CRYSTALLOGRAPHY ONLINE Workshop

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

BILBAO CRYSTALLOGRAPHIC SERVER

Leioa, 27 June -1 July 2022

Structure Relations

Crystallography Online
Leioa, Basque Country, Spain
01/07/2022

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eman ta zabal zazu

UPV EHU

HACETTEPE UNIVERSITY

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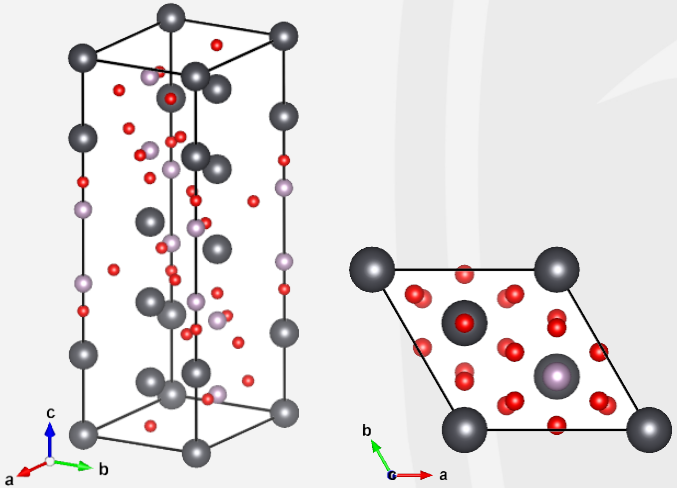
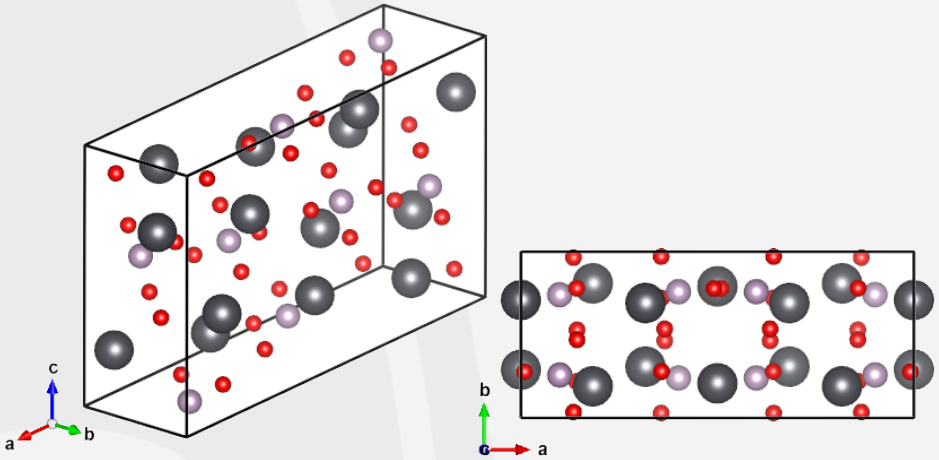
SPOT THE ~~DIFFERENCES~~ SIMILARITIES



$Pb_3(PO_4)_2$ | 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
```

Ng, H. N., & Calvo, C. (1975). Electron paramagnetic resonance and X-ray studies of the phase transformation in Pb3P2O8. Canadian Journal of Physics, 53(1), 42-51.



$Pb_3(PO_4)_2$ | 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
```

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.

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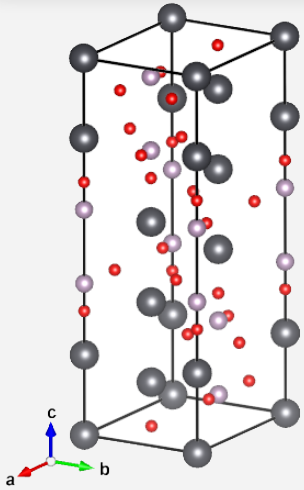
PLAN OF ATTACK

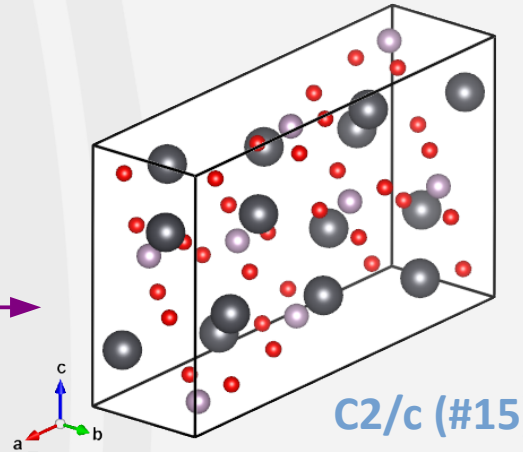


R-3m (#166)

symmetry reduction

?

affine transformation



C2/c (#15)

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INDEX

$$\left.\begin{array}{ll} f_{R\bar{3}m} = 3, & Z_{R\bar{3}m} = 3 \\ f_{C2/c} = 2, & Z_{C2/c} = 4 \end{array}\right\} i_L = \frac{f_{R\bar{3}m} \times Z_{C2/c}}{f_{C2/c} \times Z_{R\bar{3}m}} = 2$$

klassengleiche index

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

translationengleiche index

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

INDEX

$$\left.\begin{array}{ll} f_{R\bar{3}m} = 3, & Z_{R\bar{3}m} = 3 \\ f_{C2/c} = 2, & Z_{C2/c} = 4 \end{array}\right\} i_L = \frac{f_{R\bar{3}m} \times Z_{C2/c}}{f_{C2/c} \times Z_{R\bar{3}m}} = 2$$

klassengleiche index

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

translationengleiche index

Please, enter the sequential number of group as given in *International Tables for Crystallography*, Vol. A : choose 166

Please, enter the sequential number of group as given in *International Tables for Crystallography*, Vol. A : choose 15

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

The formula units (conventional) on the high symmetry structure: 3

The formula units (conventional) on the low symmetry structure: 4

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

Index of a group-subgroup pair

High symmetry Space Group: *R*-3*m* (No. 166) [hexagonal axes]
Low symmetry Space Group: *C*2/*c* (No. 15) [unique axis b]

i_L	2
i_P	3
Total index	6

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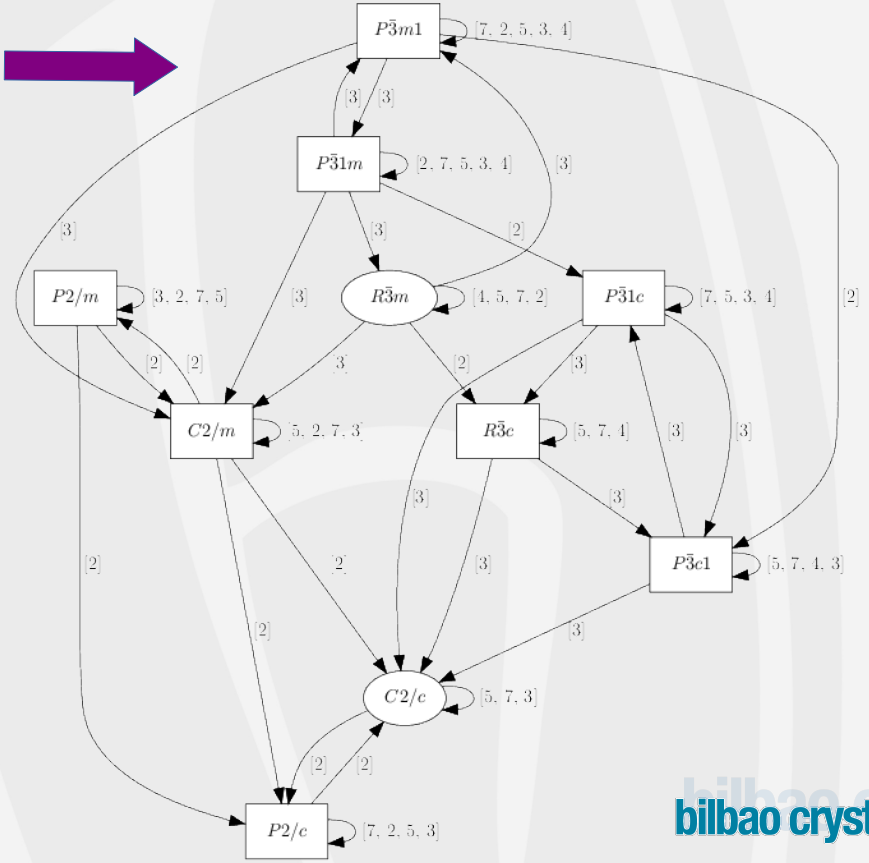
SUBGROUPGRAPH

POSSIBLE PATHS (WITHOUT 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:	166
Enter subgroup number (H) or choose it:	15
Enter the index [G:H] (optional):	

Construct the lattice

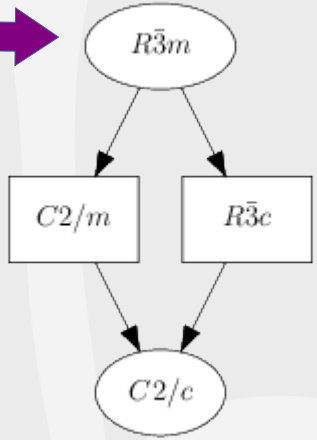


SUBGROUPGRAPH

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:	166
Enter subgroup number (H) or choose it:	15
Enter the index [G:H] (optional):	6

Construct the lattice



Classification of the subgroups of type *C2/c* (No. 15) [unique axis b] of group *R*-3*m* (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..	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..	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..	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..	Show

HERMANN

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

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13.8 5.691 9.42 90. 102.3 90.
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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
```
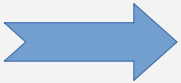

R-3m		**C2/c**	
Pb	3a	4e	Pb
	6c	8f	
P	6c	8f	P
O	6c	8f	O
	18h	8f	
		8f	
		8f	



WPASSIGN

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WYCKOFF POSITIONS SPLITTING COMPATIBILITY

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

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```

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	$\begin{pmatrix} -1/3 & -1 & 0 & 0 \\ 1/3 & -1 & 0 & 0 \\ -2/3 & 0 & 2 & 1/2 \end{pmatrix}$

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

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```

R-3m		**C2/c**	
Pb	3a	4e	Pb
	6c	8f	
P	6c	8f	P
O	6c	8f	O
	18h	8f	
		8f	
		8f	

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WYCKOFF POSITIONS SPLITTING COMPATIBILITY

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O 2 8f 0.634 0.464 0.374
O 3 8f 0.642 0.280 0.612
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```

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 [choose it]	166
Enter subgroup or [choose it]	15

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:	-1/3	-1	0
	1/3	-1	0
	-2/3	0	2
Origin shift:	0	0	0

[Show group-subgroup data.]

R-3m		C2/c	
Pb	3a	4e	Pb
	6c	8f	
P	6c	8f	P
O	6c	8f	O
	18h	8f	
		8f	
		8f	

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WYCKSPLIT

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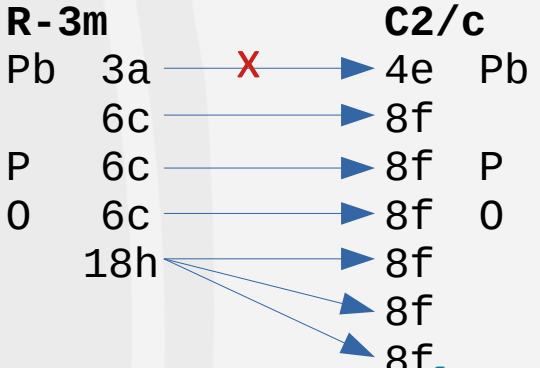
2	-1/3a+1/3b-8/3c,-a-b,2c	$\begin{pmatrix} -1/3 & -1 & 0 & 0 \\ 1/3 & -1 & 0 & 0 \\ -8/3 & 0 & 2 & 0 \end{pmatrix}$
3	-1/3a+1/3b-8/3c,-a-b,2c+1/2	$\begin{pmatrix} -1/3 & -1 & 0 & 0 \\ 1/3 & -1 & 0 & 0 \\ -8/3 & 0 & 2 & 1/2 \end{pmatrix}$
4	-1/3a+1/3b-2/3c,-a-b,2c+1/2	$\begin{pmatrix} -1/3 & -1 & 0 &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

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



[WYCKSETS]

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WYCKOFF POSITIONS SPLITTING COMPATIBILITY

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

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Pb 1 3a  0.000000  0.000000 0.000000
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$Pb_3(PO_4)_2$ | C2/c (#15)

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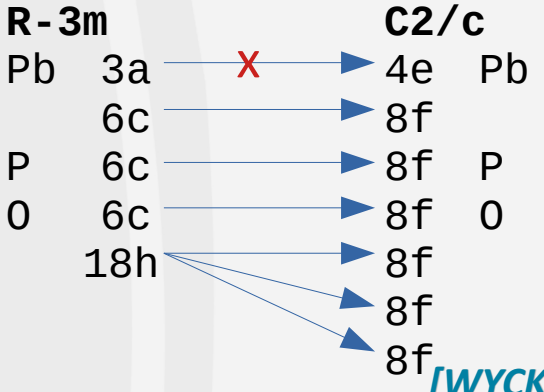
4	-1/3a+1/3b-2/3c,-a-b,2c+1/2	$\begin{pmatrix} -1/3 & -1 & 0 & 0 \\ 1/3 & -1 & 0 & 0 \\ -2/3 & 0 & 2 & 1/2 \end{pmatrix}$

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	4d 4c 4b	Relations
6	9d	8f 4e	Relations
7	6c	8f	Relations
8	3b	4e	Relations
9	3a	4a	Relations



[WYCKSETS]

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WYCKOFF POSITIONS SPLITTING COMPATIBILITY

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O 4 8f 0.491 0.222 0.420
```

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

No	Wyckoff position(s)		
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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

[WYCKSETS]

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

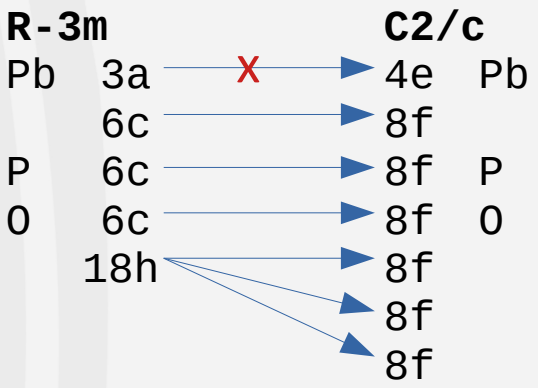
NOTE: The program uses the default choice for the group settings.

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



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WYCKOFF POSITIONS SPLITTING COMPATIBILITY

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

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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
```

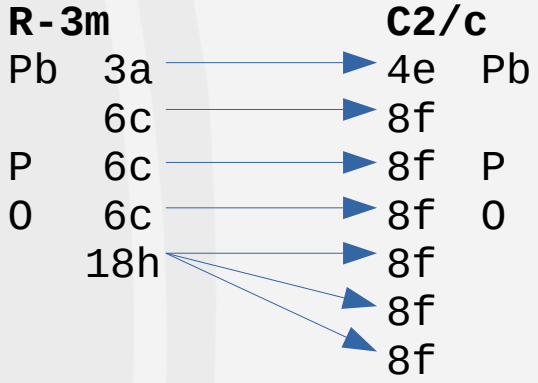
$Pb_3(PO_4)_2$ | C2/c (#15)

```
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
```

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



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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
```

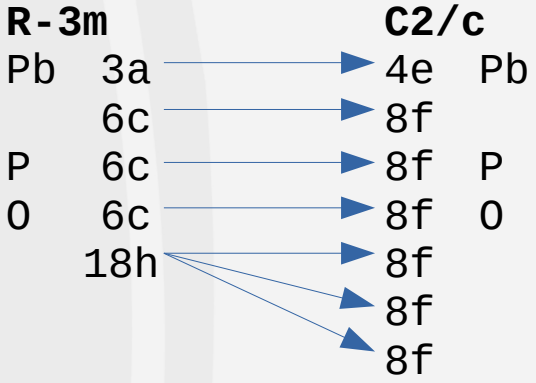
$Pb_3(PO_4)_2$ | C2/c (#15)

```
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
```

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



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WYCKOFF POSITIONS SPLITTING COMPATIBILITY

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

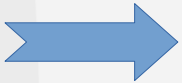
```
166
5.56 5.56 20.39 90. 90. 120.
5
Pb 1 3a  0.000000  0.000000 0.000000
Pb 2 6c  0.000000  0.000000 0.212600
P  1 6c  0.000000  0.000000 0.402100
O  1 6c  0.000000  0.000000 0.329000
O  2 18h 0.181000 -0.181000 0.096000
```

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

$Pb_3(PO_4)_2$ | 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
```

R-3m		C2/c	
Pb	3a	4e	Pb
	6c	8f	
P	6c	8f	P
O	6c	8f	O
	18h	8f	
		8f	
		8f	



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LATTICE COMPATIBILITY

CELLTRAN

Cell Parameters: 5.56 5.56 20.39 90. 90. 120. Centering R

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

in abc form: -1/3a+1/3b-8/3c,-a-b,2c+1/2 Ex: c,a,b (read by columns)

Linear part

or in matrix form:

1	0	0
0	1	0
0	0	1

Show

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

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.

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LATTICE COMPATIBILITY (TRMAT1)

CELLTRAN

Cell Parameters: 5.56 5.56 20.39 90. 90. 120. Centering R

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

in abc form: -1/3a+1/3b-8/3c,-a-b,2c+1/2 Ex: c,a,b (read by columns)

Linear part

or in matrix form:

1	0	0
0	1	0
0	0	1

Show

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

choose 15

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_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)	$\begin{bmatrix} u_{11} & 0 & u_{13} \\ 0 & \pm 1 & 0 \\ g_{31} & 0 & u_{33} \end{bmatrix} \begin{bmatrix} 1/4u_1 \\ 1/4u_2 \\ 1/2n_3 \end{bmatrix}$

n: integer
u: odd
g: even
det(N) = ±1

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

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

Δ: 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

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LATTICE COMPATIBILITY

CELLTRAN

Cell Parameters: 5.56 5.56 20.39 90. 90. 120. Centering R

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

in abc form: -1/3a+1/3b-8/3c,-a-b,2c+1/2 Ex: c,a,b (read by columns)

or in matrix form: Linear part

1	0	0
0	1	0
0	0	1

Show

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_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)	$\begin{bmatrix} u_{11} & 0 & u_{13} \\ 0 & \pm 1 & 0 \\ g_{31} & 0 & u_{33} \end{bmatrix} \begin{bmatrix} 1/4u_1 \\ 1/4u_2 \\ 1/2n_3 \end{bmatrix}$

n: integer
u: odd
g: even
det(N) = ±1

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

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

Δ: 4.17000 0.13100 4.54700 0. 1. 0.

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

NORMALIZER

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

choose 15

Choose:

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

Strain: 0.20528

STRAIN

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LATTICE COMPATIBILITY

CELLTRAN

Cell Parameters: 5.56 5.56 20.39 90. 90. 120. Centering R

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

in abc form: -1/3a+1/3b-2/3c,-a-b,2c+1/2 Ex: c,a,b (read by columns)

Linear part

or in matrix form:

1	0	0
0	1	0
0	0	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

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

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

n: integer
u: odd
g: even
det(N) = ±1

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

Δ: 0.16720 0.13100 0.21230 0. 1. 0.

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

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

choose 15

Choose:

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

NORMALIZER

Strain: 0.01160

STRAIN

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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.        ]]
```

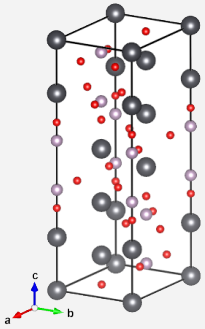
WP Splitting compatible Group – Subgroup TrMat

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

Lattice compatible element of Affine Normalizer

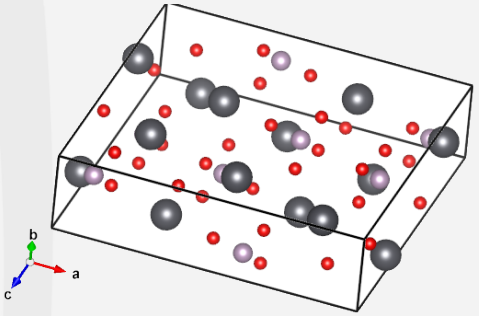
$x-3z+\frac{1}{4}, -y+\frac{1}{4}, -z$

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



```
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
```



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

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

TRANSTRU

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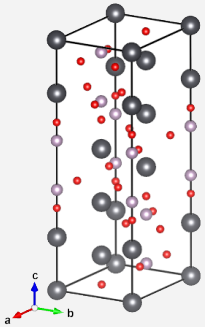
COMPATIBLE TRANSFORMATION MATRIX TO SUBGROUP



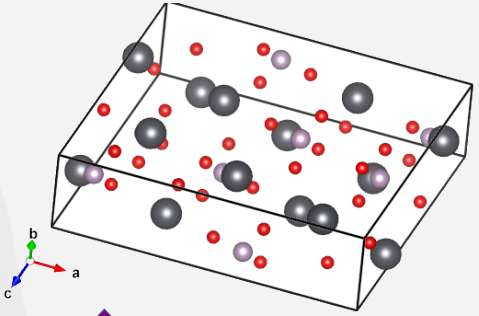
```
166
5.56 5.56 20.39 90. 90. 120.
5
Pb 1 3a  0.000000  0.000000 0.000000
Pb 2 6c  0.000000  0.000000 0.212600
P  1 6c  0.000000  0.000000 0.402100
O  1 6c  0.000000  0.000000 0.329000
O  2 18h 0.181000 -0.181000 0.096000
```

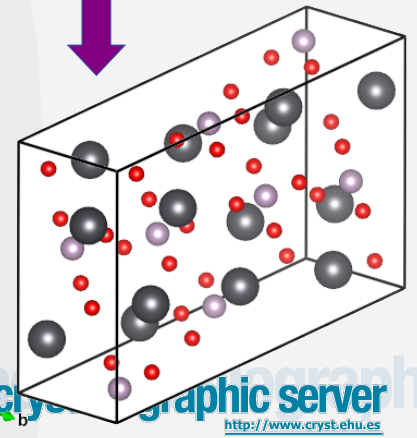
$Pb_3(PO_4)_2$ | R-3m (#166)

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

```
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)

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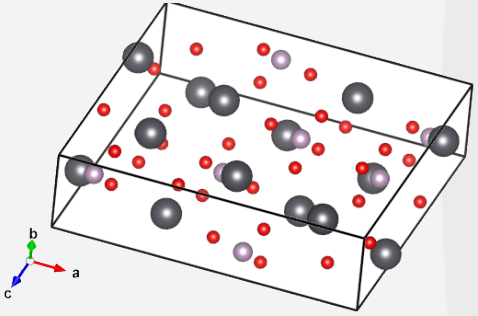
ATOMIC POSITIONS MATCHING

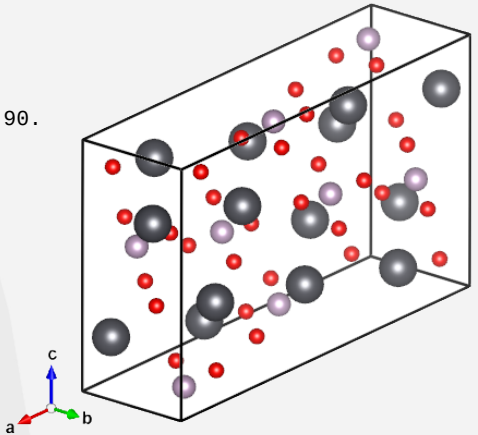



```
15
13.967 5.560 9.630 90. 103.29 90.
7
Pb 1 4e 0.499999 0.250000 0.249999
Pb 2 8f 0.181099 0.250000 0.143699
P  1 8f 0.896849 0.250000 0.048949
O  1 8f 0.006499 0.250000 0.085499
O  2 8f 0.355999 0.750000 0.882999
O  3 8f 0.355999 0.021500 0.611500
O  4 8f 0.644001 0.478500 0.888499
```

$Pb_3(PO_4)_2$ | (#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)

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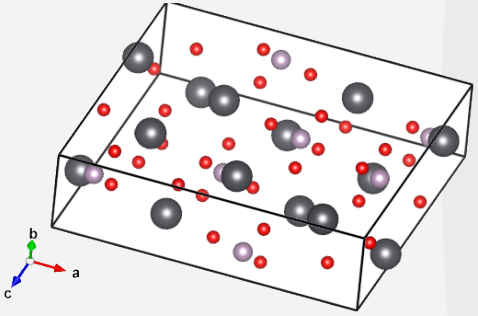
ATOMIC POSITIONS MATCHING

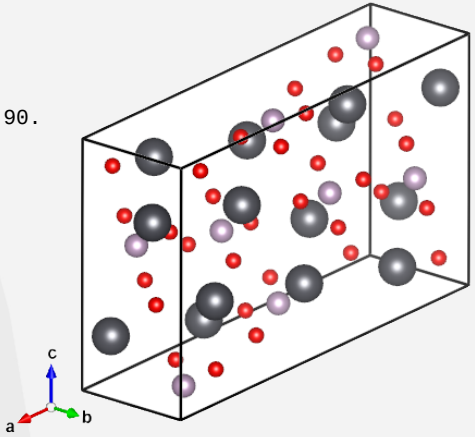



```
15
13.967 5.560 9.630 90. 103.29 90.
7
Pb 1 4e 0.499999 0.250000 0.249999
Pb 2 8f 0.181099 0.250000 0.143699
P  1 8f 0.896849 0.250000 0.048949
O  1 8f 0.006499 0.250000 0.085499
O  2 8f 0.355999 0.750000 0.882999
O  3 8f 0.355999 0.021500 0.611500
O  4 8f 0.644001 0.478500 0.888499
```

$Pb_3(PO_4)_2$ | (#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)



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
```

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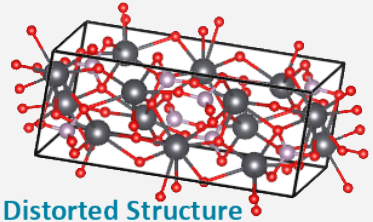
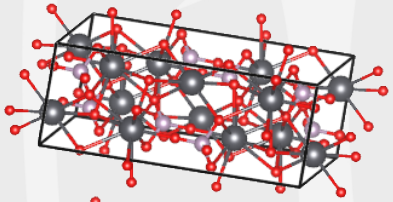
EQUIVSTRU

ATOMIC POSITIONS MATCHING

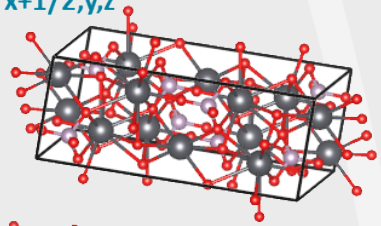


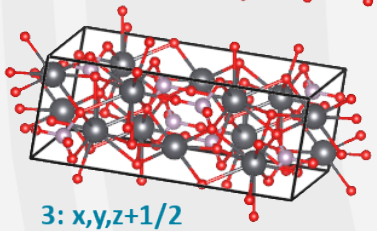
Distorted Structure

1: x,y,z

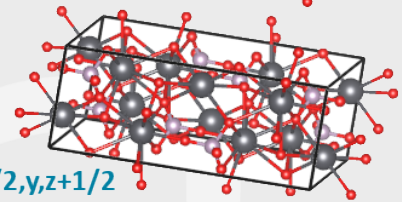


2: x+1/2,y,z





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: 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

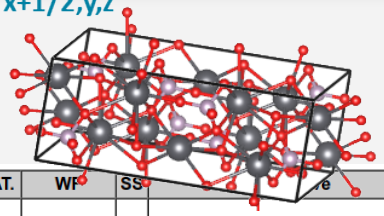
Normalizer coset representative: x+1/2,y,z+1/2

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

2: x+1/2,y,z



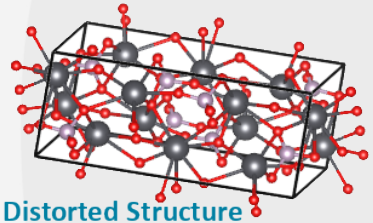
AT.	WP	SS	Representative	Atomic orbit
Pb1	4e (0,y,1/4)	2	(0.000000,0.250000,0.249999)	(0.000000,0.250000,0.249999) (0.000000,0.750000,0.750001) (0.499999,0.750000,0.249999) (0.500001,0.250000,0.750001)
Pb2	8f (x,y,z)	1	(0.681099,0.250000,0.143699)	(0.681099,0.250000,0.143699) (0.318901,0.250000,0.356301) (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)	(0.396849,0.250000,0.048949) (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)

Equivalent description 2

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

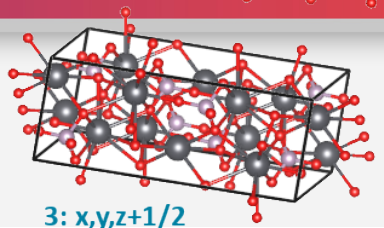
Click here to get more information about the transformation: show hide

```
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
```



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
```



3: x,y,z+1/2

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 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
```

FINAL TRANSFORMATION MATRIX

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

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

The sought transformation matrix!

WP Splitting compatible Group – Subgroup TrMat

Lattice compatible element of Affine Normalizer

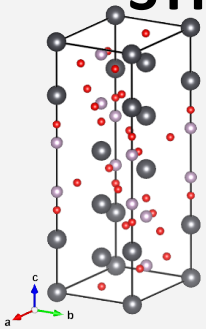
Lattice compatible element of Euclidean Normalizer

$-\frac{1}{3}a+\frac{1}{3}b-\frac{2}{3}c, -a-b, 2c; 0, 0, \frac{1}{2}$ $\qquad$ $x-3z+\frac{1}{4}, -y+\frac{1}{4}, -z$ $\qquad$ $x+\frac{1}{2}, y, z$ $\qquad$ $-\frac{1}{3}a+\frac{1}{3}b-\frac{2}{3}c, a+b, a-b; -\frac{1}{2}, 0, 0$

```
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.        ]]
```

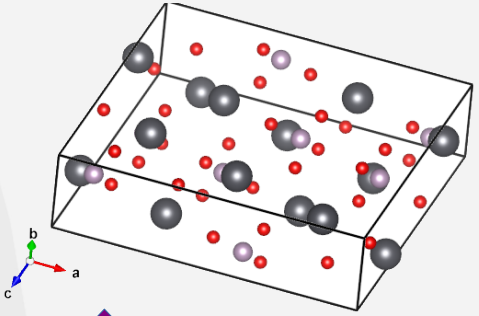
HIGH SYMMETRY STRUCTURE DEFINED IN LOW SYMMETRY STRUCTURE'S SETTING (COMPATIBLE LATTICE & POSITIONS)



```
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
```

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

```
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
```

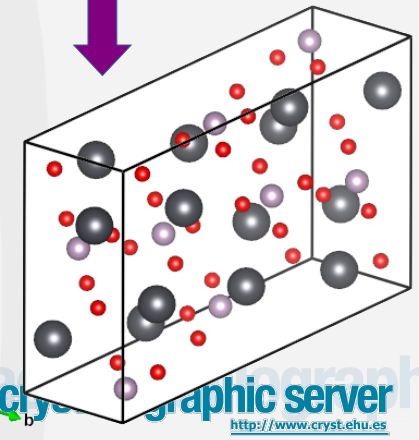


$Pb_3(PO_4)_2$ | (#166 → #15)

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

TRANSTRU

```
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)

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COMPARISON OF THE TWO STRUCTURES

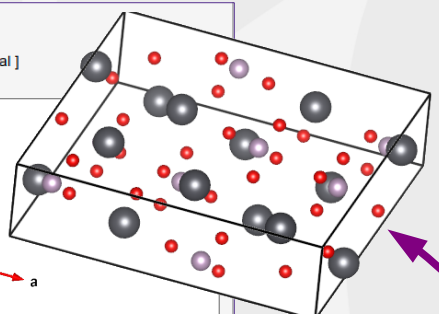
Structure Data [in CIF format]

Choose File | No file chosen

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

Structure 1

```
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
```



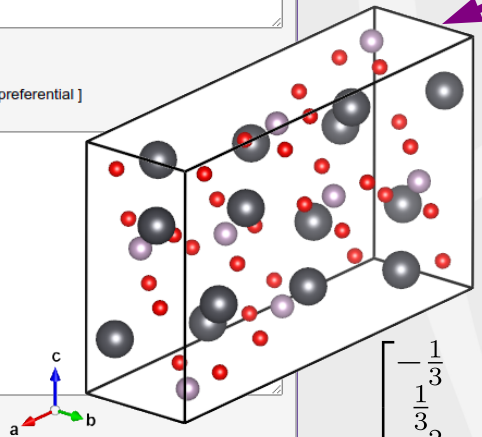
Structure Data [in CIF format]

Choose File | No file chosen

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

Structure 2

```
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: 1 Å

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

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

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

Atom pairings and distances

Atom Mappings					
WP		Atom	Coordinates in S_1	Atom	Coordinates in S_2
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)

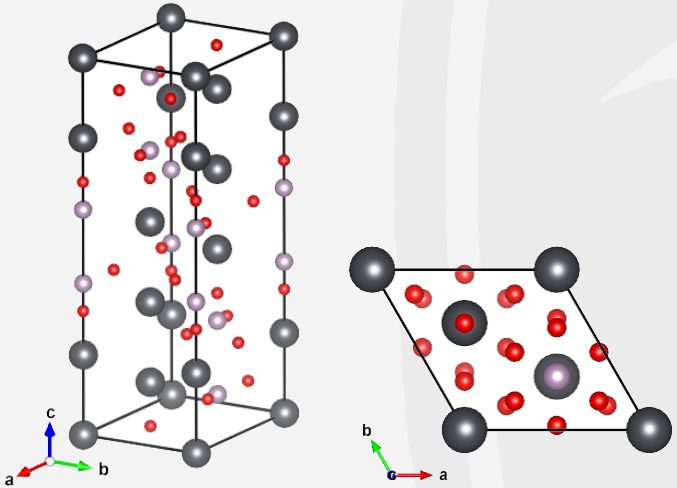
WP		Atom	Atomic Displacements			
			u_x	u_y	u_z	|u|
4e	(0,y,1/4)	Pb1	0.0000	0.0410	0.0000	0.2280
8f	(x,y,z)	Pb2	0.0019	0.0590	0.0043	0.3309
8f	(x,y,z)	P1	0.0042	-0.0090	0.0040	0.0797
8f	(x,y,z)	O1	0.0025	-0.0280	-0.0055	0.1706
8f	(x,y,z)	O2	0.0020	0.0300	0.0050	0.1741
8f	(x,y,z)	O3	0.0010	0.0085	-0.0035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

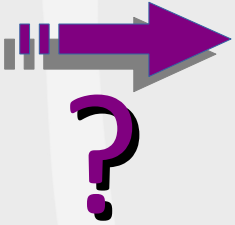
NOTE: u_x, u_y and u_z are given in relative units. |u| is the absolute distance given in Å

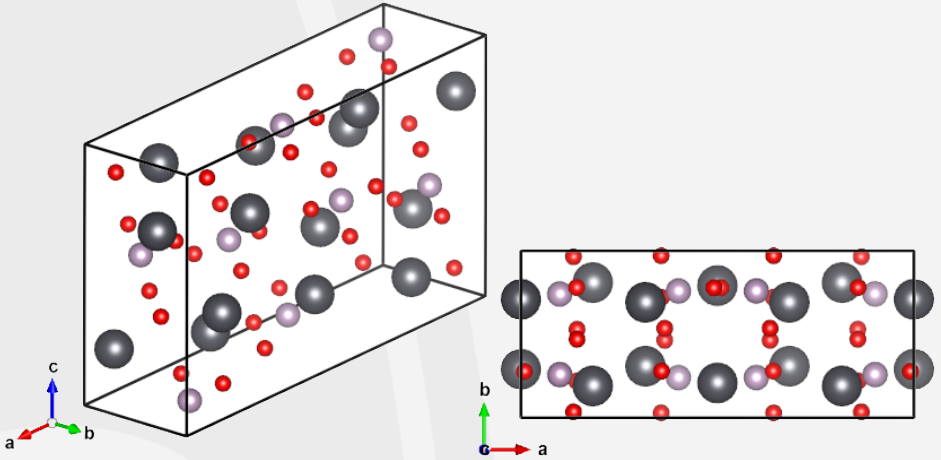
Evaluation of the structure similarity

S	$d_{max.}$ (Å)	$d_{av.}$ (Å)	Δ
0.0116	0.3309	0.1726	0.066

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







$Pb_3(PO_4)_2$ | 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
```

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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] Choose File No file chosen

BCS Format

```
# 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
# [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
```

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

BCS Format

```
# 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
# [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 0.291 0.25
Pb    2   8f    0.317 0.309 0.352
```

Calculation parameters:

Enter the allowed tolerance (a b c α β γ): 2 2 3 2 2 2

Enter the maximum distance allowed between the paired atoms: 1.5 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 : a,b,c;0,0,0

Find compatible transformation matrixes

[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:

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

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_1	Atom	Coordinates in S_2	
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)

WP	Atom	Atomic Displacements			
		u_x	u_y	u_z	|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_x, u_y and u_z are given in relative units. |u| is the absolute distance given in Å

Evaluation of the Global Distortion

S	$d_{max.}$ (Å)	$d_{av.}$ (Å)	Δ
0.0116	0.3386	0.1753	0.066

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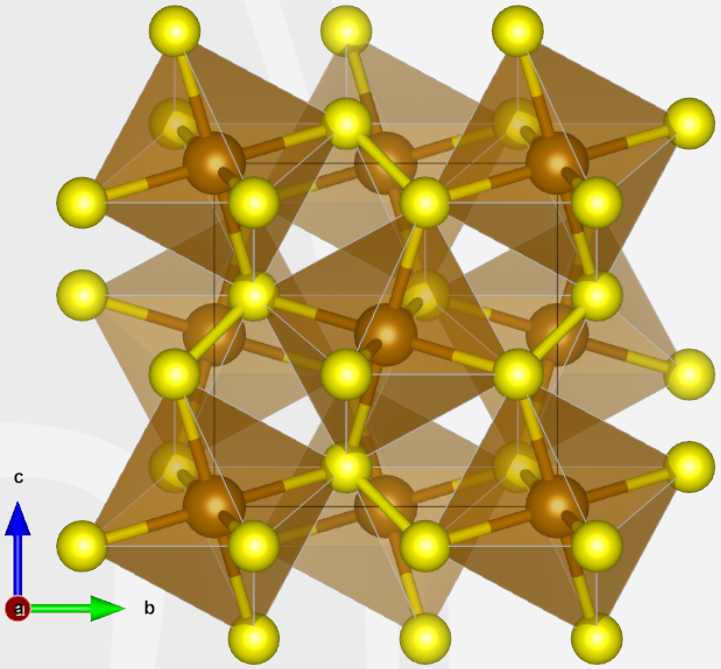
TRANSLATIONENGLEICHE MAXIMAL SUBGROUPS

FeS_2 (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
```

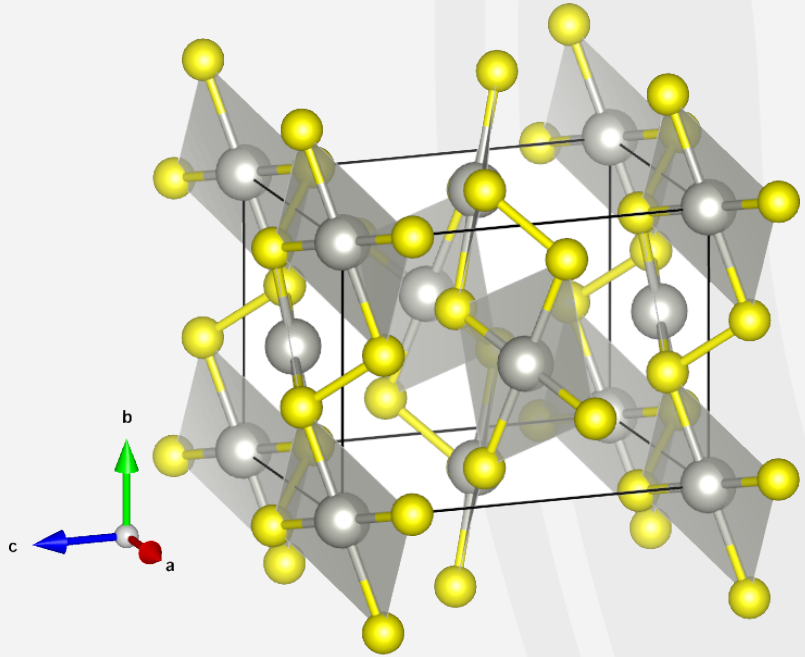
AT.	WP	SS	Representative	Atomic orbit
Fe1	4a (0,0,0)	.-3.	(0.000000,0.000000,0.000000)	(0.000000,0.000000,0.000000) (0.500000,0.000000,0.500000) (0.000000,0.500000,0.500000) (0.500000,0.500000,0.000000)
S1	8c (x,x,x)	.3.	(0.384730,0.384730,0.384730)	(0.384730,0.384730,0.384730) (0.115270,0.615270,0.884730) (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 2)." Dalton Transactions 48, no. 28 (2019): 10703-10713.

TRANSLATIONENGLEICHE MAXIMAL SUBGROUPS

PdS_2 | 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 PdX2 (X= P, S and Se). Journal of Physics and Chemistry of Solids, 71(1), 42-46.

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 -0.391000 -0.084000
```

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)

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

[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)

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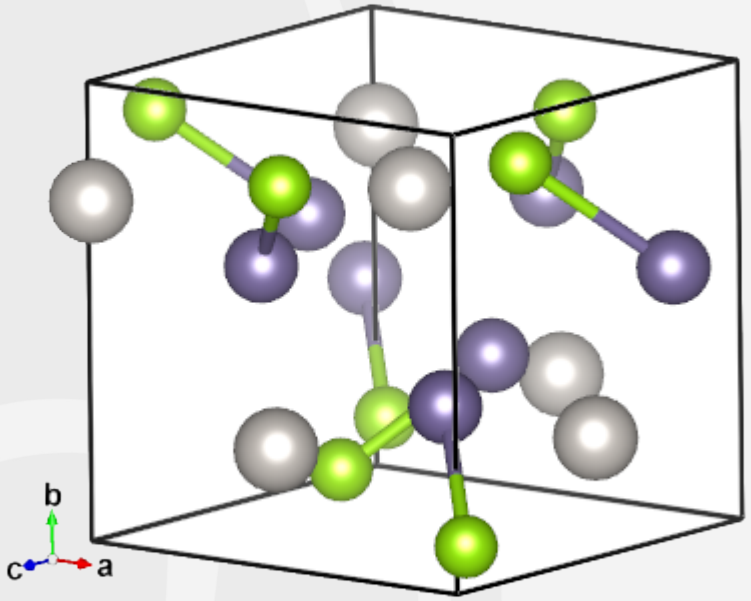
TRANSLATIONENGLEICHE MAXIMAL SUBGROUPS

PtGeSe | $Pca2_1$ (#29)

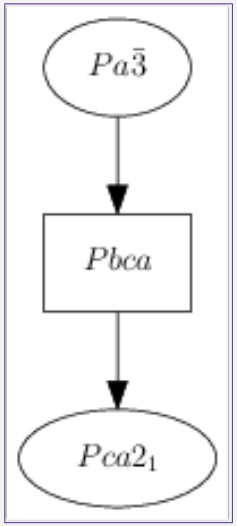
```
29
6.015 6.072 5.992 90. 90. 90.
3
Pt 1 4a 0.008600 0.742000 0.000000
Ge 1 4a 0.383300 0.136400 0.616800
Se 1 4a 0.619800 0.375900 0.382000
```

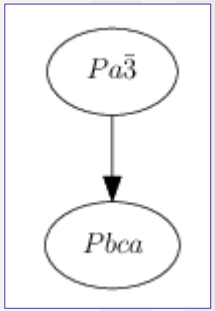
AT.	WP	SS	Representative	Atomic orbit
Pt1	4a (x,y,z)	1	(0.008600,0.742000,0.000000)	(0.008600,0.742000,0.000000) (0.991400,0.258000,0.500000) (0.508600,0.258000,0.000000) (0.491400,0.742000,0.500000)
Ge1	4a (x,y,z)	1	(0.383300,0.136400,0.616800)	(0.383300,0.136400,0.616800) (0.616700,0.863600,0.116800) (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]

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

Transform structure

Transformation matrix: a,b,c

High symmetry structure

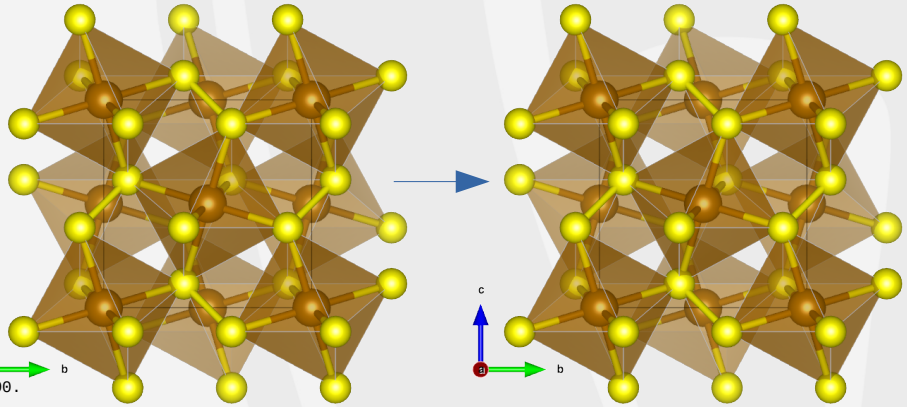
```
205
5.4178 5.4178 5.4178 90. 90. 90.
2
Fe      1       4a      0.000000        0.000000        0.000000
S       1       8c      0.384730        0.384730        0.384730
```

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_2 (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_2 | 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
```

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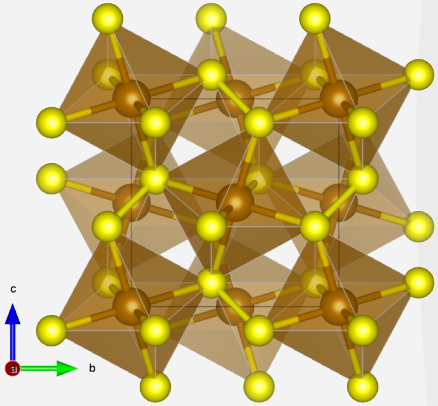
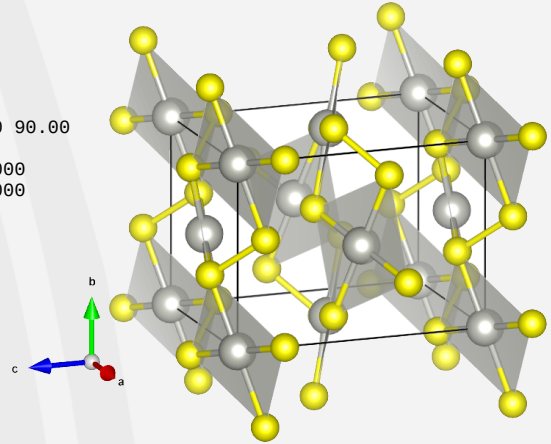


FeS_2 | Pbca (#61)

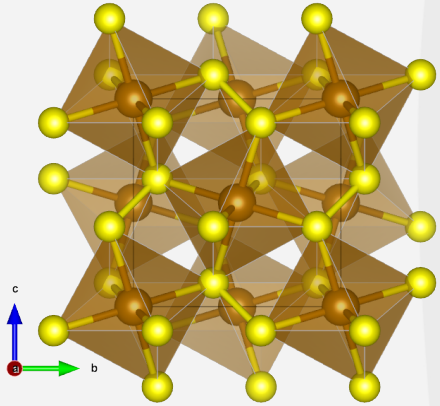
```
61
5.4178 5.4178 5.4178 90. 90. 90.
2
Fe 1 4a 0.000000 0.000000 0.000000
S  1 8c 0.384730 0.384730 0.384730
```

PdS_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
```



TRANSLATIONENGLEICHE MAXIMAL SUBGROUPS

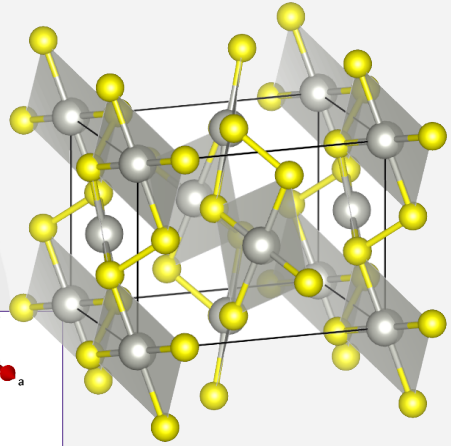


FeS_2 | Pbca (#61)

```
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_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
```



Strain Tensor

Unit cell 1: $[a_1]$ $[b_1]$ $[c_1]$ $[\alpha_1]$ $[\beta_1]$ $[\gamma_1]$

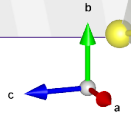
5.4650 5.5380 7.5250 90.00 90.00 90.00

Unit cell 2: $[a_2]$ $[b_2]$ $[c_2]$ $[\alpha_2]$ $[\beta_2]$ $[\gamma_2]$

5.4178 5.4178 5.4178 90. 90. 90.

Show

Finite Lagrangian Strain Tensor (finite deformation)




```
[ -0.008599  0.000000  0.000000 ]
[  0.000000 -0.021469  0.000000 ]
[  0.000000  0.000000 -0.240819 ]
```

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

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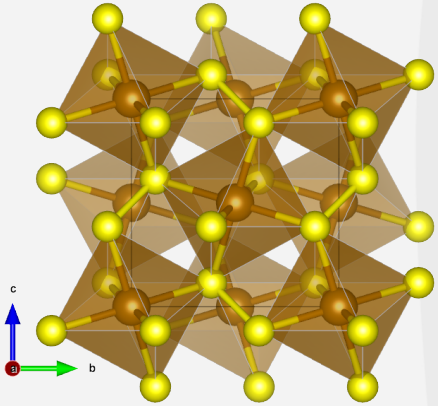
TRANSLATIONENGLEICHE MAXIMAL SUBGROUPS

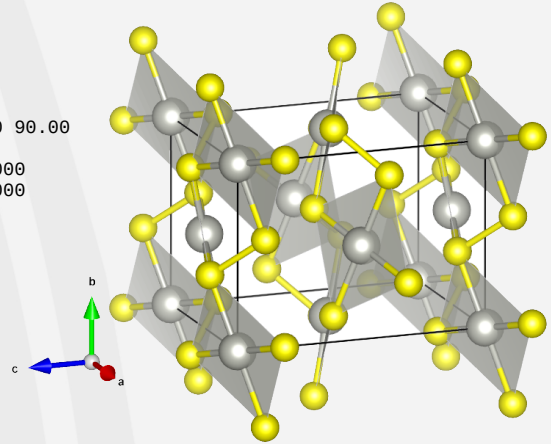


FeS_2 | Pbca (#61)

```
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_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
```



Atom pairings and distances

Atom Mappings					
WP		Atom	Coordinates in S_1	Atom	Coordinates in S_2
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_x	u_y	u_z	|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_x, u_y and u_z are given in relative units. |u| is the absolute distance given in Å

Evaluation of the structure similarity

S	$d_{max.}$ (Å)	$d_{av.}$ (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 ($d_{max.}$) shows the maximal displacement between the atomic positions of the paired atoms. The **maximum distance ($d_{max.}$)** in this case is: **0.1833 Å**
- The arithmetic mean (d_{av}) of the distance. In this case, the **arithmetic mean (d_{av})** 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): .5 .5 3 5 5 5

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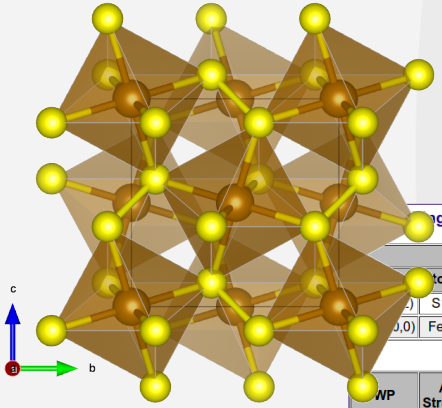
TRANSLATIONENGLEICHE MAXIMAL SUBGROUPS

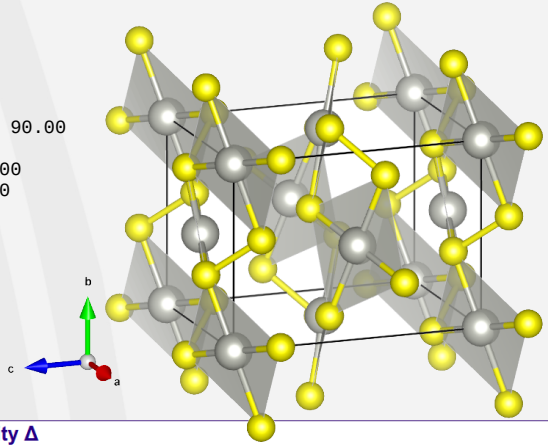


FeS_2 | Pbca (#61)

```
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_2 | Pbca (#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
```



gs and distances

Atom Mappings					
tom	Coordinates in S_1		Atom	Coordinates in S_2	
S1	(0.384730,0.384730,0.384730)		S1	(0.396000,0.391000,0.416000)	
0,0) Fe1	(0.000000,0.000000,0.000000)		Pd1	(0.000000,0.000000,0.000000)	

WP		Atom Structure1	Atom Structure2	Atomic Displacements			
				u_x	u_y	u_z	|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_x, u_y and u_z are given in relative units. |u| is the absolute distance given in Å

Evaluation of the structure similarity

S	$d_{max.}$ (Å)	$d_{av.}$ (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 ($\mathbf{d_{max.}}$) shows the maximal displacement between the atomic positions of the paired atoms. The **maximum distance** ($\mathbf{d_{max.}}$) in this case is: **0.1833 Å**
- The arithmetic mean ($\mathbf{d_{av}}$) of the distance. In this case, the **arithmetic mean** ($\mathbf{d_{av}}$) 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**.

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:

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

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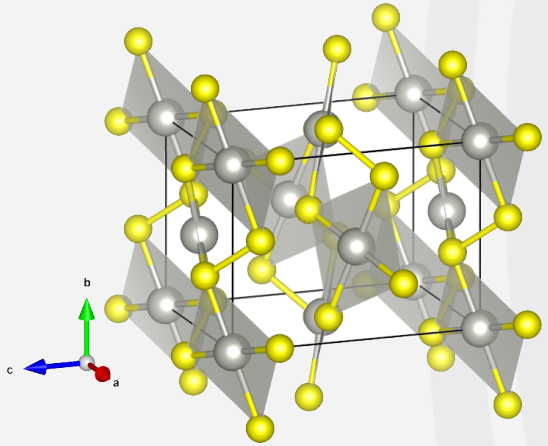


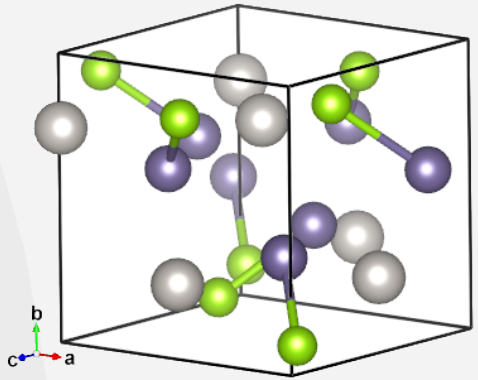
PdS_2 | Pbca (#61)

```
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
```

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)

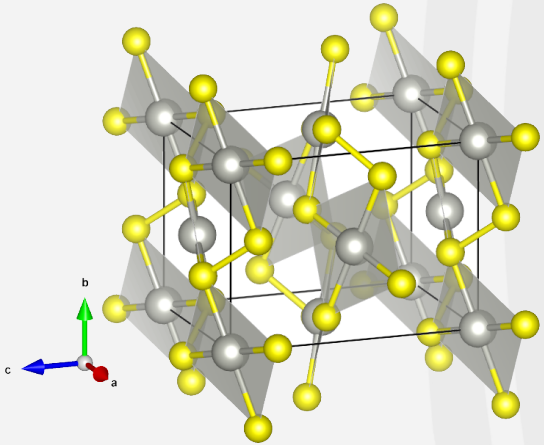
PtGeSe | $Pca2_1$ (#29)

```
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
```



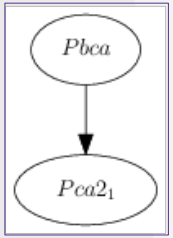
AT.	WP	SS	Representative	Atomic orbit
Pt1	4a (x,y,z)	1	(0.008600,0.742000,0.000000)	(0.008600,0.742000,0.000000) (0.991400,0.258000,0.500000) (0.508600,0.258000,0.000000) (0.491400,0.742000,0.500000)
Ge1	4a (x,y,z)	1	(0.383300,0.136400,0.616800)	(0.383300,0.136400,0.616800) (0.616700,0.863600,0.116800) (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)

TRANSLATIONENGLEICHE MAXIMAL SUBGROUPS



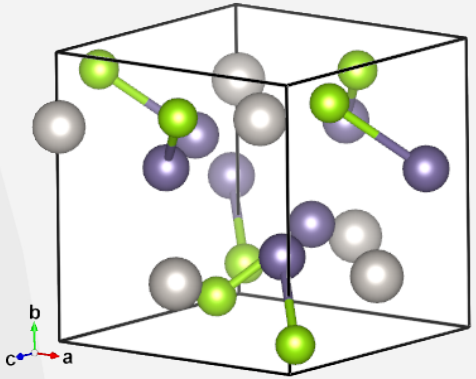
PdS_2 | Pbca (#61)

```
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
```



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
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]

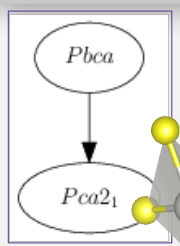
$$\begin{pmatrix} 0 & 1 & 0 & 1/4 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

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

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

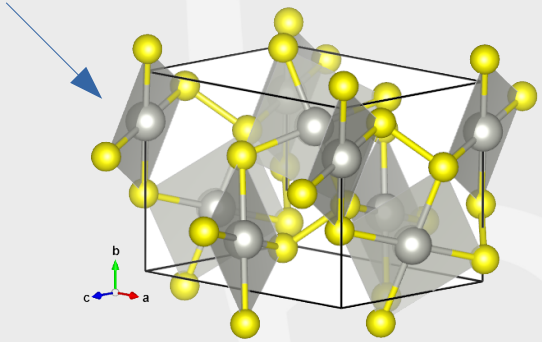
AT.	WP	SS	Representative	Atomic orbit
Pt1	4a (x,y,z)	1	(0.008600,0.742000,0.000000)	(0.008600,0.742000,0.000000) (0.991400,0.258000,0.500000) (0.508600,0.258000,0.000000) (0.491400,0.742000,0.500000)
Ge1	4a (x,y,z)	1	(0.383300,0.136400,0.616800)	(0.383300,0.136400,0.616800) (0.616700,0.863600,0.116800) (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 0.60400
```

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

061 029 [2]

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

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

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

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

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

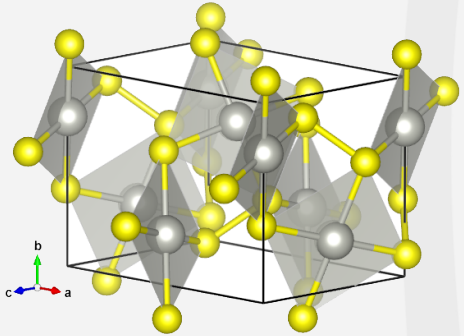
```
029
7.525000 5.538000 5.465000 90.000000 90.000000 90.000000
3
Pd      1       4a      0.500000        0.250000        0.000000
S       1       4a      0.916000        0.359000        0.896000
S       1_2     4a      0.416000        0.141000        0.604000
```

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

TRANSLATIONENGLEICHE MAXIMAL SUBGROUPS



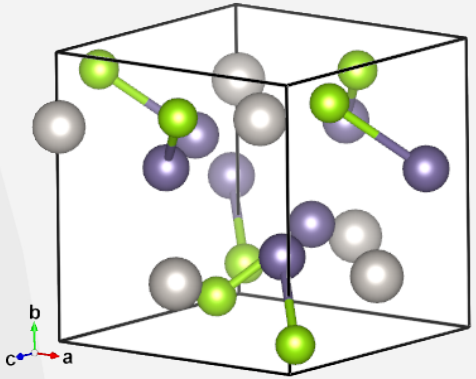
PdS_2 | $Pca2_1$ (#29)

```
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 0.60400
```

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)

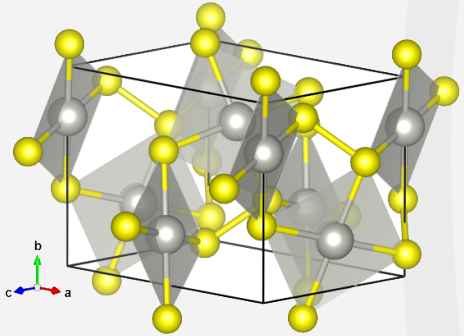
PtGeSe | $Pca2_1$ (#29)

```
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)

TRANSLATIONENGLEICHE MAXIMAL SUBGROUPS



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3
Pd 1 4a 0.500000 0.250000 0.000000
S  1 4a 0.916000 0.359000 0.896000
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```

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```
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Ge 1 4a 0.383300 0.136400 0.616800
Se 1 4a 0.619800 0.375900 0.382000
```
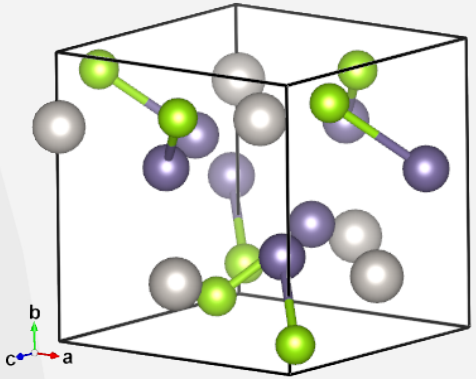
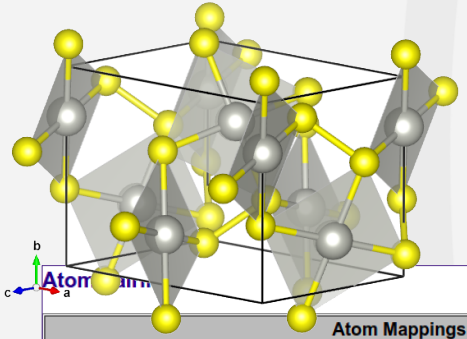



AT.	WP	SS	Representative	Atomic orbit
Pd1	4a (x,y,z)	1	(0.500000,0.250000,0.000000)	(0.500000,0.250000,0.000000) (0.500000,0.750000,0.500000) (0.000000,0.750000,0.000000) (0.000000,0.250000,0.500000)
S1	4a (x,y,z)	1	(0.916000,0.359000,0.896000)	(0.916000,0.359000,0.896000) (0.084000,0.641000,0.396000)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

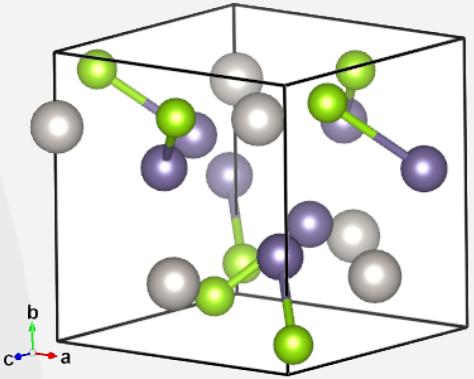
AT.	WP	SS	Representative	Atomic orbit
Pt1	4a (x,y,z)	1	(0.008600,0.742000,0.000000)	(0.008600,0.742000,0.000000) (0.991400,0.258000,0.500000) (0.508600,0.258000,0.000000) (0.491400,0.742000,0.500000)
Ge1	4a (x,y,z)	1	(0.383300,0.136400,0.616800)	(0.383300,0.136400,0.616800) (0.616700,0.863600,0.116800) (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_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 0.60400
```



$PtGeSe$ | $Pca2_1$ (#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
```

Atom Mappings

WP		Atom	Coordinates in S_1	Atom	Coordinates in S_2
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_x	u_y	u_z	|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

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

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

Evaluation of the structure similarity

S	$d_{max.}$ (Å)	$d_{av.}$ (Å)	Δ
0.1022	0.2947	0.2103	0.961

default

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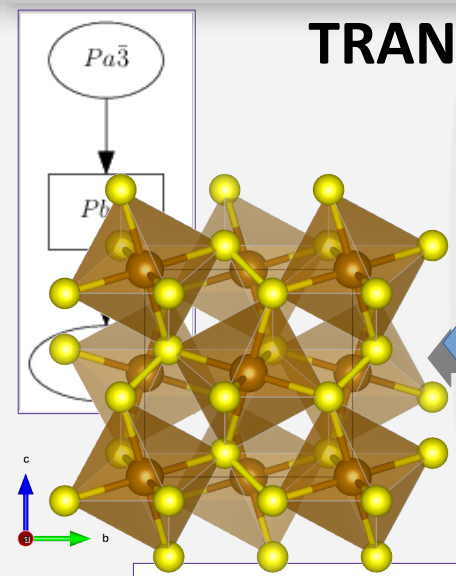
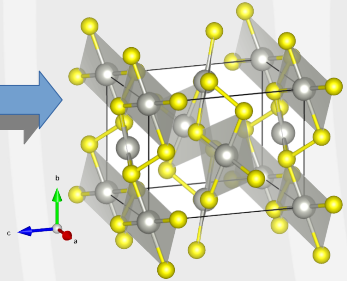
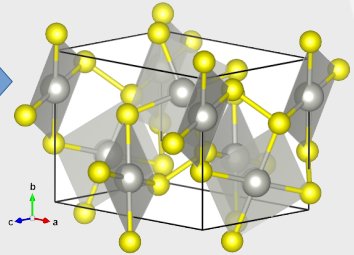
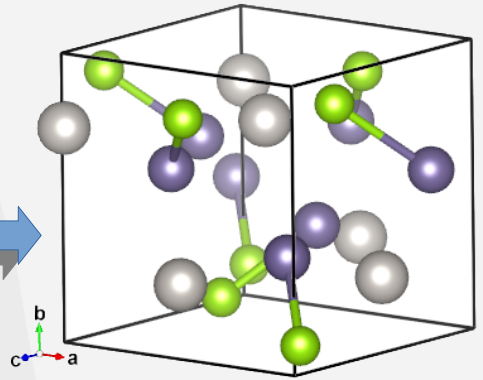
TRANSLATIONENGLEICHE MAXIMAL SUBGROUPS









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_2 | 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_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 0.60400
```

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
```

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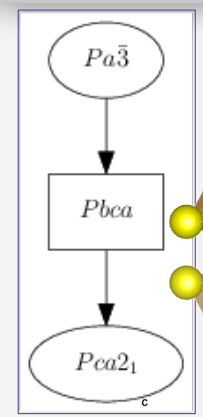
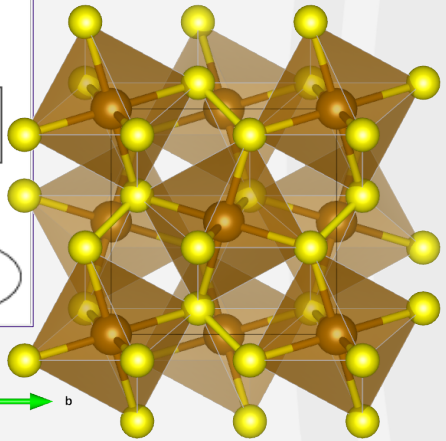
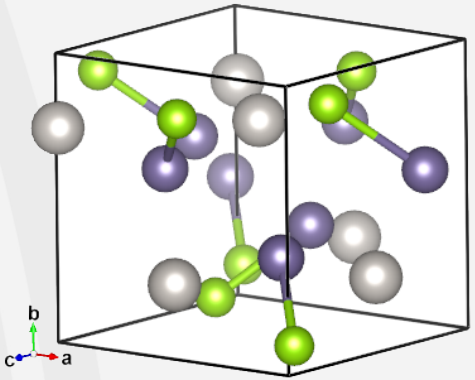




```
In [2]: P_205_061 = np.array([[1,0,0,0],\
                             [0,1,0,0],\
                             [0,0,1,0],\
                             [0,0,0,1]])
        print(P_205_061)

[[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]]
```

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



FeS_2 (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
```

$PtGeSe$ | $Pca2_1$ (#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
```

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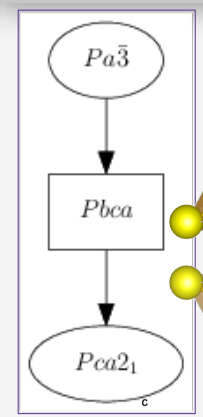

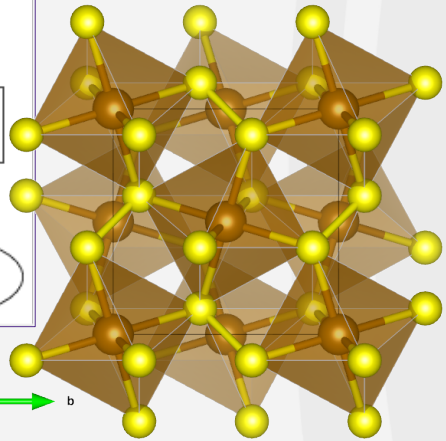

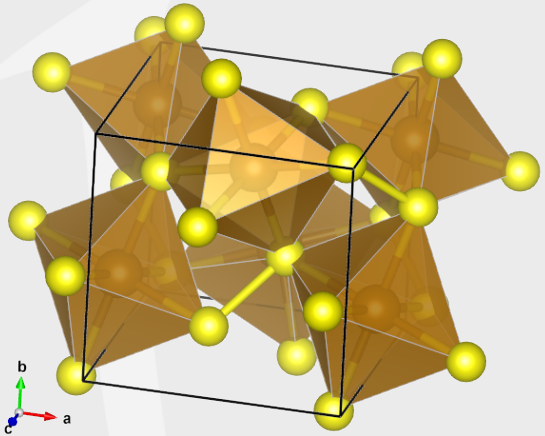

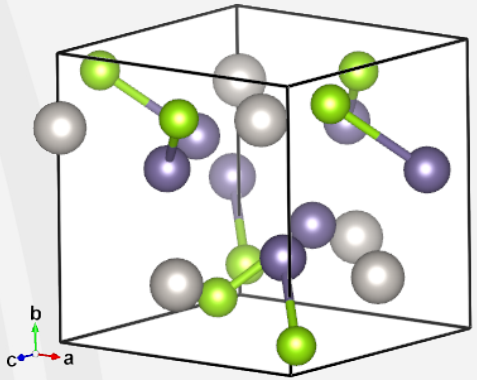

FeS_2 (Pyrite) | Pa-3 (#205)

```
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_2 | $Pca2_1$ (#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 | $Pca2_1$ (#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
```

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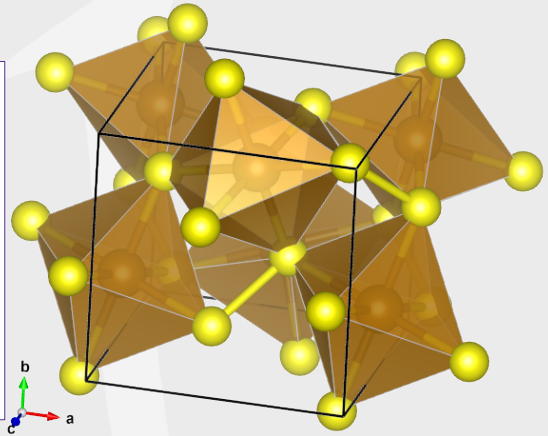
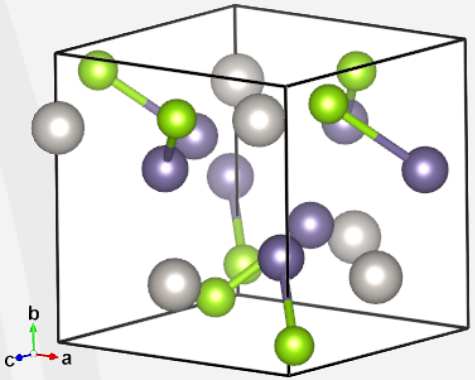
AT.	WP	SS	Representative	Atomic orbit
Fe1	4a (x,y,z)	1	(0.000000,0.750000,0.000400)	(0.000000,0.750000,0.000400) (0.000000,0.250000,0.500400) (0.500000,0.250000,0.000400) (0.500000,0.750000,0.500400)
S1	4a (x,y,z)	1	(0.384730,0.134730,0.615670)	(0.384730,0.134730,0.615670) (0.615270,0.865270,0.115670) (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_2 | $Pca2_1$ (#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 | $Pca2_1$ (#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
```

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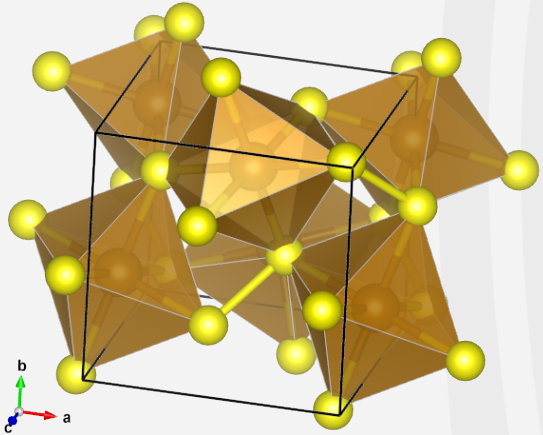
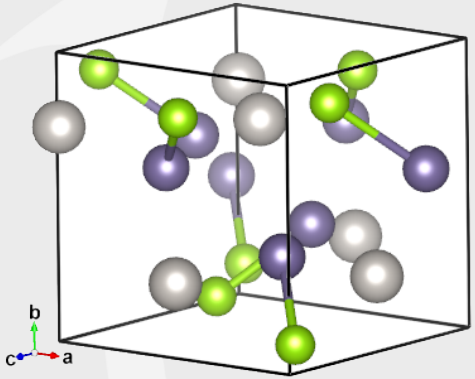
TRANSLATIONENGLEICHE MAXIMAL SUBGROUPS





FeS_2 | $Pca2_1$ (#29)

```
29
5.4178 5.4178 5.4178 90. 90. 90.
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 | $Pca2_1$ (#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
```

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

Matrix form:

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

Atom pairings and distances

Atom Mappings					
WP		Atom	Coordinates in S_1	Atom	Coordinates in S_2
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_x	u_y	u_z	|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_x, u_y and u_z are given in relative units. |u| is the absolute distance given in Å

Evaluation of the structure similarity

S	$d_{max.}$ (Å)	$d_{av.}$ (Å)	Δ
0.0686	0.0714	0.0533	0.018

1^{st}: PtGeSe, 2^{nd}: FeS_2

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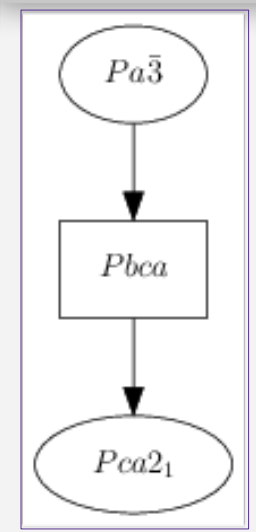
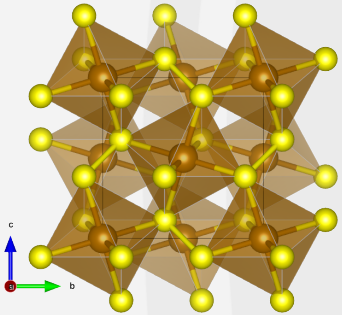
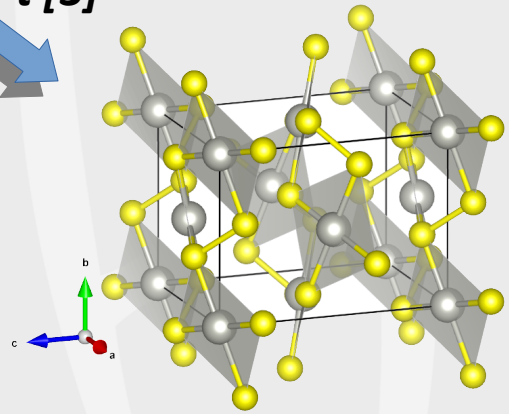


TRANSLATIONENGLEICHE MAXIMAL SUBGROUPS



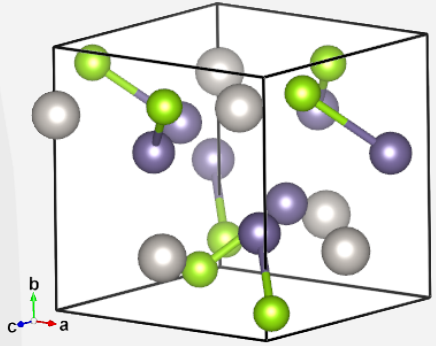
FeS_2 (Pyrite) | Pa-3 (#205)

t [3]



PdS_2 | Pbca (#61)

t [2]



PtGeSe | $Pca2_1$ (#29)

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

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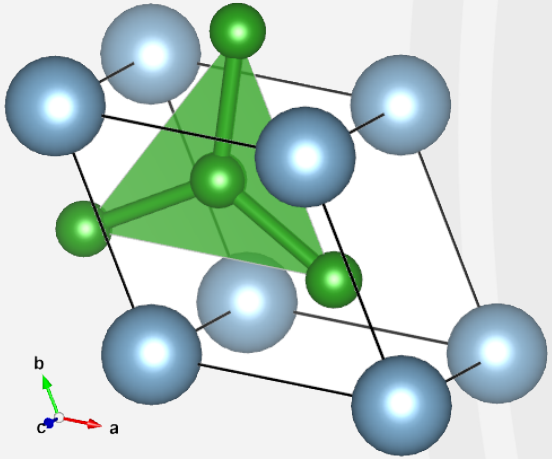
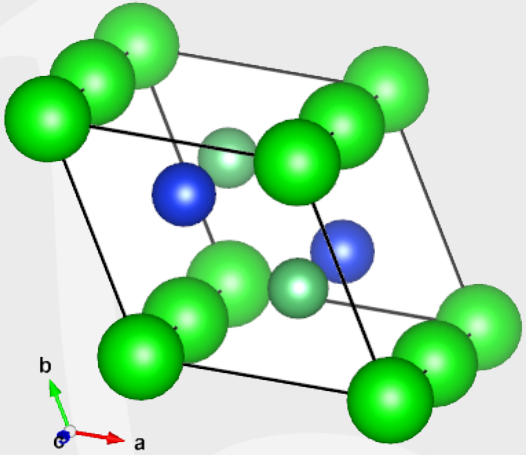
KLASSENGLEICHE MAXIMAL SUBGROUPS



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
```

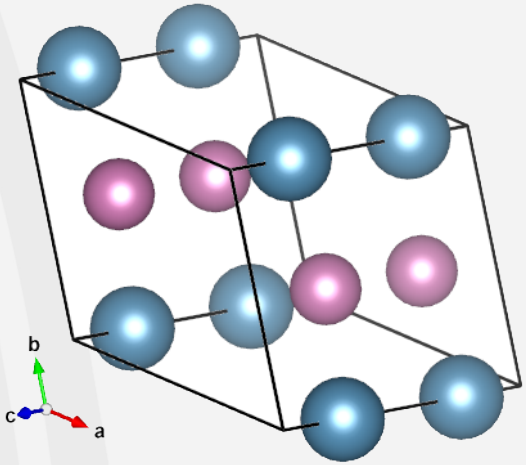
Alarco, J. A., Talbot, P. C., & Mackinnon, I. D. (2015). Phonon anomalies predict superconducting T c for AlB 2-type structures. Physical Chemistry Chemical Physics, 17(38), 25090-25099.



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
```

Rudy, E., Benesovsky, F., Nowotny, H., & Toth, L. E. (1961). Die Kristallstruktur von HfBe2, HfBe13 und HfBeSi; Teilsysteme: MeBe2-MeB2-MeSi2 (Me= Zr, Hf). Monatshefte für Chemie und verwandte Teile anderer Wissenschaften, 92(3), 692-700.



$CaIn_2$ | $P6_3/mmc$ (#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
```

Wendorff, M., & Roehr, C. (2005). Binary Indides AInx (x: 1, 2, 4; A: Ca, Sr, Ba, K, Rb)—Studies on Structural Chemistry and Chemical Bonding. ChemInform, 36(16).

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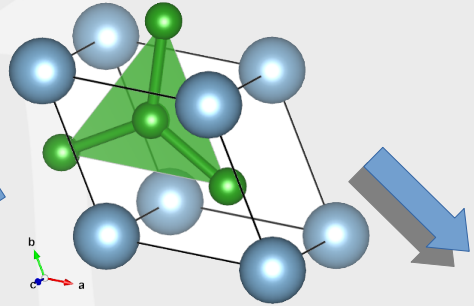
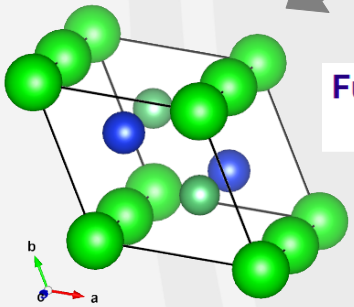
KLASSENGLEICHE MAXIMAL SUBGROUPS

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
```



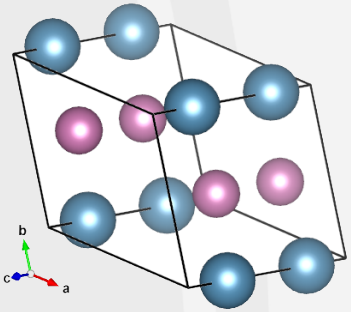


Full Set of Possible Transformations for the chain 191 194 [2]

191 194 [2]

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

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



$ZrBeSi$ | $P6_3/mmc$ (#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
```

$CaIn_2$ | $P6_3/mmc$ (#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
```

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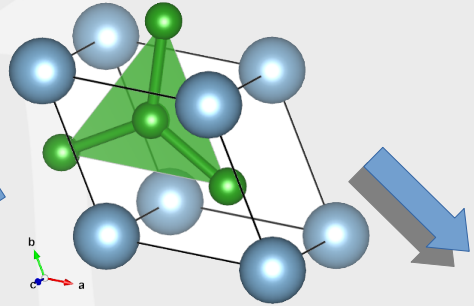
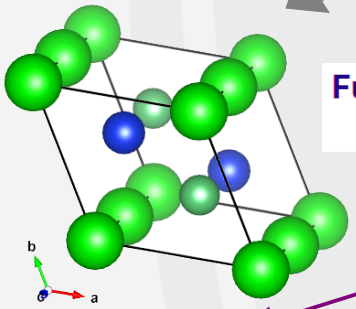
KLASSENGLEICHE MAXIMAL SUBGROUPS

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
```



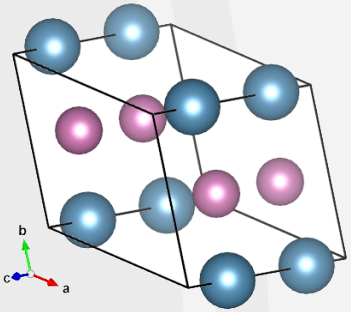


Full Set of Possible Transformations for the chain 191 194 [2]

191 194 [2]

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

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



$ZrBeSi$ | $P6_3/mmc$ (#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
```

$CaIn_2$ | $P6_3/mmc$ (#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
```

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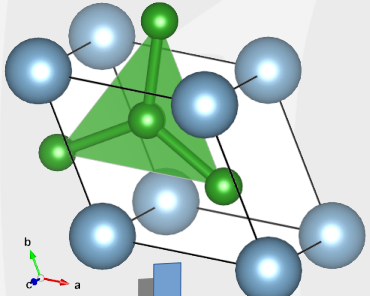
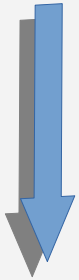
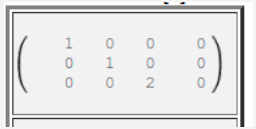
KLASSENGLEICHE MAXIMAL SUBGROUPS

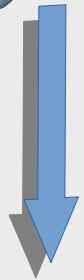
AlB_2 | P6/mmm (#191)

```
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
```



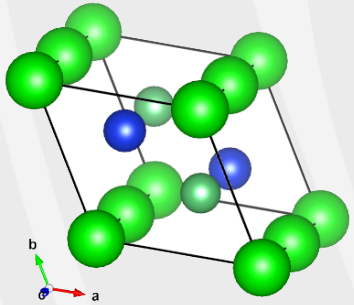






$ZrBeSi$ | $P6_3/mmc$ (#194)

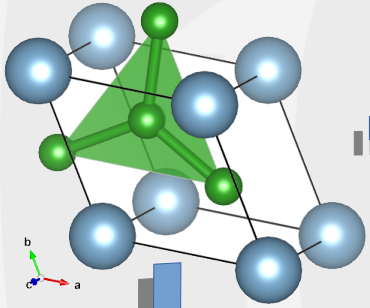
```
194
3.722 3.722 7.232 90. 90. 120.
3
Zr 1 2a 0 0 0
Be 1 2c 0.3333 0.6667 0.250
Si 2 2d 0.3333 0.6667 0.750
```

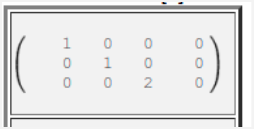


KLASSENGLEICHE MAXIMAL SUBGROUPS

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
```

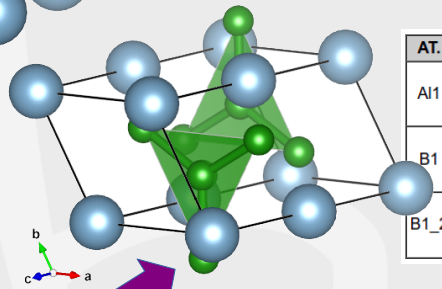




$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix}$$

AlB_2 | $P6_3/mmc$ (#194)

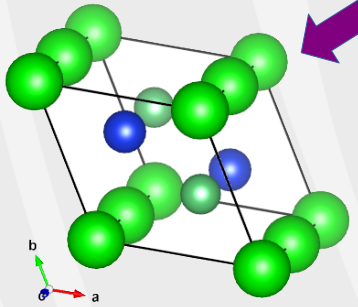
```
194
3.003900 3.003900 6.561200 90 90 120
3
Al 1 2a 0.000000 0.000000 0.000000
B  1 2c 0.333333 0.666667 0.250000
B  2 2d 0.666667 0.333333 0.250000
```



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 | $P6_3/mmc$ (#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
```



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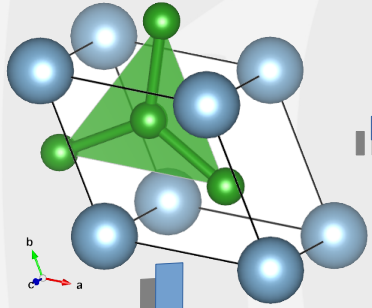
KLASSENGLEICHE MAXIMAL SUBGROUPS

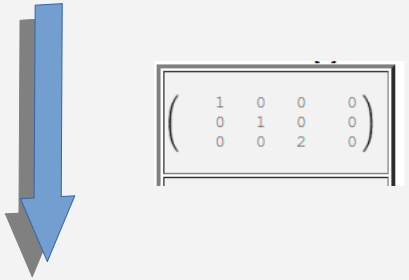
AlB_2 | P6/mmm (#191)

```
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
```

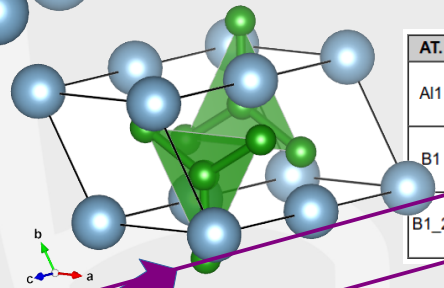


AlB_2 | $P6_3/mmc$ (#194)

```
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
```



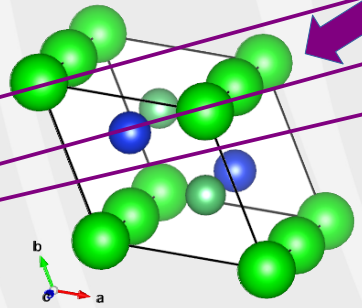
$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix}$$



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)

$ZrBeSi$ | $P6_3/mmc$ (#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
```



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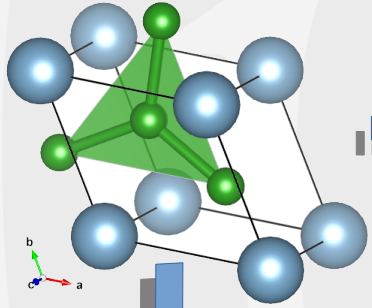
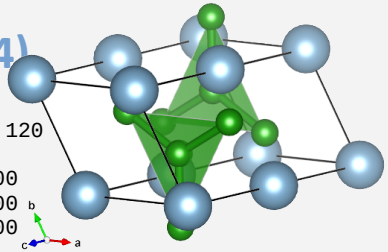
KLASSENGLEICHE MAXIMAL SUBGROUPS

AlB_2 | P6/mmm (#191)

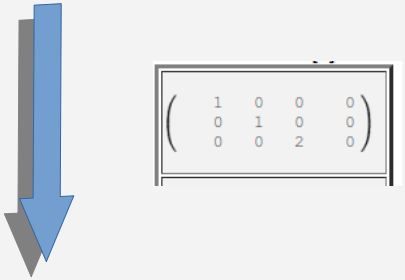
```
191
3.00390 3.00390 3.28060 90 90 120
2
Al 1 1a 0.000000 0.000000 0.000000
B  1 2d 0.333333 0.666667 0.500000
```

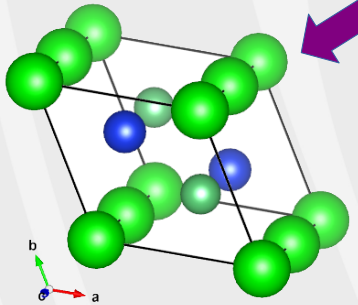




AlB_2 | $P6_3/mmc$ (#194)

```
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
```





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
```

WP		Atom Structure1	Atom Structure2	Atomic Displacements			
				u_x	u_y	u_z	|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_x, u_y and u_z are given in relative units. |u| is the absolute distance given in Å

Evaluation of the structure similarity

S	$d_{max.}$ (Å)	$d_{av.}$ (Å)	Δ
0.0873	0	0.0000	0.124

default

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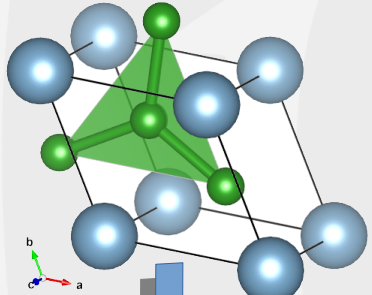
KLASSENGLEICHE MAXIMAL SUBGROUPS

AlB_2 | P6/mmm (#191)

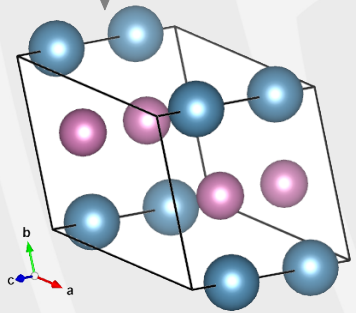
```
191
3.00390 3.00390 3.28060 90 90 120
2
Al 1 1a 0.000000 0.000000 0.000000
B  1 2d 0.333333 0.666667 0.500000
```



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

$CaIn_2$ | $P6_3/mmc$ (#194)

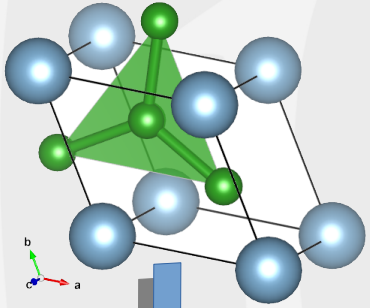
```
194
4.892 4.892 7.739 90.00 90.00 120.00
2
In 1 4f 0.6667 0.3333 0.04763
Ca 1 2b 0.0000 0.0000 0.2500
```



KLASSENGLEICHE MAXIMAL SUBGROUPS

AlB_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] Choose File No file chosen

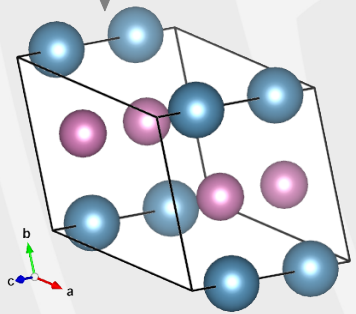
BCS Format

```
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
```

What if we don't know the transformation matrix?

$CaIn_2$ | $P6_3/mmc$ (#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] Choose File No file chosen

BCS Format

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

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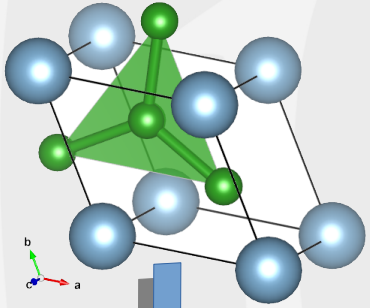
KLASSENGLEICHE MAXIMAL SUBGROUPS

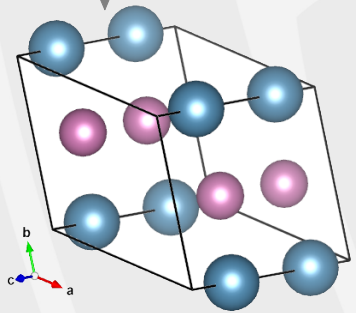
AlB_2 | P6/mmm (#191)

```
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
```



$CaIn_2$ | $P6_3/mmc$ (#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
```



High symmetry structure

Enter the formula units in the **high symmetry structure**
(Leave blank for auto-detection via the volume information) 1

Structure Data [CIF format] Choose File No file chosen

BCS Format

```
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
```

Low symmetry structure:

Enter the formula units in the **low symmetry structure**
(Leave blank for auto-detection via the volume information) 2

Structure Data [CIF format] Choose File No file chosen

BCS Format

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

Enter the allowed tolerance (a b c α β γ): 222222

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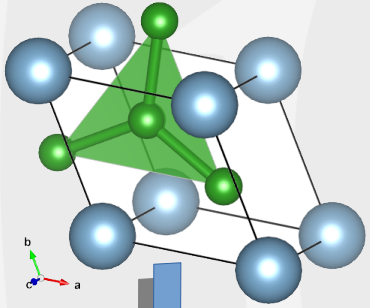
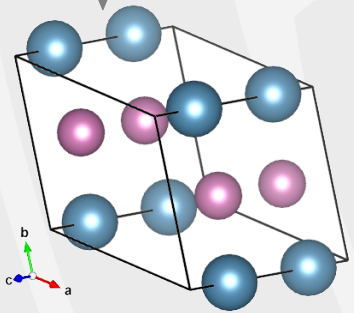
KLASSENGLEICHE MAXIMAL SUBGROUPS

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
```





$CaIn_2$ | $P6_3/mmc$ (#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
```

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_1	Atom	Coordinates in S_2
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_x	u_y	u_z	|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

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

S	$d_{max.}$ (Å)	$d_{av.}$ (Å)	Δ
0.1541	0.3686	0.2457	0.443

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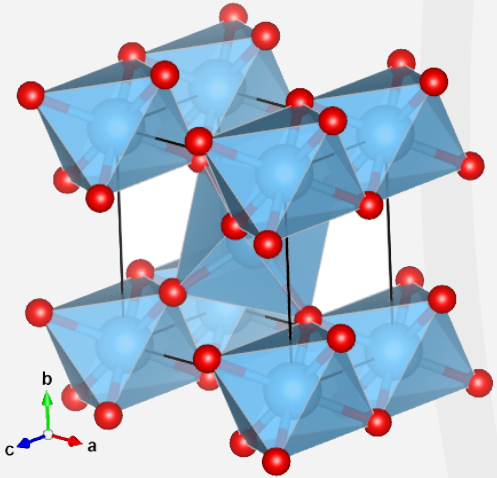
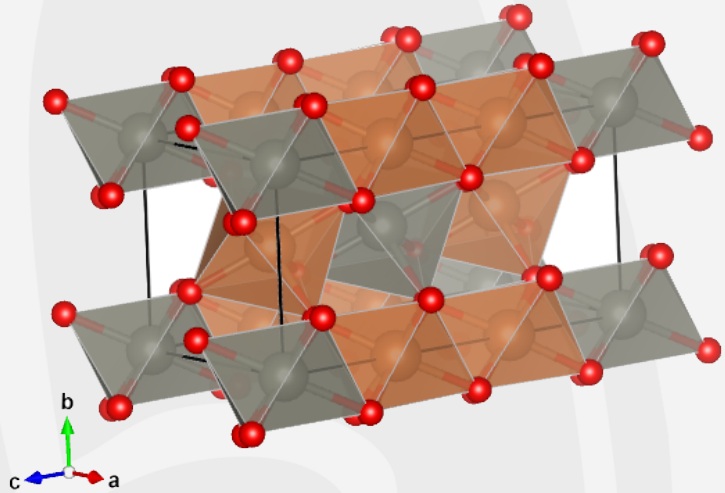
ISOMORPHIC MAXIMAL SUBGROUPS



TiO_2 (Rutile) | $P4_2/mnm$ (#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 (TiO2) prepared by high-temperature ultracentrifugation. Crystal Growth & Design, 17(4), 1460-1464.



$ZnSb_2O_6$ (Odonezite/Trirutile) | $P4_2/mnm$ (#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, Sapioris, Durango, Mexico: new data and structure refinement. The Canadian Mineralogist, 40(4), 1207-1210.

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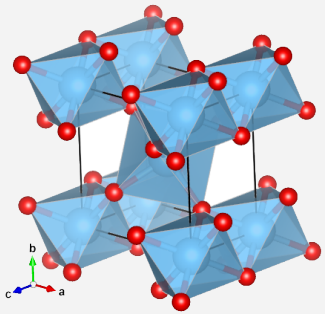
ISOMORPHIC MAXIMAL SUBGROUPS



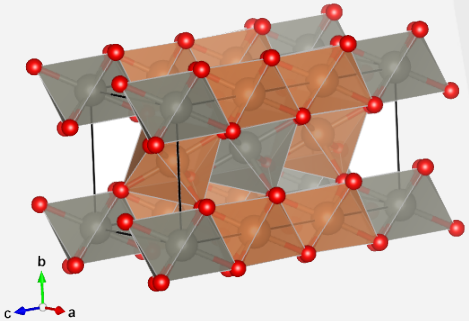
TiO_2 (Rutile) | $P4_2/mnm$ (#136)

High symmetry structure

Enter the formula units in the **high symmetry structure**
(Leave blank for auto-detection via the volume information) 2

Structure Data [CIF format] Choose File 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
```



$ZnSb_2O_6$ (Odonezite/Trirutile) | $P4_2/mnm$ (#136)

Low symmetry structure:

Enter the formula units in the **low symmetry structure**
(Leave blank for auto-detection via the volume information) 6

Structure Data [CIF format] Choose File No file chosen

BCS Format

```
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 8j 0.304 0.304 0.325
```

Enter the allowed tolerance (a b c α β γ): 2 2 2 2 2 2

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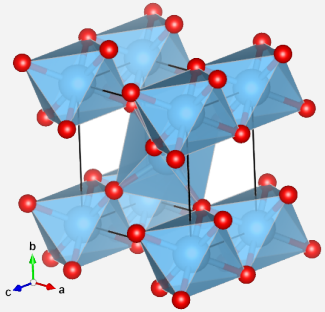
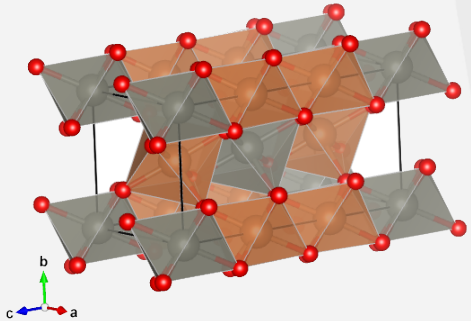
ISOMORPHIC MAXIMAL SUBGROUPS



TiO_2 (Rutile) | $P4_2/mnm$ (#136)



$ZnSb_2O_6$ (Odonezite) | $P4_2/mnm$ (#136)

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

Matrix form:

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

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_1	Atom	Coordinates in S_2
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_x	u_y	u_z	|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_x, u_y and u_z are given in relative units. |u| is the absolute distance given in Å

S	$d_{max.}$ (Å)	$d_{av.}$ (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 ($d_{max.}$) shows the maximal displacement between the atomic positions of the paired atoms. The **maximum distance ($d_{max.}$)** in this case is: **0.0774 Å**
- The average distance (d_{av}) 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_{av})** 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**.

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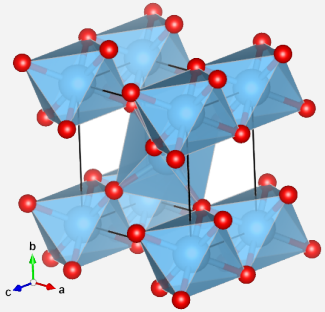
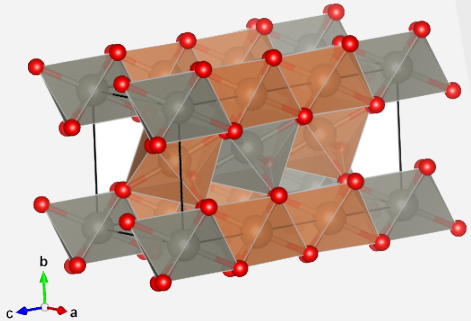
ISOMORPHIC MAXIMAL SUBGROUPS



TiO_2 (Rutile) | $P4_2/mnm$ (#136)



$ZnSb_2O_6$ (Odonezite) | $P4_2/mnm$ (#136)

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

Matrix form:

(**P**,p)= (1 0 0 / 0 1 0 / 0 0 3)

Description of the Hi… Low Symmetry Struc…

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

Atom pairings and di…

	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_x, u_y and u_z are given in relative units. |u| is the absolute distance given in Å

Maximal subgroups of group $P4_2/mnm$ (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	*Pnnm*	2	t	show..
2	65	*Cmmm*	2	t	show..
3	84	$P4_2/m$	2	t	show..
4	94	$P4_22_12$	2	t	show..
5	102	$P4_2nm$	2	t	show..
6	113	$P\text{-}42_1m$	2	t	show..
7	118	$P\text{-}4n2$	2	t	show..
8	136	$P4_2/mnm$	3	k	show..
9	136	$P4_2/mnm$	5	k	show..
10	136	$P4_2/mnm$	7	k	show..
11	136	$P4_2/mnm$	9	k	show..

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

S	$d_{max.}$ (Å)	$d_{av.}$ (Å)	Δ
	0.0515	0.038	

…he spontaneous strain (sum of the squared …d by 3). For the given two structures, the …**145**.

… the maximal displacement between the …The **maximum distance ($d_{max.}$)** in this case …

…e average over the primitive unit cell of the …he paired atoms. For this case the **average** …

…ff *et al.*, 1998) is a function of the differences …cities of the sites) and the ratios of the …ctures (the comparison being between the …e low symmetry structure's setting and the …**asure of compatibility (Δ)** calculated for this …

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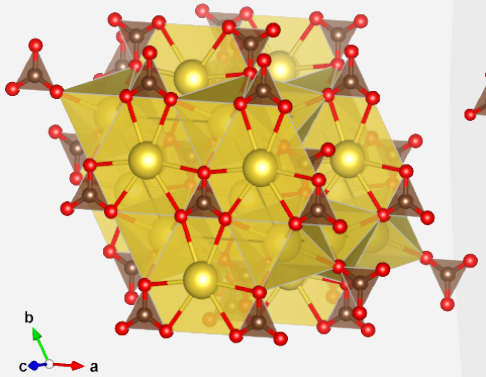
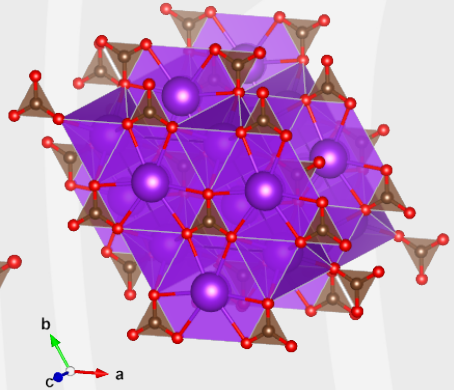
COMMON SUPERGROUP



α-Na_2CO_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
```

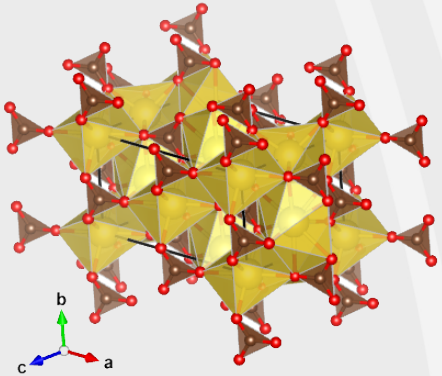
Swainson, I. P., Dove, M. T., & Harris, M. J. (1995). Neutron powder diffraction study of the ferroelastic phase transition and lattice melting in sodium carbonate, Na2CO3. Journal of Physics: Condensed Matter, 7(23), 4395.



α-K_2CO_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
```

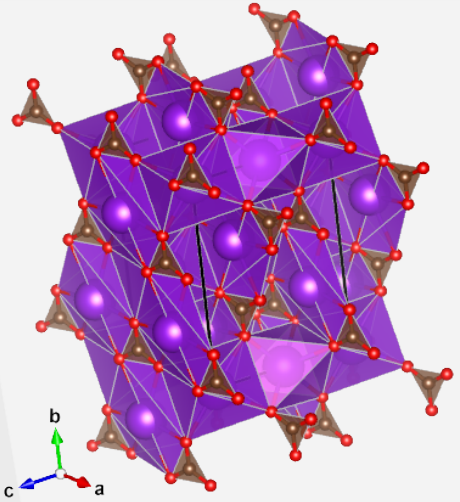
Becht, H. Y., & Struikmans, R. (1976). A monoclinic high-temperature modification of potassium carbonate. Acta Crystallographica Section B: Structural Crystallography and Crystal Chemistry, 32(12), 3344-3346.



β-Na_2CO_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.

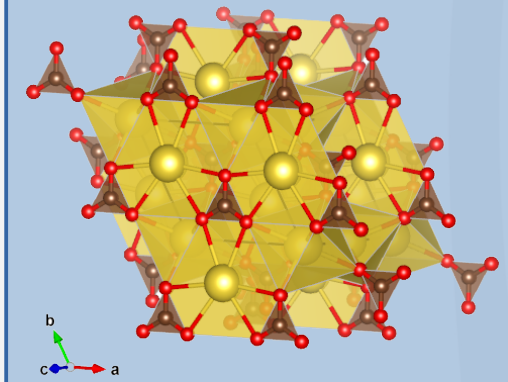


β-K_2CO_3 | C2/c (#12)

```
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

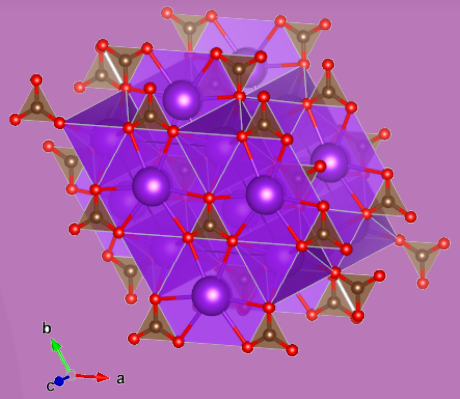


AT.	WP	SS	Representative	Atomic orbit
Na1	2a (0,0,0)	-3m.	(0.000000,0.000000,0.000000)	(0.000000,0.000000,0.000000) (0.000000,0.000000,0.500000)
Na2	2c (1/3,2/3,1/4)	-6m2	(0.666667,0.333333,0.750000)	(0.666667,0.333333,0.750000) (0.333333,0.666667,0.250000)
C1	2d (1/3,2/3,3/4)	-6m2	(0.666667,0.333333,0.250000)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

α-Na_2CO_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
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)



α-K_2CO_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
```

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COMMON SUPERGROUP

Enter the allowed tolerance (a b c α β γ): 1 1 1 1 12 1

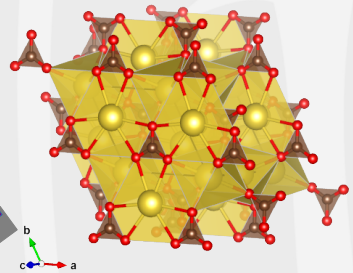
Description of the High Symmetry Structure in the most similar configuration to the Low Symmetry Structure

```
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
```

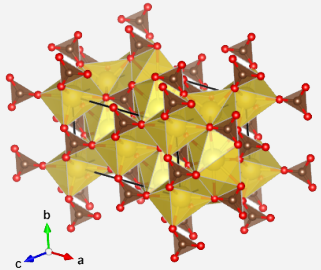
Transformation Matrix (P,p): (a-b,-a-b,-c;0,0,-1/2)

Matrix form:

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



α-Na_2CO_3 | $P6_3/mmc$ (#194)



β-Na_2CO_3 | C2/c (#12)

WP		Atom	Atomic Displacements			
			u_x	u_y	u_z	|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_x, u_y and u_z are given in relative units. |u| is the absolute distance given in Å

Evaluation of the Global Distortion

S	$d_{max.}$ (Å)	$d_{av.}$ (Å)	Δ
0.0665	0.4432	0.1614	0.081

Enter the allowed tolerance (a b c α β γ): 1 1 1 1 7 1

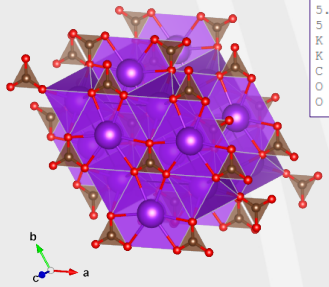
Description of the High Symmetry Structure in the most similar configuration to the Low Symmetry Structure

```
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:

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



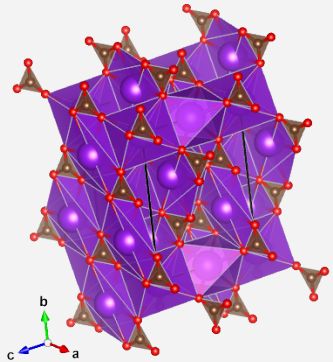
α-K_2CO_3 | $P6_3/mmc$ (#194)

WP		Atom	Atomic Displacements			
			u_x	u_y	u_z	|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_x, u_y and u_z are given in relative units. |u| is the absolute distance given in Å

Evaluation of the Global Distortion

S	$d_{max.}$ (Å)	$d_{av.}$ (Å)	Δ
0.0295	0.3083	0.1072	0.028



β-K_2CO_3 | C2/c (#12)

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APPLICATION TO THE GLASERITES FAMILY

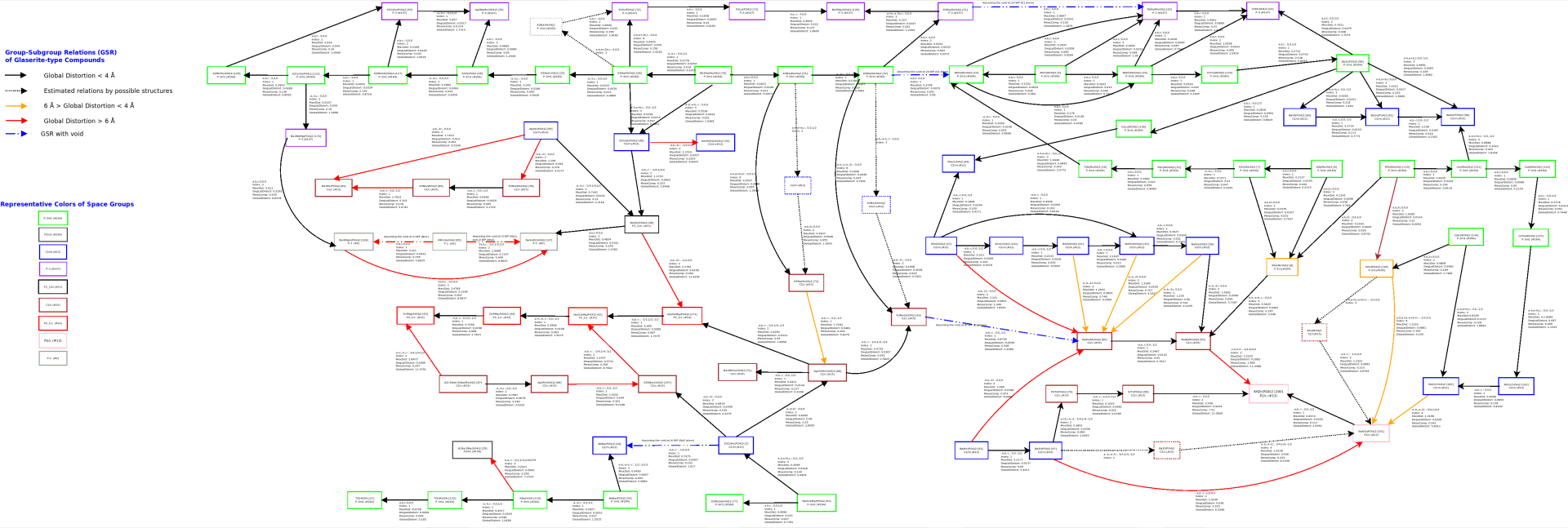
$K_3Na(SO_4)_2$

$X_{(;1)}Y_{(;2)}[M(TO_4)_2]$

No	General formula	Conditions	Examples		Ref.	Number of GTC
			Long formula	Short formula		
1	$XY_2[M(TO_4)_2]$	X≠Y≠M≠T	$BaNa_2[Mg(PO_4)_2]$	$BaNa_2Mg(PO_4)_2$	[12]	12
2	$XY_2[M(TO_4)_2]$	X=Y≠M≠T	$AgAg_2[Fe(VO_4)_2]$	$Ag_3Fe(VO_4)_2$	[29]	31
3	$XY_2[M(TO_4)_2]$	X≠Y; X=M; Y≠M≠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≠M≠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≠X2≠M≠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≠Y2;Y2=M≠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≠M≠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≠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≠T1; T1≠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≠M1≠M2≠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≠T	$TlTl_2[Tl(WO_4)_2]$= $Tl_4(WO_4)_2$	Tl_2WO_4	[37]	2
12	$XY_2H[M(TO_4)_2]$	X=Y≠M≠T	$NaNa_2H[Mg(PO_4)_2]$	$Na_3HMg(PO_4)_2$	[38]	5
13	$XY_{\square}H[M(TO_4)_2]$	X≠M≠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



$$K_3Na(SO_4)_2$$

$$X_{(;1)}Y_{(;2)}[M(TO_4)_2]$$

Albay, S. (2019) "Classification of the Glaserite Structures Family by means of Group Theory", M.S. Thesis, Hacettepe University

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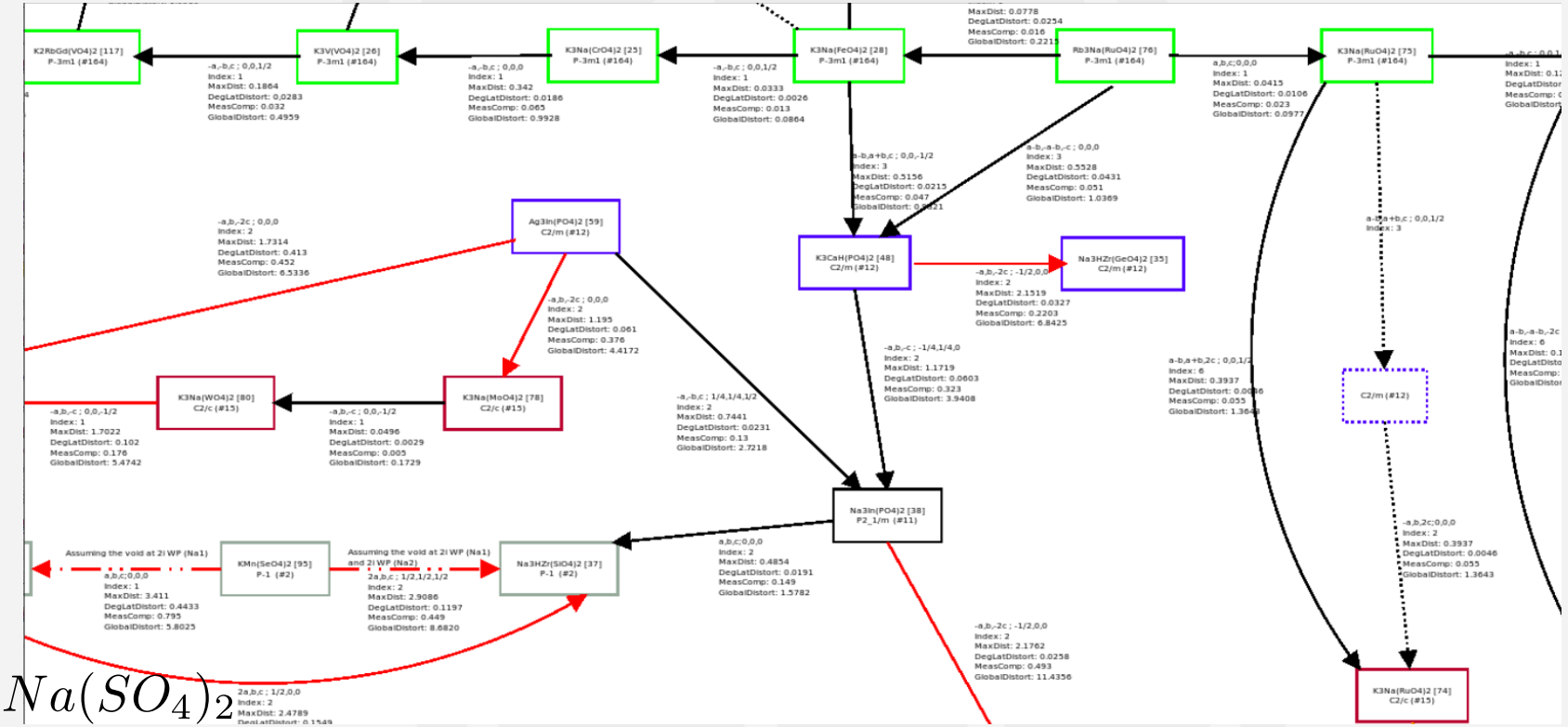
APPLICATION TO THE GLASERITES FAMILY



$$K_3Na(SO_4)_2$$

$$X_{(;1)}Y_{(;2)}[M(TO_4)_2]$$

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THANK YOU

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