

---

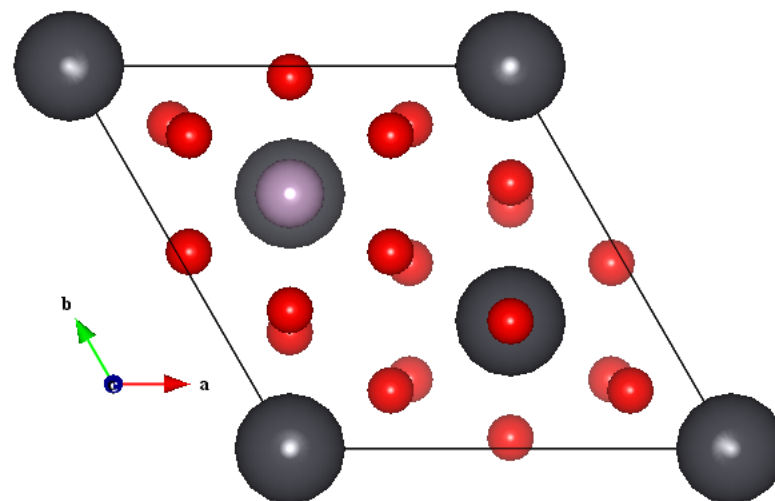
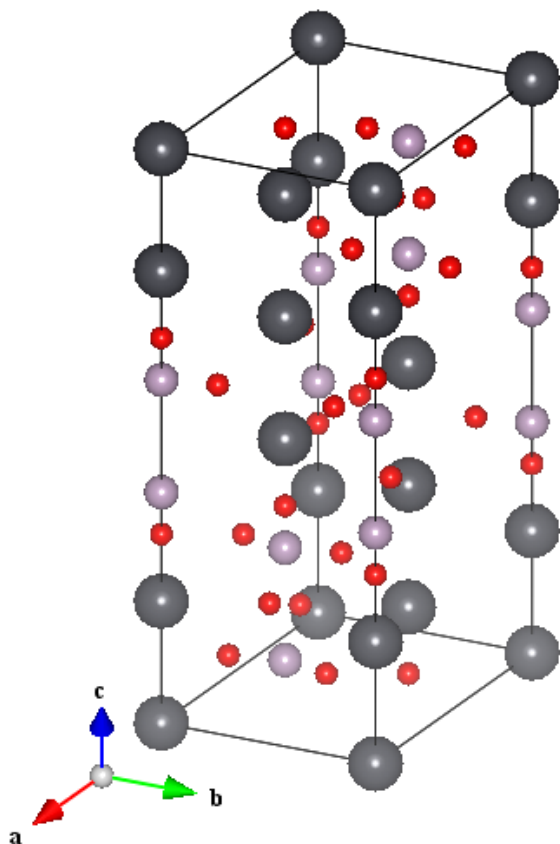
# Obtaining the transformation matrix connecting two group-subgroup related structures

---

*E.S. Tasci, Gemma de la Flor, M.I. Aroyo*

**Bilbao Crystallographic Server Team (<http://www.cryst.ehu.es>)**  
**Condensed Matter Physics, University of the Basque Country**  
08/2011, IUCr Mieres 2011: Crystallographic Computing School  
emre.tasci@ehu.es

# Structure Data



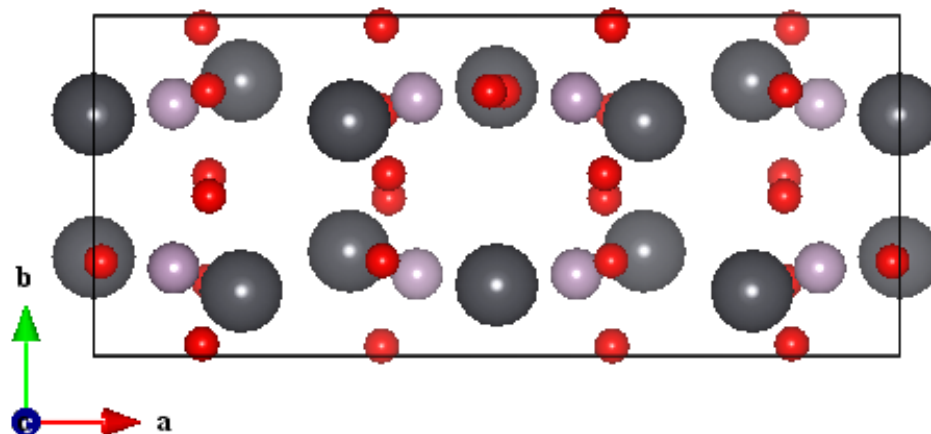
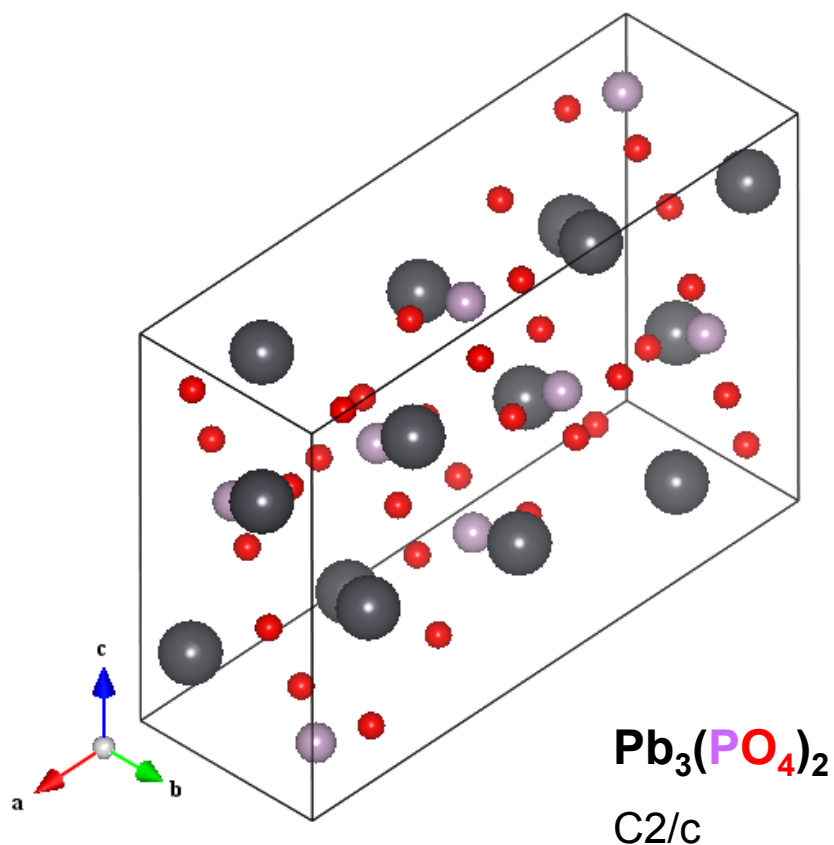
R-3m

		166				
		5.56	5.56	20.39	90	90 120
		5				
Pb	1	3a	0	0	0	
Pb	2	6c	0	0	0.2126	
P	1	6c	0	0	0.4021	
O	1	6c	0	0	0.3290	
O	2	18h	0.1810	-0.1810	0.0960	

H.N. Ng, C. Calvo

Can. J. Phys. **53** 42-51 (1975)

# Structure Data

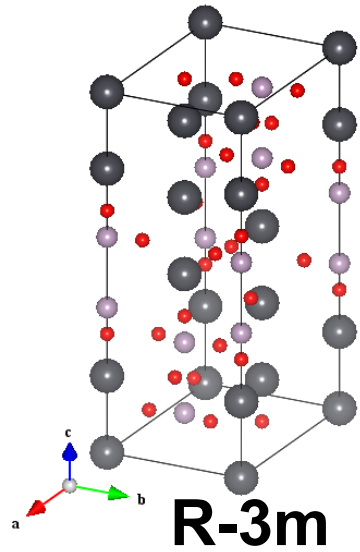


15					
13.80	5.691	9.42	90	102.3	90
7					
Pb	1	4e	0.000	0.291	0.250
Pb	2	8f	0.317	0.309	0.352
P	1	8f	0.599	0.241	0.447
O	1	8f	0.643	0.030	0.392
O	2	8f	0.634	0.464	0.374
O	3	8f	0.642	0.280	0.612
O	4	8f	0.491	0.222	0.420

Guimares, D.M.C.

Acta Cryst. A **35** 108-114 (1979)

# Plan of Attack

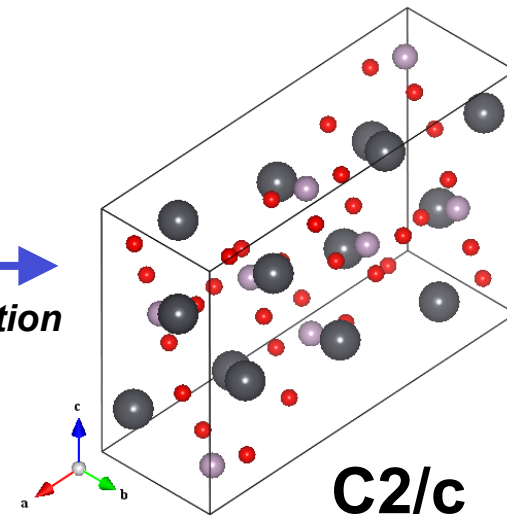


*Symmetry Reduction*



**C2/c**

*Affine Transformation*



---

# How do we relate these structures?

**1.Index**

2.Path

3.Wyckoff Splitting Compatibility

4.Lattice Compatibility

5.Atomic positions match

# How do we...?

## 1. Index

$$\left. \begin{array}{l} f_{R-3m} = 3 \quad Z_{R-3m} = 3 \\ f_{C2/c} = 2 \quad Z_{C2/c} = 4 \end{array} \right\} i_l = \frac{f_{R-3m} \times Z_{C2/c}}{f_{C2/c} \times Z_{R-3m}} = 2$$

$$\left. \begin{array}{l} [PG_{R-3m}] = [-3m] = 12 \\ [PG_{C2/c}] = [2/m] = 4 \end{array} \right\} i_p = \frac{[PG_{R-3m}]}{[PG_{C2/c}]} = 3$$

$$i = i_l \times i_p = 6$$

### Index of a group-subgroup pair

High symmetry Space Group: 166 ( $R-3m$ ) [hexagonal axes]

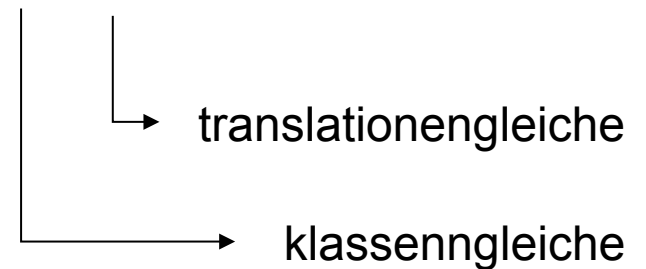
Low symmetry Space Group: 15 ( $C2/c$ ) [unique axis b]

$i_L$  2

$i_P$  3

Total index 6

**INDEX**



---

# How do we relate these structures?

1. Index ✓ 6

**2. Possible Paths**

3. Wyckoff Splitting Compatibility

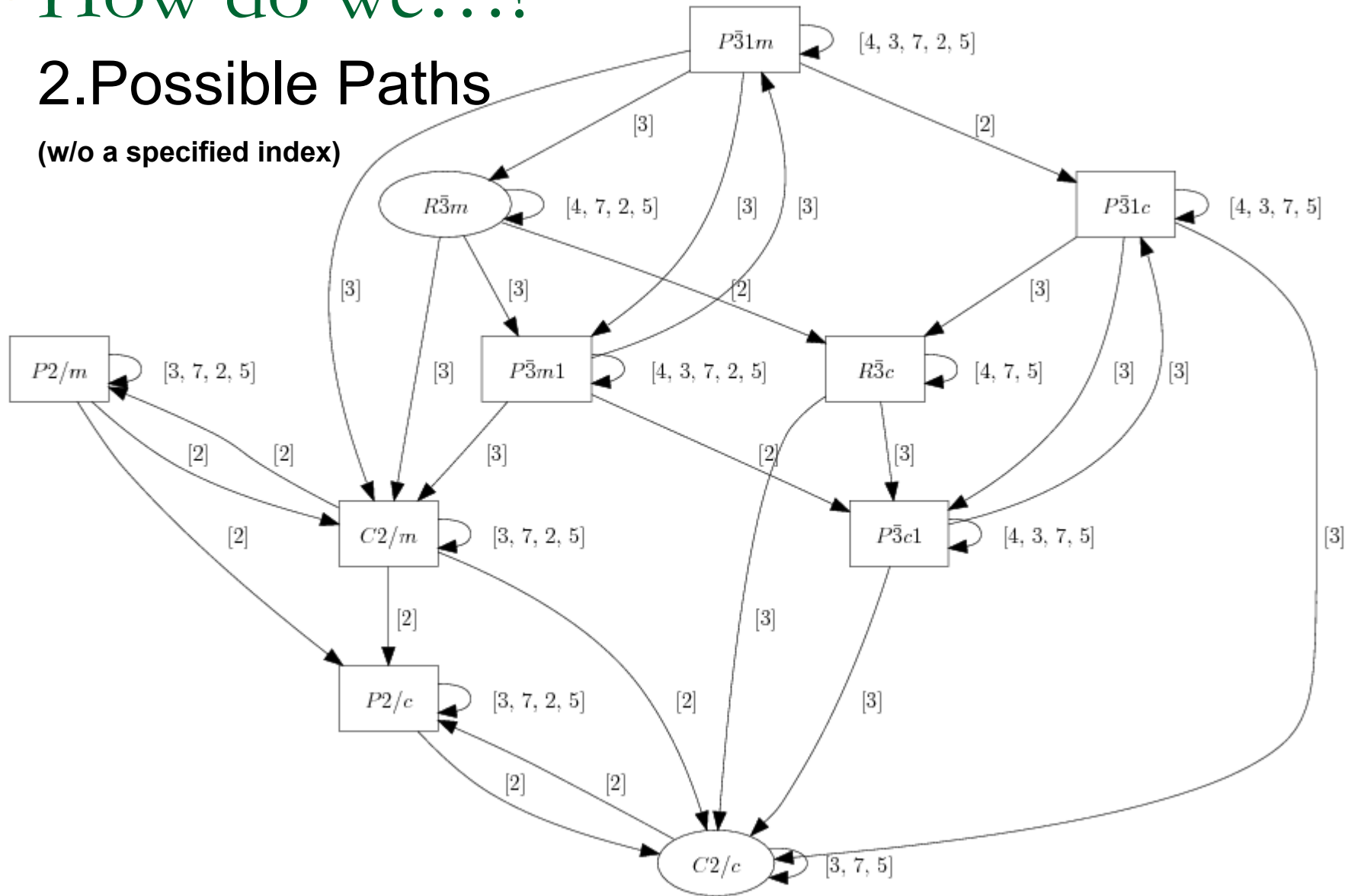
4. Lattice Compatibility

5. Atomic positions match

# How do we...?

## 2. Possible Paths

(w/o a specified index)

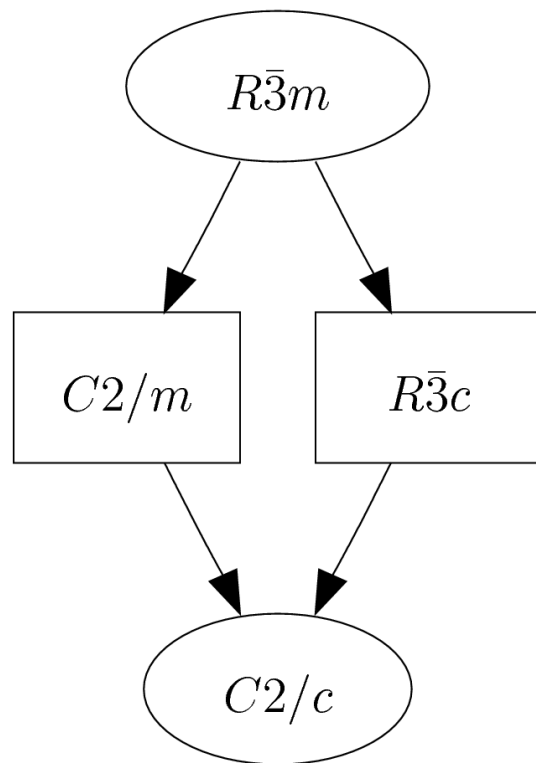


**SUBGROUPGRAPH**



# How do we...?

## 2. Possible Paths



**SUBGROUPGRAPH**

Classification of the subgroups of type 15 ( $C2/c$ ) [unique axis  $b$ ] of group 166 ( $R-3m$ ) [hexagonal axes] with index 6

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

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

Classes representatives

Class #	Transformation Matrix	Matrix Representation	WP Splitting	Symmetry Modes	All subgroups
1	$-1/3a+1/3b-8/3c,-a-b,2c+1/2$	$\begin{pmatrix} -1/3 & -1 & 0 & 0 \\ 1/3 & -1 & 0 & 0 \\ -8/3 & 0 & 2 & 1/2 \end{pmatrix}$	go to Splitting..	go to Symmodes..	Show
2	$-1/3a+1/3b-2/3c,-a-b,2c$	$\begin{pmatrix} -1/3 & -1 & 0 & 0 \\ 1/3 & -1 & 0 & 0 \\ -2/3 & 0 & 2 & 0 \end{pmatrix}$	go to Splitting..	go to Symmodes..	Show
3	$-1/3a+1/3b-8/3c,-a-b,2c$	$\begin{pmatrix} -1/3 & -1 & 0 & 0 \\ 1/3 & -1 & 0 & 0 \\ -8/3 & 0 & 2 & 0 \end{pmatrix}$	go to Splitting..	go to Symmodes..	Show
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**

# How do we relate these structures?

1. Index ✓ 6

2. Possible Paths ✓

R-3m → R-3c → C2/c

R-3m → C2/m → C2/c

## 3. Wyckoff Splitting Compatibility

$$\begin{pmatrix} -1/3 & -1 & 0 & 0 \\ 1/3 & -1 & 0 & 0 \\ -8/3 & 0 & 2 & 1/2 \end{pmatrix}$$

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

$$\begin{pmatrix} -1/3 & -1 & 0 & 0 \\ 1/3 & -1 & 0 & 0 \\ -8/3 & 0 & 2 & 0 \end{pmatrix}$$

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

4. Lattice Compatibility

5. Atomic positions match

# How do we...?

## 3. Wyckoff Splitting Compatibility

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

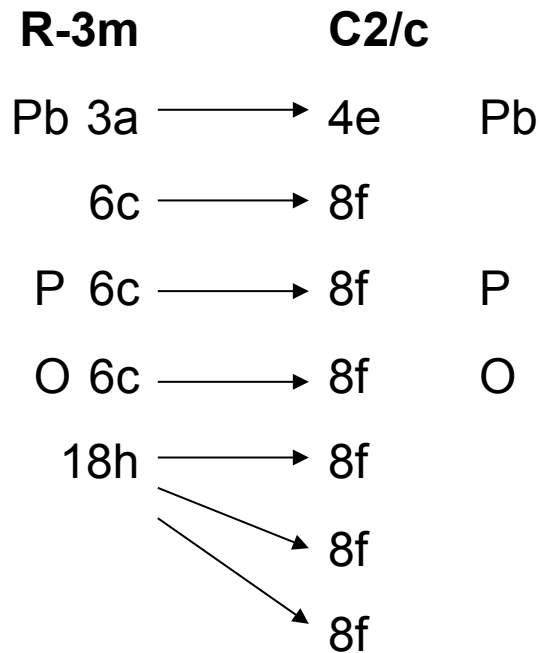
WPASSIGN

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

HERMANN

# How do we...?

## 3. Wyckoff Splitting Compatibility



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

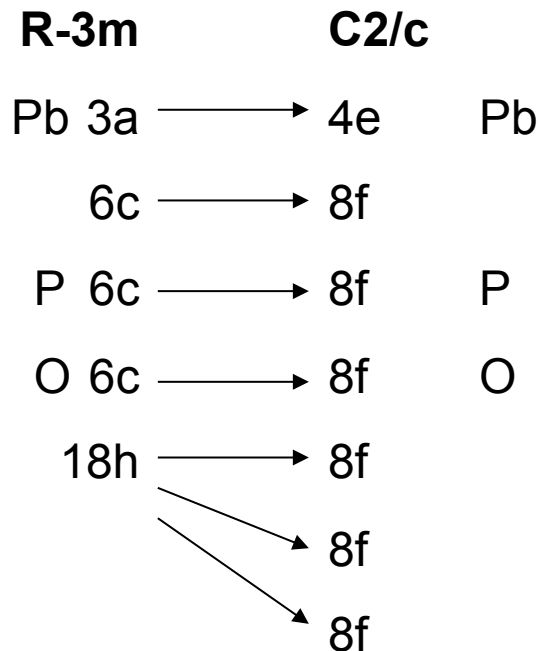
### Result from splitting

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 4e 8f 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

**WYCKSPLIT**

# How do we...?

## 3. Wyckoff Splitting Compatibility



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

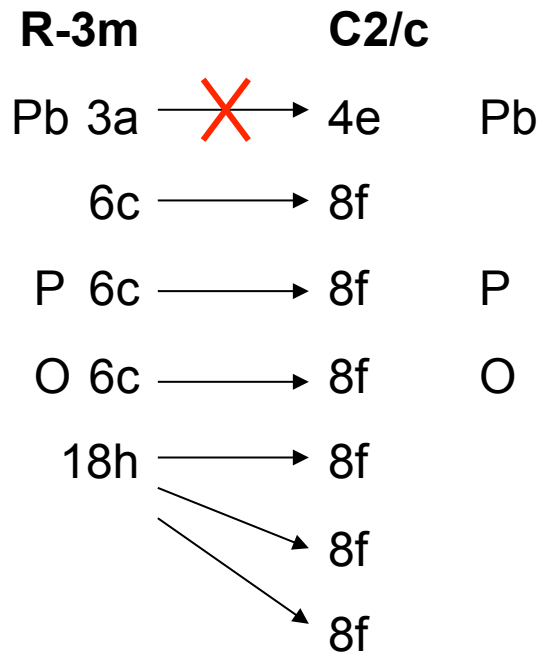
Result from splitting

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

WYCKSPLIT

# How do we...?

## 3. Wyckoff Splitting Compatibility



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

Result from splitting

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

**WYCKSPLIT**

# Wyckoff Sets

## Wyckoff Sets of Space Group 15 (C2/c) [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

**WYCKSETS**

# How do we...?

## 3. Wyckoff Splitting Compatibility

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

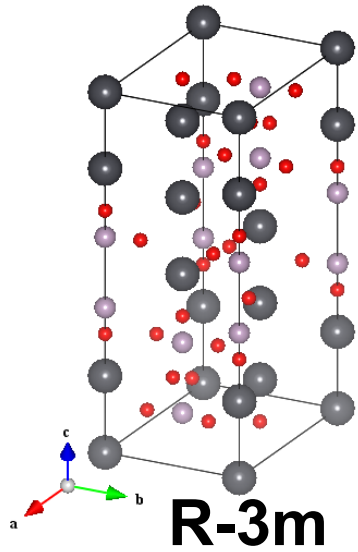
Subgroup #	Transformation Matrix	Matrix Representation
1	$-1/3a+1/3b-2/3c,-a-b,2c+1/2$	$\begin{pmatrix} -1/3 & -1 & 0 & 0 \\ 1/3 & -1 & 0 & 0 \\ -2/3 & 0 & 2 & 1/2 \end{pmatrix}$
2	$-1/3a-2/3b-2/3c,a,2c+1/2$	$\begin{pmatrix} -1/3 & 1 & 0 & 0 \\ -2/3 & 0 & 0 & 0 \\ -2/3 & 0 & 2 & 1/2 \end{pmatrix}$
3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



HERMANN / SUBGROUPGRAPH

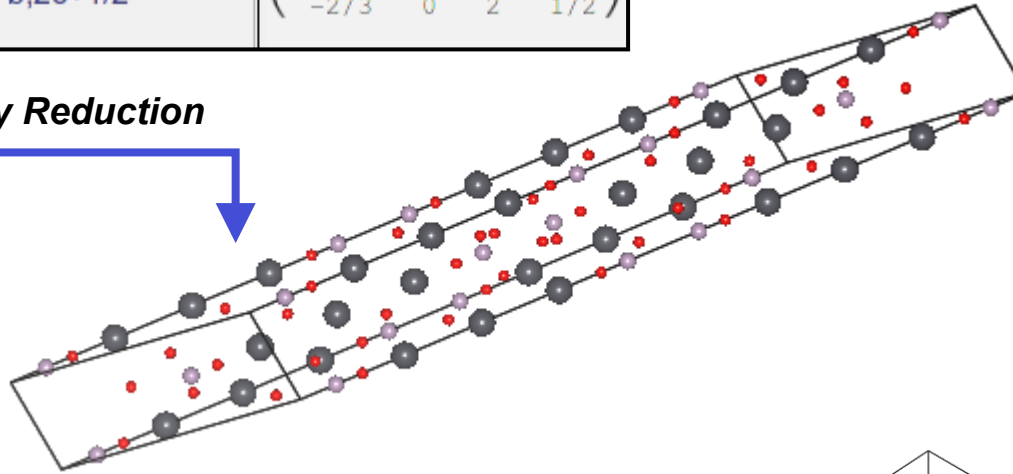


# Plan of Attack (revisited)



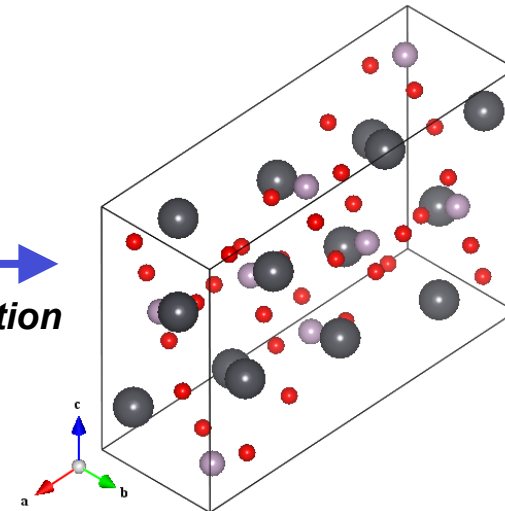
$-1/3a+1/3b-2/3c, -a-b, 2c+1/2$	$\begin{pmatrix} -1/3 & -1 & 0 & 0 \\ 1/3 & -1 & 0 & 0 \\ -2/3 & 0 & 2 & 1/2 \end{pmatrix}$
---------------------------------	---

**Symmetry Reduction**



**C2/c**

**Affine Transformation**



015					
13.97	5.56	40.78	90.00	166.71	90.00
7					
Pb	1	4e	0.0000	0.0000	0.7500
Pb	2	8f	0.0000	0.0000	0.8563
P	1	8f	0.0000	0.0000	0.9511
O	1	8f	0.0000	0.0000	0.9145
O	2	8f	0.9570	0.5000	0.1170
O	2_2	8f	0.7715	0.2285	0.3885
O	2_3	8f	0.2285	0.7715	0.1115

# How do we relate these structures?

1. Index ✓ 6

2. Possible Paths ✓

R-3m → R-3c → C2/c

R-3m → C2/m → C2/c

3. Wyckoff Splitting Compatibility

$$\begin{pmatrix} -1/3 & -1 & 0 & 0 \\ 1/3 & -1 & 0 & 0 \\ -8/3 & 2 & 1/2 & 0 \end{pmatrix}$$

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

$$\begin{pmatrix} -1/3 & 0 & 0 & 0 \\ 1/3 & 0 & 0 & 0 \\ -8/3 & 2 & 0 & 0 \end{pmatrix}$$

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

4. Lattice Compatibility

5. Atomic positions match

# How do we...?

## 4. Lattice Compatibility

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

**CELLTRAN**

R-3m
5.56 5.56 20.39 90.0 90.0 120.0

C2/c
13.97 5.56 40.78 90.0 166.71 90.00



C2/c
13.80 5.69 9.42 90.0 102.3 90.0

# How do we...?

## 4. Lattice Compatibility

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

R-3m
5.56 5.56 20.39 90.0 90.0 120.0

**CELLTRAN**

C2/c
13.97 5.56 40.78 90.0 166.71 90.00

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

$$\begin{pmatrix} 1 & 0 & -3 & 1/4 \\ 0 & -1 & 0 & 1/4 \\ 0 & 0 & -1 & 0 \end{pmatrix}$$

C2/c
13.97 5.56 9.63 90.0 103.23 90.0

C2/c
13.80 5.69 9.42 90.0 102.3 90.0

**NORMALIZER**

# How do we relate these structures?

1. Index ✓ 6

2. Possible Paths ✓

R-3m → R-3c → C2/c

R-3m → C2/m → C2/c

3. Wyckoff Splitting Compatibility ✓

4. Lattice Compatibility (Aff. Norm.  $x-3z+1/4, -b+1/4, -c$ )

$$\begin{pmatrix} -1/3 & 0 & 0 \\ 1/3 & - & 0 \\ -8/3 & 2 & 1/2 \end{pmatrix}$$

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

$$\begin{pmatrix} -1/3 & 0 & 0 \\ 1/3 & 0 & 0 \\ -8/3 & 2 & 0 \end{pmatrix}$$

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



5. Atomic positions match

# How do we relate these structures?

1. Index ✓ 6

2. Possible Paths ✓

R-3m → R-3c → C2/c

R-3m → C2/m → C2/c

3. Wyckoff Splitting Compatibility ✓

4. Lattice Compatibility (Aff. Norm.  $x-3z+1/4, -b+1/4, -c$ )

$$\begin{pmatrix} -1/3 & 0 & 0 \\ 1/3 & - & 0 \\ -8/3 & 2 & 1/2 \end{pmatrix}$$

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

$$\begin{pmatrix} -1/3 & 0 & 0 \\ 1/3 & 0 & 0 \\ -8/3 & 2 & 0 \end{pmatrix}$$

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

5. Atomic positions match

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

# How do we...?

## 5. Atomic positions match

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					
13.80	5.691	9.42	90	102.3	90
7					
Pb	1	4e	0.000	0.291	0.250
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

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

015					
13.97	5.56	9.63	90.0	103.23	90.0
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	2_2	8f	0.355999	0.021500	0.611500
O	2_3	8f	0.644001	0.478500	0.888499

**TRANSTRU**

# How do we...?

## 5. Atomic positions match

```

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
13.80 5.691 9.42 90 102.3 90
7
Pb 1 4e 0.000 0.291 0.250
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
    
```

$$\begin{bmatrix} -\frac{1}{3} & 1 & 1 & -\frac{1}{3} \\ \frac{1}{3} & 1 & -1 & -\frac{1}{6} \\ -\frac{2}{3} & 0 & 0 & \frac{1}{3} \end{bmatrix} \text{TRANSTRU}$$

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

```

015
13.97 5.56 9.63 90.0 103.23 90.0
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 2_2 8f 0.355999 0.021500 0.611500
O 2_3 8f 0.644001 0.478500 0.888499
    
```

```

015
13.97 5.56 9.63 90.0 103.23 90.0
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 2_2 8f 0.644001 0.478500 0.388500
O 2_3 8f 0.644001 0.021500 0.388499
    
```





# Comparison of nearly identical crystal structures

Maximum distance  $\Delta$ : 0.3309 Å

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

COMPSTRU

Atom Mappings						
WP	Atom	Coordinates in S <sub>1</sub>		Atom	Coordinates in S <sub>2</sub>	
4e	(0,y,1/4)	Pb1	(0.499999,0.250000,0.249999)	Pb1	(0.500000,0.291000,0.250000)	
8f	(x,y,z)	Pb2	(0.181099,0.250000,0.143699)	Pb2	(0.183000,0.309000,0.148000)	
8f	(x,y,z)	P1	(0.896849,0.250000,0.048949)	P1	(0.901000,0.241000,0.053000)	
8f	(x,y,z)	O1	(0.006499,0.250000,0.085499)	O4	(0.009000,0.222000,0.080000)	
8f	(x,y,z)	O2	(0.355999,0.750000,0.882999)	O3	(0.358000,0.780000,0.888000)	
8f	(x,y,z)	O2_2	(0.355999,0.021500,0.611500)	O2	(0.366000,0.036000,0.626000)	
8f	(x,y,z)	O2_3	(0.644001,0.478500,0.888499)	O1	(0.643000,0.470000,0.892000)	

WP	Atom	Atomic Displacements				
		u <sub>x</sub>	u <sub>y</sub>	u <sub>z</sub>	u	
4e	(0,y,1/4)	Pb1	0.0000	0.0410	0.0000	0.2280
8f	(x,y,z)	Pb2	0.0019	0.0590	0.0043	0.3309
8f	(x,y,z)	P1	0.0042	-0.0090	0.0041	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)	O2_2	0.0100	0.0145	0.0145	0.1912
8f	(x,y,z)	O2_3	-0.0010	-0.0085	0.0035	0.0615

# Transformation Matrix

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

# **Bilbao Crystallographic Server Team**

**Mois I. Aroyo**

**J. Manuel Perez-Mato**

**Emre S. Tasci**

**Gemma de la Flor**

**Samuel Vidal Gallego**



## Assignment of Wyckoff Positions

### Atoms Data:

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) (0.500000, 0.750000, 0.249999) (0.500000, 0.250000, 0.750001)
Pb2	8f (x,y,z)	1	(0.318901, 0.250000, 0.356301)	(0.318901, 0.250000, 0.356301) (0.681099, 0.250000, 0.143699) (0.681099, 0.750000, 0.643699) (0.318901, 0.750000, 0.856301) (0.818901, 0.750000, 0.356301) (0.181099, 0.750000, 0.143699) (0.181099, 0.250000, 0.643699) (0.818901, 0.250000, 0.856301)
P1	8f (x,y,z)	1	(0.603151, 0.250000, 0.451051)	(0.603151, 0.250000, 0.451051) (0.396849, 0.250000, 0.048949) (0.396849, 0.750000, 0.548949) (0.603151, 0.750000, 0.951051) (0.103151, 0.750000, 0.451051) (0.896849, 0.750000, 0.048949) (0.896849, 0.250000, 0.548949) (0.103151, 0.250000, 0.951051)

O1	8f (x,y,z)	1	(0.493501, 0.250000, 0.414501)	(0.493501, 0.250000, 0.414501) (0.506499, 0.250000, 0.085499) (0.506499, 0.750000, 0.585499) (0.493501, 0.750000, 0.914501) (0.993501, 0.750000, 0.414501) (0.006499, 0.750000, 0.085499) (0.006499, 0.250000, 0.585499) (0.993501, 0.250000, 0.914501)
O2	8f (x,y,z)	1	(0.644001, 0.250000, 0.617001)	(0.644001, 0.250000, 0.617001) (0.355999, 0.250000, 0.882999) (0.355999, 0.750000, 0.382999) (0.644001, 0.750000, 0.117001) (0.144001, 0.750000, 0.617001) (0.855999, 0.750000, 0.882999) (0.855999, 0.250000, 0.382999) (0.144001, 0.250000, 0.117001)
O22	8f (x,y,z)	1	(0.644001, 0.478500, 0.388500)	(0.644001, 0.478500, 0.388500) (0.355999, 0.478500, 0.111500) (0.355999, 0.521500, 0.611500) (0.644001, 0.521500, 0.888500) (0.144001, 0.978500, 0.388500) (0.855999, 0.978500, 0.111500) (0.855999, 0.021500, 0.611500) (0.144001, 0.021500, 0.888500)
O23	8f (x,y,z)	1	(0.644001, 0.021500, 0.388499)	(0.644001, 0.021500, 0.388499) (0.355999, 0.021500, 0.111501) (0.355999, 0.978500, 0.611501) (0.644001, 0.978500, 0.888499) (0.144001, 0.521500, 0.388499) (0.855999, 0.521500, 0.111501) (0.855999, 0.478500, 0.611501) (0.144001, 0.478500, 0.888499)

# Bilbao Crystallographic Server

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



**bilbao crystallographic server**



[ The crystallographic site at the Condensed Matter Physics Dept. of the University of the Basque Country ]

[ Space Groups ] [ Layer Groups ] [ Rod Groups ] [ Frieze Groups ] [ Wyckoff Sets ]



**IT On 2011**  
Workshop on the Online Edition of International Tables for Crystallography  
31 August - 3 September 2011  
Bilbao / SPAIN



**Aperiodic Crystals for Beginners**  
IUCr Satellite Meeting  
31 August - 1 September 2011  
Alcalá de Henares / SPAIN

## Sections

### Retrieval Tools

Group-Subgroup  
Representations  
Solid State  
Structure Utilities  
Subperiodic  
Incommensurate Structures Database

## Space Groups Retrieval Tools

<b>GENPOS</b>	Generators and General Positions of Space Groups
<b>WYCKPOS</b>	Wyckoff Positions of Space Groups
<b>HKLCD</b>	Reflection conditions of Space Groups
<b>MAXSUB</b>	Maximal Subgroups of Space Groups
<b>SERIES</b>	Series of Maximal Isomorphic Subgroups of Space Groups
<b>WYCKSETS</b>	Equivalent Sets of Wyckoff Positions
<b>NORMALIZER</b>	Normalizers of Space Groups
<b>KVEC</b>	The k-vector types and Brillouin zones of Space Groups
<b>SYMMETRY OPERATIONS</b>	Geometric interpretation of matrix column representations of symmetry operations

## Group - Subgroup Relations of Space Groups

<b>SUBGROUPGRAPH</b>	Lattice of Maximal Subgroups
<b>HERMANN</b>	Distribution of subgroups in conjugated classes
<b>COSETS</b>	Coset decomposition for a group-subgroup pair
<b>WYCKSPLIT</b>	The splitting of the Wyckoff Positions
<b>MINSUP</b>	Minimal Supergroups of Space Groups
<b>SUPERGROUPS</b>	Supergroups of Space Groups
<b>CELLSUB</b>	List of subgroups for a given k-index.
<b>CELLSUPER</b>	List of supergroups for a given k-index.
<b>NONCHAR</b>	Non Characteristic orbits.
<b>COMMONSUBS</b>	Common Subgroups of Space Groups
<b>COMMONSUPER</b>	Common Supergroups of Two Space Groups
<b>INDEX</b>	Index of a group subgroup pair

## Contact us

### About us

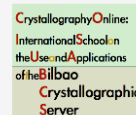
### Links

### Publications

### How to cite the server

### Tutorials

Material from the school on the server (June 2009)



## News:

- **BUGFIX: AMPLIMODES**  
03/2011: A bug occurring in the selection of representatives has been fixed.
- **DOPE**  
03/2011: New version of DOPE.
- **BUGFIX: AMPLIMODES**  
03/2011: A bug concerning AMPLIMODES for FullProf has been fixed.
- **BUGFIX: AMPLIMODES**  
02/2011: A bug concerning AMPLIMODES for FullProf has been fixed.
- **New article**  
02/2011: 'A new computer tool at the Bilbao Crystallographic Server to detect and characterize pseudosymmetry'. Z. Krist. (2011) 226(2), 183-188

## Representation Theory Applications

<b>REPRES</b>	Space Groups Representations
<b>DIRPRO</b>	Direct Products of Space Group Irreducible Representations
<b>CORREL</b>	Correlations Between Representations
<b>POINT</b>	Point Group Tables
<b>SITESYM</b>	Site-symmetry induced representations of Space Groups

## Solid State Theory Applications

<b>SAM</b>	Spectral Active Modes (IR and RAMAN Selection Rules)
<b>NEUTRON</b>	Neutron Scattering Selection Rules
<b>SYMMODES</b>	Primary and Secondary Modes for a Group - Subgroup pair
<b>AMPLIMODES</b>	Symmetry Mode Analysis
<b>PSEUDO</b>	Pseudosymmetry Search in a Structure
<b>DOPE</b>	Degree of Pseudosymmetry Estimation
<b>TRANPATH</b>	Transition Paths (Group not subgroup relations)

## Structure Utilities

<b>CELLTRAN</b>	Transform Unit Cells
<b>STRAIN</b>	Strain Tensor Calculation
<b>WPASSIGN</b>	Assignment of Wyckoff Positions
<b>TRANSTRU</b>	Transform structures.
<b>SETSTRU</b>	Alternative Settings for a given Crystal Structure
<b>EQUIVSTRU</b>	Equivalent Descriptions for a given Crystal Structure
<b>VISUALIZE</b>	Visualize structures using Jmol
<b>COMPSTRU</b>	Comparison of Nearly Identical Crystal Structures

## Subperiodic Groups: Layer, Rod and Frieze Groups Retrieval Tools

<b>GENPOS</b>	Generators and General Positions of Subperiodic Groups
<b>WYCKPOS</b>	Wyckoff Positions of Subperiodic Groups
<b>MAXSUB</b>	Maximal Subgroups of Subperiodic Groups