Obtaining the transformation matrix connecting two group-subgroup related structures

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08/2011, IUCr Mieres 2011: Crystallographic Computing School
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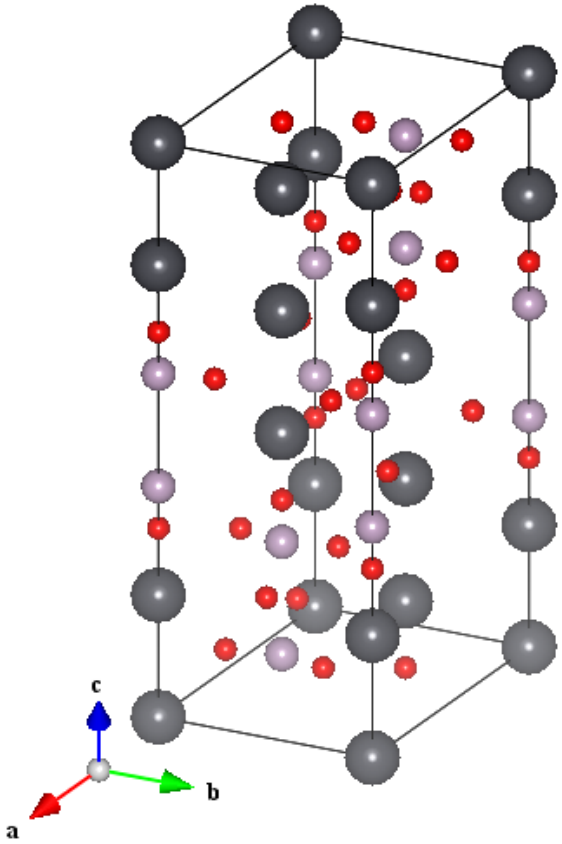
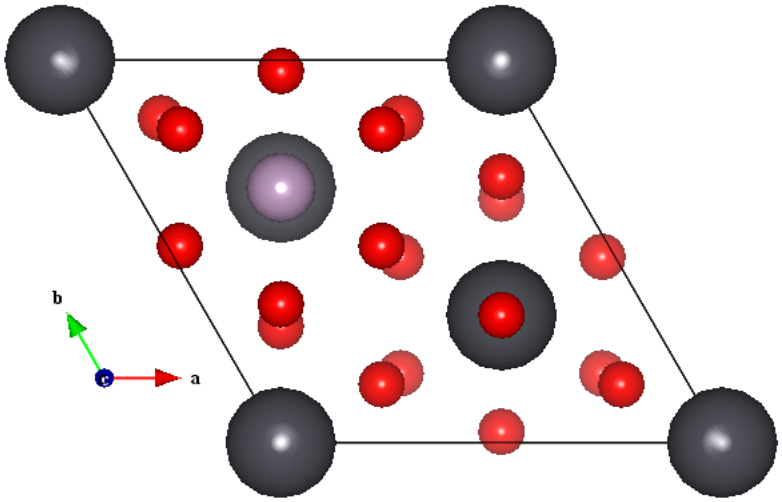
Structure Data





$Pb_3(PO_4)_2$

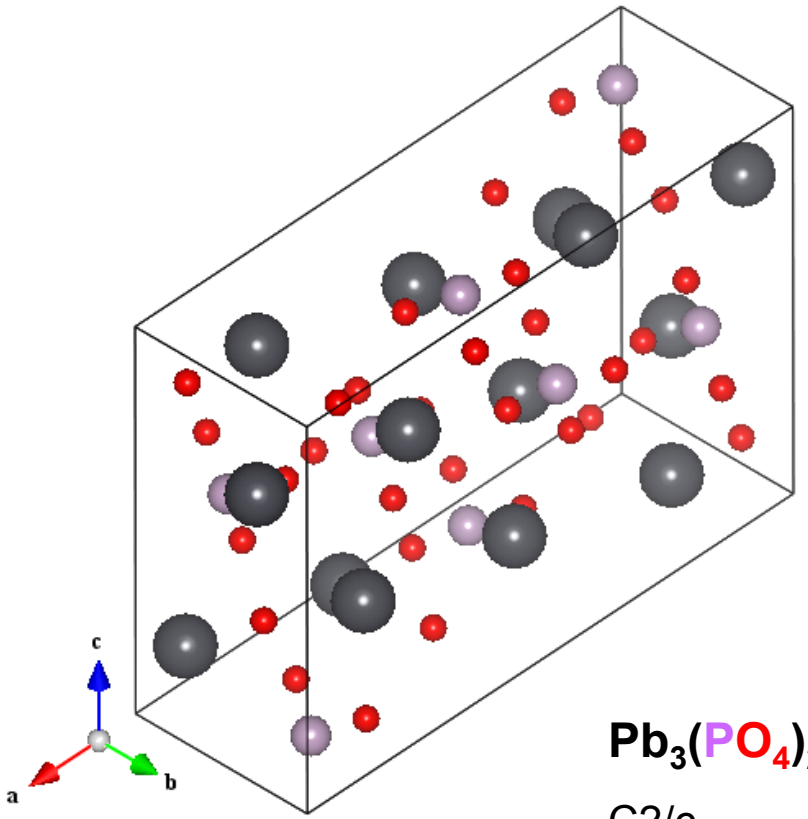
R-3m

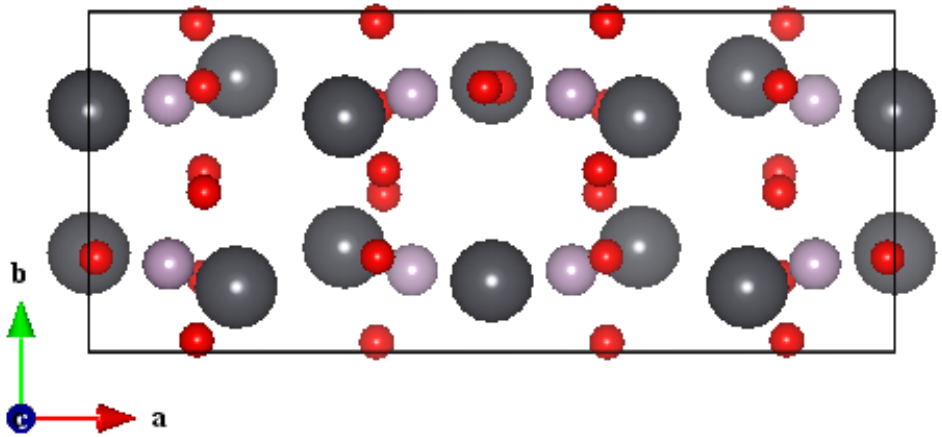
```
166
5.56 5.56 20.39 90 90 120
5
Pb 1    3a     0         0         0
Pb 2    6c     0         0         0.2126
P  1    6c     0         0         0.4021
O  1    6c     0         0         0.3290
O  2    18h    0.1810 -0.1810   0.0960
```

H.N. Ng, C. Calvo

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

Structure Data





$Pb_3(PO_4)_2$

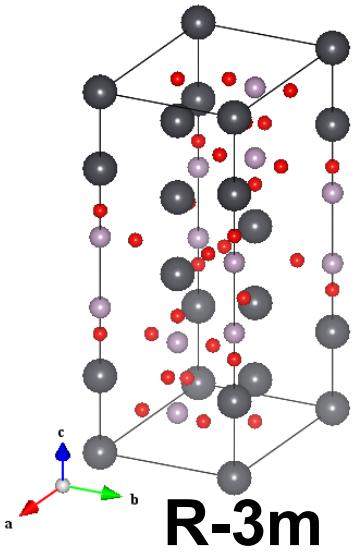
C2/c

```
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



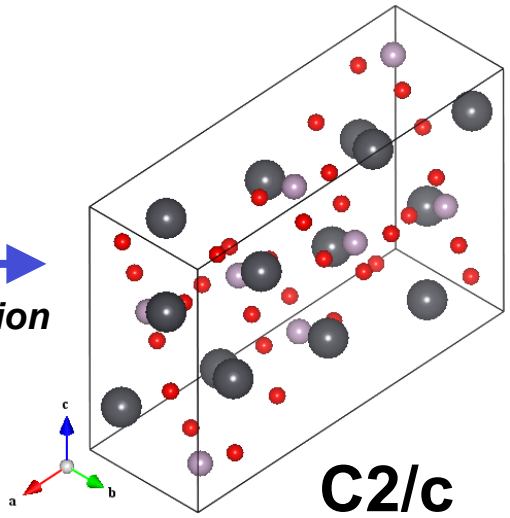
R-3m

Symmetry Reduction

?

C2/c

Affine Transformation



C2/c

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

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

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

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

translationengleiche

klassenngleiche

Index of a group-subgroup pair

High symmetry Space Group: 166 (*R*-3*m*) [hexagonal axes]	
Low symmetry Space Group: 15 (*C*2/*c*) [unique axis b]	
i_L	2
i_P	3
Total index	6

INDEX

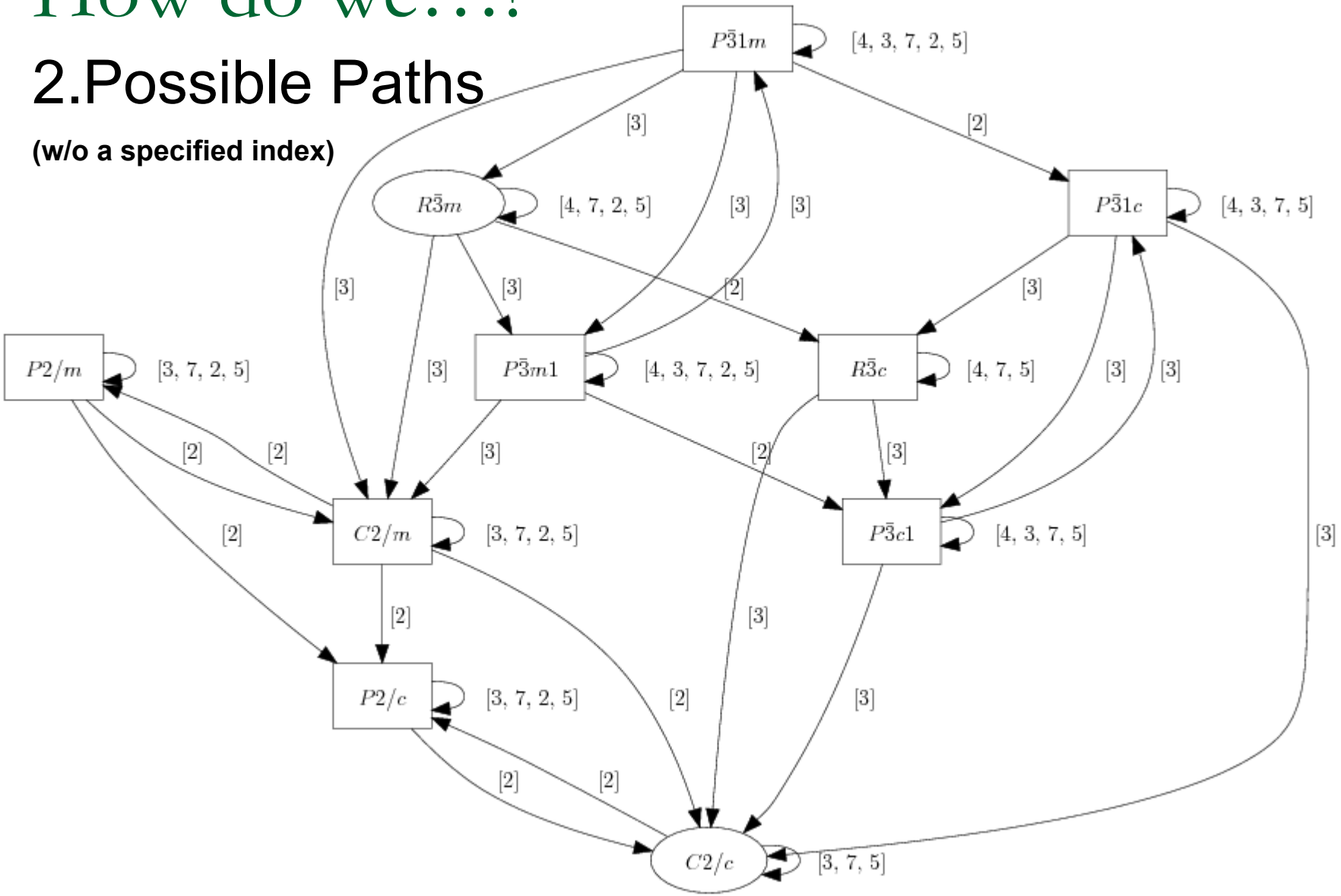
How do we relate these structures?

1. Index ✓ 6
2. **Possible Paths**
3. Wyckoff Splitting Compatibility
4. Lattice Compatibility
5. Atomic positions match

How do we…?

2.Possible Paths

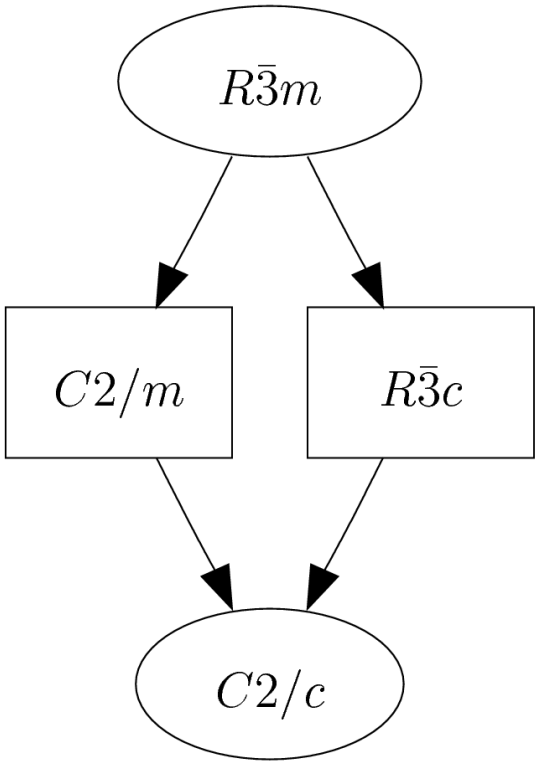
(w/o a specified index)



SUBGROUPGRAPH

How do we…?

2.Possible Paths



Classification of the subgroups of type 15 (*C2/c*) [unique axis b] of group 166 (*R*-3*m*) [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-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

SUBGROUPGRAPH

HERMANN

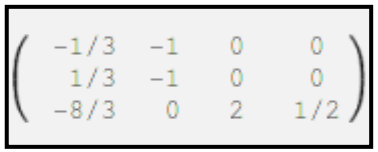
How do we relate these structures?

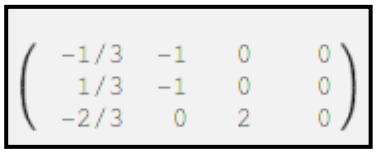
1. Index ✓ 6
2. Possible Paths ✓

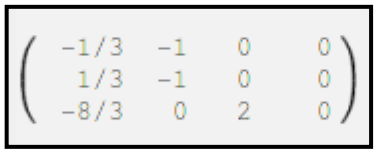
   R-3m → R-3c → C2/c

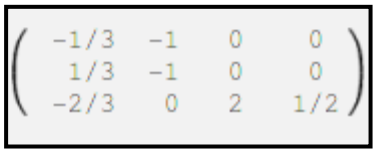
   R-3m → C2/m → C2/c

3. Wyckoff Splitting Compatibility









4. Lattice Compatibility
5. Atomic positions match

How do we…?

3.Wyckoff Splitting Compatibility

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

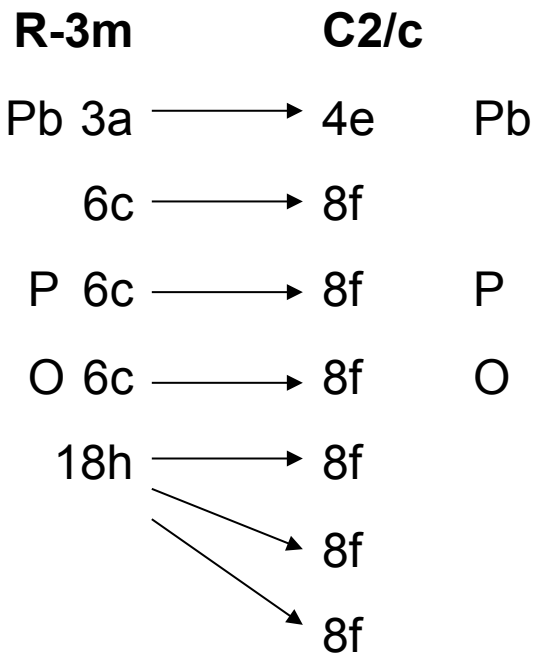
WPASSIGN

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

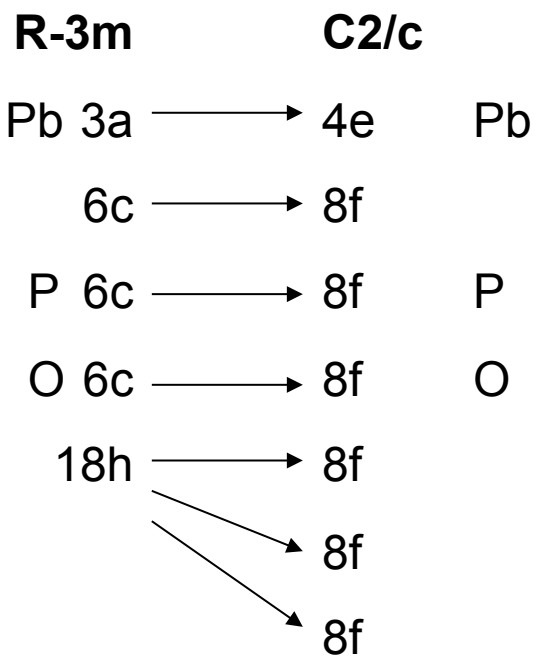
Result from splitting

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

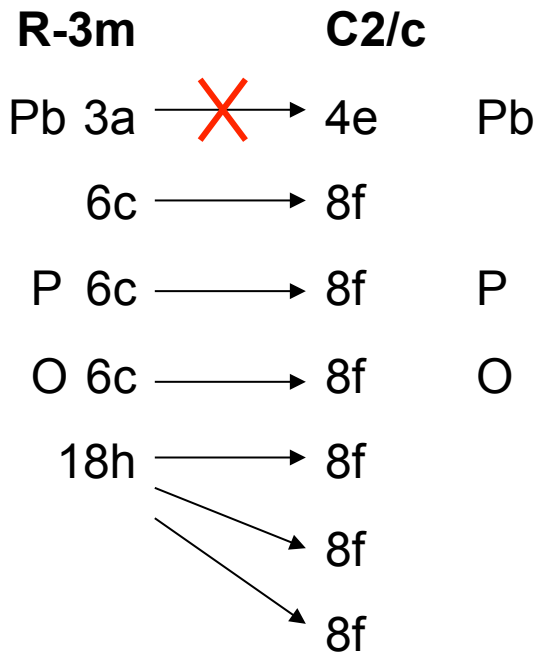
Result from splitting

No	Wyckoff position(s)		
	Group	Subgroup	More...
1	36i	8f 8f 8f 8f 8f 8f	Relations
2	18h	8f 8f 8f	Relations
3	18g	8f 8f 8f	Relations
4	18f	8f 4e 8f 4e	Relations
5	9e	4c 4e 4d	Relations
6	9d	8f 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	$\begin{pmatrix} -1/3 & -1 & 0 & 0 \\ 1/3 & -1 & 0 & 0 \\ -2/3 & 0 & 2 & 0 \end{pmatrix}$

Result from splitting

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

WYCKSPLIT

Wyckoff Sets

Wyckoff Sets of Space Group 15 (*C*2/*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…?

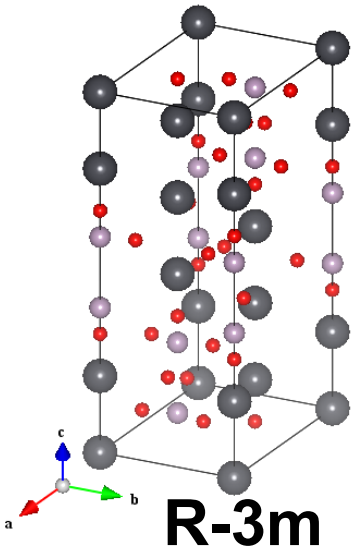
3.Wyckoff Splitting Compatibility

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

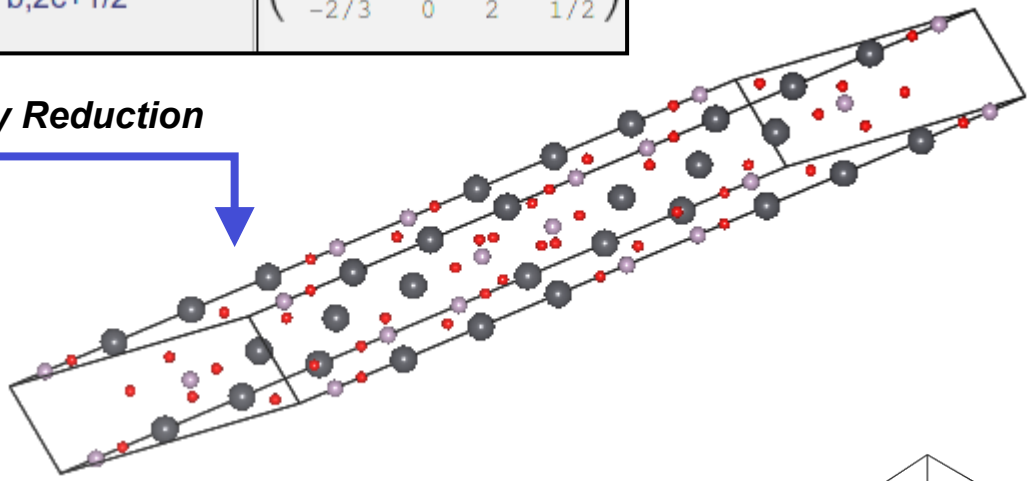
Plan of Attack (revisited)

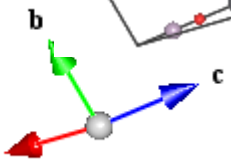


R-3m

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

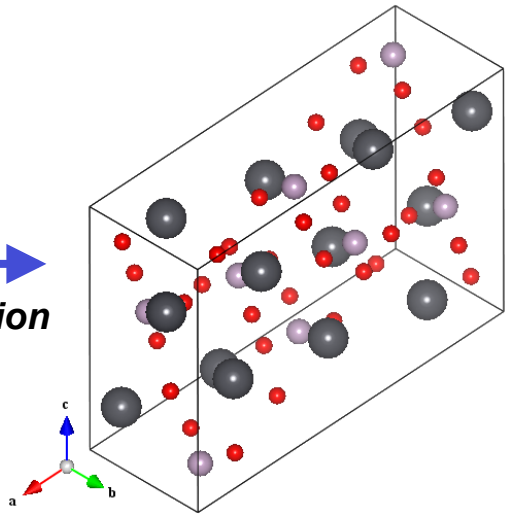
Symmetry Reduction





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

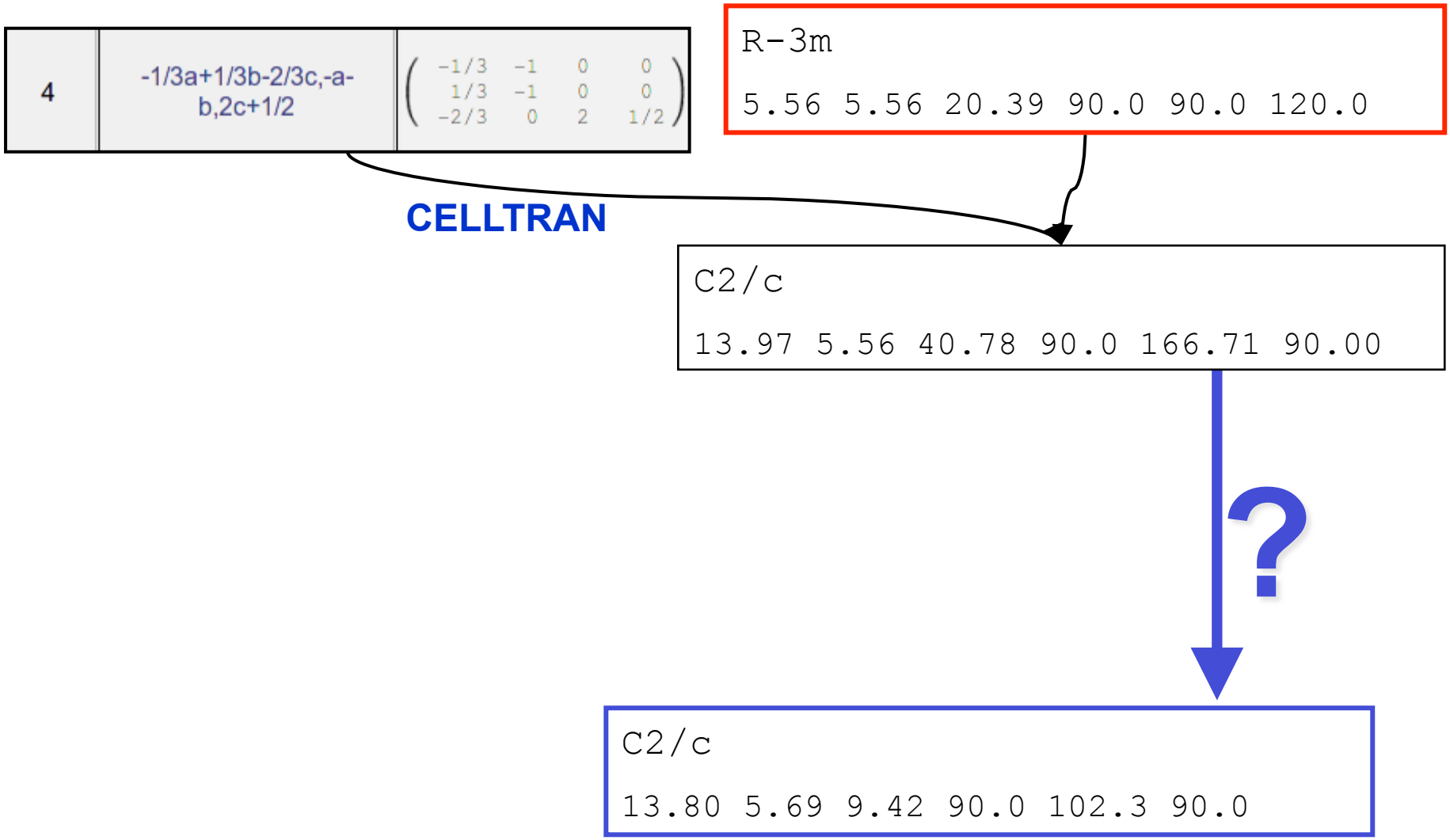
3. Wyckoff Splitting Compatibility

4. Lattice Compatibility

5. Atomic positions match

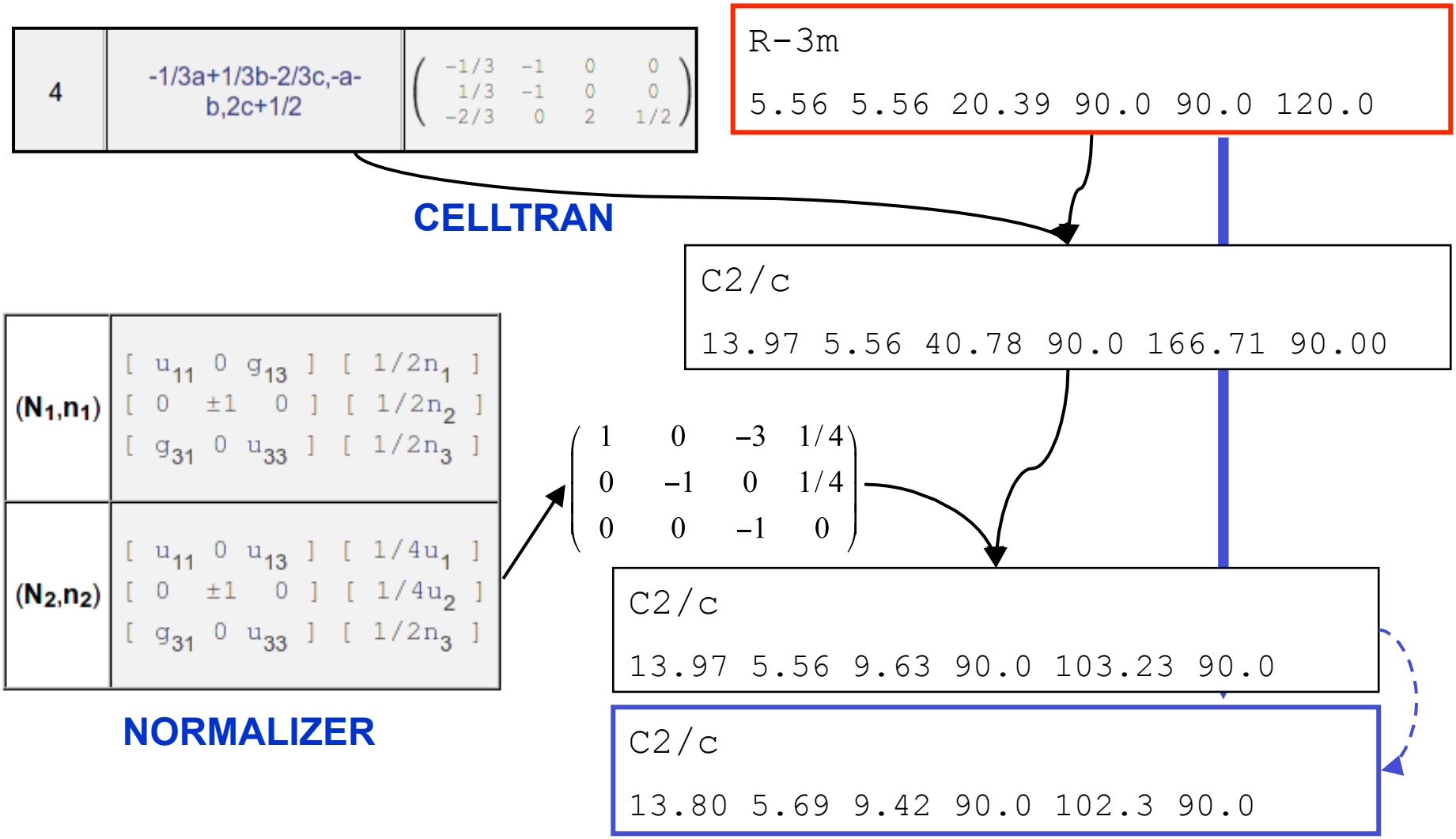
How do we…?

4.Lattice Compatibility



How do we…?

4.Lattice Compatibility



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)

5. Atomic positions match

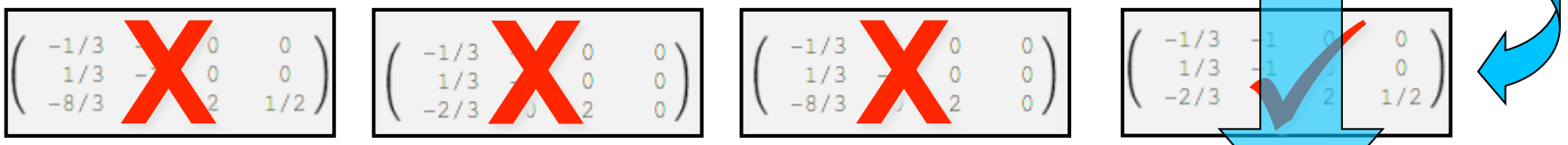
How do we relate these structures?

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)



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
```

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

```
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
```

```
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
```

$_2$

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

TRANSTRU

```
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
```

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

COMPSTRU

```
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
```

```
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 Δ: 0.3309 Å

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

COMPSTRU

Atom Mappings					
WP		Atom	Coordinates in S_1	Atom	Coordinates in S_2
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_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	0.0041	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

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

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

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