations
4	18f	8f 8f 4e 4e	Relations
5	9e	4c 4d 4e	Relations
6	9d	8f 4b	Relations
7	6c	8f	Relations
8	3b	4a	Relations
9	3a	4e	Relations



# WYCKOFF POSITIONS SPLITTING COMPATIBILITY

## $Pb_3(PO_4)_2$ | R-3m (#166)

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 -0.181000 0.096000

## $Pb_3(PO_4)_2$ | C2/c (#15)

15  
 13.8 5.691 9.42 90. 102.3 90.  
 7  
 Pb 1 4e 0 0.291 0.25  
 Pb 2 8f 0.317 0.309 0.352  
 P 1 8f 0.599 0.241 0.447  
 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

Class #	Transformation Matrix	Matrix Representation
1	$\begin{pmatrix} -1/3a+1/3b-2/3c, -a-b, c \end{pmatrix}$	$\begin{pmatrix} -1/3 & -1 & 0 & 0 \\ 1/3 & -1 & 0 & 0 \\ -2/3 & 0 & 2 & 0 \end{pmatrix}$
2	$\begin{pmatrix} -1/3a+1/3b-8/3c, -a-b, c \end{pmatrix}$	$\begin{pmatrix} -1/3 & -1 & 0 & 0 \\ 1/3 & -1 & 0 & 0 \\ -8/3 & 0 & 2 & 0 \end{pmatrix}$
3	$\begin{pmatrix} -1/3a+1/3b-8/3c, -a-b, 2c+1/2 \end{pmatrix}$	$\begin{pmatrix} -1/3 & -1 & 0 & 0 \\ 1/3 & -1 & 0 & 0 \\ -8/3 & 0 & 2 & 1/2 \end{pmatrix}$
4	$\begin{pmatrix} -1/3a+1/3b-2/3c, -a-b, 2c+1/2 \end{pmatrix}$	$\begin{pmatrix} -1/3 & -1 & 0 & 0 \\ 1/3 & -1 & 0 & 0 \\ -2/3 & 0 & 2 & 1/2 \end{pmatrix}$

R-3m

Pb 3a

6c

P 6c

O 6c

18h

C2/c

4e Pb

8f

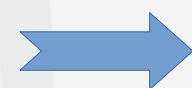
8f P

8f O

8f

8f

8f





# LATTICE COMPATIBILITY

Cell Parameters:  Centering

Please, define the linear part of the transformation matrix that relates the group and the subgroup bases

in abc form:  Ex: c,a,b (read by columns)

Linear part

or in matrix form:

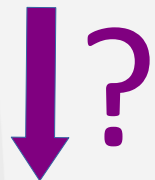
<input type="text" value="1"/>	<input type="text" value="0"/>	<input type="text" value="0"/>
<input type="text" value="0"/>	<input type="text" value="1"/>	<input type="text" value="0"/>
<input type="text" value="0"/>	<input type="text" value="0"/>	<input type="text" value="1"/>

3	$-1/3a+1/3b-8/3c,-a-b,2c+1/2$	$\begin{pmatrix} -1/3 & -1 & 0 & 0 \\ 1/3 & -1 & 0 & 0 \\ -8/3 & 0 & 2 & 1/2 \end{pmatrix}$
---	-------------------------------	---

**R-3m (#166)** 5.56 5.56 20.39 90. 90. 120.



**C2/c (#15)** 54.468 5.560 40.780 90.00 176.62 90.00



**C2/c (#15)** 13.8 5.691 9.42 90. 102.3 90.

## Transform Structure

```

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 -0.181000 0.096000
    
```

Low symmetry  
Space Group  
ITA number

15

Transformation  
Matrix:

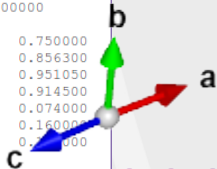
In matrix form:

	Linear part			Origin Shift
	<input type="text" value="-1/3"/>	<input type="text" value="-1"/>	<input type="text" value="0"/>	<input type="text" value="0"/>
	<input type="text" value="1/3"/>	<input type="text" value="-1"/>	<input type="text" value="0"/>	<input type="text" value="0"/>
	<input type="text" value="-8/3"/>	<input type="text" value="0"/>	<input type="text" value="2"/>	<input type="text" value="0.5"/>

## Low symmetry structure

```

015
54.468010 5.560000 40.779999 90.000000 176.621307 90.000000
7
Pb 1 4e 0.000000 0.000000 0.750000
Pb 2 8f 0.000000 0.000000 0.856300
P 1 8f 0.000000 0.000000 0.951050
O 1 8f 0.000000 0.000000 0.914500
O 2 8f 0.957000 0.500000 0.074000
O 2_2 8f 0.771500 0.228500 0.160000
O 2_3 8f 0.271500 0.271500 0.000000
    
```

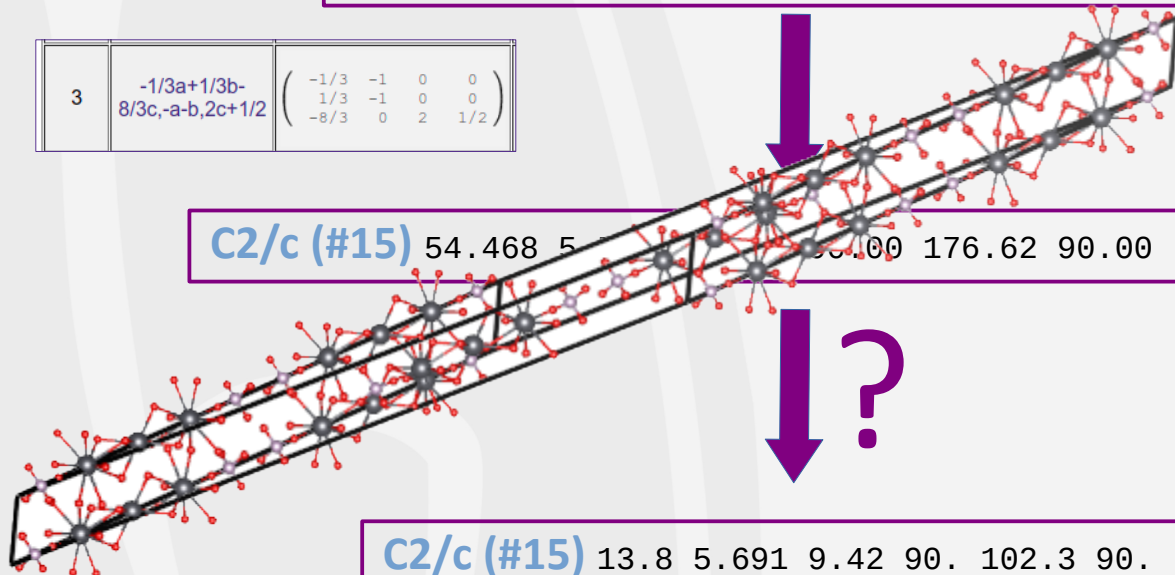


**R-3m (#166)** 5.56 5.56 20.39 90. 90. 120.

3	$\begin{matrix} -1/3a+1/3b- \\ 8/3c,-a-b,2c+1/2 \end{matrix}$	$\begin{pmatrix} -1/3 & -1 & 0 & 0 \\ 1/3 & -1 & 0 & 0 \\ -8/3 & 0 & 2 & 1/2 \end{pmatrix}$
---	---	---

**C2/c (#15)** 54.468 5.560000 40.779999 90.000000 176.62 90.00

**C2/c (#15)** 13.8 5.691 9.42 90. 102.3 90.



# LATTICE COMPATIBILITY

Cell Parameters:  Centering

Please, define the linear part of the transformation matrix that relates the group and the subgroup bases

in abc form:  Ex: c,a,b (read by columns)

Linear part

or in matrix form:

<input type="text" value="1"/>	<input type="text" value="0"/>	<input type="text" value="0"/>
<input type="text" value="0"/>	<input type="text" value="1"/>	<input type="text" value="0"/>
<input type="text" value="0"/>	<input type="text" value="0"/>	<input type="text" value="1"/>

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

Choose:

Euclidean (general metric):

Enhanced Euclidean (specialized metric):

Affine:

**NORMALIZER**

**R-3m (#166)** 5.56 5.56 20.39 90. 90. 120.

3	-1/3a+1/3b-8/3c,-a-b,2c+1/2	$\begin{pmatrix} -1/3 & -1 & 0 & 0 \\ 1/3 & -1 & 0 & 0 \\ -8/3 & 0 & 2 & 1/2 \end{pmatrix}$
---	-----------------------------	---



**C2/c (#15)** 54.468 5.560 40.780 90.00 176.62 90.00

(N <sub>1</sub> ,n <sub>1</sub> )	$\begin{bmatrix} u_{11} & 0 & g_{13} \\ 0 & \pm 1 & 0 \\ g_{31} & 0 & u_{33} \end{bmatrix}$	$\begin{bmatrix} 1/2n_1 \\ 1/2n_2 \\ 1/2n_3 \end{bmatrix}$
(N <sub>2</sub> ,n <sub>2</sub> )	$\begin{bmatrix} u_{11} & 0 & u_{13} \\ 0 & \pm 1 & 0 \\ g_{31} & 0 & u_{33} \end{bmatrix}$	$\begin{bmatrix} 1/4u_1 \\ 1/4u_2 \\ 1/2n_3 \end{bmatrix}$

$$\begin{bmatrix} 3 & 0 & -1 & \frac{1}{4} \\ 0 & -1 & 0 & \frac{1}{4} \\ 4 & 0 & -1 & 0 \end{bmatrix}$$



**C2/c (#15)** 9.630 5.560 13.967 90.00 103.29 90.00

n: integer  
u: odd  
g: even  
det(N) = ±1

$\Delta$ : 4.17000 0.13100 4.54700 0. 1. 0.

**C2/c (#15)** 13.8 5.691 9.42 90. 102.3 90.

Strain: 0.20528  
**STRAIN**

# LATTICE COMPATIBILITY

Cell Parameters:  Centering  ▾

Please, define the linear part of the transformation matrix that relates the group and the subgroup bases

in abc form:  Ex: c,a,b (read by columns)

Linear part

or in matrix form:

<input type="text" value="1"/>	<input type="text" value="0"/>	<input type="text" value="0"/>
<input type="text" value="0"/>	<input type="text" value="1"/>	<input type="text" value="0"/>
<input type="text" value="0"/>	<input type="text" value="0"/>	<input type="text" value="1"/>

**R-3m (#166)** 5.56 5.56 20.39 90. 90. 120.

4	$-1/3a+1/3b-2/3c,-a-b,2c+1/2$	$\begin{pmatrix} -1/3 & -1 & 0 & 0 \\ 1/3 & -1 & 0 & 0 \\ -2/3 & 0 & 2 & 1/2 \end{pmatrix}$
---	-------------------------------	---



**C2/c (#15)** 13.9672 5.5600 40.7800 90.00 166.71 90.00

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

Choose:

- Euclidean (general metric):
- Enhanced Euclidean (specialized metric):
- Affine:

$(N_1, n_1)$	$\begin{bmatrix} u_{11} & 0 & g_{13} \\ 0 & \pm 1 & 0 \\ g_{31} & 0 & u_{33} \end{bmatrix}$	$\begin{bmatrix} 1/2n_1 \\ 1/2n_2 \\ 1/2n_3 \end{bmatrix}$
$(N_2, n_2)$	$\begin{bmatrix} u_{11} & 0 & u_{13} \\ 0 & \pm 1 & 0 \\ g_{31} & 0 & u_{33} \end{bmatrix}$	$\begin{bmatrix} 1/4u_1 \\ 1/4u_2 \\ 1/2n_3 \end{bmatrix}$

$$\begin{bmatrix} 1 & 0 & -3 & \frac{1}{4} \\ 0 & -1 & 0 & \frac{1}{4} \\ 0 & 0 & -1 & 0 \end{bmatrix}$$



**C2/c (#15)** 13.9672 5.5600 9.6323 90.00 103.29 90.00

n: integer  
u: odd  
g: even  
det(N) = ±1

Δ: 0.16720 0.13100 0.21230 0. 1. 0.

**C2/c (#15)** 13.8 5.691 9.42 90. 102.3 90.

Strain: 0.01160

**STRAIN**

**NORMALIZER**

# COMPATIBLE TRANSFORMATION MATRIX TO SUBGROUP

4	$-1/3a+1/3b-2/3c, -a-b, 2c+1/2$	$\begin{pmatrix} -1/3 & -1 & 0 & 0 \\ 1/3 & -1 & 0 & 0 \\ -2/3 & 0 & 2 & 1/2 \end{pmatrix}$
---	---------------------------------	---

$$\begin{bmatrix} 1 & 0 & -3 & \frac{1}{4} \\ 0 & -1 & 0 & \frac{1}{4} \\ 0 & 0 & -1 & 0 \end{bmatrix} = \begin{bmatrix} -\frac{1}{3} & 1 & 1 & -\frac{1}{3} \\ \frac{1}{3} & 1 & -1 & -\frac{1}{6} \\ -\frac{2}{3} & 0 & 0 & \frac{1}{3} \end{bmatrix}$$

```
P_166_015_WP = np.array([[ -1/3, -1, 0, 0 ],\
                          [ 1/3, -1, 0, 0 ],\
                          [ -2/3, 0, 2, 1/2 ],\
                          [ 0, 0, 0, 1 ]])
Affine_Normalizer_Element = np.array([[ 1, 0, -3, 1/4 ],\
                                       [ 0, -1, 0, 1/4 ],\
                                       [ 0, 0, -1, 0 ],\
                                       [ 0, 0, 0, 1 ]])
P_166_015_WP_Lattice = np.dot(P_166_015_WP, Affine_Normalizer_Element)
print(P_166_015_WP_Lattice)
```

```
[[-0.33333333  1.          1.          -0.33333333]
 [ 0.33333333  1.         -1.         -0.16666667]
 [-0.66666667  0.          0.          0.33333333]
 [ 0.          0.          0.          1.          ]]
```

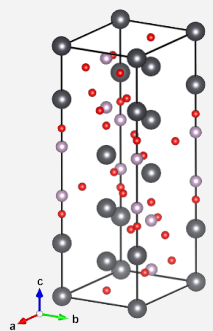
**WP Splitting compatible Group – Subgroup TrMat**      **Lattice compatible element of Affine Normalizer**



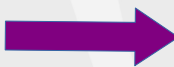
$$-\frac{1}{3}a + \frac{1}{3}b - \frac{2}{3}c, -a - b, 2c; 0, 0, \frac{1}{2}$$

$$x - 3z + \frac{1}{4}, -y + \frac{1}{4}, -z$$

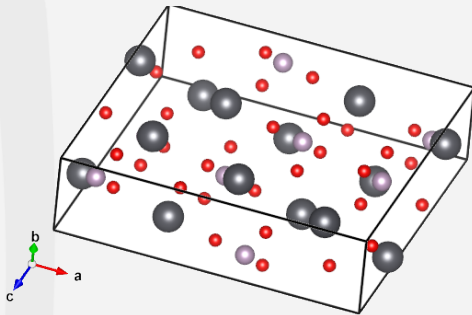
$$-\frac{1}{3}a + \frac{1}{3}b - \frac{2}{3}c, a + b + c, a - b; -\frac{1}{3}, -\frac{1}{6}, \frac{1}{3}$$



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 -0.181000 0.096000



15  
13.967 5.560 9.630 90. 103.29 90.  
7  
Pb 1 4e 0.499999 0.250000 0.249999  
Pb 2 8f 0.181099 0.250000 0.143699  
P 1 8f 0.896849 0.250000 0.048949  
O 1 8f 0.006499 0.250000 0.085499  
O 2 8f 0.355999 0.750000 0.882999  
O 3 8f 0.355999 0.021500 0.611500  
O 4 8f 0.644001 0.478500 0.888499



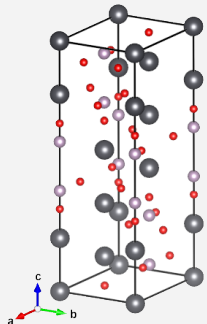
**Pb<sub>3</sub>(PO<sub>4</sub>)<sub>2</sub> | R-3m (#166)**

$$-1/3a+1/3b-2/3c, a+b, a-b; -1/3, -1/6, 1/3$$

**TRANSTRU**

**bilbao crystallographic server**  
<http://www.cryst.ehu.es>

# COMPATIBLE TRANSFORMATION MATRIX TO SUBGROUP



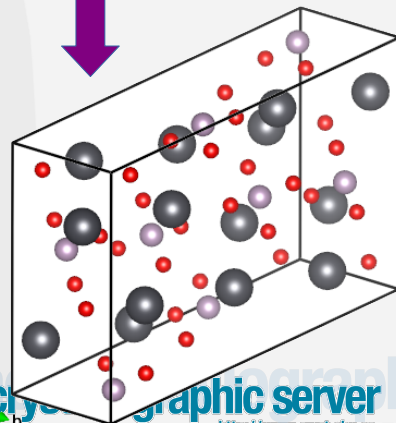
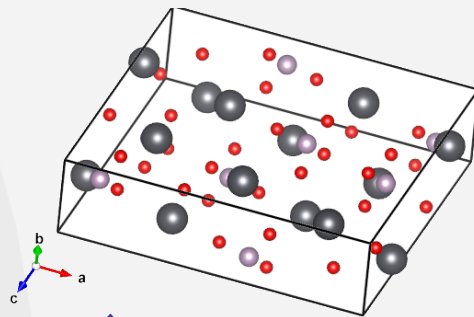
```

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 -0.181000 0.096000
    
```



```

15
13.967 5.560 9.630 90. 103.29 90.
7
Pb 1 4e 0.499999 0.250000 0.249999
Pb 2 8f 0.181099 0.250000 0.143699
P 1 8f 0.896849 0.250000 0.048949
O 1 8f 0.006499 0.250000 0.085499
O 2 8f 0.355999 0.750000 0.882999
O 3 8f 0.355999 0.021500 0.611500
O 4 8f 0.644001 0.478500 0.888499
    
```



$\text{Pb}_3(\text{PO}_4)_2$  | R-3m (#166)

$-1/3a+1/3b-2/3c, a+b, a-b; -1/3, -1/6, 1/3$

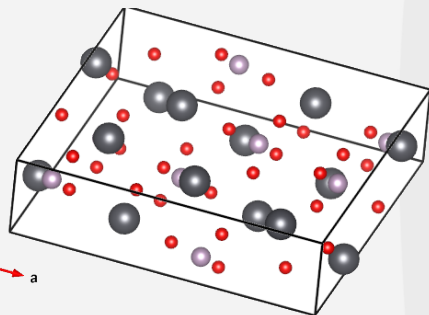
$\text{Pb}_3(\text{PO}_4)_2$  | (#166 → #15)

```

15
13.8 5.691 9.42 90. 102.3 90.
7
Pb 1 4e 0 0.291 0.25
Pb 2 8f 0.317 0.309 0.352
P 1 8f 0.599 0.241 0.447
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
    
```

$\text{Pb}_3(\text{PO}_4)_2$  | C2/c (#15)

# ATOMIC POSITIONS MATCHING



```

15
13.967 5.560 9.630 90. 103.29 90.
7
Pb 1 4e 0.499999 0.250000 0.249999
Pb 2 8f 0.181099 0.250000 0.143699
P 1 8f 0.896849 0.250000 0.048949
O 1 8f 0.006499 0.250000 0.085499
O 2 8f 0.355999 0.750000 0.882999
O 3 8f 0.355999 0.021500 0.611500
O 4 8f 0.644001 0.478500 0.888499
    
```

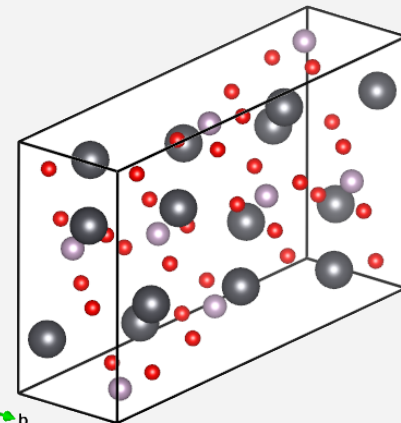
$Pb_3(PO_4)_2$  | (#166 - #15)



```

15
13.8 5.691 9.42 90. 102.3 90.
7
Pb 1 4e 0 0.291 0.25
Pb 2 8f 0.317 0.309 0.352
P 1 8f 0.599 0.241 0.447
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
    
```

$Pb_3(PO_4)_2$  | C2/c (#15)

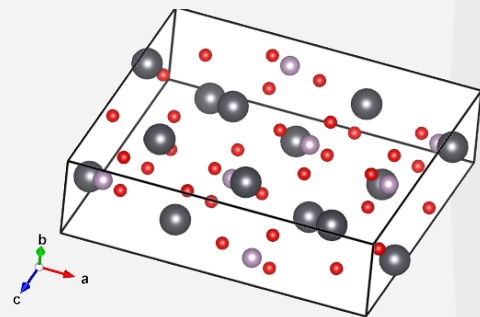


AT.	WP	SS	Representative	Atomic orbit
Pb1	4e (0,y,1/4)	2	(0.499999, 0.250000, 0.249999)	(0.499999, 0.250000, 0.249999) (0.500001, 0.750000, 0.750001) (0.000000, 0.750000, 0.249999) (0.000000, 0.250000, 0.750001)
Pb2	8f (x,y,z)	1	(0.181099, 0.250000, 0.143699)	(0.181099, 0.250000, 0.143699) (0.818901, 0.250000, 0.356301) (0.818901, 0.750000, 0.856301) (0.181099, 0.750000, 0.643699) (0.681099, 0.750000, 0.143699) (0.318901, 0.750000, 0.356301) (0.318901, 0.250000, 0.856301) (0.681099, 0.250000, 0.643699)
P1	8f (x,y,z)	1	(0.896849, 0.250000, 0.048949)	(0.896849, 0.250000, 0.048949) (0.103151, 0.250000, 0.451051) (0.103151, 0.750000, 0.951051) (0.896849, 0.750000, 0.548949) (0.396849, 0.750000, 0.048949) (0.603151, 0.750000, 0.451051) (0.603151, 0.250000, 0.951051) (0.396849, 0.250000, 0.548949)
				(0.006499, 0.250000, 0.085499) (0.993501, 0.250000, 0.414501)



AT.	WP	SS	Representative	Atomic orbit
Pb1	4e (0,y,1/4)	2	(0.000000, 0.291000, 0.250000)	(0.000000, 0.291000, 0.250000) (0.000000, 0.709000, 0.750000) (0.500000, 0.791000, 0.250000) (0.500000, 0.209000, 0.750000)
Pb2	8f (x,y,z)	1	(0.317000, 0.309000, 0.352000)	(0.317000, 0.309000, 0.352000) (0.683000, 0.309000, 0.148000) (0.683000, 0.691000, 0.648000) (0.317000, 0.691000, 0.852000) (0.817000, 0.809000, 0.352000) (0.183000, 0.809000, 0.148000) (0.183000, 0.191000, 0.648000) (0.817000, 0.191000, 0.852000)
P1	8f (x,y,z)	1	(0.599000, 0.241000, 0.447000)	(0.599000, 0.241000, 0.447000) (0.401000, 0.241000, 0.053000) (0.401000, 0.759000, 0.553000) (0.599000, 0.759000, 0.947000) (0.099000, 0.741000, 0.447000) (0.901000, 0.741000, 0.053000) (0.901000, 0.259000, 0.553000) (0.099000, 0.259000, 0.947000)
				(0.643000, 0.030000, 0.392000) (0.357000, 0.030000, 0.108000)

## ATOMIC POSITIONS MATCHING



```

15
13.967 5.560 9.630 90. 103.29 90.
7
Pb 1 4e 0.499999 0.250000 0.249999
Pb 2 8f 0.181099 0.250000 0.143699
P 1 8f 0.896849 0.250000 0.048949
O 1 8f 0.006499 0.250000 0.085499
O 2 8f 0.355999 0.750000 0.882999
O 3 8f 0.355999 0.021500 0.611500
O 4 8f 0.644001 0.478500 0.888499

```

$\text{Pb}_3(\text{PO}_4)_2$  | (#166 - #15)

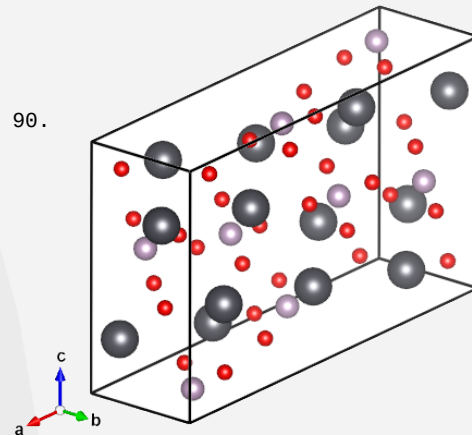


```

15
13.8 5.691 9.42 90. 102.3 90.
7
Pb 1 4e 0.291 0.25
Pb 2 8f 0.317 0.309 0.352
P 1 8f 0.599 0.241 0.447
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

```

$\text{Pb}_3(\text{PO}_4)_2$  | C2/c (#15)



## Equivalent description 2

Normalizer coset representative:  $x+1/2,y,z$

Click here to get more information about the transformation: [show](#) [hide](#)

```

15
13.9670 5.5600 9.6300 90.00 103.29 90.00
7
Pb 1 - -0.000001 0.250000 0.249999
Pb 2 - -0.318901 0.250000 0.143699
P 1 - 0.396849 0.250000 0.048949
O 1 - -0.493501 0.250000 0.085499
O 2 - -0.144001 0.750000 0.882999
O 3 - -0.144001 0.021500 0.611500
O 4 - 0.144001 0.478500 0.888499

```

## Equivalent description 3

Normalizer coset representative:  $x,y,z+1/2$

Click here to get more information about the transformation: [show](#) [hide](#)

```

15
13.9670 5.5600 9.6300 90.00 103.29 90.00
7
Pb 1 - 0.499999 0.250000 -0.250001
Pb 2 - 0.181099 0.250000 -0.356301
P 1 - 0.896849 0.250000 -0.451051
O 1 - 0.006499 0.250000 -0.414501
O 2 - 0.355999 0.750000 0.382999
O 3 - 0.355999 0.021500 0.111500
O 4 - 0.644001 0.478500 0.388499

```

## Equivalent description 4

Normalizer coset representative:  $x+1/2,y,z+1/2$

Click here to get more information about the transformation: [show](#) [hide](#)

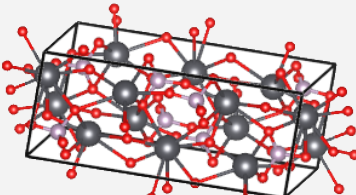
```

15
13.9670 5.5600 9.6300 90.00 103.29 90.00
7
Pb 1 - -0.000001 0.250000 -0.250001
Pb 2 - -0.318901 0.250000 -0.356301
P 1 - 0.396849 0.250000 -0.451051
O 1 - -0.493501 0.250000 -0.414501
O 2 - -0.144001 0.750000 0.382999
O 3 - -0.144001 0.021500 0.111500
O 4 - 0.144001 0.478500 0.388499

```

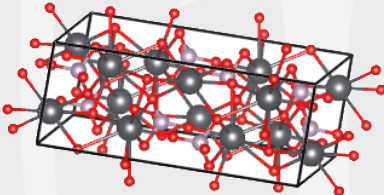


# ATOMIC POSITIONS MATCHING

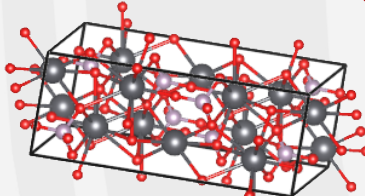
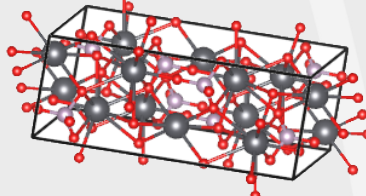


Distorted Structure

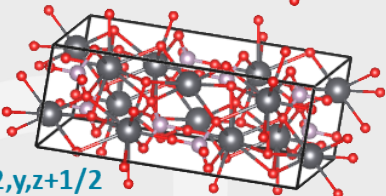
1:  $x,y,z$



2:  $x+1/2,y,z$



3:  $x,y,z+1/2$



4:  $x+1/2,y,z+1/2$

**Equivalent description 2**

Normalizer coset representative:  $x+1/2,y,z$

Click here to get more information about the transformation:

```

15
13.9670 5.5600 9.6300 90.00 103.29 90.00
7
Pb 1 - -0.000001 0.250000 0.249999
Pb 2 - -0.318901 0.250000 0.143699
P 1 - -0.396849 0.250000 0.048949
O 1 - -0.493501 0.250000 0.085499
O 2 - -0.144001 0.750000 0.882999
O 3 - -0.144001 0.021500 0.611500
O 4 - 0.144001 0.478500 0.888499
  
```

**Equivalent description 3**

Normalizer coset representative:  $x,y,z+1/2$

Click here to get more information about the transformation:

```

15
13.9670 5.5600 9.6300 90.00 103.29 90.00
7
Pb 1 - -0.499999 0.250000 -0.250001
Pb 2 - -0.181099 0.250000 -0.356301
P 1 - -0.896849 0.250000 -0.451051
O 1 - -0.006499 0.250000 -0.414501
O 2 - -0.355999 0.750000 0.382999
O 3 - -0.355999 0.021500 0.111500
O 4 - 0.644001 0.478500 0.388499
  
```

**Equivalent description 4**

Normalizer coset representative:  $x+1/2,y,z+1/2$

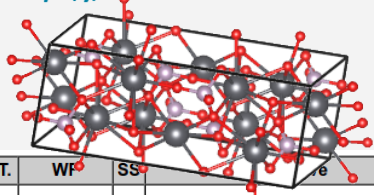
Click here to get more information about the transformation:

```

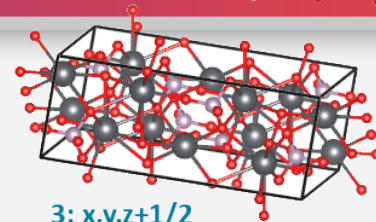
15
13.9670 5.5600 9.6300 90.00 103.29 90.00
7
Pb 1 - -0.000001 0.250000 -0.250001
Pb 2 - -0.318901 0.250000 -0.356301
P 1 - -0.396849 0.250000 -0.451051
O 1 - -0.493501 0.250000 -0.414501
O 2 - -0.144001 0.750000 0.382999
O 3 - -0.144001 0.021500 0.111500
O 4 - 0.144001 0.478500 0.388499
  
```

# ATOMIC POSITIONS MATCHING

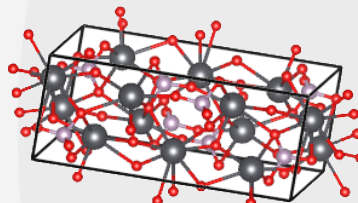
2:  $x+1/2, y, z$



AT.	WP	SS	Atomic orbit
Pb1	4e (0,y,1/4)	2	(0.000000, 0.250000, 0.249999) (0.000000, 0.750000, 0.750001) (0.499999, 0.750000, 0.249999) (0.500001, 0.250000, 0.750001)
Pb2	8f (x,y,z)	1	(0.681099, 0.250000, 0.143699) (0.318901, 0.250000, 0.356301) (0.318901, 0.750000, 0.856301) (0.681099, 0.750000, 0.643699) (0.181099, 0.750000, 0.143699) (0.818901, 0.750000, 0.356301) (0.818901, 0.250000, 0.856301) (0.181099, 0.250000, 0.643699)
P1	8f (x,y,z)	1	(0.396849, 0.250000, 0.048949) (0.603151, 0.250000, 0.451051) (0.603151, 0.750000, 0.951051) (0.396849, 0.750000, 0.548949) (0.896849, 0.750000, 0.048949) (0.103151, 0.750000, 0.451051) (0.103151, 0.250000, 0.951051) (0.896849, 0.250000, 0.548949)



3:  $x, y, z+1/2$



Distorted Structure

```

15
13.8 5.691 9.42 90. 102.3 90.
7
Pb 1 4e 0 0.291 0.25
Pb 2 8f 0.317 0.309 0.352
P 1 8f 0.599 0.241 0.447
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
    
```

AT.	WP	SS	Representative	Atomic orbit
Pb1	4e (0,y,1/4)	2	(0.499999, 0.250000, 0.749999)	(0.499999, 0.250000, 0.749999) (0.500001, 0.750000, 0.250001) (0.000000, 0.750000, 0.749999) (0.000000, 0.250000, 0.250001)
Pb2	8f (x,y,z)	1	(0.181099, 0.250000, 0.643699)	(0.181099, 0.250000, 0.643699) (0.818901, 0.250000, 0.856301) (0.818901, 0.750000, 0.356301) (0.181099, 0.750000, 0.143699) (0.681099, 0.750000, 0.643699) (0.318901, 0.750000, 0.856301) (0.318901, 0.250000, 0.356301) (0.681099, 0.250000, 0.143699)
P1	8f (x,y,z)	1	(0.896849, 0.250000, 0.548949)	(0.896849, 0.250000, 0.548949) (0.103151, 0.250000, 0.951051) (0.103151, 0.750000, 0.451051) (0.896849, 0.750000, 0.048949) (0.396849, 0.750000, 0.548949) (0.603151, 0.750000, 0.951051) (0.603151, 0.250000, 0.451051) (0.396849, 0.250000, 0.048949)

## Equivalent description 2

Normalizer coset representative:  $x+1/2, y, z$

Click here to get more information about the transformation:

```

15
13.9670 5.5600 9.6300 90.00 103.29 90.00
7
Pb 1 - -0.000001 0.250000 0.249999
Pb 2 - -0.318901 0.250000 0.143699
P 1 - 0.396849 0.250000 0.048949
O 1 - -0.493501 0.250000 0.085499
O 2 - -0.144001 0.750000 0.882999
O 3 - -0.144001 0.021500 0.611500
O 4 - 0.144001 0.478500 0.888499
    
```

## Equivalent description 3

Normalizer coset representative:  $x, y, z+1/2$

Click here to get more information about the transformation:

```

15
13.9670 5.5600 9.6300 90.00 103.29 90.00
7
Pb 1 - 0.499999 0.250000 -0.250001
Pb 2 - 0.181099 0.250000 -0.356301
P 1 - 0.896849 0.250000 -0.451051
O 1 - 0.006499 0.250000 -0.414501
O 2 - 0.355999 0.750000 0.382999
O 3 - 0.355999 0.021500 0.111500
O 4 - 0.644001 0.478500 0.388499
    
```

bill

# FINAL TRANSFORMATION MATRIX

4	$-1/3a+1/3b-2/3c,-a-b,2c+1/2$	$\begin{pmatrix} -1/3 & -1 & 0 & 0 \\ 1/3 & -1 & 0 & 0 \\ -2/3 & 0 & 2 & 1/2 \end{pmatrix}$
---	-------------------------------	---

$$\begin{bmatrix} 1 & 0 & -3 & \frac{1}{4} \\ 0 & -1 & 0 & \frac{1}{4} \\ 0 & 0 & -1 & 0 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 0 & 0 & \frac{1}{2} \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

$$= \begin{bmatrix} -\frac{1}{3} & 1 & 1 & -\frac{1}{2} \\ \frac{1}{3} & 1 & -1 & 0 \\ -\frac{2}{3} & 0 & 0 & 0 \end{bmatrix}$$

*The sought transformation matrix!*

**WP Splitting compatible Group  
– Subgroup TrMat**

**Lattice compatible element  
of Affine Normalizer**

**Lattice compatible element  
of Euclidean Normalizer**

$$-\frac{1}{3}a + \frac{1}{3}b - \frac{2}{3}c, -a - b, 2c; 0, 0, \frac{1}{2}$$

$$x - 3z + \frac{1}{4}, -y + \frac{1}{4}, -z$$

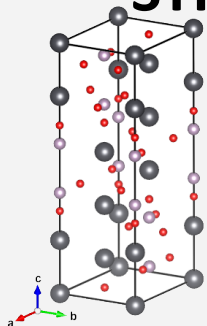
$$x + \frac{1}{2}, y, z$$

$$-\frac{1}{3}a + \frac{1}{3}b - \frac{2}{3}c, a + b, a - b; -\frac{1}{2}, 0, 0$$

```
Euclidean_Normalizer_Element = np.eye(4,4)
Euclidean_Normalizer_Element[0,3] = 0.5
P_166_015_WP_Lattice_Positions = np.dot(P_166_015_WP_Lattice,\
                                         Euclidean_Normalizer_Element)
P_166_015_WP_Lattice_Positions[
    np.isclose(P_166_015_WP_Lattice_Positions,np.zeros((4,4)))] = 0
print(P_166_015_WP_Lattice_Positions)
```

```
[[-0.33333333  1.         1.         -0.5        ]
 [ 0.33333333  1.        -1.         0.         ]
 [-0.66666667  0.         0.         0.         ]
 [ 0.          0.         0.         1.         ]]
```

# HIGH SYMMETRY STRUCTURE DEFINED IN LOW SYMMETRY STRUCTURE'S SETTING (COMPATIBLE LATTICE & POSITIONS)



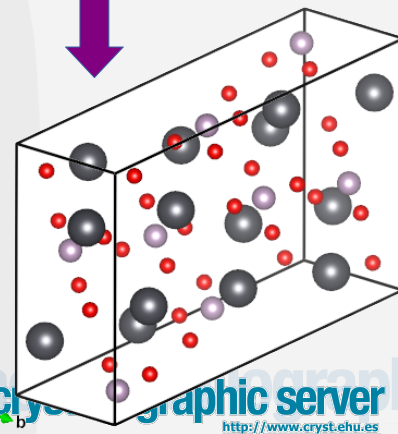
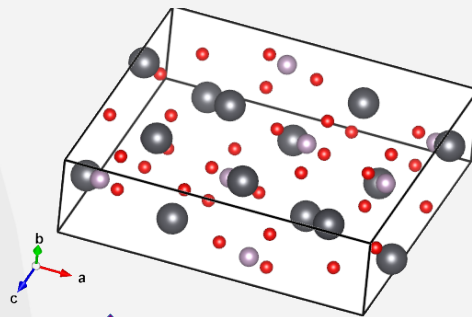
```

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 -0.181000 0.096000
    
```



```

15
13.967 5.560 9.630 90. 103.29 90.
7
Pb 1 4e 0.000000 0.250000 0.250000
Pb 2 8f 0.681100 0.250000 0.143700
P 1 8f 0.396850 0.250000 0.048950
O 1 8f 0.506500 0.250000 0.085500
O 2 8f 0.856000 0.750000 0.883000
O 3 8f 0.856000 0.521500 0.111500
O 4 8f 0.144000 0.978500 0.388500
    
```



$-1/3a+1/3b-2/3c, a+b, a-b; -1/2, 0, 0$

**TRANSTRU**

$Pb_3(PO_4)_2$  | (#166 → #15)

```

15
13.8 5.691 9.42 90. 102.3 90.
7
Pb 1 4e 0 0.291 0.25
Pb 2 8f 0.317 0.309 0.352
P 1 8f 0.599 0.241 0.447
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
    
```

$Pb_3(PO_4)_2$  | C2/c (#15)

# COMPARISON OF THE TWO STRUCTURES

Structure Data  No file chosen  
 [in CIF format] HINT: [ The option for a given filename is preferential ]

```

15
13.967 5.560 9.630 90. 103.29 90.
7
Pb 1 4e 0.000000 0.250000 0.250000
Pb 2 8f 0.681100 0.250000 0.143700
P 1 8f 0.396850 0.250000 0.048950
O 1 8f 0.506500 0.250000 0.085500
O 2 8f 0.856000 0.750000 0.883000
O 3 8f 0.856000 0.521500 0.111500
O 4 8f 0.144000 0.978500 0.388500
    
```

Structure Data  No file chosen  
 [in CIF format] HINT: [ The option for a given filename is preferential ]

```

15
13.8 5.691 9.42 90. 102.3 90.
7
Pb 1 4e 0 0.291 0.25
Pb 2 8f 0.317 0.309 0.352
P 1 8f 0.599 0.241 0.447
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
    
```

Enter the maximum distance allowed between the paired atoms:  Å

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

$$\begin{bmatrix} -\frac{1}{3} & 1 & 1 & -\frac{1}{2} \\ \frac{1}{3} & 1 & -1 & 0 \\ \frac{2}{3} & 0 & 0 & 0 \end{bmatrix}$$

$$-\frac{1}{3}a + \frac{1}{3}b - \frac{2}{3}c, a + b, a - b; -\frac{1}{2}, 0, 0$$

## Atom pairings and distances

Atom Mappings					
WP	Atom	Coordinates in S <sub>1</sub>		Atom	Coordinates in S <sub>2</sub>
4e	(0,y,1/4)	Pb1	(0.000000,0.250000,0.250000)	Pb1	(0.000000,0.291000,0.250000)
8f	(x,y,z)	Pb2	(0.681100,0.250000,0.143700)	Pb2	(0.683000,0.309000,0.148000)
8f	(x,y,z)	P1	(0.396850,0.250000,0.048950)	P1	(0.401000,0.241000,0.053000)
8f	(x,y,z)	O1	(0.506500,0.250000,0.085500)	O4	(0.509000,0.222000,0.080000)
8f	(x,y,z)	O2	(0.856000,0.750000,0.883000)	O3	(0.858000,0.780000,0.888000)
8f	(x,y,z)	O3	(0.856000,0.521500,0.111500)	O1	(0.857000,0.530000,0.108000)
8f	(x,y,z)	O4	(0.144000,0.978500,0.388500)	O2	(0.134000,0.964000,0.374000)

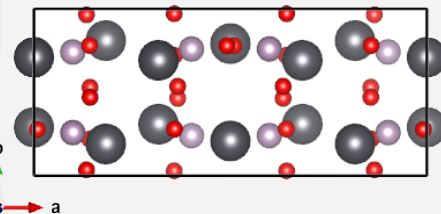
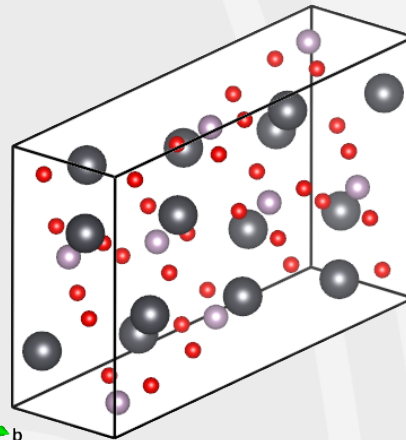
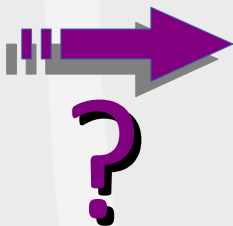
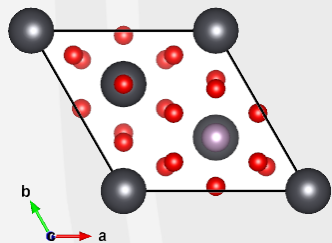
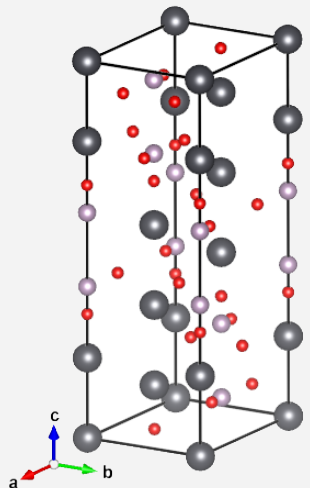
WP	Atom	Atomic Displacements				
		u <sub>x</sub>	u <sub>y</sub>	u <sub>z</sub>	u	
4e	(0,y,1/4)	Pb1	0.0000	0.0410	0.0000	0.2280
8f	(x,y,z)	Pb2	0.0019	0.0590	0.0043	0.3309
8f	(x,y,z)	P1	0.0042	-0.0090	0.0040	0.0797
8f	(x,y,z)	O1	0.0025	-0.0280	-0.0055	0.1706
8f	(x,y,z)	O2	0.0020	0.0300	0.0050	0.1741
8f	(x,y,z)	O3	0.0010	0.0085	-0.0035	0.0615
8f	(x,y,z)	O4	-0.0100	-0.0145	-0.0145	0.1912

NOTE: u<sub>x</sub>, u<sub>y</sub> and u<sub>z</sub> are given in relative units. |u| is the absolute distance given in Å

## Evaluation of the structure similarity

S	d <sub>max</sub> (Å)	d <sub>av</sub> (Å)	Δ
0.0116	0.3309	0.1726	0.066

# IF ONLY WE HAD A DIRECT WAY OF DOING IT...



$\text{Pb}_3(\text{PO}_4)_2$  | R-3m (#166)

```

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 -0.181000 0.096000
    
```

$\text{Pb}_3(\text{PO}_4)_2$  | C2/c (#15)

```

15
13.8 5.691 9.42 90. 102.3 90.
7
Pb 1 4e 0 0.291 0.25
Pb 2 8f 0.317 0.309 0.352
P 1 8f 0.599 0.241 0.447
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
    
```

# IF ONLY WE HAD A DIRECT WAY OF DOING IT...

Spoiler Alert: **STRUCTURE RELATIONS!** (*This case is actually the default case! 8*)

**High symmetry structure**

Enter the formula units in the **high symmetry structure**  
(Leave blank for auto-detection via the volume information)

Structure  
Data [CIF format]  No file chosen

```
# Space Group ITA number
166
# Lattice parameters
5.56 5.56 20.39 90 90 120
# Number of independent atoms in the asymmetric unit
5
BCS
Format # [atom type] [number] [WP] [x] [y] [z]
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
```

**Calculation parameters:**

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

Enter the maximum distance allowed between the paired atoms:  Å

One or both of the structures are given in a non-standard setting?  No  Yes

**Calculation method:**

The group-subgroup transformation matrices are automatically fetched from the database.

User defined group-subgroup **transformation matrix** :

[Index: 6] (Calculated formula units -- High Sym. Structure: 3; Low Sym. Structure: 4)

**Transformation Matrix (P,p):** (-1/3a+1/3b-2/3c,a+b,a-b;-1/2,0,0)

Matrix form:

$$(P,p) = \begin{pmatrix} -1/3 & 1 & 1 & -1/2 \\ 1/3 & 1 & -1 & 0 \\ -2/3 & 0 & 0 & 0 \end{pmatrix}$$

## Description of the High Symmetry Structure in the most similar configuration to the Low Symmetry Structure

```
015
13.967220 5.560000 9.630202 90.000000 103.286987 90.000000
7
Pb 1 4e 0.000000 0.250000 0.249999
Pb 2 8f 0.318901 0.250000 0.356301
P 1 8f 0.603151 0.250000 0.451051
O 1 8f 0.493501 0.250000 0.414501
O 2 8f 0.644001 0.250000 0.617001
O 22 8f 0.644001 0.478500 0.388500
O 23 8f 0.644001 0.021500 0.388499
```

## Atom pairings and distances

Atom Mappings						
WP	Atom	Coordinates in S <sub>1</sub>		Atom	Coordinates in S <sub>2</sub>	
8f	(x,y,z)	O23	(0.644001,0.021500,0.388499)	O1	(0.643000,0.030000,0.392000)	
8f	(x,y,z)	O22	(0.644001,0.478500,0.388500)	O2	(0.634000,0.464000,0.374000)	
8f	(x,y,z)	O2	(0.644001,0.250000,0.617001)	O3	(0.642000,0.280000,0.612000)	
8f	(x,y,z)	O1	(0.493501,0.250000,0.414501)	O4	(0.491000,0.222000,0.420000)	
8f	(x,y,z)	P1	(0.603151,0.250000,0.451051)	P1	(0.599000,0.241000,0.447000)	
4e	(0,y,1/4)	Pb1	(0.000000,0.250000,0.249999)	Pb1	(0.000000,0.291000,0.250000)	
8f	(x,y,z)	Pb2	(0.318901,0.250000,0.356301)	Pb2	(0.317000,0.309000,0.352000)	

Atomic Displacements						
WP	Atom	u <sub>x</sub>	u <sub>y</sub>	u <sub>z</sub>	u	
8f	(x,y,z)	O23	0.0010	-0.0085	-0.0035	0.0617
8f	(x,y,z)	O22	0.0100	0.0145	0.0145	0.1910
8f	(x,y,z)	O2	0.0020	-0.0300	0.0050	0.1777
8f	(x,y,z)	O1	0.0025	0.0280	-0.0055	0.1733
8f	(x,y,z)	P1	0.0042	0.0090	0.0041	0.0802
4e	(0,y,1/4)	Pb1	0.0000	-0.0410	-0.0000	0.2333
8f	(x,y,z)	Pb2	0.0019	-0.0590	0.0043	0.3386

NOTE: u<sub>x</sub>, u<sub>y</sub> and u<sub>z</sub> are given in relative units. |u| is the absolute distance given in Å

## Evaluation of the Global Distortion

S	d <sub>max</sub> (Å)	d <sub>av</sub> (Å)	Δ
0.0116	0.3386	0.1753	0.066

**Low symmetry structure:**

Enter the formula units in the **low symmetry structure**  
(Leave blank for auto-detection via the volume information)

Structure  
Data [CIF format]  No file chosen

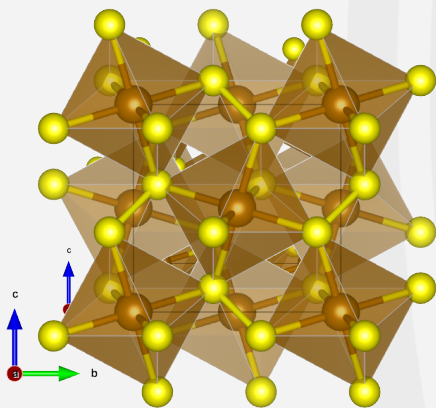
```
# Space Group ITA number
15
# Lattice parameters
13.80 5.691 9.42 90 102.3 90
# Number of independent atoms in the asymmetric unit
7
BCS
Format # [atom type] [number] [WP] [x] [y] [z]
O 1 8f 0.643 0.030 0.392
O 2 8f 0.634 0.464 0.374
O 3 8f 0.642 0.280 0.612
O 4 8f 0.491 0.222 0.420
P 1 8f 0.599 0.241 0.447
Pb 1 4e 0.0291 0.25
Pb 2 8f 0.317 0.309 0.352
```

## FURTHER CASE STUDIES

- Translationengleiche Maximal Subgroups
- Klassengleiche Maximal Subgroups
- Isomorphic Maximal Subgroups
- Common Supergroup

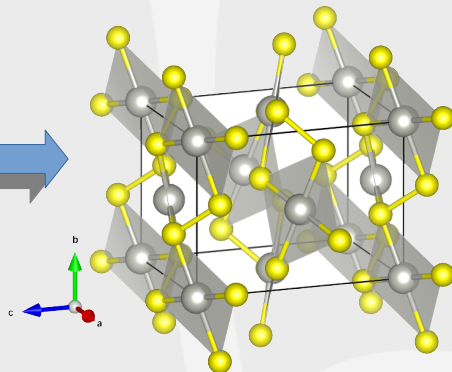


# TRANSLATIONENGLEICHE MAXIMAL SUBGROUPS



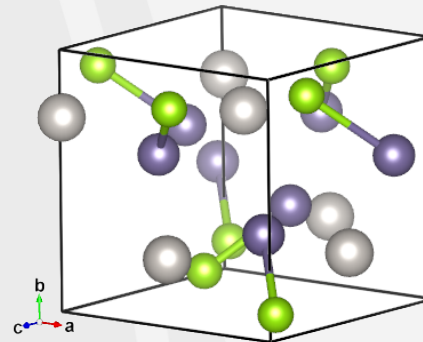
**FeS<sub>2</sub> (Pyrite) | Pa-3 (#205)**

205  
 5.4178 5.4178 5.4178 90. 90. 90.  
 2  
 Fe 1 4a 0.000000 0.000000 0.000000  
 S 1 8c 0.384730 0.384730 0.384730



**PdS<sub>2</sub> | Pbc<sub>a</sub> (#61)**

61  
 5.4650 5.5380 7.5250 90.00 90.00 90.00  
 2  
 Pd 1 4a 0.000000 0.500000 0.500000  
 S 1 8c 0.104000 0.609000 0.916000



**PtGeSe | Pca2<sub>1</sub> (#29)**

29  
 6.015 6.072 5.992 90. 90. 90.  
 3  
 Pt 1 4a 0.008600 0.742000 0.000000  
 Ge 1 4a 0.383300 0.136400 0.616800  
 Se 1 4a 0.619800 0.375900 0.382000

# TRANSLATIONENGLEICHE MAXIMAL SUBGROUPS

## FeS<sub>2</sub> (Pyrite) | Pa-3 (#205)

205

5.4178 5.4178 5.4178 90. 90. 90.

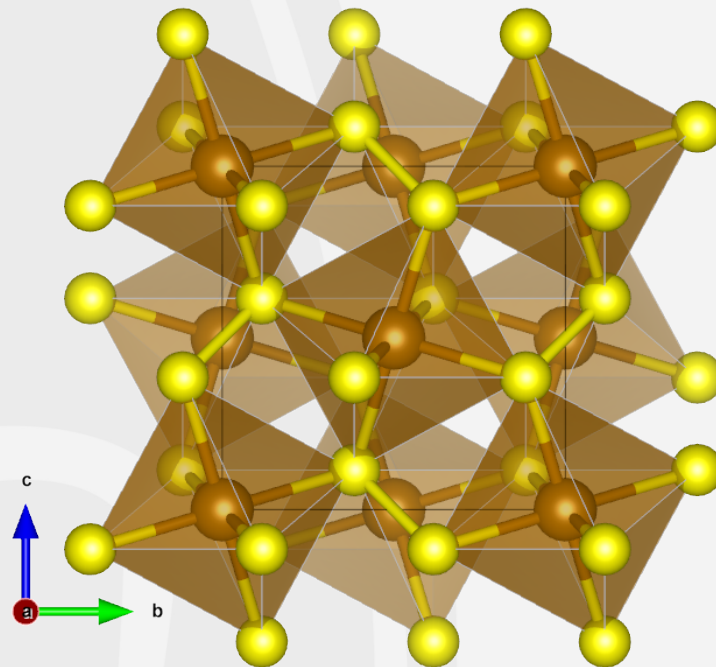
2

Fe 1 4a 0.000000 0.000000 0.000000

S 1 8c 0.384730 0.384730 0.384730

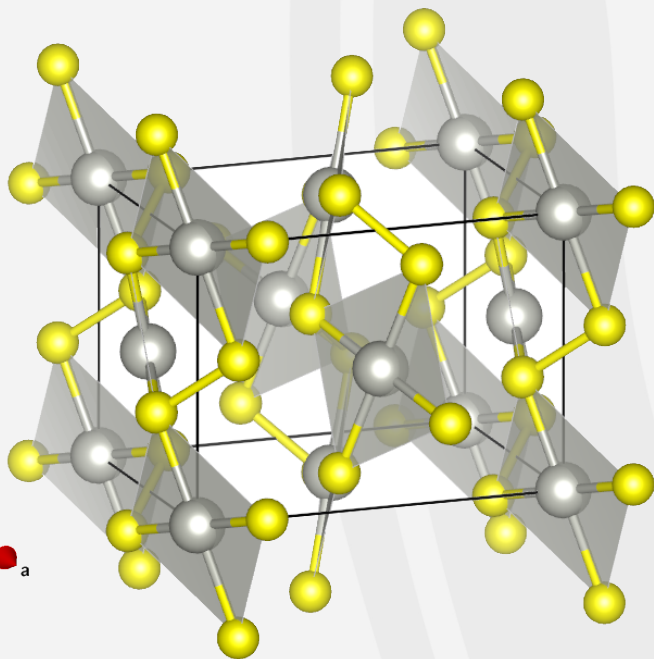
AT.	WP	SS	Representative	Atomic orbit
Fe1	4a (0,0,0)	-.3.	(0.000000, 0.000000, 0.000000)	(0.000000, 0.000000, 0.000000) (0.500000, 0.000000, 0.500000) (0.000000, 0.500000, 0.500000) (0.500000, 0.500000, 0.000000)
S1	8c (x,x,x)	.3.	(0.384730, 0.384730, 0.384730)	(0.384730, 0.384730, 0.384730) (0.115270, 0.615270, 0.884730) (0.615270, 0.884730, 0.115270) (0.884730, 0.115270, 0.615270) (0.615270, 0.615270, 0.615270) (0.884730, 0.384730, 0.115270) (0.384730, 0.115270, 0.884730) (0.115270, 0.884730, 0.384730)

Zuñiga-Puelles, E., R. Cardoso-Gil, M. Bobnar, I. Veremchuk, C. Himcinschi, C. Hennig, J. Kortus, G. Heide, and R. Gumeniuk. "Structural stability and thermoelectric performance of high quality synthetic and natural pyrites (FeS<sub>2</sub>)." *Dalton Transactions* 48, no. 28 (2019): 10703-10713.



# TRANSLATIONENGLEICHE MAXIMAL SUBGROUPS

$\text{PdS}_2$  |  $\text{Pbca}$  (#61)



61  
 5.465 5.538 7.525 90. 90. 90.  
 2  
 Pd 1 4a 0 0 0  
 S 1 8c 0.104 0.109 0.416

AT.	WP	SS	Representative	Atomic orbit
Pd1	4a (0,0,0)	-1	(0.000000, 0.000000, 0.000000)	(0.000000, 0.000000, 0.000000) (0.500000, 0.000000, 0.500000) (0.000000, 0.500000, 0.500000) (0.500000, 0.500000, 0.000000)
S1	8c (x,y,z)	1	(0.104000, 0.109000, 0.416000)	(0.104000, 0.109000, 0.416000) (0.396000, 0.891000, 0.916000) (0.896000, 0.609000, 0.084000) (0.604000, 0.391000, 0.584000) (0.896000, 0.891000, 0.584000) (0.604000, 0.109000, 0.084000) (0.104000, 0.391000, 0.916000) (0.396000, 0.609000, 0.416000)

Hamidani, A., Bennecer, B., & Zanat, K. (2010). Structural and electronic properties of the pseudo-binary compounds  $\text{PdX}_2$  ( $X = \text{P}$ ,  $\text{S}$  and  $\text{Se}$ ). *Journal of Physics and Chemistry of Solids*, 71(1), 42-46.

# TRANSLATIONENGLICHE MAXIMAL SUBGROUPS

## PdS<sub>2</sub> | Pbc<sub>a</sub> (#61)

61  
 5.465 5.538 7.525 90. 90. 90.  
 2  
 Pd 1 4a 0 0 0  
 S 1 8c 0.104 0.109 0.416

AT.	WP	SS	Representative	Atomic orbit
Pd1	4a (0,0,0)	-1	(0.000000, 0.000000, 0.000000)	(0.000000, 0.000000, 0.000000) (0.500000, 0.000000, 0.500000) (0.000000, 0.500000, 0.500000) (0.500000, 0.500000, 0.000000)
S1	8c (x,y,z)	1	(0.104000, 0.109000, 0.416000)	(0.104000, 0.109000, 0.416000) (0.396000, 0.891000, 0.916000) (0.896000, 0.609000, 0.084000) (0.604000, 0.391000, 0.584000) (0.896000, 0.891000, 0.584000) (0.604000, 0.109000, 0.084000) (0.104000, 0.391000, 0.916000) (0.396000, 0.609000, 0.416000)

$$x, y + \frac{1}{2}, z + \frac{1}{2}$$

[Normalizer]

61  
 5.4650 5.5380 7.5250 90.00 90.00 90.00  
 2  
 Pd 1 4a 0.000000 0.500000 0.500000  
 S 1 8c 0.104000 0.609000 0.916000

AT.	WP	SS	Representative	Atomic orbit
Pd1	4a (0,0,0)	-1	(0.000000, 0.500000, 0.500000)	(0.000000, 0.500000, 0.500000) (0.500000, 0.500000, 0.000000) (0.000000, 0.000000, 0.000000) (0.500000, 0.000000, 0.500000)
S1	8c (x,y,z)	1	(0.104000, 0.609000, 0.916000)	(0.104000, 0.609000, 0.916000) (0.396000, 0.391000, 0.416000) (0.896000, 0.109000, 0.584000) (0.604000, 0.891000, 0.084000) (0.896000, 0.391000, 0.084000) (0.604000, 0.609000, 0.584000) (0.104000, 0.891000, 0.416000) (0.396000, 0.109000, 0.916000)

# TRANSLATIONENGLEICHE MAXIMAL SUBGROUPS

## PtGeSe | $Pca2_1$ (#29)

29

6.015 6.072 5.992 90. 90. 90.

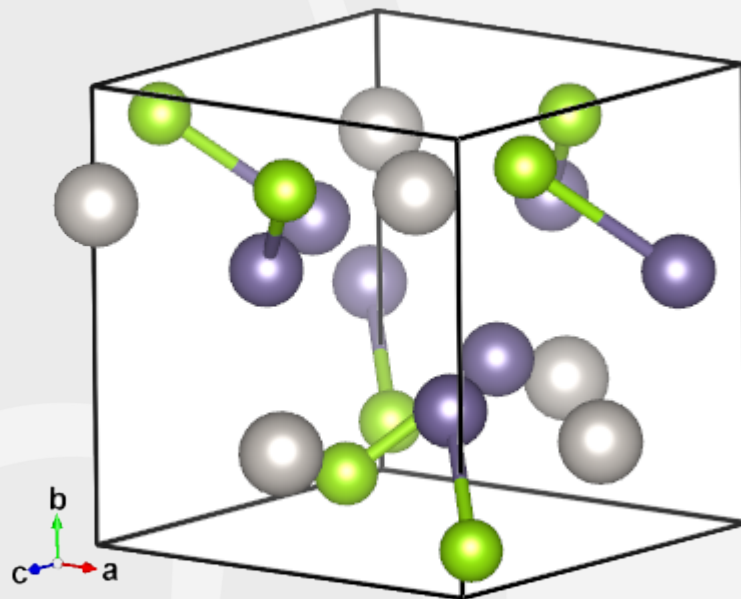
3

Pt 1 4a 0.008600 0.742000 0.000000

Ge 1 4a 0.383300 0.136400 0.616800

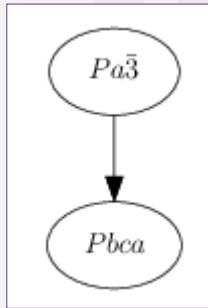
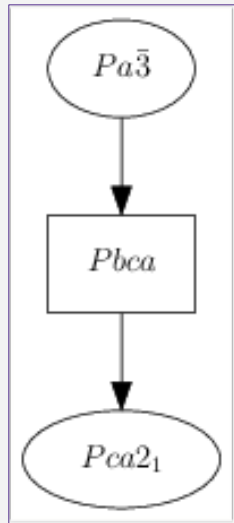
Se 1 4a 0.619800 0.375900 0.382000

AT.	WP	SS	Representative	Atomic orbit
Pt1	4a (x,y,z)	1	(0.008600, 0.742000, 0.000000)	(0.008600, 0.742000, 0.000000) (0.991400, 0.258000, 0.500000) (0.508600, 0.258000, 0.000000) (0.491400, 0.742000, 0.500000)
Ge1	4a (x,y,z)	1	(0.383300, 0.136400, 0.616800)	(0.383300, 0.136400, 0.616800) (0.616700, 0.863600, 0.116800) (0.883300, 0.863600, 0.616800) (0.116700, 0.136400, 0.116800)
Se1	4a (x,y,z)	1	(0.619800, 0.375900, 0.382000)	(0.619800, 0.375900, 0.382000) (0.380200, 0.624100, 0.882000) (0.119800, 0.624100, 0.382000) (0.880200, 0.375900, 0.882000)



Abrahams, S. C., & Bernstein, J. L. (1977). Note on the crystal structure of ferroelastic PtGeSe. *Acta Crystallographica Section B: Structural Crystallography and Crystal Chemistry*, 33(1), 301-302.

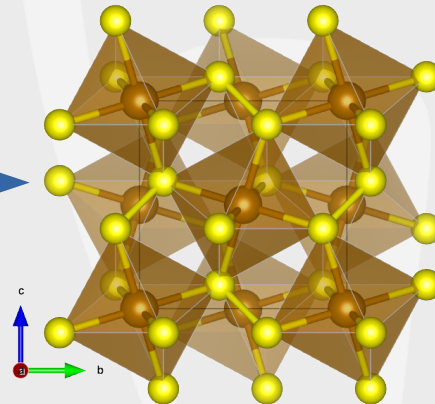
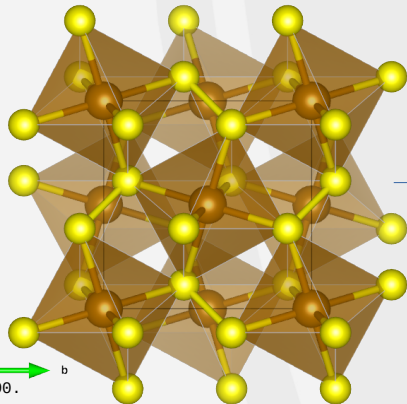
# TRANSLATIONENGLEICHE MAXIMAL SUBGROUPS



Full Set of Possible Transformations  
for the chain 205 061 [3]

# 205 061 [3]

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



**FeS<sub>2</sub> (Pyrite) | Pa-3 (#205)**  
 205  
 5.4178 5.4178 5.4178 90. 90. 90.  
 2  
 Fe 1 4a 0.000000 0.000000 0.000000  
 S 1 8c 0.384730 0.384730 0.384730

## Transform structure

Transformation matrix: a,b,c

### High symmetry structure

205  
 5.4178 5.4178 5.4178 90. 90. 90.  
 2  
 Fe 1 4a 0.000000 0.000000 0.000000  
 S 1 8c 0.384730 0.384730 0.384730

[Visualize this structure](#) [CIF File](#) [Cartesian Coordinates](#)

### Low symmetry structure

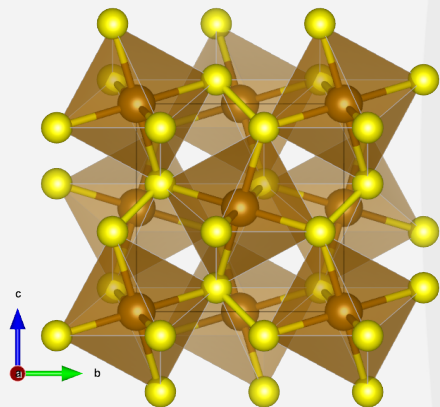
061  
 5.417800 5.417800 5.417800 90.000000 90.000000 90.000000  
 2  
 Fe 1 4a 0.000000 0.000000 0.000000  
 S 1 8c 0.384730 0.384730 0.384730

[Visualize this structure](#) [CIF File](#) [Cartesian Coordinates](#)

### FeS<sub>2</sub> | Pbcu (#61)

61  
 5.4178 5.4178 5.4178 90. 90. 90.  
 2  
 Fe 1 4a 0.000000 0.000000 0.000000  
 S 1 8c 0.384730 0.384730 0.384730

# TRANSLATIONENGLEICHE MAXIMAL SUBGROUPS

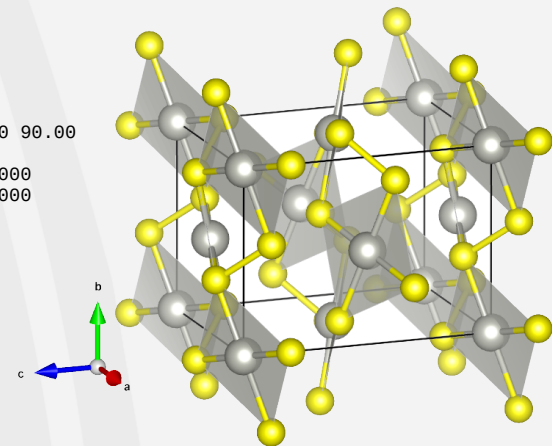


## FeS<sub>2</sub> | Pbca (#61)

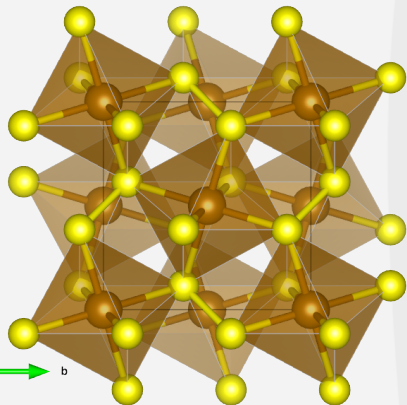
61  
5.4178 5.4178 5.4178 90. 90. 90.  
2  
Fe 1 4a 0.000000 0.000000 0.000000  
S 1 8c 0.384730 0.384730 0.384730

## PdS<sub>2</sub> | Pbca (#61)

61  
5.4650 5.5380 7.5250 90.00 90.00 90.00  
2  
Pd 1 4a 0.000000 0.500000 0.500000  
S 1 8c 0.104000 0.609000 0.916000



# TRANSLATIONENGLEICHE MAXIMAL SUBGROUPS

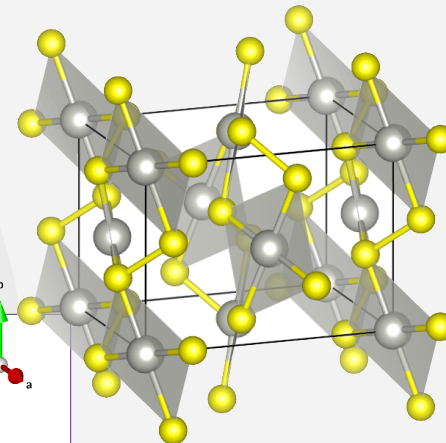


## FeS<sub>2</sub> | Pbc<sub>a</sub> (#61)

61  
 5.4178 5.4178 5.4178 90. 90. 90.  
 2  
 Fe 1 4a 0.000000 0.000000 0.000000  
 S 1 8c 0.384730 0.384730 0.384730

## PdS<sub>2</sub> | Pbc<sub>a</sub> (#61)

61  
 5.4650 5.5380 7.5250 90.00 90.00 90.00  
 2  
 Pd 1 4a 0.000000 0.500000 0.500000  
 S 1 8c 0.104000 0.609000 0.916000



### Finite Lagrangian Strain Tensor (finite deformation)

$$\begin{bmatrix} -0.008599 & 0.000000 & 0.000000 \\ 0.000000 & -0.021469 & 0.000000 \\ 0.000000 & 0.000000 & -0.240819 \end{bmatrix}$$

### Eigenvalues

-0.02147 -0.00860 -0.24082

### Degree of lattice distortion

0.08064

**Note:** The finite Lagrangian strain tensor can be calculated according to the formula:  $S = 0.5 (e + e^T + e^T e)$ , where,  $e = R_2 R_1^{-1} - I$  and,  $R_1$  and  $R_2$  are the standard root tensors of cell 1 and 2, and  $I$  is a 3x3 identity matrix

**Note:** The degree of lattice distortion is described here as the spontaneous strain (square root of the sum of squared eigenvalues of strain tensor) divided by 3

## Strain Tensor

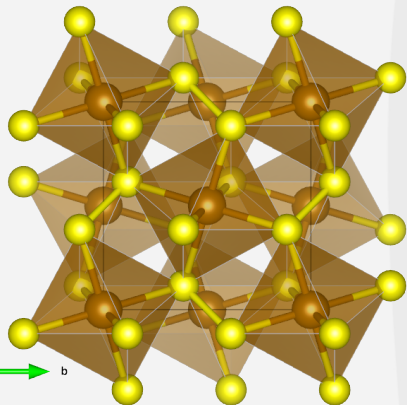
Unit cell 1:

Unit cell 2:

Show



# TRANSLATIONENGLEICHE MAXIMAL SUBGROUPS



## FeS<sub>2</sub> | Pbc<sub>a</sub> (#61)

61  
 5.4178 5.4178 5.4178 90. 90. 90.  
 2  
 Fe 1 4a 0.000000 0.000000 0.000000  
 S 1 8c 0.384730 0.384730 0.384730

## PdS<sub>2</sub> | Pbc<sub>a</sub> (#61)

61  
 5.4650 5.5380 7.5250 90.00 90.00 90.00  
 2  
 Pd 1 4a 0.000000 0.500000 0.500000  
 S 1 8c 0.104000 0.609000 0.916000

### Atom pairings and distances

Atom Mappings						
WP	Atom	Coordinates in S <sub>1</sub>		Atom	Coordinates in S <sub>2</sub>	
8c	(x,y,z)	S1	(0.384730,0.384730,0.384730)	S1	(0.396000,0.391000,0.416000)	
4a	(0,0,0)	Fe1	(0.000000,0.000000,0.000000)	Pd1	(0.000000,0.000000,0.000000)	

WP	Atom Structure1	Atom Structure2	Atomic Displacements				
			u <sub>x</sub>	u <sub>y</sub>	u <sub>z</sub>	u	
8c	(x,y,z)	S1	S1	0.0113	0.0063	0.0313	0.1833
4a	(0,0,0)	Fe1	Pd1	0.0000	0.0000	0.0000	0.0000

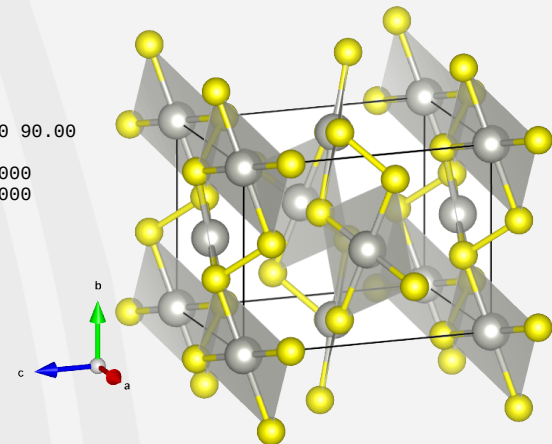
NOTE: u<sub>x</sub>, u<sub>y</sub> and u<sub>z</sub> are given in relative units. |u| is the absolute distance given in Å

### Evaluation of the structure similarity

S	d <sub>max</sub> (Å)	d <sub>av</sub> (Å)	Δ
0.0806	0.1833	0.1222	0.440

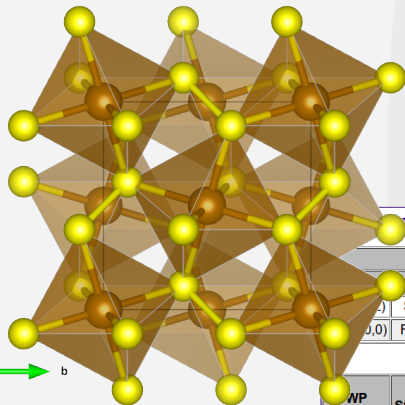
Transformation matrix (P, p): a,b,c ; 0,0,0

- Lattice and atomic position criteria:
  - The degree of lattice distortion (S) is the spontaneous strain (sum of the squared eigenvalues of the strain tensor divided by 3). For the given two structures, the degree of lattice distortion (S) is **0.0806**.
  - The maximum distance (d<sub>max</sub>) shows the maximal displacement between the atomic positions of the paired atoms. The maximum distance (d<sub>max</sub>) in this case is: **0.1833 Å**
- The arithmetic mean (d<sub>av</sub>) of the distance. In this case, the arithmetic mean (d<sub>av</sub>) is **0.1222 Å**
- The measure of similarity (Δ) (Bergerhoff *et al.*, 1998) is a function of the differences in atomic positions (weighted by the multiplicities of the sites) and the ratios of the corresponding lattice parameters of the structures. The measure of similarity (Δ) calculated for this case is **0.440**.



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

# TRANSLATIONENGLEICHE MAXIMAL SUBGROUPS



## FeS<sub>2</sub> | Pbc<sub>a</sub> (#61)

61  
 5.4178 5.4178 5.4178 90. 90. 90.  
 2  
 Fe 1 4a 0.000000 0.000000 0.000000  
 S 1 8c 0.384730 0.384730 0.384730

### Atom mappings and distances

Atom Mappings			
Atom	Coordinates in S <sub>1</sub>	Atom	Coordinates in S <sub>2</sub>
S	(0.384730,0.384730,0.384730)	S1	(0.396000,0.391000,0.416000)
Fe1	(0.000000,0.000000,0.000000)	Pd1	(0.000000,0.000000,0.000000)

WP	Atom Structure1	Atom Structure2	Atomic Displacements			
			u <sub>x</sub>	u <sub>y</sub>	u <sub>z</sub>	u
8c (x,y,z)	S1	S1	0.0113	0.0063	0.0313	0.1833
4a (0,0,0)	Fe1	Pd1	0.0000	0.0000	0.0000	0.0000

NOTE: u<sub>x</sub>, u<sub>y</sub> and u<sub>z</sub> are given in relative units. |u| is the absolute distance given in Å

### Evaluation of the structure similarity

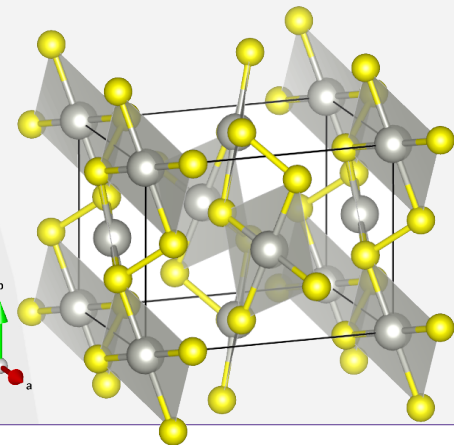
S	d <sub>max</sub> (Å)	d <sub>av</sub> (Å)	Δ
0.0806	0.1833	0.1222	0.440

Transformation matrix (P, p): a,b,c ; 0,0,0

- Lattice and atomic position criteria:
  - The degree of lattice distortion (S) is the spontaneous strain (sum of the squared eigenvalues of the strain tensor divided by 3). For the given two structures, the **degree of lattice distortion (S)** is **0.0806**.
  - The maximum distance (d<sub>max</sub>) shows the maximal displacement between the atomic positions of the paired atoms. The **maximum distance (d<sub>max</sub>)** in this case is: **0.1833 Å**
- The arithmetic mean (d<sub>av</sub>) of the distance. In this case, the **arithmetic mean (d<sub>av</sub>)** is **0.1222 Å**
- The measure of similarity (Δ) (Bergerhoff *et al.*, 1998) is a function of the differences in atomic positions (weighted by the multiplicities of the sites) and the ratios of the corresponding lattice parameters of the structures. The **measure of similarity (Δ)** calculated for this case is **0.440**.

## PdS<sub>2</sub> | Pbc<sub>a</sub> (#61)

061  
 5.4650 5.5380 7.5250 90.00 90.00 90.00  
 2  
 Pd 1 4a 0.000000 0.500000 0.500000  
 S 1 8c 0.104000 0.609000 0.916000



### Measure of similarity Δ

The measure of similarity is defined as

$$\Delta = [2^{1/2}\Delta(c) + 1] \Delta(d) - 1$$

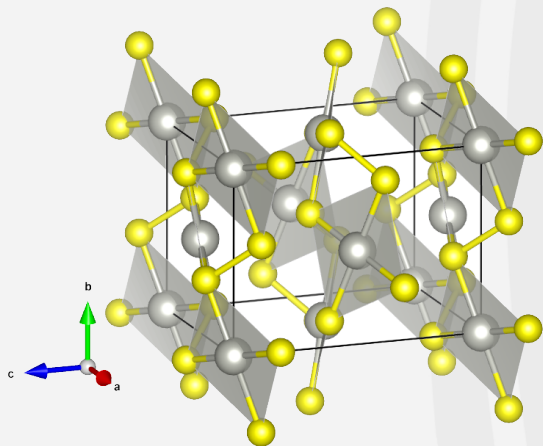
- Δ(c) is the sum of the weighted mean differences of the atomic coordinates of the structure 1 and 2:

$$\Delta(c) = \frac{\sum m[(x_1 - x_2)^2 + (y_1 - y_2)^2 + (z_1 - z_2)^2]^{1/2}}{\sum m}$$

- Δ(d) is the relation between the axial ratios of the structures 1 and 2:

$$\Delta(d) = \frac{[(b_1/a_1)(c_1/a_1)]}{[(b_2/a_2)(c_2/a_2)]}$$

# TRANSLATIONENGLEICHE MAXIMAL SUBGROUPS

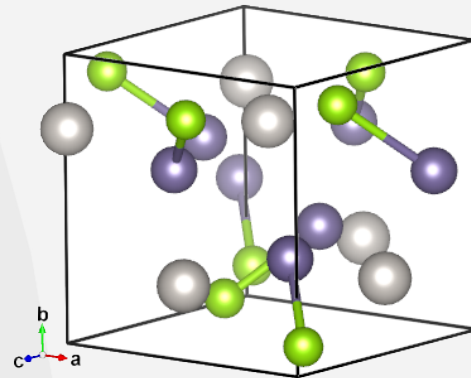


## PdS<sub>2</sub> | Pbc<sub>a</sub> (#61)

61  
 5.4650 5.5380 7.5250 90.00 90.00 90.00  
 2  
 Pd 1 4a 0.000000 0.500000 0.500000  
 S 1 8c 0.104000 0.609000 0.916000

## PtGeSe | Pca2<sub>1</sub> (#29)

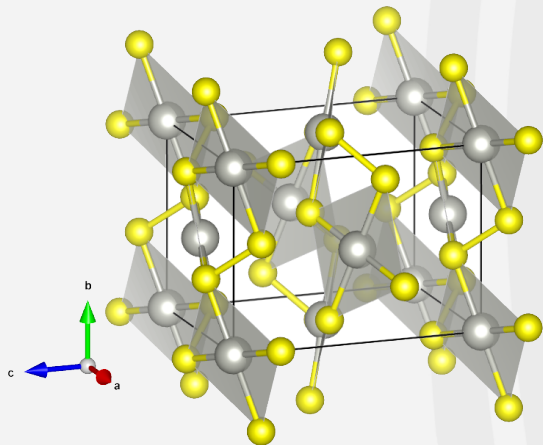
29  
 6.015 6.072 5.992 90. 90. 90.  
 3  
 Pt 1 4a 0.008600 0.742000 0.000000  
 Ge 1 4a 0.383300 0.136400 0.616800  
 Se 1 4a 0.619800 0.375900 0.382000



AT.	WP	SS	Representative	Atomic orbit
Pd1	4a (0,0,0)	-1	(0.000000, 0.500000, 0.500000)	(0.000000, 0.500000, 0.500000) (0.500000, 0.500000, 0.000000) (0.000000, 0.000000, 0.000000) (0.500000, 0.000000, 0.500000)
S1	8c (x,y,z)	1	(0.104000, 0.609000, 0.916000)	(0.104000, 0.609000, 0.916000) (0.396000, 0.391000, 0.416000) (0.896000, 0.109000, 0.584000) (0.604000, 0.891000, 0.084000) (0.896000, 0.391000, 0.084000) (0.604000, 0.609000, 0.584000) (0.104000, 0.891000, 0.416000) (0.396000, 0.109000, 0.916000)

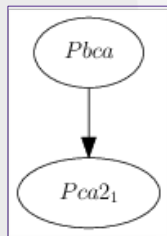
AT.	WP	SS	Representative	Atomic orbit
Pt1	4a (x,y,z)	1	(0.008600, 0.742000, 0.000000)	(0.008600, 0.742000, 0.000000) (0.991400, 0.258000, 0.500000) (0.508600, 0.258000, 0.000000) (0.491400, 0.742000, 0.500000)
Ge1	4a (x,y,z)	1	(0.383300, 0.136400, 0.616800)	(0.383300, 0.136400, 0.616800) (0.616700, 0.863600, 0.116800) (0.883300, 0.863600, 0.616800) (0.116700, 0.136400, 0.116800)
Se1	4a (x,y,z)	1	(0.619800, 0.375900, 0.382000)	(0.619800, 0.375900, 0.382000) (0.380200, 0.624100, 0.882000) (0.119800, 0.624100, 0.382000) (0.880200, 0.375900, 0.882000)

# TRANSLATIONENGLEICHE MAXIMAL SUBGROUPS



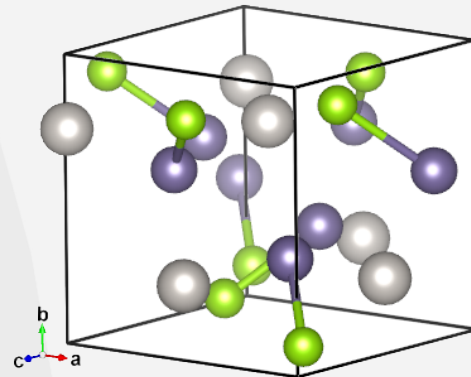
## PdS<sub>2</sub> | Pbc<sub>a</sub> (#61)

61  
 5.4650 5.5380 7.5250 90.00 90.00 90.00  
 2  
 Pd 1 4a 0.000000 0.500000 0.500000  
 S 1 8c 0.104000 0.609000 0.916000



## PtGeSe | Pca2<sub>1</sub> (#29)

29  
 6.015 6.072 5.992 90. 90. 90.  
 3  
 Pt 1 4a 0.008600 0.742000 0.000000  
 Ge 1 4a 0.383300 0.136400 0.616800  
 Se 1 4a 0.619800 0.375900 0.382000



AT.	WP	SS	Representative	Atomic orbit
Pd1	4a (0,0,0)	-1	(0.000000, 0.500000, 0.500000)	(0.000000, 0.500000, 0.500000) (0.500000, 0.500000, 0.000000) (0.000000, 0.000000, 0.000000) (0.500000, 0.000000, 0.500000)
S1	8c (x,y,z)	1	(0.104000, 0.609000, 0.916000)	(0.104000, 0.609000, 0.916000) (0.396000, 0.391000, 0.416000) (0.896000, 0.109000, 0.584000) (0.604000, 0.891000, 0.084000) (0.896000, 0.391000, 0.084000) (0.604000, 0.609000, 0.584000) (0.104000, 0.891000, 0.416000) (0.396000, 0.109000, 0.916000)

### Full Set of Possible Transformations for the chain 061 029 [2]

# 061 029 [2]

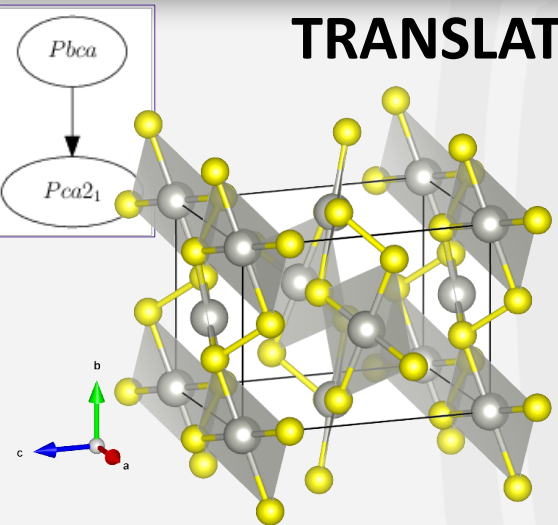
$$\begin{pmatrix} 0 & 1 & 0 & 1/4 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1/4 \end{pmatrix}$$

$$\begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 1/4 \\ 1 & 0 & 0 & 0 \end{pmatrix}$$

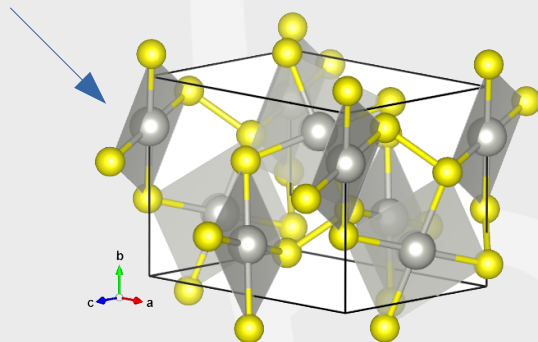
AT.	WP	SS	Representative	Atomic orbit
Pt1	4a (x,y,z)	1	(0.008600, 0.742000, 0.000000)	(0.008600, 0.742000, 0.000000) (0.991400, 0.258000, 0.500000) (0.508600, 0.258000, 0.000000) (0.491400, 0.742000, 0.500000)
Ge1	4a (x,y,z)	1	(0.383300, 0.136400, 0.616800)	(0.383300, 0.136400, 0.616800) (0.616700, 0.863600, 0.116800) (0.883300, 0.863600, 0.616800) (0.116700, 0.136400, 0.116800)
Se1	4a (x,y,z)	1	(0.619800, 0.375900, 0.382000)	(0.619800, 0.375900, 0.382000) (0.380200, 0.624100, 0.882000) (0.119800, 0.624100, 0.382000) (0.880200, 0.375900, 0.882000)

# TRANSLATIONENGLEICHE MAXIMAL SUBGROUPS



## $PdS_2$ | $Pbca$ (#61)

```
61
5.4650 5.5380 7.5250 90.00 90.00 90.00
2
Pd 1 4a 0.000000 0.500000 0.500000
S 1 8c 0.104000 0.609000 0.916000
```



## $PdS_2$ | $Pca2_1$ (#29)

```
29
7.5250 5.5380 5.4650 90.00 90.00 90.00
3
Pd 1 4a 0.500000 0.250000 0.000000
S 1 4a 0.916000 0.359000 0.896000
S 2 4a 0.416000 0.141000 0.604000
```

## Transform structure

Transformation matrix:  $c, b+0.25, -a$

## High symmetry structure

```
61
5.4650 5.5380 7.5250 90.00 90.00 90.00
2
Pd 1 4a 0.000000 0.500000 0.500000
S 1 8c 0.104000 0.609000 0.916000
```

[Visualize this structure](#) [CIF File](#) [Cartesian Coordinates](#)

## Low symmetry structure

```
029
7.525000 5.538000 5.465000 90.000000 90.000000 90.000000
3
Pd 1 4a 0.500000 0.250000 0.000000
S 1 4a 0.916000 0.359000 0.896000
S 1_2 4a 0.416000 0.141000 0.604000
```

[Visualize this structure](#) [CIF File](#) [Cartesian Coordinates](#)

Space Group: 29

Lattice Parameters: 7.525000 5.538000 5.465000 90 90 90

AT	#	WP	Coordinates		
Pd	1	4a	1/2	1/4	0
S	1	4a	0.91600	0.35900	0.89600
S	1_2	4a	0.41600	0.14100	0.60400

## Full Set of Possible Transformations for the chain 061 029 [2]

# 061 029 [2]

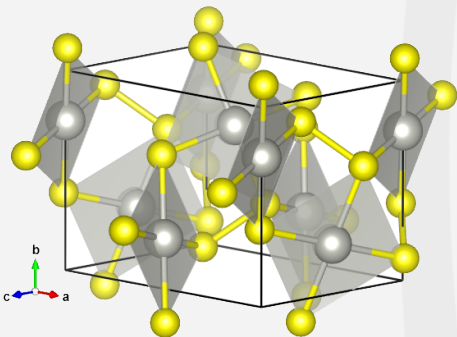
$$\begin{pmatrix} 0 & 1 & 0 & 1/4 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1/4 \end{pmatrix}$$

$$\begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 1/4 \\ 1 & 0 & 0 & 0 \end{pmatrix}$$

$c, b, -a; 0, \frac{1}{4}, 0$

# TRANSLATIONENGLEICHE MAXIMAL SUBGROUPS

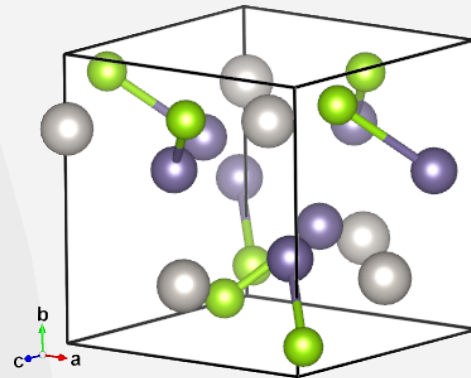


## PdS<sub>2</sub> | Pca2<sub>1</sub> (#29)

29  
 7.5250 5.5380 5.4650 90.00 90.00 90.00  
 3  
 Pd 1 4a 0.500000 0.250000 0.000000  
 S 1 4a 0.916000 0.359000 0.896000  
 S 2 4a 0.416000 0.141000 0.604000

## PtGeSe | Pca2<sub>1</sub> (#29)

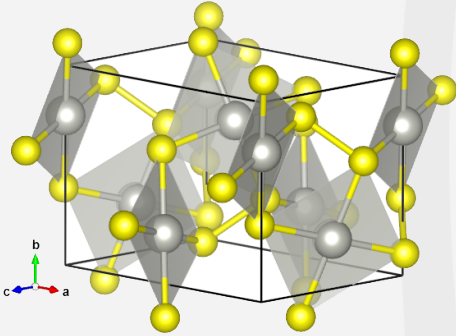
29  
 6.015 6.072 5.992 90. 90. 90.  
 3  
 Pt 1 4a 0.008600 0.742000 0.000000  
 Ge 1 4a 0.383300 0.136400 0.616800  
 Se 1 4a 0.619800 0.375900 0.382000



AT.	WP	SS	Representative	Atomic orbit
Pd1	4a (x,y,z)	1	(0.500000, 0.250000, 0.000000)	(0.500000, 0.250000, 0.000000) (0.500000, 0.750000, 0.500000) (0.000000, 0.750000, 0.000000) (0.000000, 0.250000, 0.500000)
S1	4a (x,y,z)	1	(0.916000, 0.359000, 0.896000)	(0.916000, 0.359000, 0.896000) (0.084000, 0.641000, 0.396000) (0.416000, 0.641000, 0.896000) (0.584000, 0.359000, 0.396000)
S2	4a (x,y,z)	1	(0.416000, 0.141000, 0.604000)	(0.416000, 0.141000, 0.604000) (0.584000, 0.859000, 0.104000) (0.916000, 0.859000, 0.604000) (0.084000, 0.141000, 0.104000)

AT.	WP	SS	Representative	Atomic orbit
Pt1	4a (x,y,z)	1	(0.008600, 0.742000, 0.000000)	(0.008600, 0.742000, 0.000000) (0.991400, 0.258000, 0.500000) (0.508600, 0.258000, 0.000000) (0.491400, 0.742000, 0.500000)
Ge1	4a (x,y,z)	1	(0.383300, 0.136400, 0.616800)	(0.383300, 0.136400, 0.616800) (0.616700, 0.863600, 0.116800) (0.883300, 0.863600, 0.616800) (0.116700, 0.136400, 0.116800)
Se1	4a (x,y,z)	1	(0.619800, 0.375900, 0.382000)	(0.619800, 0.375900, 0.382000) (0.380200, 0.624100, 0.882000) (0.119800, 0.624100, 0.382000) (0.880200, 0.375900, 0.882000)

# TRANSLATIONENGLEICHE MAXIMAL SUBGROUPS

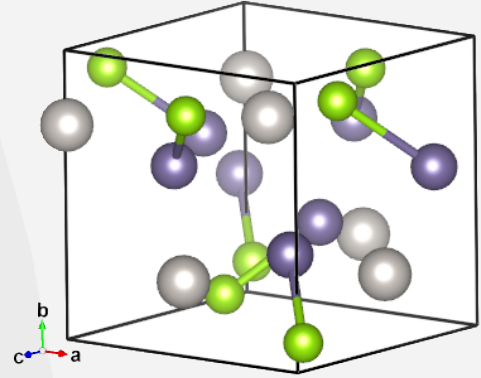


## PdS<sub>2</sub> | Pca2<sub>1</sub> (#29)

29  
 7.5250 5.5380 5.4650 90.00 90.00 90.00  
 3  
 Pd 1 4a 0.500000 0.250000 0.000000  
 S 1 4a 0.916000 0.359000 0.896000  
 S 2 4a 0.416000 0.141000 0.604000

## PtGeSe | Pca2<sub>1</sub> (#29)

29  
 6.015 6.072 5.992 90. 90. 90.  
 3  
 Pt 1 4a 0.008600 0.742000 0.000000  
 Ge 1 4a 0.383300 0.136400 0.616800  
 Se 1 4a 0.619800 0.375900 0.382000



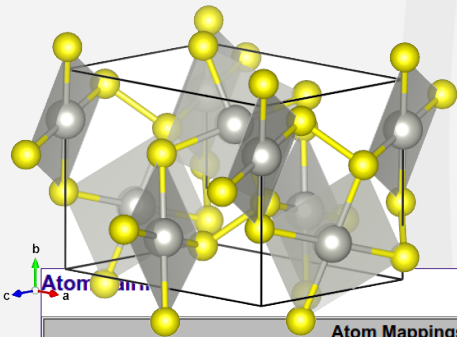
AT.	WP	SS	Representative	Atomic orbit
Pd1	4a (x,y,z)	1	(0.500000, 0.250000, 0.000000)	(0.500000, 0.250000, 0.000000) (0.500000, 0.750000, 0.500000) (0.000000, 0.750000, 0.000000) (0.000000, 0.250000, 0.500000)
S1	4a (x,y,z)	1	(0.916000, 0.359000, 0.896000)	(0.916000, 0.359000, 0.896000) (0.084000, 0.641000, 0.396000) (0.416000, 0.641000, 0.896000) (0.584000, 0.359000, 0.396000)
S2	4a (x,y,z)	1	(0.416000, 0.141000, 0.604000)	(0.416000, 0.141000, 0.604000) (0.584000, 0.859000, 0.104000) (0.916000, 0.859000, 0.604000) (0.084000, 0.141000, 0.104000)

AT.	WP	SS	Representative	Atomic orbit
Pt1	4a (x,y,z)	1	(0.008600, 0.742000, 0.000000)	(0.008600, 0.742000, 0.000000) (0.991400, 0.258000, 0.500000) (0.508600, 0.258000, 0.000000) (0.491400, 0.742000, 0.500000)
Ge1	4a (x,y,z)	1	(0.383300, 0.136400, 0.616800)	(0.383300, 0.136400, 0.616800) (0.616700, 0.863600, 0.116800) (0.883300, 0.863600, 0.616800) (0.116700, 0.136400, 0.116800)
Se1	4a (x,y,z)	1	(0.619800, 0.375900, 0.382000)	(0.619800, 0.375900, 0.382000) (0.380200, 0.624100, 0.882000) (0.119800, 0.624100, 0.382000) (0.880200, 0.375900, 0.882000)

# TRANSLATIONENGLEICHE MAXIMAL SUBGROUPS

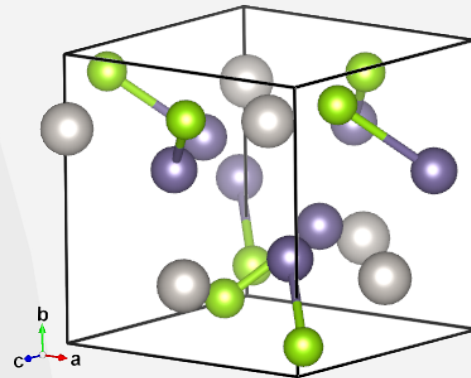
## PdS<sub>2</sub> | Pca2<sub>1</sub> (#29)

29  
 7.5250 5.5380 5.4650 90.00 90.00 90.00  
 3  
 Pd 1 4a 0.500000 0.250000 0.000000  
 S 1 4a 0.916000 0.359000 0.896000  
 S 2 4a 0.416000 0.141000 0.604000



## PtGeSe | Pca2<sub>1</sub> (#29)

29  
 6.015 6.072 5.992 90. 90. 90.  
 3  
 Pt 1 4a 0.008600 0.742000 0.000000  
 Ge 1 4a 0.383300 0.136400 0.616800  
 Se 1 4a 0.619800 0.375900 0.382000



### Atom Mappings

WP	Atom	Coordinates in S <sub>1</sub>	Atom	Coordinates in S <sub>2</sub>
4a	(x,y,z)	S2 (0.416000,0.141000,0.604000)	Ge1	(0.383300,0.136400,0.617200)
4a	(x,y,z)	S1 (0.916000,0.359000,0.896000)	Se1	(0.880200,0.375900,0.882400)
4a	(x,y,z)	Pd1 (0.500000,0.250000,0.000000)	Pt1	(0.508600,0.258000,0.000400)

WP	Atom Structure1	Atom Structure2	Atomic Displacements				
			u <sub>x</sub>	u <sub>y</sub>	u <sub>z</sub>	u	
4a	(x,y,z)	S2	Ge1	-0.0327	-0.0046	0.0132	0.2577
4a	(x,y,z)	S1	Se1	-0.0358	0.0169	-0.0136	0.2947
4a	(x,y,z)	Pd1	Pt1	0.0086	0.0080	0.0004	0.0785

Transformation matrix (P, p): a,b,c ; 0,0,-0.00040

NOTE: u<sub>x</sub>, u<sub>y</sub> and u<sub>z</sub> are given in relative units. |u| is the absolute distance given in Å

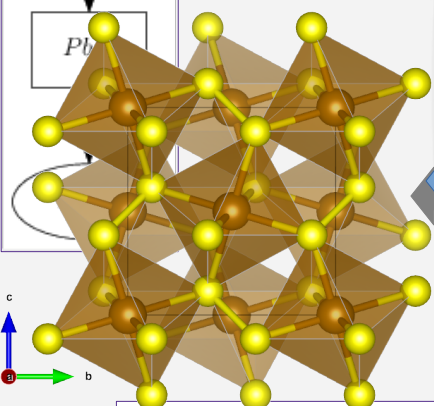
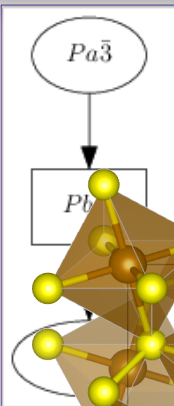
### Evaluation of the structure similarity

S	d <sub>max.</sub> (Å)	d <sub>av.</sub> (Å)	Δ
0.1022	0.2947	0.2103	0.961

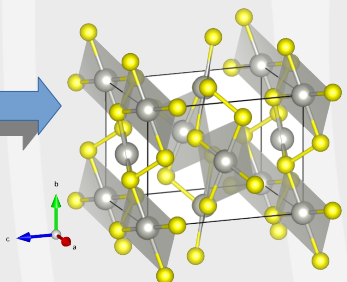
default



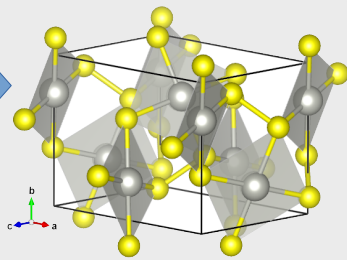
# TRANSLATIONENGLEICHE MAXIMAL SUBGROUPS



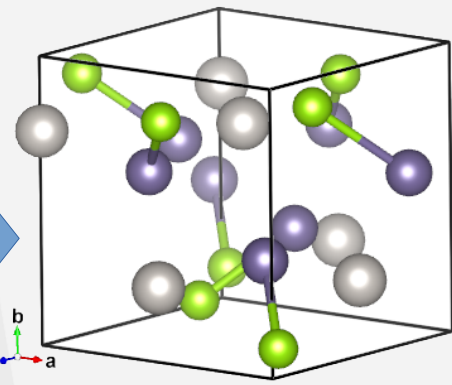
Transformation matrix (P, p): a,b,c ; 0,0,0



Transformation matrix: c,b+0.25,-a



Transformation matrix (P, p): a,b,c ; 0,0,-0.00040



## FeS<sub>2</sub> | Pbca (#61)

61  
 5.4178 5.4178 5.4178 90. 90. 90.  
 2  
 Fe 1 4a 0.000000 0.000000 0.000000  
 S 1 8c 0.384730 0.384730 0.384730

## PdS<sub>2</sub> | Pbca (#61)

61  
 5.4650 5.5380 7.5250 90.00 90.00  
 90.00  
 2  
 Pd 1 4a 0.000000 0.500000 0.500000  
 S 1 8c 0.104000 0.609000 0.916000

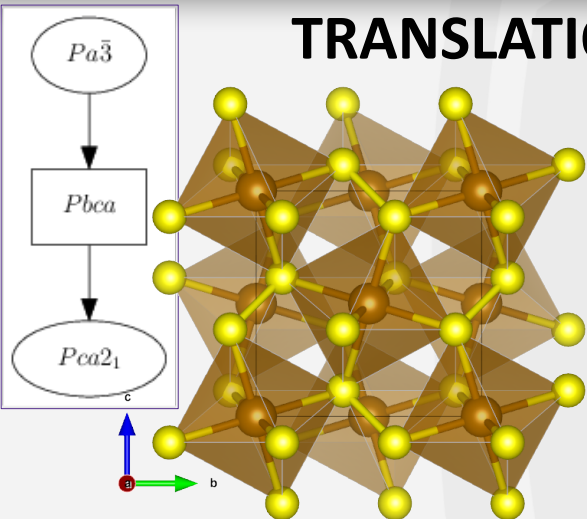
## PdS<sub>2</sub> | Pca2<sub>1</sub> (#29)

29  
 7.5250 5.5380 5.4650 90.00 90.00 90.00  
 3  
 Pd 1 4a 0.500000 0.250000 0.000000  
 S 1 4a 0.916000 0.359000 0.896000  
 S 2 4a 0.416000 0.141000 0.60400

## PtGeSe | Pca2<sub>1</sub> (#29)

29  
 6.015 6.072 5.992 90. 90. 90.  
 3  
 Pt 1 4a 0.008600 0.742000 0.000000  
 Ge 1 4a 0.383300 0.136400 0.616800  
 Se 1 4a 0.619800 0.375900 0.382000

# TRANSLATIONS



## FeS<sub>2</sub> (Pyrite) | Pa-3 (#205)

205  
 5.4178 5.4178 5.4178 90. 90. 90.  
 2  
 Fe 1 4a 0.000000 0.000000 0.000000  
 S 1 8c 0.384730 0.384730 0.384730

```
In [2]: P_205_061 = np.array([[1,0,0,0],\
                             [0,1,0,0],\
                             [0,0,1,0],\
                             [0,0,0,1]])
print(P_205_061)
```

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

```
In [3]: P_061_029 = np.array([[0,0,-1,0],\
                               [0,1,0,0.25],\
                               [1,0,0,0],\
                               [0,0,0,1]])
with np.printoptions(formatter=\
                      {'float': '{: 0.5f}'.format}):
print(P_061_029)
```

```
[[ 0.00000  0.00000 -1.00000  0.00000]
 [ 0.00000  1.00000  0.00000  0.25000]
 [ 1.00000  0.00000  0.00000  0.00000]
 [ 0.00000  0.00000  0.00000  1.00000]]
```

```
In [4]: P_029_029 = np.array([[1,0,0,0],\
                               [0,1,0,0],\
                               [0,0,1,-0.0004],\
                               [0,0,0,1]])
with np.printoptions(formatter=\
                      {'float': '{: 0.5f}'.format}):
print(P_061_029)
```

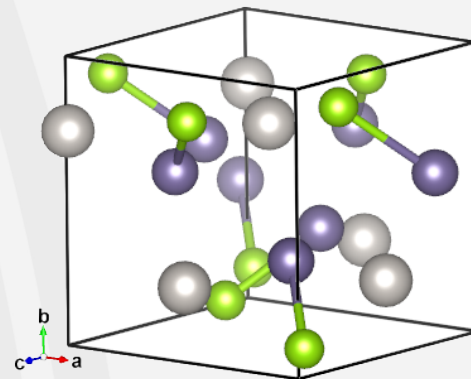
```
[[ 0.00000  0.00000 -1.00000  0.00000]
 [ 0.00000  1.00000  0.00000  0.25000]
 [ 1.00000  0.00000  0.00000  0.00000]
 [ 0.00000  0.00000  0.00000  1.00000]]
```

```
In [5]: P = np.linalg.multi_dot(\
        (P_205_061,P_061_029,P_029_029))
with np.printoptions(formatter=\
                      {'float': '{: 0.5f}'.format}):
print(P)
```

```
[[ 0.00000  0.00000 -1.00000  0.00040]
 [ 0.00000  1.00000  0.00000  0.25000]
 [ 1.00000  0.00000  0.00000  0.00000]
 [ 0.00000  0.00000  0.00000  1.00000]]
```

$c, b, -a; 0.0004, \frac{1}{4}, 0$

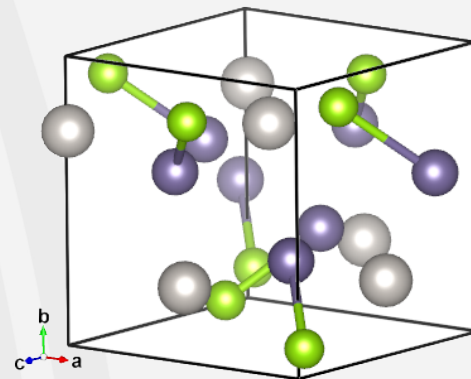
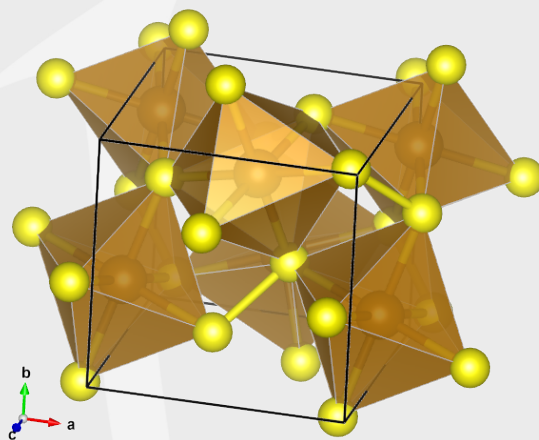
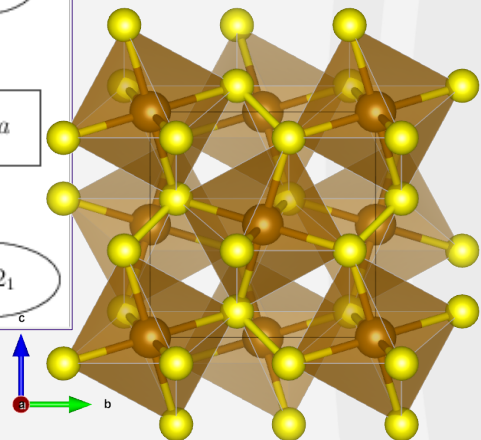
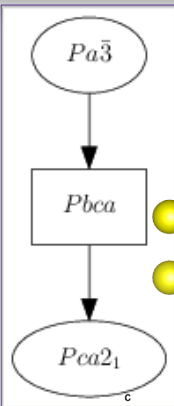
# LOCAL SUBGROUPS



## PtGeSe | Pca2<sub>1</sub> (#29)

29  
 6.015 6.072 5.992 90. 90. 90.  
 3  
 Pt 1 4a 0.008600 0.742000 0.000000  
 Ge 1 4a 0.383300 0.136400 0.616800  
 Se 1 4a 0.619800 0.375900 0.382000

# TRANSLATIONENGLEICHE MAXIMAL SUBGROUPS



**FeS<sub>2</sub> (Pyrite) | Pa-3 (#205)**

205  
5.4178 5.4178 5.4178 90. 90. 90.  
2  
Fe 1 4a 0.000000 0.000000 0.000000  
S 1 8c 0.384730 0.384730 0.384730



**FeS<sub>2</sub> | Pca2<sub>1</sub> (#29)**

29  
5.4178 5.4178 5.4178 90.00 90.00 90.00  
3  
Fe 1 4a 0.000000 0.750000 0.000400  
S 1 4a 0.384730 0.134730 0.615670  
S 2 4a 0.884730 0.365270 0.885130

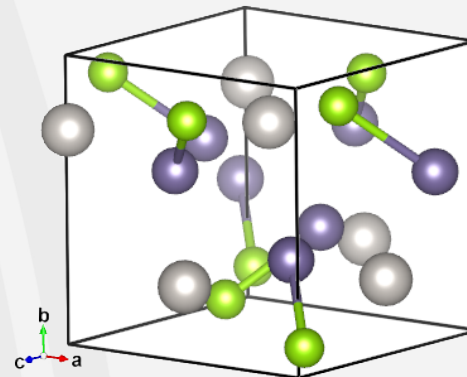
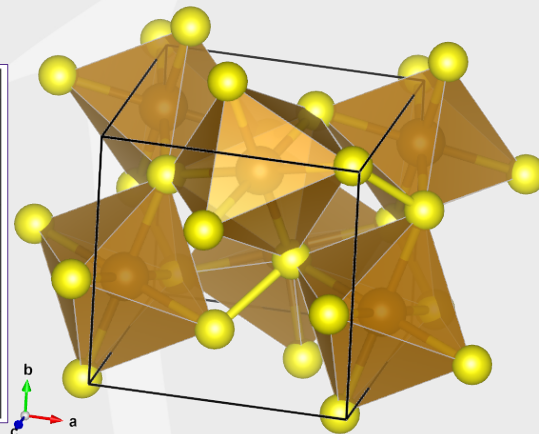


**PtGeSe | Pca2<sub>1</sub> (#29)**

29  
6.015 6.072 5.992 90. 90. 90.  
3  
Pt 1 4a 0.008600 0.742000 0.000000  
Ge 1 4a 0.383300 0.136400 0.616800  
Se 1 4a 0.619800 0.375900 0.382000

# TRANSLATIONENGLEICHE MAXIMAL SUBGROUPS

AT.	WP	SS	Representative	Atomic orbit
Fe1	4a (x,y,z)	1	(0.000000, 0.750000, 0.000400)	(0.000000, 0.750000, 0.000400) (0.000000, 0.250000, 0.500400) (0.500000, 0.250000, 0.000400) (0.500000, 0.750000, 0.500400)
S1	4a (x,y,z)	1	(0.384730, 0.134730, 0.615670)	(0.384730, 0.134730, 0.615670) (0.615270, 0.865270, 0.115670) (0.884730, 0.865270, 0.615670) (0.115270, 0.134730, 0.115670)
S1_2	4a (x,y,z)	1	(0.884730, 0.365270, 0.885130)	(0.884730, 0.365270, 0.885130) (0.115270, 0.634730, 0.385130) (0.384730, 0.634730, 0.885130) (0.615270, 0.365270, 0.385130)



**FeS<sub>2</sub> | Pca2<sub>1</sub> (#29)**

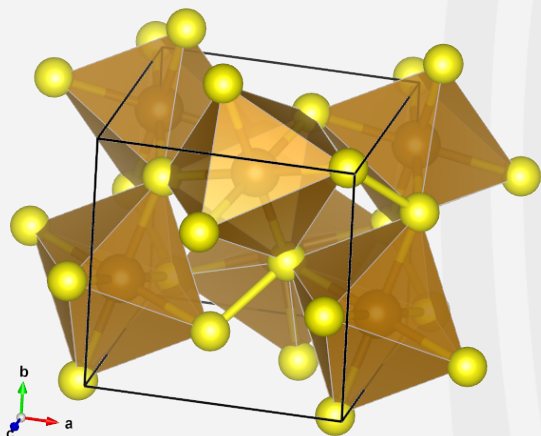
29  
5.4178 5.4178 5.4178 90.00 90.00 90.00  
3  
Fe 1 4a 0.000000 0.750000 0.000400  
S 1 4a 0.384730 0.134730 0.615670  
S 2 4a 0.884730 0.365270 0.885130



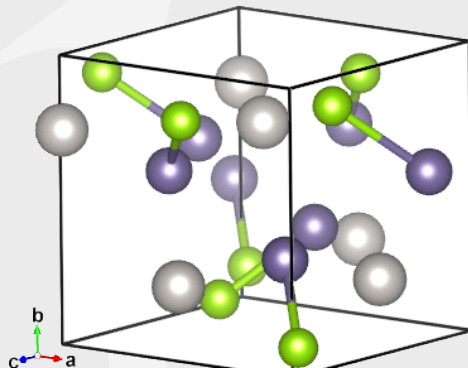
**PtGeSe | Pca2<sub>1</sub> (#29)**

29  
6.015 6.072 5.992 90. 90. 90.  
3  
Pt 1 4a 0.008600 0.742000 0.000000  
Ge 1 4a 0.383300 0.136400 0.616800  
Se 1 4a 0.619800 0.375900 0.382000

# TRANSLATIONENGLEICHE MAXIMAL SUBGROUPS



**FeS<sub>2</sub> | Pca2<sub>1</sub> (#29)**



**PtGeSe | Pca2<sub>1</sub> (#29)**

Transformation matrix (P, p): a,b,c ; 0,0,0.00080

Matrix form:

$$(P, p) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0.00080 \end{pmatrix}$$

## Atom pairings and distances

Atom Mappings						
WP	Atom	Coordinates in S <sub>1</sub>		Atom	Coordinates in S <sub>2</sub>	
4a	(x,y,z)	Ge1	(0.383300,0.136400,0.616800)	S1	(0.384730,0.134730,0.614870)	
4a	(x,y,z)	Pt1	(0.008600,0.742000,0.000000)	Fe1	(0.000000,0.750000,0.999600)	
4a	(x,y,z)	Se1	(0.619800,0.375900,0.382000)	S2	(0.615270,0.365270,0.384330)	

WP	Atom Structure1	Atom Structure2	Atomic Displacements				
			u <sub>x</sub>	u <sub>y</sub>	u <sub>z</sub>	u	
4a	(x,y,z)	Ge1	S1	0.0014	-0.0017	-0.0019	0.0176
4a	(x,y,z)	Pt1	Fe1	-0.0086	0.0080	-0.0004	0.0710
4a	(x,y,z)	Se1	S2	-0.0045	-0.0106	0.0023	0.0714

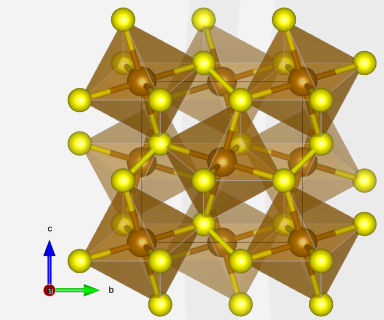
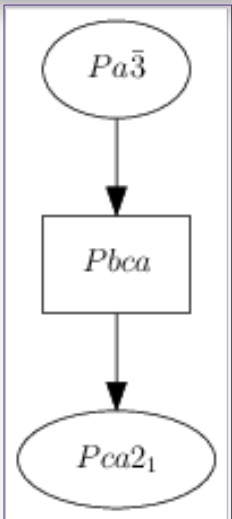
NOTE: u<sub>x</sub>, u<sub>y</sub> and u<sub>z</sub> are given in relative units. |u| is the absolute distance given in Å

## Evaluation of the structure similarity

S	d <sub>max</sub> (Å)	d <sub>av</sub> (Å)	Δ
0.0686	0.0714	0.0533	0.018

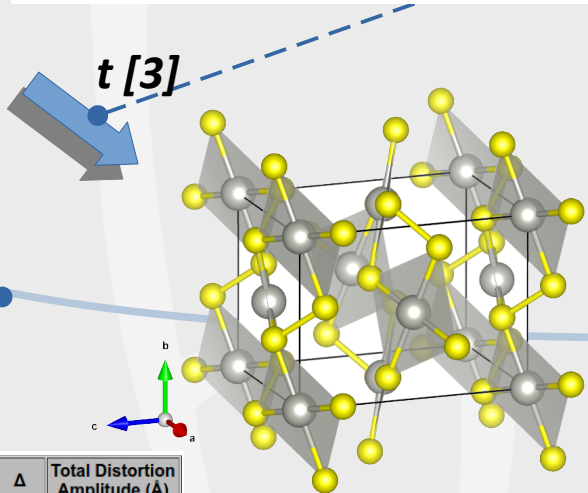
1<sup>st</sup>: PtGeSe, 2<sup>nd</sup>: FeS<sub>2</sub>

# TRANSLATIONENGLEICHE MAXIMAL SUBGROUPS

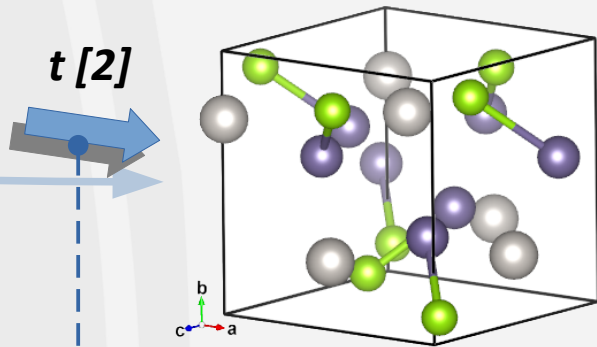


FeS<sub>2</sub> (Pyrite) | Pa-3 (#205)

Transformation Matrix	Matrix Form	S	d <sub>max</sub> (Å)	d <sub>avg</sub> (Å)	Axes ratios	Δ	Total Distortion Amplitude (Å)
a,b,c ; 0,1/2,1/2 <a href="#">Details</a>	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1/2 \\ 0 & 0 & 1 & 1/2 \end{pmatrix}$	0.0806	0.2457	0.1638	1.013 1.359 0.726	0.440	0.6949



PdS<sub>2</sub> | Pbca (#61)



PtGeSe | Pca2<sub>1</sub> (#29)

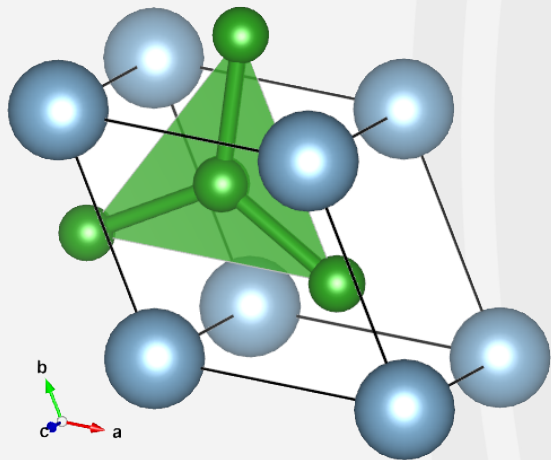
Transformation Matrix	Matrix Form	S	d <sub>max</sub> (Å)	d <sub>avg</sub> (Å)	Axes ratios	Δ	Total Distortion Amplitude (Å)
-b,a,c ; 3/4,-1/2,0.00040 <a href="#">Details</a>	$\begin{pmatrix} 0 & 1 & 0 & 3/4 \\ -1 & 0 & 0 & -1/2 \\ 0 & 0 & 1 & 0.00040 \end{pmatrix}$	0.0554	0.0714	0.0533	1.009 0.987 1.004	0.018	0.2044

Transformation Matrix	Matrix Form	S	d <sub>max</sub> (Å)	d <sub>avg</sub> (Å)	Axes ratios	Δ	Total Distortion Amplitude (Å)
c,b,-a ; -0.00040,3/4,1/2 <a href="#">Details</a>	$\begin{pmatrix} 0 & 0 & -1 & -0.00040 \\ 0 & 1 & 0 & 3/4 \\ 1 & 0 & 0 & 1/2 \end{pmatrix}$	0.1022	0.2521	0.1790	1.372 1.000 0.729	0.961	0.6762

<https://www.cryst.ehu.es/cryst/rel3.html>

<http://www.cryst.ehu.es>

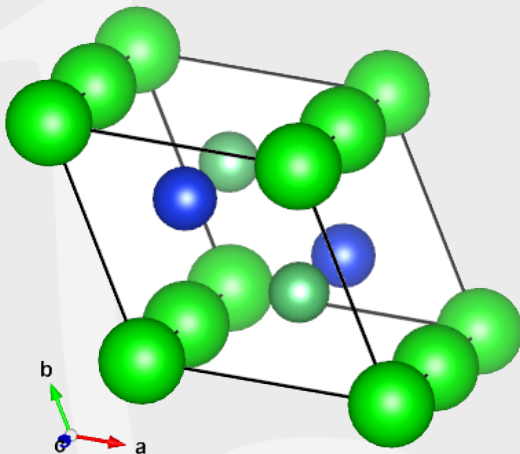
# KLASSENGLEICHE MAXIMAL SUBGROUPS



## AlB<sub>2</sub> | P6/mmm (#191)

191  
 3.00390 3.00390 3.28060 90 90 120  
 2  
 Al 1 1a 0.000000 0.000000 0.000000  
 B 1 2d 0.333333 0.666667 0.500000

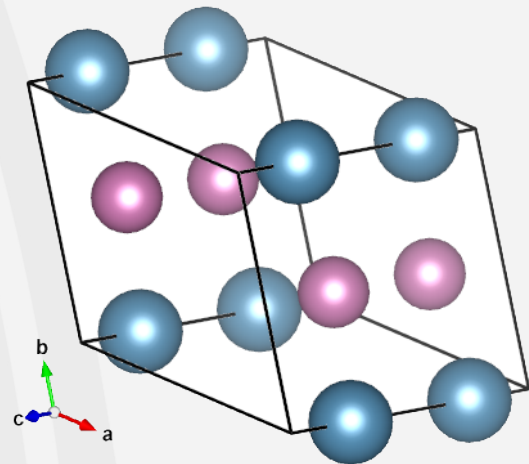
Alarco, J. A., Talbot, P. C., & Mackinnon, I. D. (2015). Phonon anomalies predict superconducting  $T_c$  for AlB<sub>2</sub>-type structures. *Physical Chemistry Chemical Physics*, 17(38), 25090-25099.



## ZrBeSi | P6<sub>3</sub>/mmc (#194)

194  
 3.722 3.722 7.232 90. 90. 120.  
 3  
 Zr 1 2a 0 0 0  
 Be 1 2c 0.3333 0.6667 0.250  
 Si 2 2d 0.3333 0.6667 0.750

Rudy, E., Benesovsky, F., Nowotny, H., & Toth, L. E. (1961). Die Kristallstruktur von HfBe<sub>2</sub>, HfBe<sub>13</sub> und HfBeSi; Teilsysteme: MeBe<sub>2</sub>-MeB<sub>2</sub>-MeSi<sub>2</sub> (Me= Zr, Hf). *Monatshefte für Chemie und verwandte Teile anderer Wissenschaften*, 92(3), 692-700.



## CaIn<sub>2</sub> | P6<sub>3</sub>/mmc (#194)

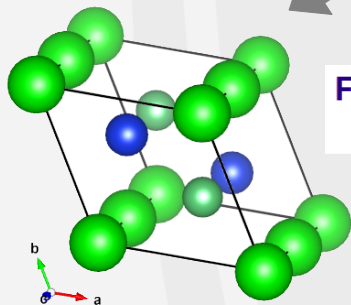
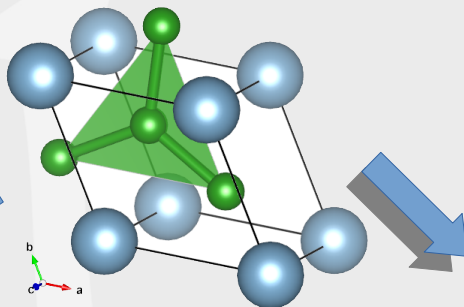
194  
 4.892 4.892 7.739 90.00 90.00 120.00  
 2  
 In 1 4f 0.6667 0.3333 0.04763  
 Ca 1 2b 0.0000 0.0000 0.2500

Wendorff, M., & Roehr, C. (2005). Binary Inides Al<sub>n</sub>x (x: 1, 2, 4; A: Ca, Sr, Ba, K, Rb)—Studies on Structural Chemistry and Chemical Bonding. *Cheminform*, 36(16).

# KLASSENGLEICHE MAXIMAL SUBGROUPS

## $\text{AlB}_2$ | $P6/mmm$ (#191)

191  
 3.00390 3.00390 3.28060 90 90 120  
 2  
 Al 1 1a 0.000000 0.000000 0.000000  
 B 1 2d 0.333333 0.666667 0.500000



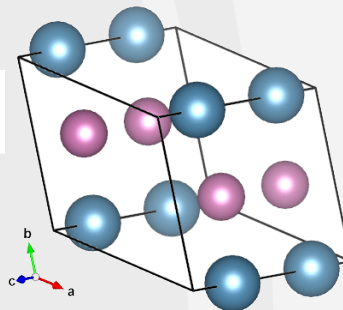
## $\text{ZrBeSi}$ | $P6_3/mmc$ (#194)

194  
 3.722 3.722 7.232 90. 90. 120.  
 3  
 Zr 1 2a 0 0 0  
 Be 1 2c 0.3333 0.6667 0.250  
 Si 2 2d 0.3333 0.6667 0.750

Full Set of Possible Transformations  
 for the chain 191 194 [2]

# 191 194 [2]

$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix}$
$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$



## $\text{CaIn}_2$ | $P6_3/mmc$ (#194)

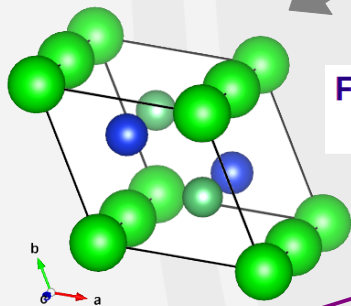
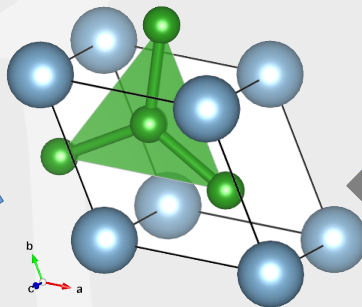
194  
 4.892 4.892 7.739 90.00 90.00 120.00  
 2  
 In 1 4f 0.6667 0.3333 0.04763  
 Ca 1 2b 0.0000 0.0000 0.2500



# KLASSENGLEICHE MAXIMAL SUBGROUPS

## $\text{AlB}_2$ | $P6/mmm$ (#191)

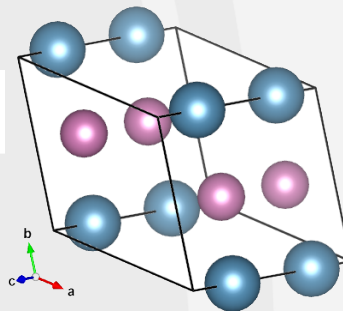
191  
 3.00390 3.00390 3.28060 90 90 120  
 2  
 Al 1 1a 0.000000 0.000000 0.000000  
 B 1 2d 0.333333 0.666667 0.500000



Full Set of Possible Transformations  
for the chain 191 194 [2]

# 191 194 [2]

$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix}$
$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$



## $\text{ZrBeSi}$ | $P6_3/mmc$ (#194)

194  
 3.722 3.722 7.232 90. 90. 120.  
 3  
 Zr 1 2a 0 0 0  
 Be 1 2c 0.3333 0.6667 0.250  
 Si 2 2d 0.3333 0.6667 0.750

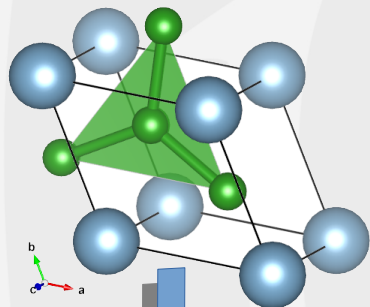
## $\text{CaIn}_2$ | $P6_3/mmc$ (#194)

194  
 4.892 4.892 7.739 90.00 90.00 120.00  
 2  
 In 1 4f 0.6667 0.3333 0.04763  
 Ca 1 2b 0.0000 0.0000 0.2500

# KLASSENGLEICHE MAXIMAL SUBGROUPS

## AlB<sub>2</sub> | P6/mmm (#191)

191  
 3.00390 3.00390 3.28060 90 90 120  
 2  
 Al 1 1a 0.000000 0.000000 0.000000  
 B 1 2d 0.333333 0.666667 0.500000

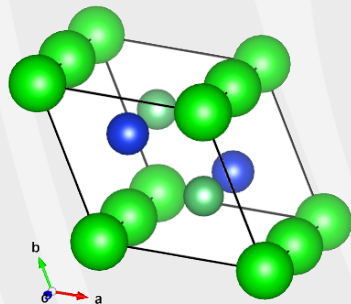


$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix}$$



## ZrBeSi | P6<sub>3</sub>/mmc (#194)

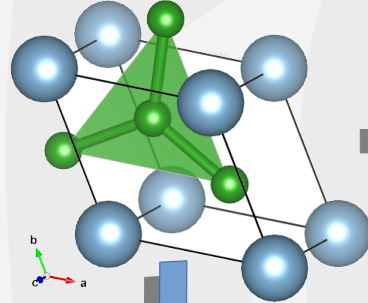
194  
 3.722 3.722 7.232 90. 90. 120.  
 3  
 Zr 1 2a 0 0 0  
 Be 1 2c 0.3333 0.6667 0.250  
 Si 2 2d 0.3333 0.6667 0.750



# KLASSENGLEICHE MAXIMAL SUBGROUPS

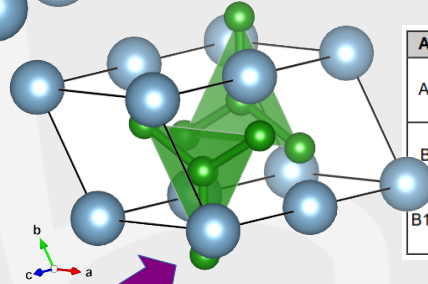
## AlB<sub>2</sub> | P6/mmm (#191)

191  
 3.00390 3.00390 3.28060 90 90 120  
 2  
 Al 1 1a 0.000000 0.000000 0.000000  
 B 1 2d 0.333333 0.666667 0.500000



## AlB<sub>2</sub> | P6<sub>3</sub>/mmc (#194)

194  
 3.003900 3.003900 6.561200 90 90 120  
 3  
 Al 1 2a 0.000000 0.000000 0.000000  
 B 1 2c 0.333333 0.666667 0.250000  
 B 2 2d 0.666667 0.333333 0.250000

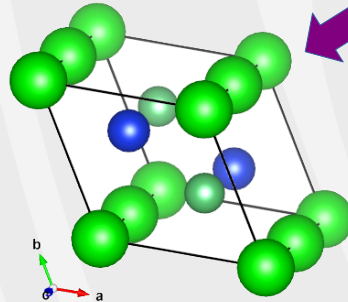


AT.	WP	SS	Representative	Atomic orbit
Al1	2a (0,0,0)	-3m.	(0.000000, 0.000000, 0.000000)	(0.000000, 0.000000, 0.000000) (0.000000, 0.000000, 0.500000)
B1	2c (1/3,2/3,1/4)	-6m2	(0.333333, 0.666667, 0.250000)	(0.333333, 0.666667, 0.250000) (0.666667, 0.333333, 0.750000)
B1_2	2d (1/3,2/3,3/4)	-6m2	(0.666667, 0.333333, 0.250000)	(0.666667, 0.333333, 0.250000) (0.333333, 0.666667, 0.750000)

1	0	0	0
0	1	0	0
0	0	2	0

## ZrBeSi | P6<sub>3</sub>/mmc (#194)

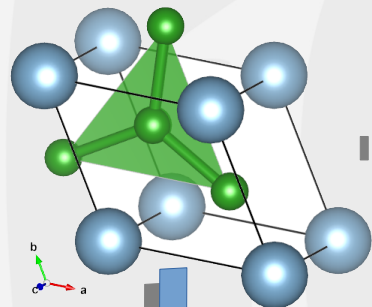
194  
 3.722 3.722 7.232 90. 90. 120.  
 3  
 Zr 1 2a 0 0 0  
 Be 1 2c 0.3333 0.6667 0.250  
 Si 2 2d 0.3333 0.6667 0.750



# KLASSENGLEICHE MAXIMAL SUBGROUPS

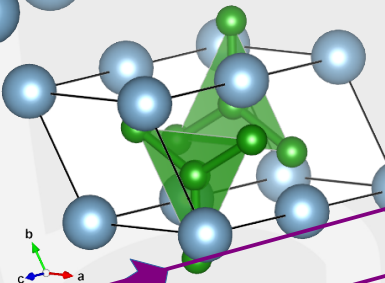
## AlB<sub>2</sub> | P6/mmm (#191)

191  
 3.00390 3.00390 3.28060 90 90 120  
 2  
 Al 1 1a 0.000000 0.000000 0.000000  
 B 1 2d 0.333333 0.666667 0.500000

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix}$$


## AlB<sub>2</sub> | P6<sub>3</sub>/mmc (#194)

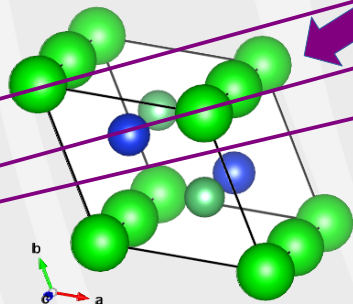
194  
 3.003900 3.003900 6.561200 90 90 120  
 3  
 Al 1 2a 0.000000 0.000000 0.000000  
 B 1 2c 0.333333 0.666667 0.250000  
 B 2 2d 0.666667 0.333333 0.250000



AT.	WP	SS	Representative	Atomic orbit
Al1	2a (0,0,0)	-3m.	(0.000000, 0.000000, 0.000000)	(0.000000, 0.000000, 0.000000) (0.000000, 0.000000, 0.500000)
B1	2c (1/3,2/3,1/4)	6m2	(0.333333, 0.666667, 0.250000)	(0.333333, 0.666667, 0.250000) (0.666667, 0.333333, 0.750000)
B1_2	2d (1/3,2/3,3/4)	6m2	(0.666667, 0.333333, 0.250000)	(0.666667, 0.333333, 0.250000) (0.333333, 0.666667, 0.750000)

## ZrBeSi | P6<sub>3</sub>/mmc (#194)

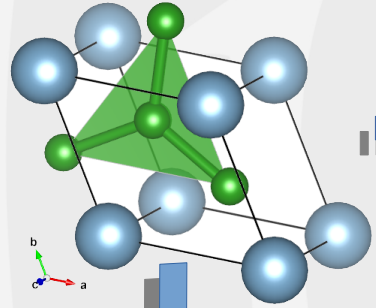
194  
 3.722 3.722 7.232 90. 90. 120.  
 3  
 Zr 1 2a 0 0 0  
 Be 1 2c 0.3333 0.6667 0.250  
 Si 2 2d 0.3333 0.6667 0.750



# KLASSENGLEICHE MAXIMAL SUBGROUPS

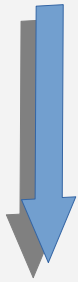
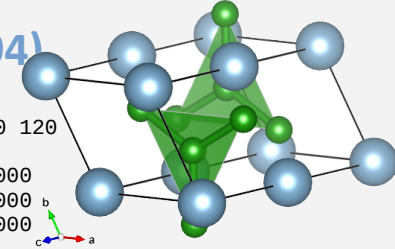
## AlB<sub>2</sub> | P6/mmm (#191)

191  
 3.00390 3.00390 3.28060 90 90 120  
 2  
 Al 1 1a 0.000000 0.000000 0.000000  
 B 1 2d 0.333333 0.666667 0.500000



## AlB<sub>2</sub> | P6<sub>3</sub>/mmc (#194)

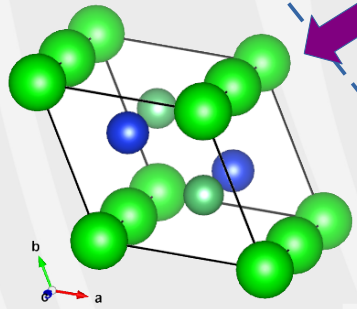
194  
 3.003900 3.003900 6.561200 90 90 120  
 3  
 Al 1 2a 0.000000 0.000000 0.000000  
 B 1 2c 0.333333 0.666667 0.250000  
 B 2 2d 0.666667 0.333333 0.250000



$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix}$$

## ZrBeSi | P6<sub>3</sub>/mmc (#194)

194  
 3.722 3.722 7.232 90. 90. 120.  
 3  
 Zr 1 2a 0 0 0  
 Be 1 2c 0.3333 0.6667 0.250  
 Si 2 2d 0.3333 0.6667 0.750



WP	Atom Structure1	Atom Structure2	Atomic Displacements				
			u <sub>x</sub>	u <sub>y</sub>	u <sub>z</sub>	u	
2a	(0,0,0)	Al1	Zr1	0.0000	0.0000	0.0000	0.0000
2c	(1/3,2/3,1/4)	B1	Be1	0.0000	0.0000	0.0000	0.0000
2d	(1/3,2/3,3/4)	B2	Si2	0.0000	0.0000	0.0000	0.0000

NOTE: u<sub>x</sub>, u<sub>y</sub> and u<sub>z</sub> are given in relative units. |u| is the absolute distance given in Å

### Evaluation of the structure similarity

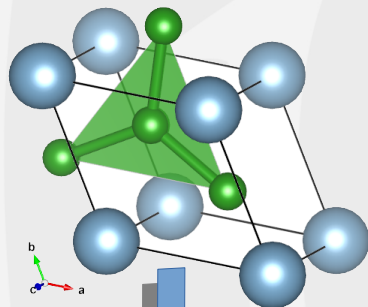
S	d <sub>max.</sub> (Å)	d <sub>av.</sub> (Å)	Δ
0.0873	0	0.0000	0.124

Transformation Matrix	Matrix Form	S	d <sub>max</sub> (Å)	d <sub>avg</sub> (Å)	Axes ratios	Δ	Total Distortion Amplitude (Å)
a,b,2c : 0,0,0 Details	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	0.0873	0	0.0000	1.000 0.890 1.124	0.124	0.0000

# KLASSENGLEICHE MAXIMAL SUBGROUPS

## AlB<sub>2</sub> | P6/mmm (#191)

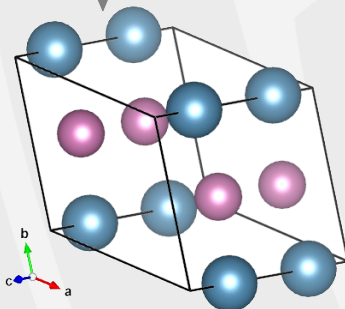
191  
 3.00390 3.00390 3.28060 90 90 120  
 2  
 Al 1 1a 0.000000 0.000000 0.000000  
 B 1 1d 0.333333 0.666667 0.500000



$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$$

## CaIn<sub>2</sub> | P6<sub>3</sub>/mmc (#194)

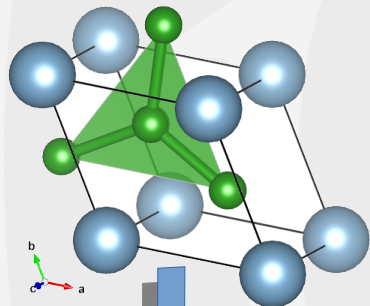
194  
 4.892 4.892 7.739 90.00 90.00 120.00  
 2  
 In 1 4f 0.6667 0.3333 0.04763  
 Ca 1 2b 0.0000 0.0000 0.2500



# KLASSENGLEICHE MAXIMAL SUBGROUPS

## $\text{AlB}_2$ | $P6/mmm$ (#191)

191  
 3.00390 3.00390 3.28060 90 90 120  
 2  
 Al 1 1a 0.000000 0.000000 0.000000  
 B 1 2d 0.333333 0.666667 0.500000



### High symmetry structure

Enter the formula units in the **high symmetry structure**  
 (Leave blank for auto-detection via the volume information)

Structure

Data

[CIF  
 format]

No file chosen

```
191
3.00390 3.00390 3.28060 90 90 120
2
Al 1 1a 0.000000 0.000000 0.000000
B 1 2d 0.333333 0.666667 0.500000
```

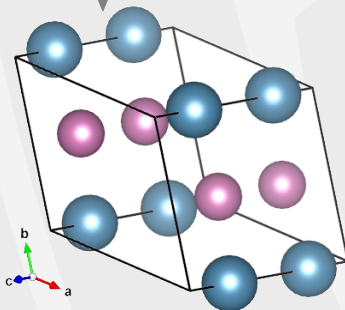
BCS

Format

*What if we  
 don't know the  
 transformation  
 matrix?*

## $\text{CaIn}_2$ | $P6_3/mmc$ (#194)

194  
 4.892 4.892 7.739 90.00 90.00 120.00  
 2  
 In 1 4f 0.6667 0.3333 0.04763  
 Ca 1 2b 0.0000 0.0000 0.2500



### Low symmetry structure:

Enter the formula units in the **low symmetry structure**  
 (Leave blank for auto-detection via the volume information)

Structure

Data

[CIF  
 format]

No file chosen

```
194
4.892 4.892 7.739 90.00 90.00 120.00
2
In 1 4f 0.6667 0.3333 0.04763
Ca 1 2b 0.0000 0.0000 0.2500
```

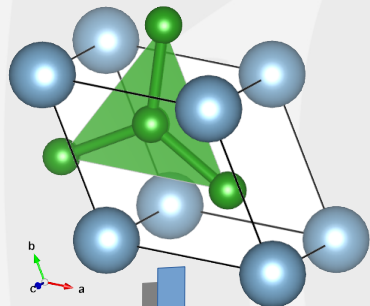
BCS

Format

# KLASSENGLEICHE MAXIMAL SUBGROUPS

## AlB<sub>2</sub> | P6/mmm (#191)

191  
 3.00390 3.00390 3.28060 90 90 120  
 2  
 Al 1 1a 0.000000 0.000000 0.000000  
 B 1 2d 0.333333 0.666667 0.500000



**High symmetry structure**

Enter the formula units in the **high symmetry structure**  
 (Leave blank for auto-detection via the volume information) ➔

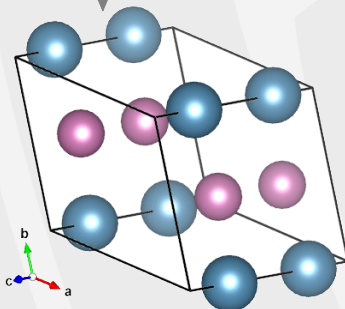
Structure Data [CIF format] Choose File No file chosen

```
191
3.00390 3.00390 3.28060 90 90 120
2
Al 1 1a 0.000000 0.000000 0.000000
B 1 2d 0.333333 0.666667 0.500000
```

BCS Format

## CaIn<sub>2</sub> | P6<sub>3</sub>/mmc (#194)

194  
 4.892 4.892 7.739 90.00 90.00 120.00  
 2  
 In 1 4f 0.6667 0.3333 0.04763  
 Ca 1 2b 0.0000 0.0000 0.2500



**Low symmetry structure:**

Enter the formula units in the **low symmetry structure**  
 (Leave blank for auto-detection via the volume information) ➔

Structure Data [CIF format] Choose File No file chosen

```
194
4.892 4.892 7.739 90.00 90.00 120.00
2
In 1 4f 0.6667 0.3333 0.04763
Ca 1 2b 0.0000 0.0000 0.2500
```

BCS Format

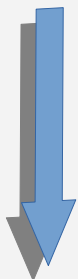
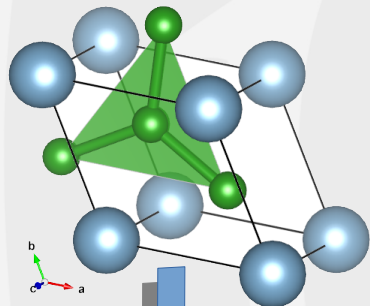
Enter the allowed tolerance (a b c α β γ):



# KLASSENGLEICHE MAXIMAL SUBGROUPS

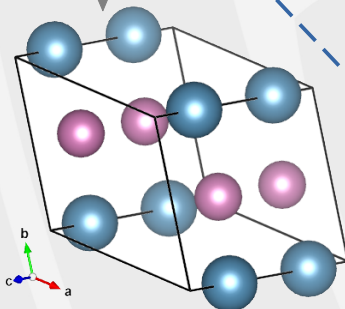
## AlB<sub>2</sub> | P6/mmm (#191)

191  
 3.00390 3.00390 3.28060 90 90 120  
 2  
 Al 1 1a 0.000000 0.000000 0.000000  
 B 1 2d 0.333333 0.666667 0.500000



## CaIn<sub>2</sub> | P6<sub>3</sub>/mmc (#194)

194  
 4.892 4.892 7.739 90.00 90.00 120.00  
 2  
 In 1 4f 0.6667 0.3333 0.04763  
 Ca 1 2b 0.0000 0.0000 0.2500



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

Matrix form:

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

Description of the High Symmetry Structure in the most similar configuration to the Low Symmetry Structure

194  
 3.003900 3.003900 6.561200 90.000000 90.000000 120.000000  
 2  
 Al 1 2b 0.000000 0.000000 0.250000  
 B 1 4f 0.666667 0.333333 0.000000

Atom pairings and distances

Atom Mappings					
WP	Atom	Coordinates in S <sub>1</sub>		Atom	Coordinates in S <sub>2</sub>
4f	(1/3,2/3,z)	B1	(0.666667,0.333333,0.000000)	B1	(0.666667,0.333333,0.047630)
2b	(0,0,1/4)	Al1	(0.000000,0.000000,0.250000)	Al1	(0.000000,0.000000,0.250000)

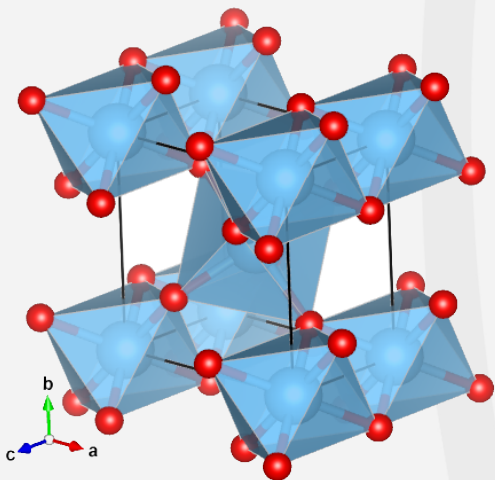
WP	Atom	Atomic Displacements				
		u <sub>x</sub>	u <sub>y</sub>	u <sub>z</sub>	u	
4f	(1/3,2/3,z)	B1	0.0000	0.0000	-0.0476	0.3686
2b	(0,0,1/4)	Al1	0.0000	0.0000	0.0000	0.0000

S	d <sub>max</sub> (Å)	d <sub>av</sub> (Å)	Δ
0.1541	0.3686	0.2457	0.443

NOTE: u<sub>x</sub>, u<sub>y</sub> and u<sub>z</sub> are given in relative units. |u| is the absolute distance given in Å

Transformation Matrix	Matrix Form	S	d <sub>max</sub> (Å)	d <sub>avg</sub> (Å)	Axes ratios	Δ	Total Distortion Amplitude (Å)
a,b,2c ; 0,0,1/2 Details	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	0.1541	0.3686	0.2457	1.000 0.724 1.381	0.443	0.7372

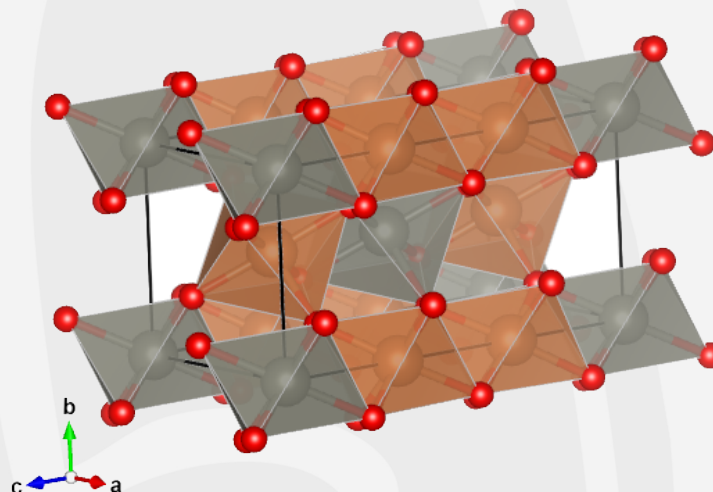
# ISOMORPHIC MAXIMAL SUBGROUPS



**TiO<sub>2</sub> (Rutile) | P4<sub>2</sub>/mnm (#136)**

136  
 4.6012 4.6012 2.9637 90. 90. 90.  
 2  
 Ti 1 2a 0 0 0  
 O 1 4f 0.3049 0.3049 0

Mashimo, T., Bagum, R., Ogata, Y., Tokuda, M., Okube, M., Sugiyama, K., ... & Yoshiasa, A. (2017). Structure of single-crystal rutile (TiO<sub>2</sub>) prepared by high-temperature ultracentrifugation. *Crystal Growth & Design*, 17(4), 1460-1464.

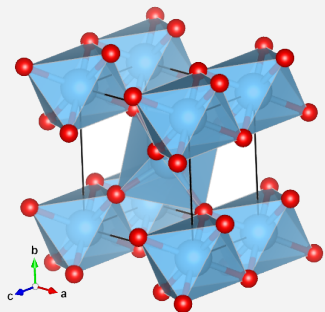


**ZnSb<sub>2</sub>O<sub>6</sub> (Odonezite/Trirutile) | P4<sub>2</sub>/mnm (#136)**

136  
 4.6638 4.6638 9.263 90 90 90  
 4  
 Zn 1 2a 0 0 0  
 Sb 1 4e 0 0 0.3322  
 O 1 4f 0.315 0.315 0  
 O 2 8j 0.304 0.304 0.325

Ercit, T. S., Foord, E. E., & Fitzpatrick, J. J. (2002). Ordoñezite from the Theodoso Soto mine, Saporis, Durango, Mexico: new data and structure refinement. *The Canadian Mineralogist*, 40(4), 1207-1210.

# ISOMORPHIC MAXIMAL SUBGROUPS



TiO<sub>2</sub> (Rutile) | P<sub>4</sub>/mnm (#136)

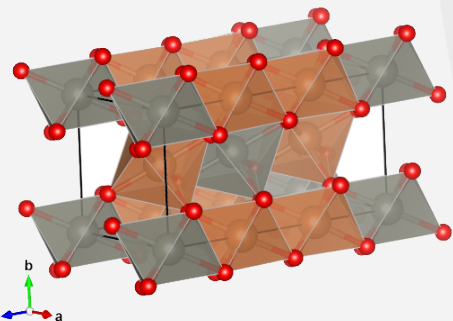
**High symmetry structure**

Enter the formula units in the **high symmetry structure**  
(Leave blank for auto-detection via the volume information)

Structure  
Data  
[CIF  
format]  No file chosen

```

136
4.6012 4.6012 2.9637 90. 90. 90.
2
Ti 1 2a 0 0 0
O 1 4f 0.3049 0.3049 0
    
```



ZnSb<sub>2</sub>O<sub>6</sub> (Odenezite/Trirutile) | P<sub>4</sub>/mnm (#136)

**Low symmetry structure:**

Enter the formula units in the **low symmetry structure**  
(Leave blank for auto-detection via the volume information)

Structure  
Data  
[CIF  
format]  No file chosen

```

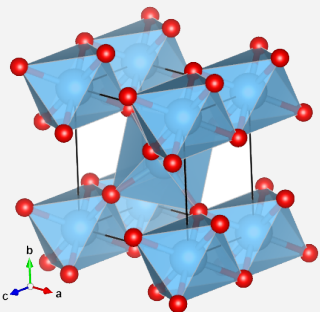
136
4.6638 4.6638 9.263 90 90 90
4
Ti 1 2a 0 0 0
Ti 2 4e 0 0 0.3322
O 1 4f 0.315 0.315 0
O 2 8i 0.304 0.304 0.325
    
```

BCS  
Format

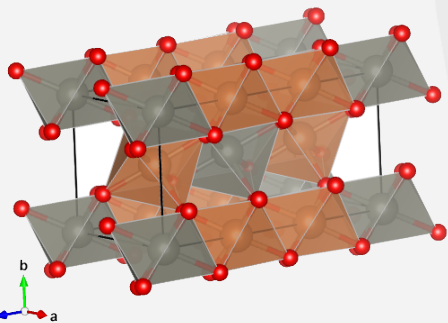


Enter the allowed tolerance (a b c α β γ):

# ISOMORPHIC MAXIMAL SUBGROUPS



TiO<sub>2</sub> (Rutile) | P<sub>4</sub><sub>2</sub>/mnm (#136)



ZnSb<sub>2</sub>O<sub>6</sub> (Odenezite) | P<sub>4</sub><sub>2</sub>/mnm (#136)

Transformation Matrix (P,p): (a,b,3c;0,0,0)

Matrix form:

$$(P,p) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 3 & 0 \end{pmatrix}$$

Description of the High Symmetry Structure in the most similar configuration to the Low Symmetry Structure

```

136
4.601200 4.601200 8.891100 90.000000 90.000000 90.000000
4
Ti 1 2a 0.000000 0.000000 0.000000
Ti 12 4e 0.000000 0.000000 0.333333
O 1 4f 0.304900 0.304900 0.000000
O 12 8j 0.304900 0.304900 0.333333
    
```

Atom pairings and distances

Atom Mappings						
WP	Atom	Coordinates in S <sub>1</sub>		Atom	Coordinates in S <sub>2</sub>	
2a	(0,0,0)	Ti1	(0.000000,0.000000,0.000000)	Ti1	(0.000000,0.000000,0.000000)	
4e	(0,0,z)	Ti12	(0.000000,0.000000,0.333333)	Ti2	(0.000000,0.000000,0.332200)	
4f	(x,x,0)	O1	(0.304900,0.304900,0.000000)	O1	(0.315000,0.315000,0.000000)	
8j	(x,x,z)	O12	(0.304900,0.304900,0.333333)	O2	(0.304000,0.304000,0.325000)	

WP	Atom	Atomic Displacements				
		u <sub>x</sub>	u <sub>y</sub>	u <sub>z</sub>	u	
2a	(0,0,0)	Ti1	0.0000	0.0000	0.0000	0.0000
4e	(0,0,z)	Ti12	0.0000	0.0000	0.0011	0.0105
4f	(x,x,0)	O1	-0.0101	-0.0101	0.0000	0.0666
8j	(x,x,z)	O12	0.0009	0.0009	0.0083	0.0774

NOTE: u<sub>x</sub>, u<sub>y</sub> and u<sub>z</sub> are given in relative units. |u| is the absolute distance given in Å

S	d <sub>max.</sub> (Å)	d <sub>av.</sub> (Å)	Δ
0.0145	0.0774	0.0515	0.038

• Lattice and atomic position criteria:

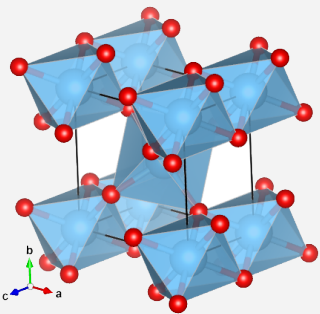
- The **degree of lattice distortion (S)** is the spontaneous strain (sum of the squared eigenvalues of the strain tensor divided by 3). For the given two structures, the **degree of lattice distortion (S)** is **0.0145**.
- The **maximum distance (d<sub>max.</sub>)** shows the maximal displacement between the atomic positions of the paired atoms. The **maximum distance (d<sub>max.</sub>)** in this case is: **0.0774 Å**
- The **average distance (d<sub>av.</sub>)** is defined as the average over the primitive unit cell of the distances between the atomic positions of the paired atoms. For this case the **average distance (d<sub>av.</sub>)** is calculated as **0.0515 Å**.
- The **measure of compatibility (Δ)** (Bergerhoff *et al.*, 1998) is a function of the differences in atomic positions (weighted by the multiplicities of the sites) and the ratios of the corresponding lattice parameters of the structures (the comparison being between the transformed high symmetry structure into the low symmetry structure's setting and the reference low symmetry structure). The **measure of compatibility (Δ)** calculated for this case is **0.038**.

Transformation Matrix	Matrix Form	S	d <sub>max</sub> (Å)	d <sub>avg</sub> (Å)	Axes ratios	Δ	Total Distortion Amplitude (Å)
a,b,3c ; 0,0,0 Details	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 3 & 0 \end{pmatrix}$	0.0145	0.0774	0.0515	1.000 1.028 0.973	0.038	0.2571

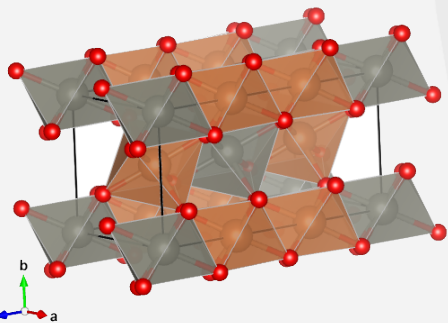
<https://www.cryst.ehu.es/cryst/re13.html>  
bilbao crystallographic server

<http://www.cryst.ehu.es>

# ISOMORPHIC MAXIMAL SUBGROUPS



TiO<sub>2</sub> (Rutile) | P<sub>4</sub>/mnm (#136)



ZnSb<sub>2</sub>O<sub>6</sub> (Odenezite) | P<sub>4</sub>/mnm (#136)

Transformation Matrix (P,p): (a,b,3c;0,0,0)

Matrix form:

$$(P,p) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 3 \end{pmatrix}$$

Description of the High Symmetry Points in the Low Symmetry Structure

136  
4.601200 4.601200 8.  
4  
Ti1 1 2a  
Ti1 12 4e  
O 1 4f  
O 12 8j

Atom pairings and distances

WP	Atom	
2a	(0,0,0)	Ti1 (0.
4e	(0,0,z)	Ti12 (0.
4f	(x,x,0)	O1 (0.
8j	(x,x,z)	O12 (0.

WP	Atom	
2a	(0,0,0)	Ti1 0.
4e	(0,0,z)	Ti12 0.
4f	(x,x,0)	O1 -0.01
8j	(x,x,z)	O12 0.0009 0.0009 0.0083 0.0774

NOTE: u<sub>x</sub>, u<sub>y</sub> and u<sub>z</sub> are given in relative units. |u<sub>j</sub>| is the absolute distance given in Å

S	d <sub>max.</sub> (Å)	d <sub>av.</sub> (Å)	Δ
		0.0515	0.038

## Maximal subgroups of group P<sub>4</sub>/mnm (No. 136)

Note: The program uses the default choice for the group settings.

In the following table the list of maximal subgroups is given. Click over "setting..." to see the possible setting(s) for the given subgroup.

N	IT number	HM symbol	Index	Type	Transformations
1	58	Pnmm	2	t	show..
2	65	Cmmm	2	t	show..
3	84	P <sub>4</sub> /m	2	t	show..
4	94	P <sub>4</sub> 2 <sub>2</sub> 12	2	t	show..
5	102	P <sub>4</sub> 2nm	2	t	show..
6	113	P-4 <sub>2</sub> 1m	2	t	show..
7	118	P-4n2	2	t	show..
8	136	P <sub>4</sub> /mnm	3	k	show..
9	136	P <sub>4</sub> /mnm	5	k	show..
10	136	P <sub>4</sub> /mnm	7	k	show..
11	136	P <sub>4</sub> /mnm	9	k	show..

t represents the *translationengleichen subgroups*  
k represents the *klassengleichen subgroups*

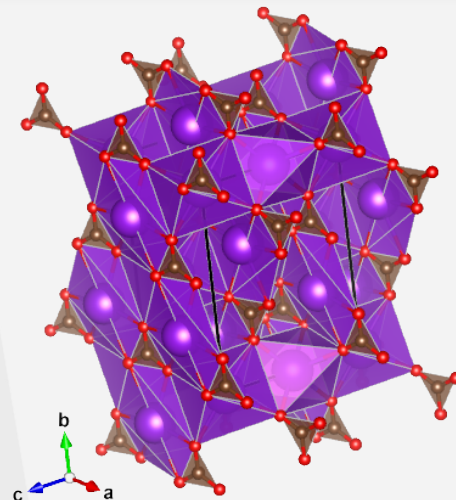
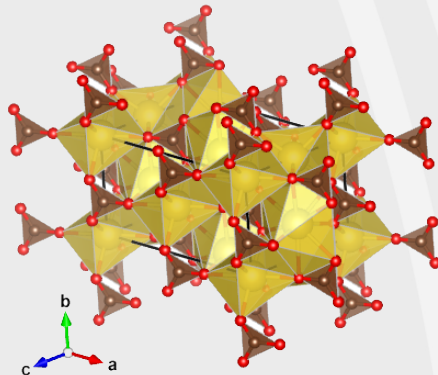
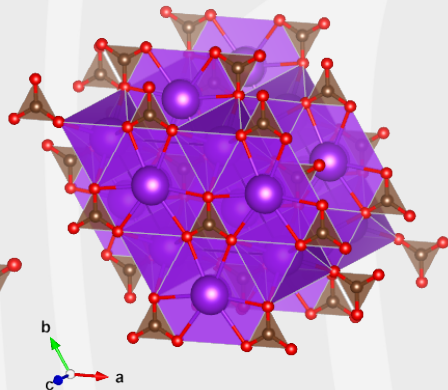
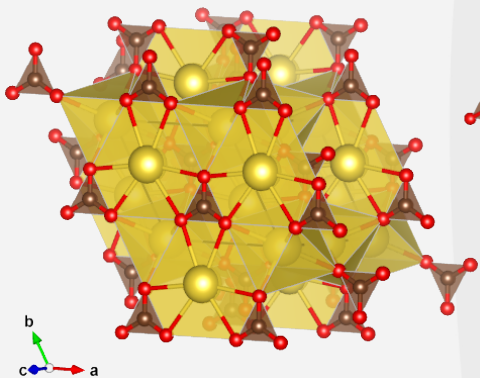
The spontaneous strain (sum of the squared displacements of the sites and divided by 3). For the given two structures, the value is 0.0145.

The maximal displacement between the paired atoms. The maximum distance (d<sub>max.</sub>) in this case is 0.0515 Å.

The average over the primitive unit cell of the squared displacement of the paired atoms. For this case the average value is 0.0038 Å<sup>2</sup>.

The compatibility (Δ) (see e.g. *Acta Cryst.* B 24, 1968) is a function of the differences between the sites and the ratios of the differences between the sites in the low symmetry structure's setting and the high symmetry structure's setting and the measure of compatibility (Δ) calculated for this case is 0.038.

# COMMON SUPERGROUP



## $\alpha\text{-Na}_2\text{CO}_3$ | $P6_3/mmc$ (#194)

194  
 5.20784 5.20784 6.45403 90. 90. 120.  
 4  
 Na 1 2a 0 0 0  
 Na 2 2c 0.6667 0.3333 0.75  
 C 1 2d 0.6667 0.3333 0.25  
 O 1 6h 0.7958 0.2042 0.25

Swanson, I. P., Dove, M. T., & Harris, M. J. (1995). Neutron powder diffraction study of the ferroelastic phase transition and lattice melting in sodium carbonate,  $\text{Na}_2\text{CO}_3$ . *Journal of Physics: Condensed Matter*, 7(23), 4395.

## $\alpha\text{-K}_2\text{CO}_3$ | $P6_3/mmc$ (#194)

194  
 5.66 5.66 7.1 90. 90. 120.  
 4  
 K 1 2a 0 0 0  
 K 2 2c 0.3333 0.6667 0.25  
 C 1 2d 0.3333 0.6667 0.75  
 O 1 6h 0.203 0.406 0.75

Becht, H. Y., & Struikmans, R. (1976). A monoclinic high-temperature modification of potassium carbonate. *Acta Crystallographica Section B: Structural Crystallography and Crystal Chemistry*, 32(12), 3344-3346.

## $\beta\text{-Na}_2\text{CO}_3$ | $C2/c$ (#12)

12  
 8.898 5.237 5.996 90. 101.87 90.  
 6  
 Na 1 2a 0 0 0  
 Na 2 2c 0 0 0.5  
 Na 3 4i 0.17125 0.5 0.74784  
 C 1 4i 0.16454 0.5 0.24887  
 O 1 8j 0.10175 0.29345 0.28667  
 O 2 4i 0.28941 0.5 0.17472

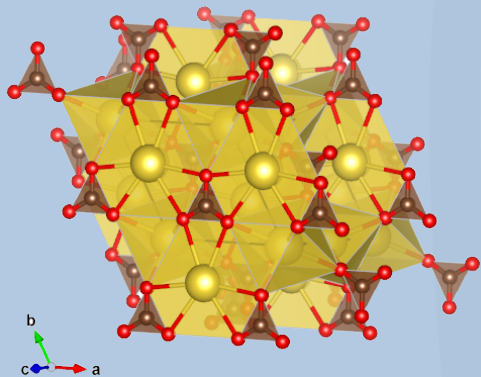
Dušek, M., Chapuis, G., Meyer, M., & Petricek, V. (2003). Sodium carbonate revisited. *Acta Crystallographica Section B: Structural Science*, 59(3), 337-352.

## $\beta\text{-K}_2\text{CO}_3$ | $C2/c$ (#12)

15  
 5.675 9.920 7.018 90. 96.8 90.  
 5  
 K 1 4a 0.5 0.5 0.5  
 K 2 4e 0 0.332 0.25  
 C 1 4e 0 0.333 0.75  
 O 1 4e 0.5 0.702 0.75  
 O 2 8f 0.678 0.895 0.707

Becht, H. Y., & Struikmans, R. (1976). A monoclinic high-temperature modification of potassium carbonate. *Acta Crystallographica Section B: Structural Crystallography and Crystal Chemistry*, 32(12), 3344-3346.

# COMMON SUPERGROUP

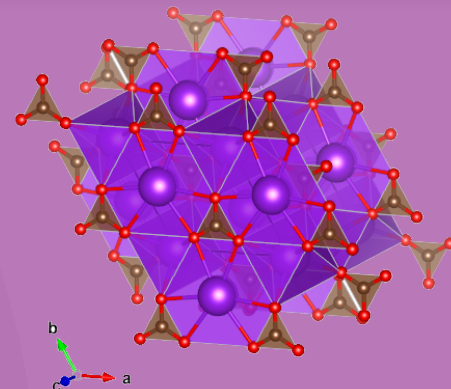


$\alpha\text{-Na}_2\text{CO}_3$  |  $P6_3/mmc$  (#194)

194  
5.20784 5.20784 6.45403 90. 90. 120.  
4  
Na 1 2a 0 0 0  
Na 2 2c 0.6667 0.3333 0.75  
C 1 2d 0.6667 0.3333 0.25  
O 1 6h 0.7958 0.2042 0.25

AT.	WP	SS	Representative	Atomic orbit
Na1	2a (0,0,0)	-3m.	(0.000000, 0.000000, 0.000000)	(0.000000, 0.000000, 0.000000) (0.000000, 0.000000, 0.500000)
Na2	2c (1/3,2/3,1/4)	-6m2	(0.666667, 0.333333, 0.750000)	(0.666667, 0.333333, 0.750000) (0.333333, 0.666667, 0.250000)
C1	2d (1/3,2/3,3/4)	-6m2	(0.666667, 0.333333, 0.250000)	(0.666667, 0.333333, 0.250000) (0.333333, 0.666667, 0.750000)
O1	6h (x,2x,1/4)	mm2	(0.795800, 0.204200, 0.250000)	(0.795800, 0.204200, 0.250000) (0.795800, 0.591600, 0.250000) (0.408400, 0.204200, 0.250000) (0.204200, 0.795800, 0.750000) (0.204200, 0.408400, 0.750000) (0.591600, 0.795800, 0.750000)

AT.	WP	SS	Representative	Atomic orbit
K1	2a (0,0,0)	-3m.	(0.000000, 0.000000, 0.000000)	(0.000000, 0.000000, 0.000000) (0.000000, 0.000000, 0.500000)
K2	2c (1/3,2/3,1/4)	-6m2	(0.333333, 0.666667, 0.250000)	(0.333333, 0.666667, 0.250000) (0.666667, 0.333333, 0.750000)
C1	2d (1/3,2/3,3/4)	-6m2	(0.333333, 0.666667, 0.750000)	(0.333333, 0.666667, 0.750000) (0.666667, 0.333333, 0.250000)
O1	6h (x,2x,1/4)	mm2	(0.203000, 0.406000, 0.750000)	(0.203000, 0.406000, 0.750000) (0.594000, 0.797000, 0.750000) (0.203000, 0.797000, 0.750000) (0.797000, 0.594000, 0.250000) (0.406000, 0.203000, 0.250000) (0.797000, 0.203000, 0.250000)



$\alpha\text{-K}_2\text{CO}_3$  |  $P6_3/mmc$  (#194)

194  
5.66 5.66 7.1 90. 90. 120.  
4  
K 1 2a 0 0 0  
K 2 2c 0.3333 0.6667 0.25  
C 1 2d 0.3333 0.6667 0.75  
O 1 6h 0.203 0.406 0.75

# COMMON SUPERGROUP

Enter the allowed tolerance (a b c  $\alpha$   $\beta$   $\gamma$ ): 1 1 1 1 2 1

Enter the allowed tolerance (a b c  $\alpha$   $\beta$   $\gamma$ ): 1 1 1 1 7 1

Description of the High Symmetry Structure in the most similar configuration to the Low Symmetry Structure

```

012
9.020244 5.207840 6.454030 90.000000 90.000000 90.000000
6
Na 1 2c 0.000000 0.000000 0.500000
Na 12 2a 0.000000 0.000000 0.000000
Na 2 4i 0.166667 0.500000 0.750000
C 1 4i 0.166667 0.500000 0.250000
O 1 4i 0.295800 0.500000 0.250000
O 12 8j 0.102100 0.306300 0.250000
    
```

Description of the High Symmetry Structure in the most similar configuration to the Low Symmetry Structure

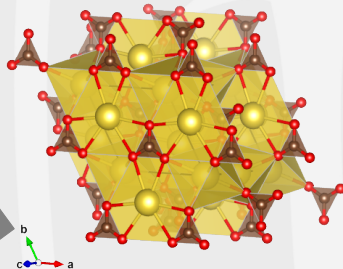
```

015
5.660000 9.803408 7.100000 90.000000 90.000000 90.000000
5
K 1 4a 0.500000 0.500000 0.500000
K 2 4e 0.000000 0.333333 0.250000
C 1 4e 0.000000 0.333333 0.750000
O 1 8f 0.695500 0.898500 0.750000
O 12 4e 0.500000 0.703000 0.750000
    
```

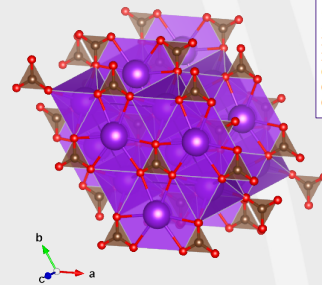
Transformation Matrix (P,p): (a-b,-a-b,-c;0,0,-1/2)

Matrix form:

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



$\alpha$ -Na<sub>2</sub>CO<sub>3</sub> | P6<sub>3</sub>/mmc (#194)

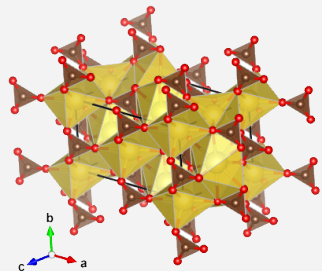


$\alpha$ -K<sub>2</sub>CO<sub>3</sub> | P6<sub>3</sub>/mmc (#194)

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

Matrix form:

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



$\beta$ -Na<sub>2</sub>CO<sub>3</sub> | C2/c (#12)

WP	Atom	Atomic Displacements				
		u <sub>x</sub>	u <sub>y</sub>	u <sub>z</sub>	u	
2a	(0,0,0)	Na12	0.0000	0.0000	0.0000	0.0000
2c	(0,0,1/2)	Na1	0.0000	0.0000	0.0000	0.0000
4i	(x,0,z)	Na2	-0.0046	0.0000	0.0022	0.0453
4i	(x,0,z)	C1	0.0021	0.0000	0.0011	0.0187
8j	(x,y,z)	O12	0.0003	0.0129	-0.0367	0.2306
4i	(x,0,z)	O1	0.0064	0.0000	0.0753	0.4432

NOTE: u<sub>x</sub>, u<sub>y</sub> and u<sub>z</sub> are given in relative units. |u| is the absolute distance given in Å

Evaluation of the Global Distortion

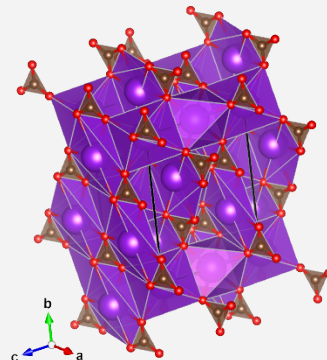
S	d <sub>max</sub> . (Å)	d <sub>av</sub> . (Å)	$\Delta$
0.0665	0.4432	0.1614	0.081

WP	Atom	Atomic Displacements				
		u <sub>x</sub>	u <sub>y</sub>	u <sub>z</sub>	u	
4a	(0,0,0)	K1	0.0000	0.0000	0.0000	0.0000
4e	(0,y,1/4)	K2	0.0000	0.0013	0.0000	0.0132
4e	(0,y,1/4)	C1	0.0000	0.0003	0.0000	0.0033
4e	(0,y,1/4)	O12	0.0000	0.0010	0.0000	0.0099
8f	(x,y,z)	O1	0.0175	0.0035	0.0430	0.3083

NOTE: u<sub>x</sub>, u<sub>y</sub> and u<sub>z</sub> are given in relative units. |u| is the absolute distance given in Å

Evaluation of the Global Distortion

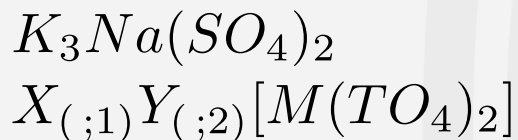
S	d <sub>max</sub> . (Å)	d <sub>av</sub> . (Å)	$\Delta$
0.0295	0.3083	0.1072	0.028



$\beta$ -K<sub>2</sub>CO<sub>3</sub> | C2/c (#12)



# APPLICATION TO THE GLASERITES FAMILY

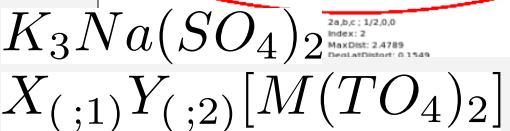
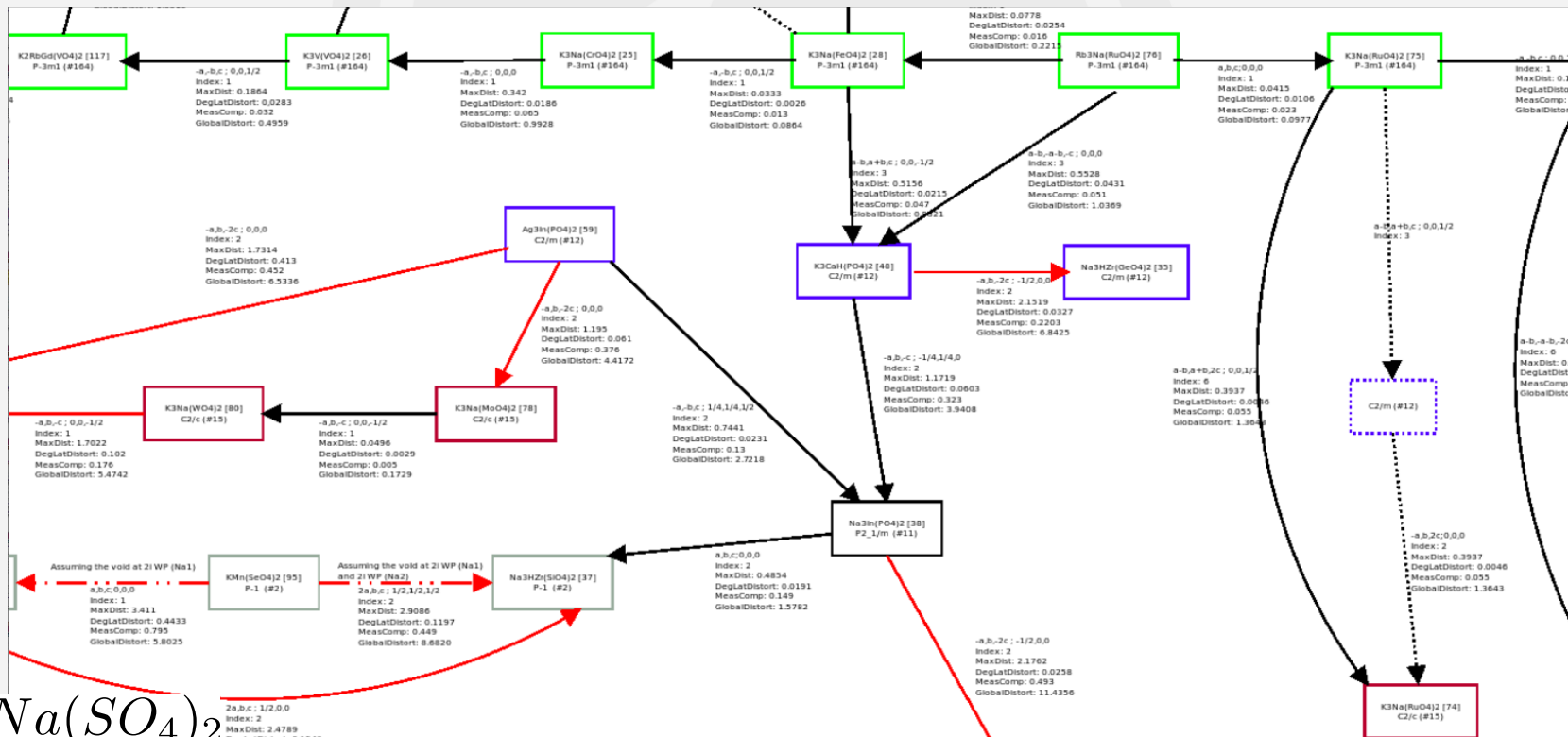


No	General formula	Conditions	Examples		Ref.	Number of GTC
			Long formula	Short formula		
1	$XY_2[M(TO_4)_2]$	$X \neq Y \neq M \neq T$	$BaNa_2[Mg(PO_4)_2]$	$BaNa_2Mg(PO_4)_2$	[12]	12
2	$XY_2[M(TO_4)_2]$	$X = Y \neq M \neq T$	$AgAg_2[Fe(VO_4)_2]$	$Ag_3Fe(VO_4)_2$	[29]	31
3	$XY_2[M(TO_4)_2]$	$X \neq Y; X = M; Y \neq M \neq T$	$NaK_2[Na(SO_4)_2] =$ $K_2Na_2(SO_4)_2$	$KNaSO_4$	[2]	1
4	$XY_{\square}[M(TO_4)_2]$	$X \neq M \neq T; Y = 0$	$Rb\square[Fe(MoO_4)_2]$	$RbFe(MoO_4)_2$	[30]	41
5	$(X1,X2)Y_{\square}[M(TO_4)_2]$	$X1 \neq X2 \neq M \neq T; Y = 0$	$(Ba_{0.3}Sr_{0.7})[Zr(PO_4)_2]$	$Ba_{0.3}Sr_{0.7}Zr(PO_4)_2$	[31]	1
6	$X(Y1,Y2)_2[M(TO_4)_2]$	$X = Y1 \neq Y2; Y2 = M \neq T$	$Ba(Ba_{0.5},Na_{0.5})_2[Na(PO_4)_2] =$ $Ba_2Na_2(PO_4)_2$	$BaNaPO_4$	[32]	4
7	$X_{\square}Y_2[M(TO_4)_2]$	$Y \neq M \neq T; X = 0$	$\square K_2[Zr(PO_4)_2]$	$K_2Zr(PO_4)_2$	[33]	1
8	$X_{\square}Y_{\square}[M(TO_4)_2]$	$M \neq T; X = 0, Y = 0$	$\square\square[Ni(ReO_4)_2]$	$Ni(ReO_4)_2$	[34]	7
9	$X_{\square}Y_{\square}[M(T1,T2O_4)_2]$	$M \neq T1; T1 \neq T2; X = 0,$ $Y = 0$	$\square\square[Zr(Mo,WO_4)_2]$	$Zr(Mo,WO_4)_2$	[35]	1
10	$XY_{\square}[(M1,M2)(TO_4)_2]$	$X \neq M1 \neq M2 \neq T; Y = 0$	$K\square[(Mg_{0.5}Zr_{0.5})(MoO_4)_2]$	$K(Mg_{0.5}Zr_{0.5})(MoO_4)_2$	[36]	1
11	$XY_2[M(TO_4)_2]$	$X = Y = M \neq T$	$TiTi_2[Tl(WO_4)_2] =$ $Tl_4(WO_4)_2$	$Tl_2WO_4$	[37]	2
12	$XY_2H[M(TO_4)_2]$	$X = Y \neq M \neq T$	$NaN_2H[Mg(PO_4)_2]$	$Na_3HMg(PO_4)_2$	[38]	5
13	$XY_{\square}H[M(TO_4)_2]$	$X \neq M \neq T; Y = 0$	$K\square H[Zr(PO_4)_2]$	$KHZr(PO_4)_2$	[39]	2

Nikolova, R., & Kostov-Kytin, V. (2013). Crystal chemistry of "glaserite" type compounds. *Bulgarian Chemical Communications*, 45(4), 418-426.



# APPLICATION TO THE GLASERITES FAMILY



**THANK YOU**

Dr. Emre S. Tasci  
emre.tasci@hacettepe.edu.tr

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*Most of the cases discussed in this presentation have been taken from Ulrich Müller's "Symmetry Relations between Crystal Structures" manuscript prepared for Summer School on Mathematical and Theoretical Crystallography (27/4 – 3/5 2008, Italy) organized by MathCryst.*

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**Bonus "Track": STRUCTURE RELATIONS new version (unpublished)**