Karlsruhe Institute of Technology

VERSAILLES 2022 ECM33

Mathematics and Computer Science for Materials Innovation: Crystal Lattice Classifications

05.09 – 09.09 2022 Liverpool

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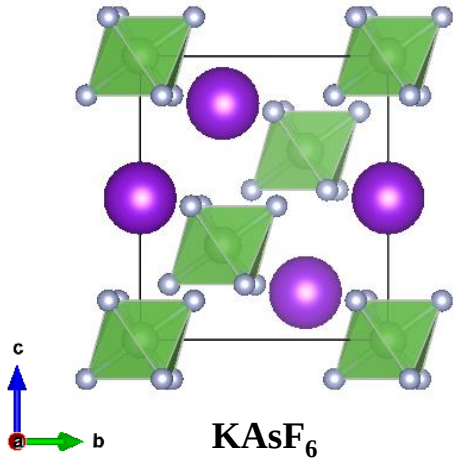
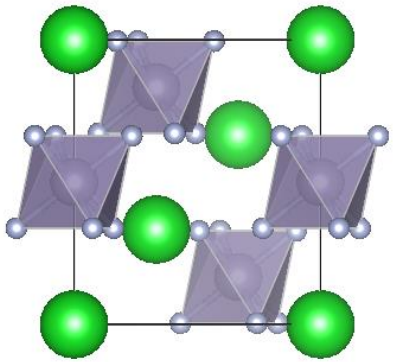
Comparison of structures by the Bilbao Crystallographic Server



$KAsF_6$

?

≈



$BaSnF_6$

Content

Crystal-structure descriptions

- Transformations between different crystal-structure descriptions
- Transformations to a lower symmetry space group
- Symmetrically equivalent descriptions

Comparison between different structure descriptions

- Comparison of structures with the same/different composition
- Comparison of chiral structures

Crystal structure description

- What type of information is necessary to describe a crystal structure?
  - Space Group
  - Lattice parameters
  - The number of independent atoms in the asymmetric unit
  - The atom type and the coordinates

```
141
6.6164  6.6164  6.0150  90  90  90
3
Zr  1   4a    0.000   0.750   0.125
Si  1   4b    0.000   0.750   0.625
O  1   16h    0.000   0.067   0.198
```

BCS format

Standard setting

The settings of space groups hat coincide with the conventional space-group descriptions found in *Volume A of International Tables for Crystallography*. For space groups with more than one description, the following settings are chosen as standard:

- *Unique axis b* and *cell choice 1* for monoclinic space groups
- *Hexagonal axes* for rhombohedral space groups
- *Origin choice 2* (origin at $\bar{1}$) for centrosymmetric space groups listed with two origin choices

What can I do if my structures are described in a non-standard setting?

Example – Structure transformation

Transform the crystal structure of manganese trifluoride MnF_3, described in the space group $I12/a1$ (No. 15), to its standard setting $C12/c1$ taking into account that the transformation matrix $(\boldsymbol{P}, \boldsymbol{p}) = \boldsymbol{-a-c, b, a};\ 0{,}0{,}0$

Initial Setting: $I12/a$ (No. 15)

15
5.5017 5.0270 7.2619 90 92.814 90
3

Mn	1	4d	0.250000	0.250000	0.250000
F	1	8f	0.072200	-0.038000	0.305700
F	2	4e	0.250000	0.136000	0.000000

$(\boldsymbol{P}, \boldsymbol{p})$

$\boldsymbol{-a-c, b, a}$

Final Setting: $C12/c1$ (No. 15)

1) Transform the unit cell parameters
2) Transform of the atomic coordinates

Example – Structure transformation

1) Transform the unit cell parameters

Calculate the metric tensor $\boldsymbol{G}$

Initial Setting: $I12/a$ (No. 15)

a	b	c	α	β	γ
5.5017	5.0270	7.2619	90	92.814	90

$$\boldsymbol{G} = \begin{pmatrix} a^2 & ab\,cos\gamma & ac\,cos\beta \\ ab\,cos\gamma & b^2 & bc\cos\alpha \\ ac\,cos\beta & bc\cos\alpha & c^2 \end{pmatrix} \Longrightarrow \boldsymbol{G} = \begin{pmatrix} 30.268703 & 0 & -1.961435 \\ 0 & 25.270726 & 0 \\ -1.961435 & 0 & 52.735192 \end{pmatrix}$$

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Example – Structure transformation

1) Transform the unit cell parameters

Transform the unit cell parameters to the standard setting

Initial Setting: $I12/a$ (No. 15)

a	b	c	α	β	γ
5.5017	5.0270	7.2619	90	92.814	90

$$\boldsymbol{P} = \begin{pmatrix} \bar{1} & 0 & 1 \\ 0 & 1 & 0 \\ \bar{1} & 0 & 0 \end{pmatrix}$$

$$\boldsymbol{G'} = \boldsymbol{P}^T \cdot \boldsymbol{G} \cdot \boldsymbol{P} = \begin{pmatrix} \bar{1} & 0 & \bar{1} \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 30.268703 & 0 & -1.961435 \\ 0 & 25.270726 & 0 \\ -1.961435 & 0 & 52.735192 \end{pmatrix} \begin{pmatrix} \bar{1} & 0 & 1 \\ 0 & 1 & 0 \\ \bar{1} & 0 & 0 \end{pmatrix}$$

$$\boldsymbol{G'} = \begin{pmatrix} 79.081024 & 0 & -28.307267 \\ 0 & 25.270726 & 0 \\ -28.307267 & 0 & 30.268703 \end{pmatrix}$$

Final Setting: $C12/c1$ (No. 15)

a	b	c	α	β	γ
8.8928	5.0270	5.5017	90	125.35	90

Example – Structure transformation

2) Transform of the atomic coordinates $\boldsymbol{x'} = \boldsymbol{P^{-1}x}$

Mn	1	4d	0.250000	0.250000	0.250000
F	1	8f	0.072200	-0.038000	0.305700
F	2	4e	0.250000	0.136000	0.000000

$$\boldsymbol{P} = \begin{pmatrix} \bar{1} & 0 & 1 \\ 0 & 1 & 0 \\ \bar{1} & 0 & 0 \end{pmatrix} \Longrightarrow \boldsymbol{P^{-1}} = \begin{pmatrix} 0 & 0 & \bar{1} \\ 0 & 1 & 0 \\ 1 & 0 & \bar{1} \end{pmatrix}$$

Mn $$x' = \begin{pmatrix} 0 & 0 & \bar{1} \\ 0 & 1 & 0 \\ 1 & 0 & \bar{1} \end{pmatrix} \begin{pmatrix} 0.25 \\ 0.25 \\ 0.25 \end{pmatrix} = \begin{pmatrix} -0.25 \\ 0.25 \\ 0 \end{pmatrix}$$

F1 $$x' = \begin{pmatrix} 0 & 0 & \bar{1} \\ 0 & 1 & 0 \\ 1 & 0 & \bar{1} \end{pmatrix} \begin{pmatrix} 0.0722 \\ -0.038 \\ 0.3057 \end{pmatrix} = \begin{pmatrix} -0.3057 \\ -0.038 \\ -0.2335 \end{pmatrix}$$

F2 $$x' = \begin{pmatrix} 0 & 0 & \bar{1} \\ 0 & 1 & 0 \\ 1 & 0 & \bar{1} \end{pmatrix} \begin{pmatrix} 0.25 \\ 0.136 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0.136 \\ 0.25 \end{pmatrix}$$

Final Setting: $C12/c1$ (No. 15)

Mn	1		-0.250000	0.250000	0.000000
F	1		-0.305700	-0.038000	-0.233500
F	2		0.000000	0.136000	0.250000

WP?

Example – Structure transformation

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

Multiplicity	Wyckoff letter	Site symmetry	Coordinates (0,0,0) + (1/2,1/2,0) +
8	f	1	(x,y,z) (-x,y,-z+1/2) (-x,-y,-z) (x,-y,z+1/2)
4	e	2	(0,y,1/4) (0,-y,3/4)
4	d	-1	(1/4,1/4,1/2) (3/4,1/4,0)
4	c	-1	(1/4,1/4,0) (3/4,1/4,1/2)
4	b	-1	(0,1/2,0) (0,1/2,1/2)
4	a	-1	(0,0,0) (0,0,1/2)

Mn 1 4d -0.250000 0.250000 0.000000
F 1 8f -0.305700 0.038000 -0.233500
F 2 4e 0.000000 0.136000 0.250000

Initial Setting: $I12/a$ (No. 15)

15
5.5017 5.0270 7.2619 90 92.814 90
3
Mn 1 4d 0.250000 0.250000 0.250000
F 1 8f 0.072200 -0.038000 0.305700
F 2 4e 0.250000 0.136000 0.000000

$(\boldsymbol{P}, \boldsymbol{p})$

Final Setting: $C12/c1$ (No. 15)

15
8.8928 5.0270 5.5017 90 125.35 90
3
Mn 1 4d -0.250000 0.250000 0.000000
F 1 8f -0.305700 0.038000 -0.233500
F 2 4e 0.000000 0.136000 0.250000

Crystal-structure descriptions

Transformation between different structure descriptions

Structure Utilities	
CELLTRAN	Transform Unit Cells
STRAIN	Strain Tensor Calculation
WPASSIGN	Assignment of Wyckoff Positions
TRANSTRU	Transform structures.
SETSTRU	Alternative Settings for a given Crystal Structure
EQUIVSTRU	Equivalent Descriptions for a given Crystal Structure
CIF2STANDARD	Transforms a given CIF (in any setting) to that of standard setting
STRCONVERT	Convert & Edit Structure Data (supports the CIF, mCIF, VESTA, VASP formats -- with magnetic information where available)
VISUALIZE	Visualize structures using Jmol
COMPSTRU	Comparison of Crystal Structures with the same Symmetry
STRUCTURE RELATIONS	Evaluation of structure relationships [transformation matrix] between group-subgroup related phases
PSEUDOLATTICE	Pseudosymmetry of a lattice and compatible supergroups

*IT*A setting structure description

SETSTRU https://www.cryst.ehu.es/cryst/setstru.html

Transform a structure to an alternative setting

Transform to an alternative setting

The program SETSTRU performs the transformations between crystal-structure descriptions referred to the so-called ITA setting of space groups.

The first step consists in the input of the structure data. The data can be given using the form or it can be loaded from a CIF file. The necessary data for the structure consists in the number of its space group in the *International Tables for Crystallography,* Vol A, the lattice parameters (in A and degrees), the number of the atoms in the asymmetric unit and the corresponding atomic positions.

Next, it is necessary to specify the initial and final settings of the structure descriptions among the listed ITA-settings of the structure's space group (e.g. to convert from **rhombohedral** to the standard **hexagonal** settings).

A detailed description of the structure with respect to the final setting of the space group is shown in the output.

Structure Data
[in CIF format]

Browse... No file selected.

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

CIF file

Structure

```
15
5.5017 5.0270 7.2619 90 92.814 90
3
Mn      1       4d      0.250000        0.250000        0.250000
F       1       8f      0.072200        -0.038000       0.305700
F       2       4e      0.250000        0.136000        0.000000
```

BCS format

Transform Structure

To transform a structure described in a *IT*A-setting into another *IT*A-setting

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*IT*A setting structure description

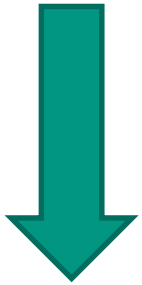
Choose the initial and final space groups symbols

The standard setting (default) of the space group 15 is *C*12/*c*1 [*cell choice 1*]

Initial	Final	Setting	P	P^{-1}
○	◉	*C* 1 2/*c* 1 [*cell choice 1*]	a,b,c	a,b,c
○	○	*A* 1 2/*a* 1 [*cell choice 1*]	c,-b,a	c,-b,a
○	○	*A* 1 2/*n* 1 [*cell choice 2*]	-a-c,b,a	c,b,-a-c
○	○	*C* 1 2/*n* 1 [*cell choice 2*]	a,-b,-a-c	a,-b,-a-c
◉	○	*I* 1 2/*a* 1 [*cell choice 3*]	c,b,-a-c	-a-c,b,a
○	○	*I* 1 2/*c* 1 [*cell choice 3*]	-a-c,-b,c	-a-c,-b,c
○	○	*A* 1 1 2/*a* [*cell choice 1*]	c,a,b	b,c,a
○	○	*B* 1 1 2/*b* [*cell choice 1*]	a,c,-b	a,-c,b
○	○	*B* 1 1 2/*n* [*cell choice 2*]	a,-a-c,b	a,c,-a-b
○	○	*A* 1 1 2/*n* [*cell choice 2*]	-a-c,a,-b	b,-c,-a-b
○	○	*I* 1 1 2/*b* [*cell choice 3*]	-a-c,c,b	-a-b,c,b
○	○	*I* 1 1 2/*a* [*cell choice 3*]	c,-a-c,-b	-a-b,-c,a
○	○	*B* 2/*b* 1 1 [*cell choice 1*]	b,c,a	c,a,b
○	○	*C* 2/*c* 1 1 [*cell choice 1*]	-b,a,c	b,-a,c
○	○	*C* 2/*n* 1 1 [*cell choice 2*]	b,a,-a-c	b,a,-b-c
○	○	*B* 2/*n* 1 1 [*cell choice 2*]	-b,-a-c,a	c,-a,-b-c
○	○	*I* 2/*c* 1 1 [*cell choice 3*]	b,-a-c,c	-b-c,a,c
○	○	*I* 2/*b* 1 1 [*cell choice 3*]	-b,c,-a-c	-b-c,-a,b

Initial Setting: $I12/a$ (No. 15)

```
15
5.5017 5.0270 7.2619 90 92.814 90
3
Mn  1  4d  0.250000  0.250000  0.250000
F   1  8f  0.072200 -0.038000  0.305700
F   2  4e  0.250000  0.136000  0.000000
```



Final Setting: $C12/c1$ (No. 15)

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ITA setting structure description

Transformation to standard setting of space group 15

Initial structure

Initial Setting: *I*12/*a*1 [cell choice 3] (No. 15)

```
15
5.5017 5.0270 7.2619 90 92.814 90
3
Mn      1       -       0.250000        0.250000        0.250000
F       1       -       0.072200        -0.038000       0.305700
F       2       -       0.250000        0.136000        0.000000
```

Final structure

Final Setting: *C*12/*c*1 [cell choice 1] (No. 15)

```
15
8.8928 5.0270 5.5017 90.00 125.35 90.00
3
Mn      1       4d      -0.250000       0.250000        0.000000
F       1       8f      -0.305700       -0.038000       -0.233500
F       2       4e      0.000000        0.136000        0.250000
```

CIF File

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

Matrix form:

```
          [   -1     0     1 ] [     0]
(P, p) =  [    0     1     0 ] [     0]
          [   -1     0     0 ] [     0]
```

Atoms Data:

The data shown in this table corresponds to the final setting which corresponds to the standard setting

AT.	WP	SS	Representative	Atomic orbit
Mn1	4d (1/4,1/4,1/2)	-1	(0.750000,0.250000,0.000000)	(0.750000,0.250000,0.000000) (0.250000,0.250000,0.500000) (0.250000,0.750000,0.000000) (0.750000,0.750000,0.500000)
F1	8f (x,y,z)	1	(0.694300,0.962000,0.766500)	(0.694300,0.962000,0.766500) (0.305700,0.962000,0.733500) (0.305700,0.038000,0.233500) (0.694300,0.038000,0.266500) (0.194300,0.462000,0.766500) (0.805700,0.462000,0.733500) (0.805700,0.538000,0.233500) (0.194300,0.538000,0.266500)
F2	4e (0,y,1/4)	2	(0.000000,0.136000,0.250000)	(0.000000,0.136000,0.250000) (0.000000,0.864000,0.750000) (0.500000,0.636000,0.250000) (0.500000,0.364000,0.750000)

This data is only calculated by the program if the final setting corresponds to the standard

Example – Scheelite

- Scheelite ($CaWO_4$) is a mineral that crystallizes in the space group $I4_1/a$ (No. 88). In the *Inorganic Crystal Structure Database* the following two descriptions of $CaWO_4$ can be found:

```
# (a) Origin choice 1
# ICSD: 15869
88
5.243  5.243  11.376  90  90  90
3
Ca 1   4b    0.0000  0.0000  0.5000
W  1   4a    0.0000  0.0000  0.0000
O  1   16 f  0.2413  0.1511  0.0861
```

```
# (b) Origin choice 2
# ICSD: 15586
88
5.243  5.243  11.376  90  90  90
3
Ca 1   4b    0.0000  0.2500  0.6250
W  1   4a    0.0000  0.2500  0.1250
O  1   16 f  0.1504  0.0085  0.2111
```

Compare the two structure descriptions

Hint: In order to compare the different data, the parameters of Structure (a) are to be transformed to 'origin at center 2/m', *i.e.* ORIGIN CHOICE 2

Example – Scheelite

 # Structure 1 – origin 1
88
5.243 5.243 11.376 90 90 90
3
Ca 1 4*b* 0.0000 0.0000 0.5000
W 1 4*a* 0.0000 0.0000 0.0000
O 1 16 *f* 0.2413 0.1511 0.0861

SETSTRU

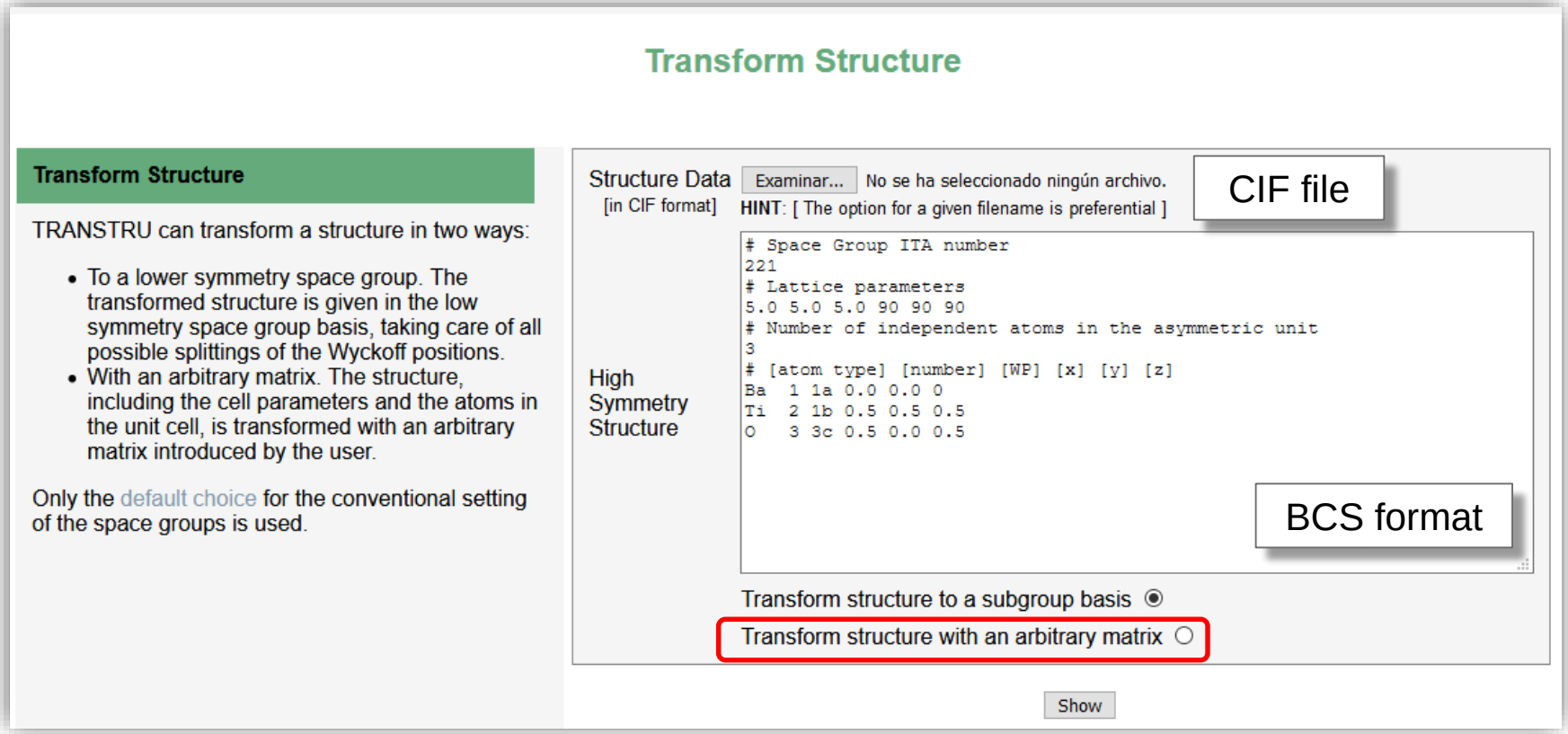
 # Structure 1 – origin 2
88
5.2430 5.2430 11.3760 90 90 90
3
Ca 1 4*b* 0.0000 -0.2500 0.375000
W 1 4*a* 0.0000 -0.2500 -0.125000
O 1 16*f* 0.2413 -0.0989 -0.038900

 # Structure 2 – origin 2
88
5.243 5.243 11.376 90 90 90
3
Ca 1 4*b* 0.0000 0.2500 0.6250
W 1 4*a* 0.0000 0.2500 0.1250
O 1 16 *f* 0.1504 0.0085 0.2111

AT.	WP	SS	Representative	Atomic orbit
Ca1	4b (0,1/4,5/8)	-4..	(0.000000,0.750000,0.375000)	(0.000000,0.750000,0.375000) (0.500000,0.250000,0.875000) (0.000000,0.250000,0.625000) (0.500000,0.750000,0.125000)
W1	4a (0,1/4,1/8)	-4..	(0.000000,0.750000,0.875000)	(0.000000,0.750000,0.875000) (0.500000,0.250000,0.375000) (0.000000,0.250000,0.125000) (0.500000,0.750000,0.625000)
O1	16f (x,y,z)	1	(0.241300,0.901100,0.961100)	(0.241300,0.901100,0.961100) (0.258700,0.098900,0.461100) (0.848900,0.491300,0.211100) (0.651100,0.508700,0.711100) (0.758700,0.098900,0.038900) (0.741300,0.901100,0.538900) (0.151100,0.508700,0.788900) (0.348900,0.491300,0.288900) (0.741300,0.401100,0.461100) (0.758700,0.598900,0.961100) (0.348900,0.991300,0.711100) (0.151100,0.008700,0.211100) (0.258700,0.598900,0.538900) (0.241300,0.401100,0.038900) (0.651100,0.008700,0.288900) (0.848900,0.991300,0.788900)

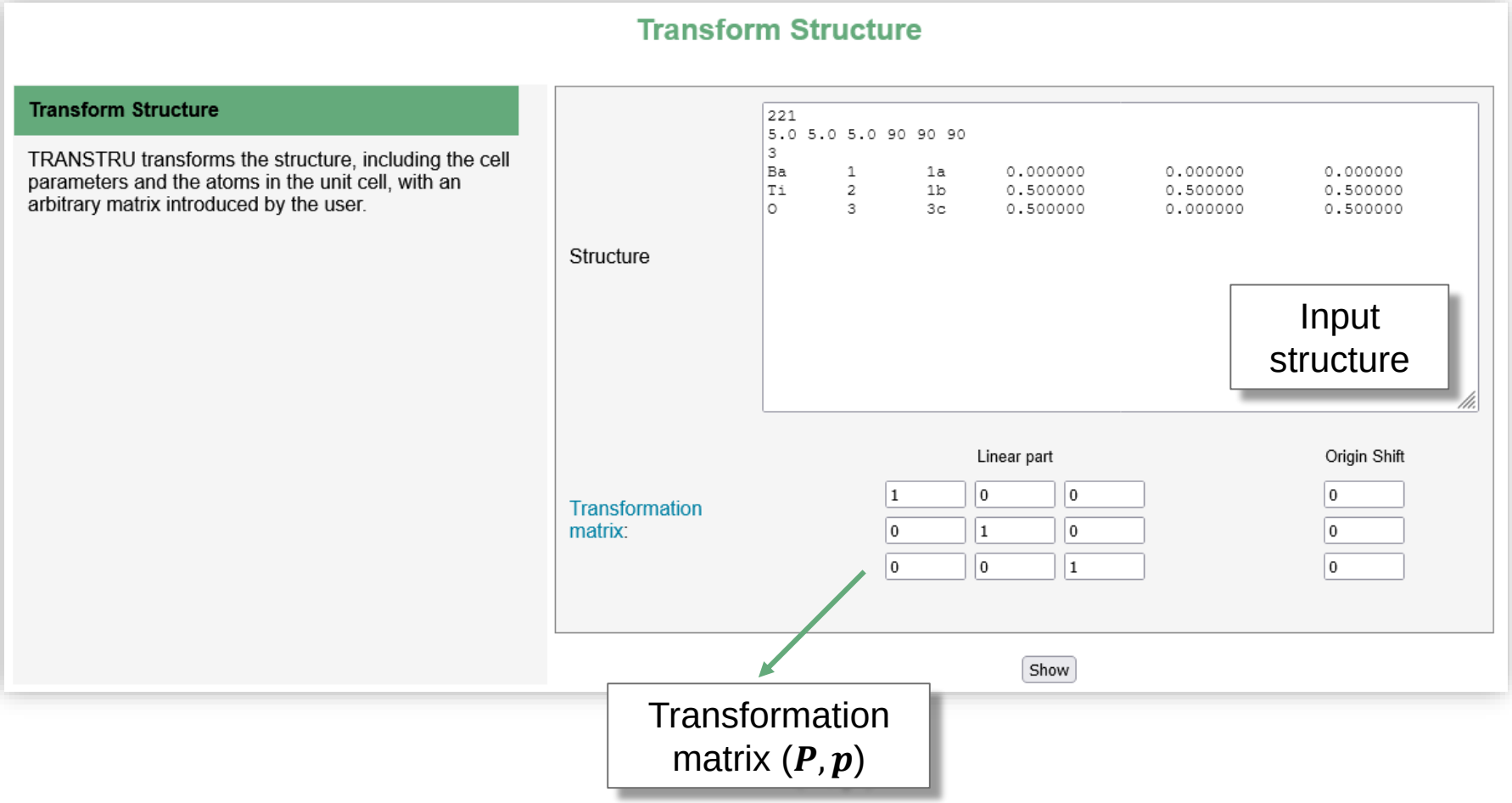
Structure transformation

TRANSTRU https://www.cryst.ehu.es/cryst/transtru.html



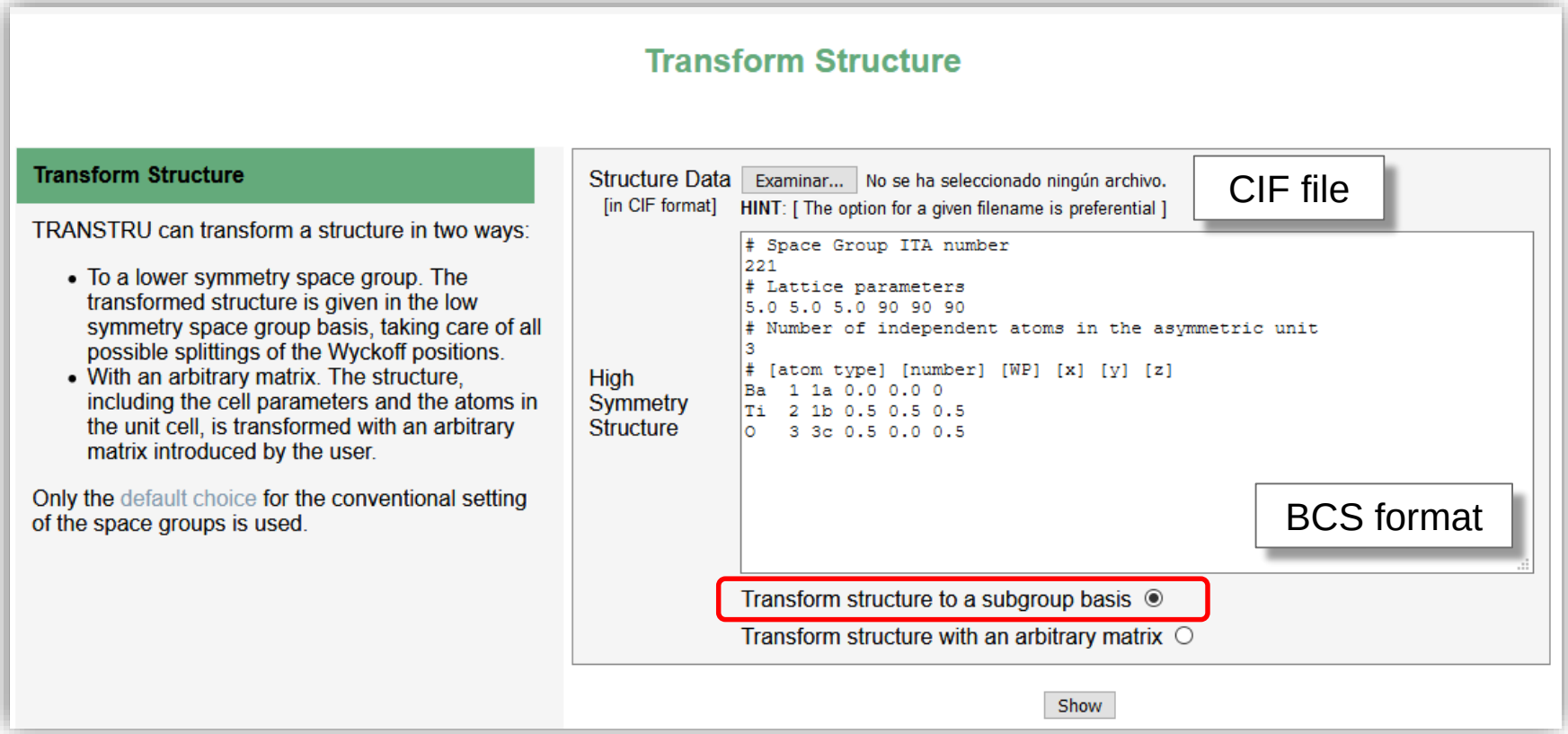
To transform a structure described in standard setting to a lower symmetry space group or with an arbitrary matrix

Structure transformation – arbitrary matrix



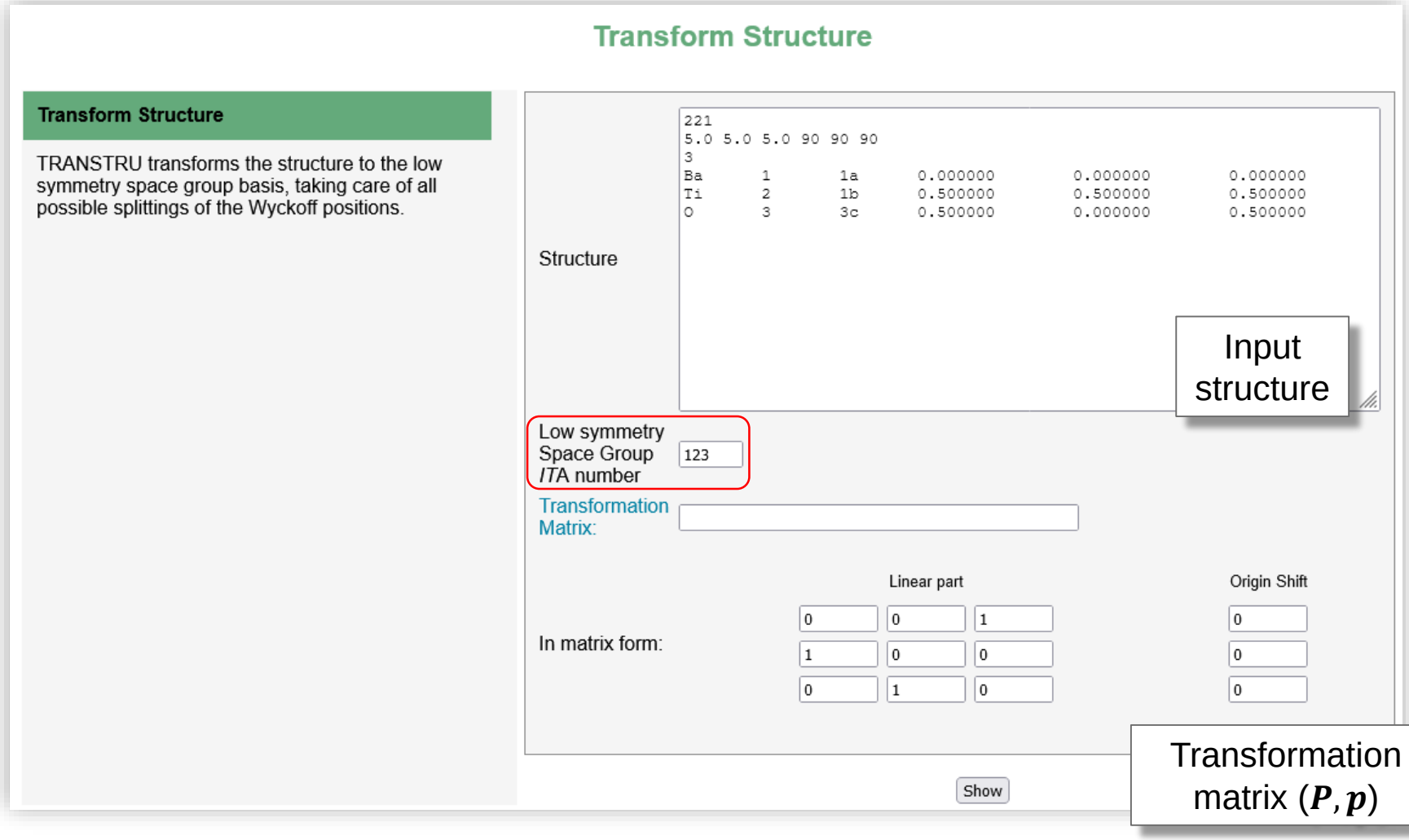
Structure transformation

TRANSTRU https://www.cryst.ehu.es/cryst/transtru.html



To transform a structure described in standard setting to a lower symmetry space group or with an arbitrary matrix

Structure transformation – lower symmetry



Output – TRANSTRU

Transform structure

Transformation matrix: b,c,a

High symmetry structure

```
221
5.0 5.0 5.0 90 90 90
3
Ba      1       1a      0.000000        0.000000        0.000000
Ti      2       1b      0.500000        0.500000        0.500000
O       3       3c      0.500000        0.000000        0.500000
```

Visualize this structure | CIF File | Cartesian Coordinates

Low symmetry structure

```
123
5.000000 5.000000 5.000000 90.000000 90.000000 90.000000
4
Ba      1       1a      0.000000        0.000000        0.000000
Ti      2       1d      0.500000        0.500000        0.500000
O       3       2e      0.000000        0.500000        0.500000
O       3_2     1c      0.500000        0.500000        0.000000
```

Visualize this structure | CIF File | Cartesian Coordinates

Space Group: 123
Lattice Parameters: 5 5 5 90 90 90

AT	#	WP	Coordinates		
Ba	1	1a	0	0	0
Ti	2	1d	1/2	1/2	1/2
O	3	2e	0	1/2	1/2
O	3_2	1c	1/2	1/2	0

Detailed information

Atoms Data:

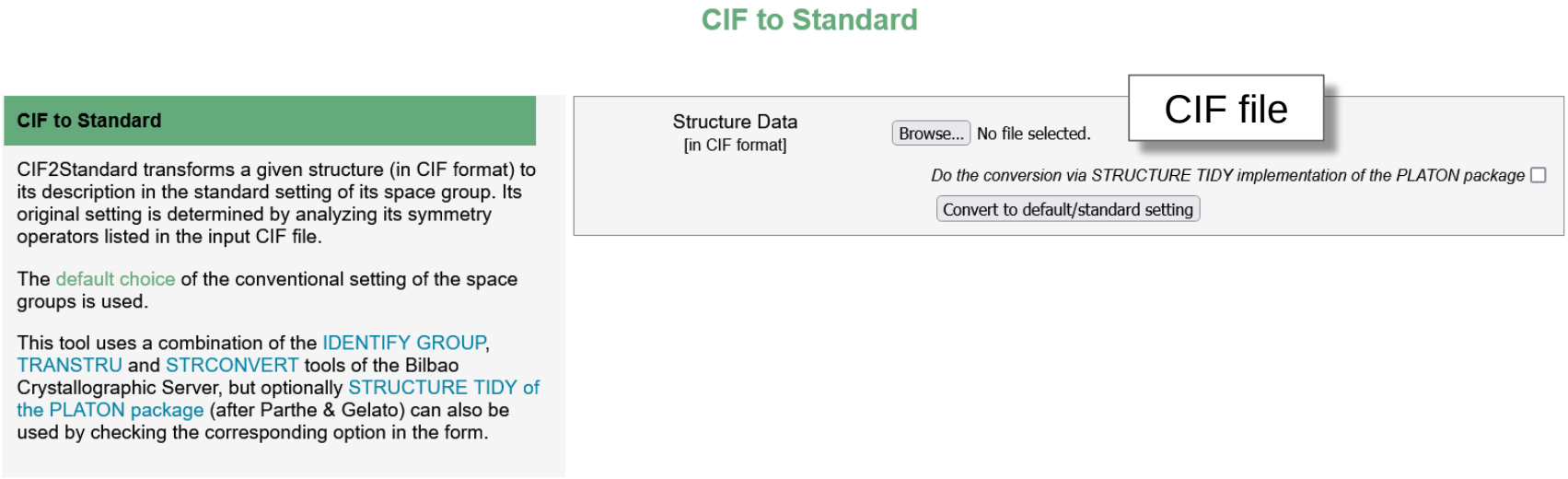
AT.	WP	SS	Representative	Atomic orbit
Ba1	1a (0,0,0)	4/mmm	(0.000000,0.000000,0.000000)	(0.000000,0.000000,0.000000)
Ti2	1d (1/2,1/2,1/2)	4/mmm	(0.500000,0.500000,0.500000)	(0.500000,0.500000,0.500000)
O3	2e (0,1/2,1/2)	mmm .	(0.000000,0.500000,0.500000)	(0.000000,0.500000,0.500000) (0.500000,0.000000,0.500000)
O3_2	1c (1/2,1/2,0)	4/mmm	(0.500000,0.500000,0.000000)	(0.500000,0.500000,0.000000)

Note: The data shown in this table are correct if the input structure is referred to standard setting.

Structure transformation – CIF2Standard

CIF2Standard https://www.cryst.ehu.es/cryst/cif2standard.html

Transform a given structure (in CIF format) to its description in the standard setting



Structure transformation – CIF2Standard

CIF to Standard Setting

The submitted structure's space group number is identified through the symmetry operators as: #15.

It has been transformed to the standard setting *C*2/*c* via the transformation matrix: a+c+1/4,b+1/4,c+1/4

```
15
8.8588 5.0084 7.2411 90.00 38.29 90.00
3
Mn      1       4a      0.000000        0.000000        0.000000
F       1       8f      0.678050        0.209720        -0.735150
F       2       4e      0.000000        -0.117620       -0.250000
```

Transform structure (standard setting)

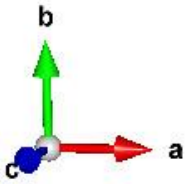
CIF file of the structure in standard setting: cif2std_13517.cif

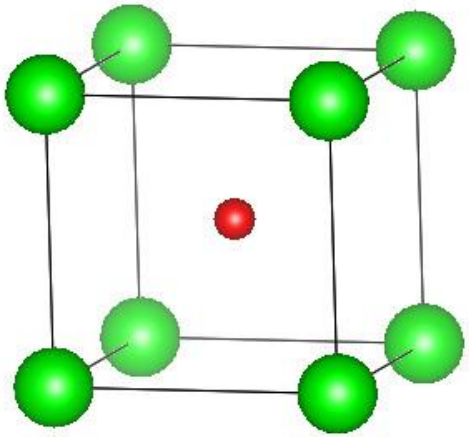
Download CIF file (standard setting)

Equivalent crystal structure descriptions

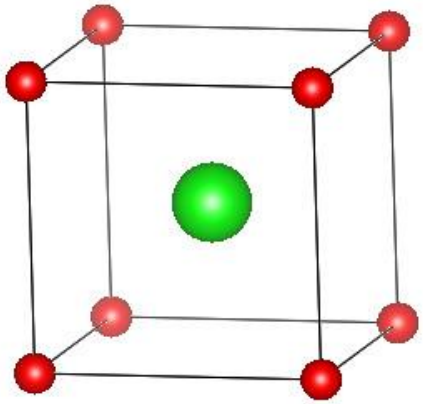
There are almost always several possible ways to describe the exactly same crystal structure

Space group $Pm\bar{3}m$ (No. 221)





Cs 1a 0 0 0
Cl 1b 0.5 0.5 0.5



Cs 1b 0.5 0.5 0.5
Cl 1a 0 0 0

How many equivalent descriptions of the structure CsCl exist?

Equivalent crystal structure descriptions

- For all space groups, except $Im\bar{3}m\ (No.229)$ and $Ia\bar{3}d\ (No.230)$, one can choose several different sets of atomic coordinates describing the same structure in the same space-group setting.

- The number of equivalent descriptions can be calculated:

$$[i] = \frac{|N_\varepsilon(G)|}{|G|}$$

$N_\varepsilon(G)$ represents the Euclidean normalizer of the space group G

- By definition, i cosets result in the coset decomposition of $N_\varepsilon(G)$ with respect to G. The cosets generate the different equivalent descriptions of a given structure

Example – CsCl

- CsCl crystallizes in space group $Pm\bar{3}m$ (No. 221)

Euclidean normalizer (general metric) of the Group *Pm*-3*m* (No. 221)

Euclidean normalizer of *Pm*-3*m* (a,b,c): *Im*-3*m* (a,b,c)

Index of *Pm*-3*m* in *Im*-3*m* (**a**,**b**,**c**): 2 with i_L=2 and i_P=1

Additional generators of *Im*-3*m* (**a**,**b**,**c**) with respect to *Pm*-3*m*

x+1/2,y+1/2,z+1/2	$\begin{pmatrix} 1 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 1/2 \\ 0 & 0 & 1 & 1/2 \end{pmatrix}$	*t* (1/2,1/2,1/2)

The cosets representatives of the Euclidean normalizer *Im*-3*m* (**a**,**b**,**c**) with respect to *Pm*-3*m*

- As $[i] = 2 \Rightarrow$ there are <u>two possible sets of coordinates</u>
- One set of cordinates is obtained from the other one according to the additional generators of $N_{\mathcal{E}}(G)$

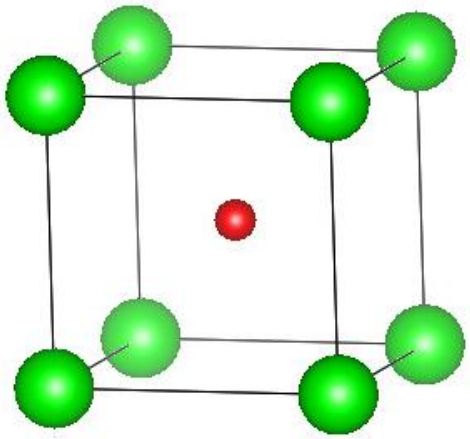
Example – CsCl

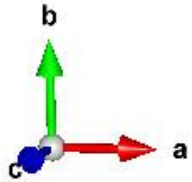
- CsCl crystallizes in space group $Pm\bar{3}m$ (No. 221)

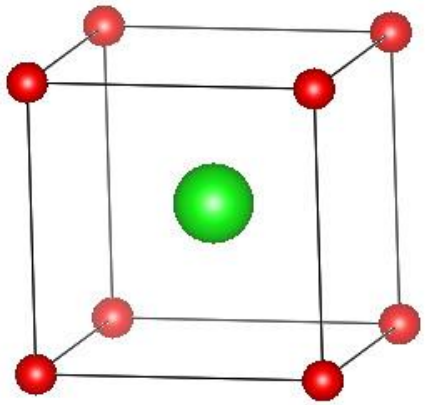
Cs	1a	0	0	0
Cl	1b	0.5	0.5	0.5

$t(1/2,1/2,1/2)$ →

Cs	1b	0.5	0.5	0.5
Cl	1a	0	0	0

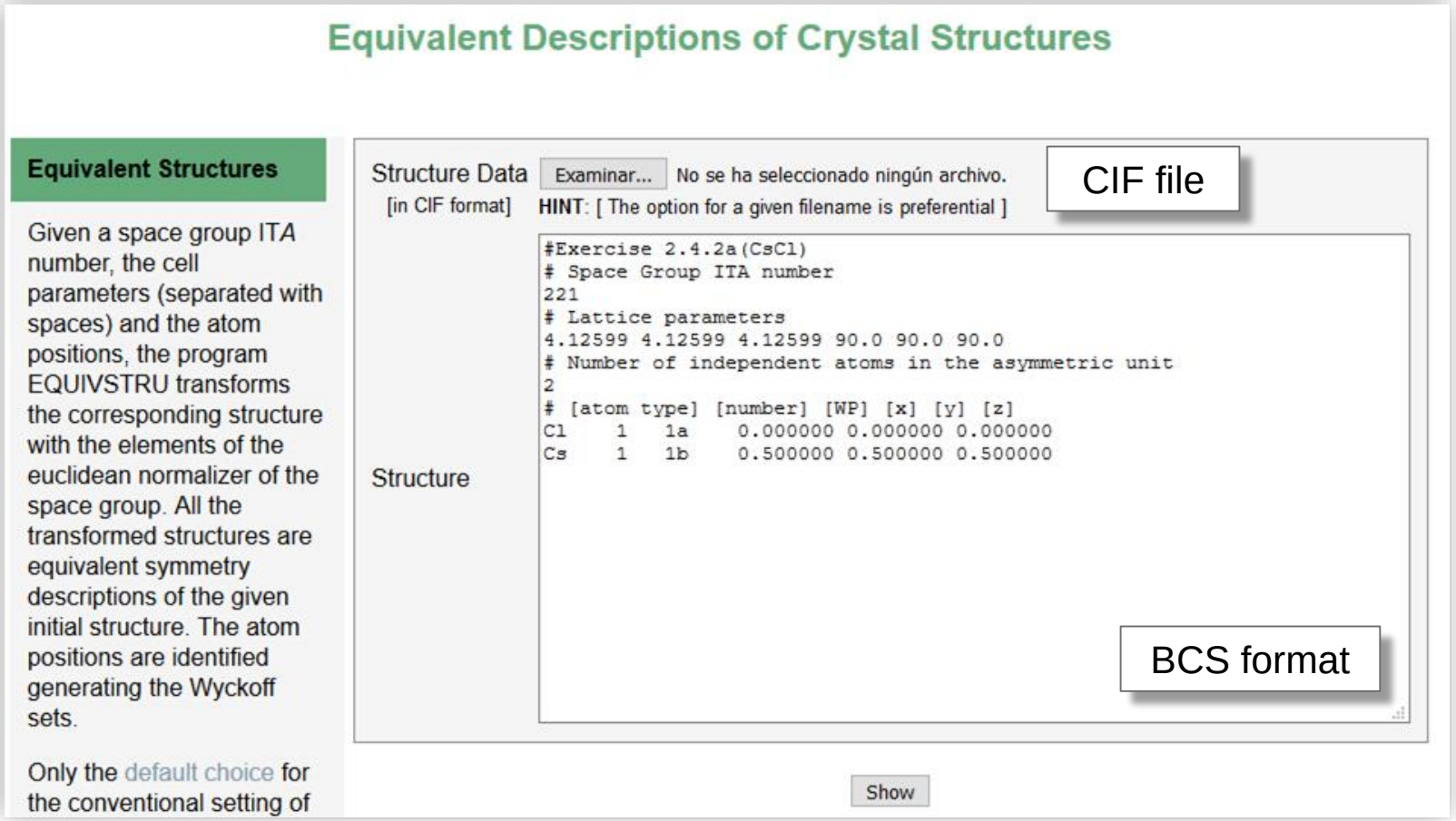




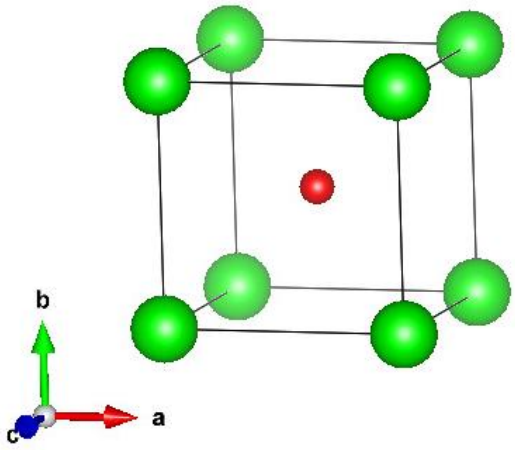


Equivalent crystal structure descriptions

EQUIVSTRU https://www.cryst.ehu.es/cryst/equivstru.html



EQUIVSTRU – Output



- **Equivalent description 1 (original input structure)**

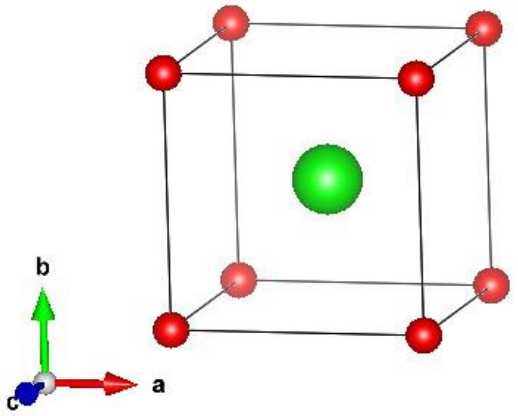
Normalizer coset representative: x,y,z

AT.	WP	SS	Representative	Atomic orbit
Cl1	1a (0,0,0)	m-3m	(0.000000,0.000000,0.000000)	(0.000000,0.000000,0.000000)
Cs1	1b (1/2,1/2,1/2)	m-3m	(0.500000,0.500000,0.500000)	(0.500000,0.500000,0.500000)

- **Equivalent description 2**

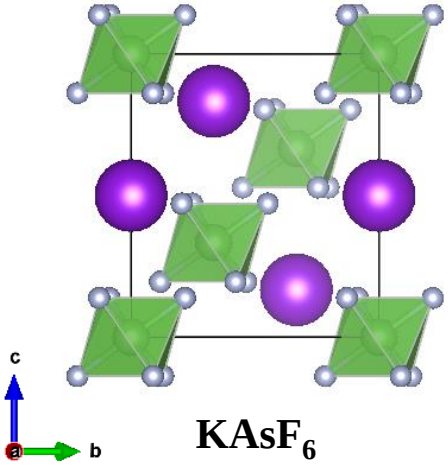
Normalizer coset representative: x+1/2,y+1/2,z+1/2

AT.	WP	SS	Representative	Atomic orbit
Cl1	1b (1/2,1/2,1/2)	m-3m	(0.500000,0.500000,0.500000)	(0.500000,0.500000,0.500000)
Cs1	1a (0,0,0)	m-3m	(0.000000,0.000000,0.000000)	(0.000000,0.000000,0.000000)

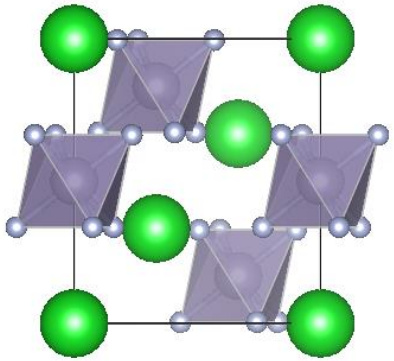


Example – similarity

Evaluate the similarity between these two structures. Try to find analogous coordinate descriptions.



$KAsF_6$



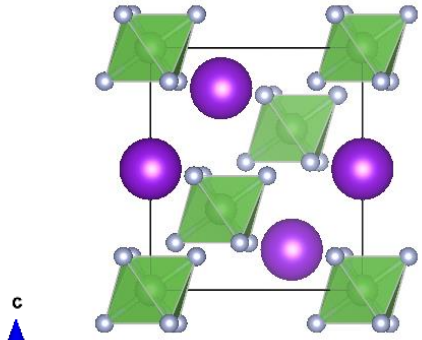
$BaSnF_6$

#ICSD: 59413
148
7.348 7.348 7.274 90. 90. 120.
3
K 1 3b 0.333333 0.666670 0.166670
As 1 3a 0.000000 0.000000 0.000000
F 1 18f 0.129200 0.216500 0.138100

#ICSD: 33788
148
7.4279 7.4279 7.418 90. 90. 120.
3
Ba 1 3a 0.000000 0.000000 0.000000
Sn 1 3b 0.000000 0.000000 0.500000
F 1 18f 0.258600 0.826200 0.004700

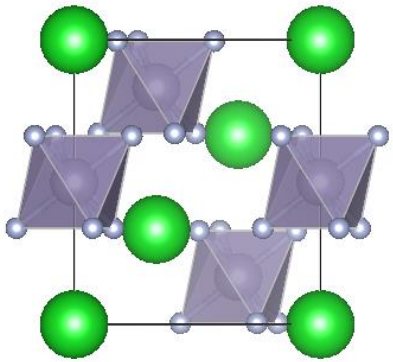
$R\bar{3}$ (No. 148) $\Longrightarrow$ 4 equivalent descriptions: $x, y, z;\ x, y, z + 1/2;\ y, x, -z;\ y, x, -z + 1/2$

Example – similarity



$KAsF_6$

#ICSD: 59413
148
7.348 7.348 7.274 90. 90. 120.
3
K 1 3b 0.333333 0.666670 0.166670
As 1 3a 0.000000 0.000000 0.000000
F 1 18f 0.129200 0.216500 0.138100

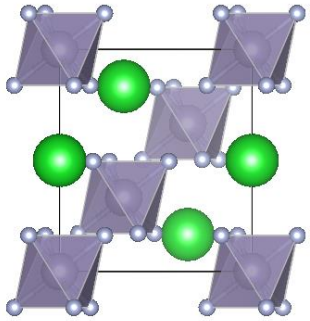


$BaSnF_6$

#ICSD: 33788
148
7.4279 7.4279 7.418 90. 90. 120.
3
Ba 1 3a 0.000000 0.000000 0.000000
Sn 1 3b 0.000000 0.000000 0.500000
F 1 18f 0.258600 0.826200 0.004700

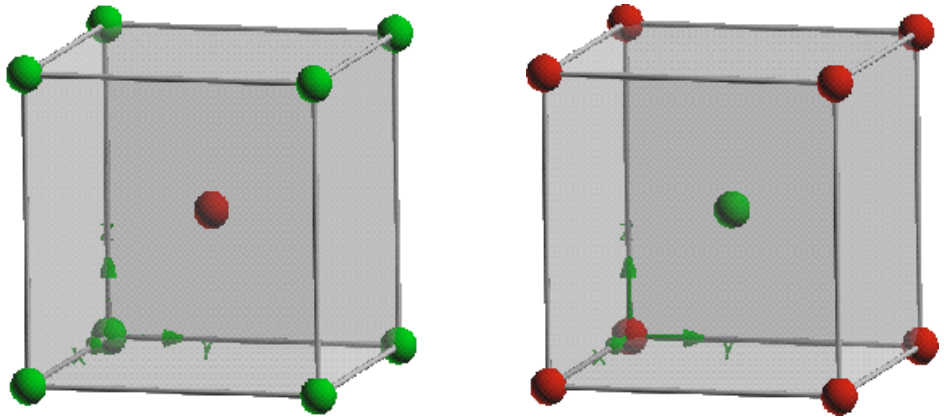
x, y, z+1/2

148
7.4279 7.4279 7.4180 90.00 90.00 120.00
3
Ba 1 3b 0.333333 0.666667 0.166667
Sn 1 3a 0.000000 0.000000 0.000000
F 1 18f 0.159533 0. 234267 0.161967



Comparison of structures

- Comparison of crystal structures is convenient to:
  - cross-check different experimental and/or theoretical structural models of the same phase coming from different sources
  - identify different phases with the same symmetry
  - classify structures into structure types
- The existence of various equivalent structure descriptions makes the comparison of different structural models a non-trivial task in general.



Are these two structures of Cs Cl similar?

Yes

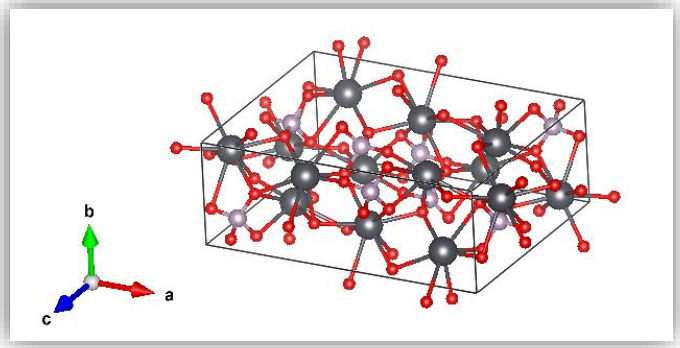
Similarity between two crystal structures

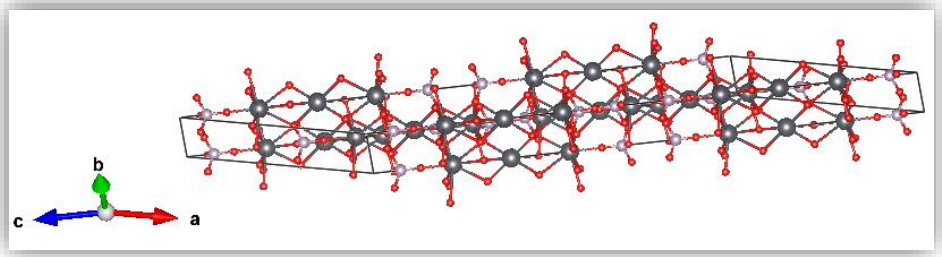
#Structure 1

```
15
13.800 5.691 9.420 90.0 102.3 90.0
7
Pb      1       4e      0.000000        0.291000        0.250000
Pb      2       8f      0.317000        0.309000        0.352000
P       1       8f      0.599000        0.241000        0.447000
O       1       8f      0.643000        0.030000        0.392000
O       2       8f      0.634000        0.464000        0.374000
O       3       8f      0.642000        0.280000        0.612000
O       4       8f      0.491000        0.222000        0.420000
```

#Structure 2

```
15
13.967 5.560 40.778 90.0 166.713 90.0
7
Pb      1       4e      0.000000        0.000000        0.750000
Pb      2       8f      0.000000        0.000000        0.856300
P       1       8f      0.000000        0.000000        0.951100
O       1       8f      0.000000        0.000000        0.914500
O       2       8f      0.271500        0.728500        0.888500
O       3       8f      0.957000        0.500000        0.117000
O       4       8f      0.728500        0.271500        0.611500
```



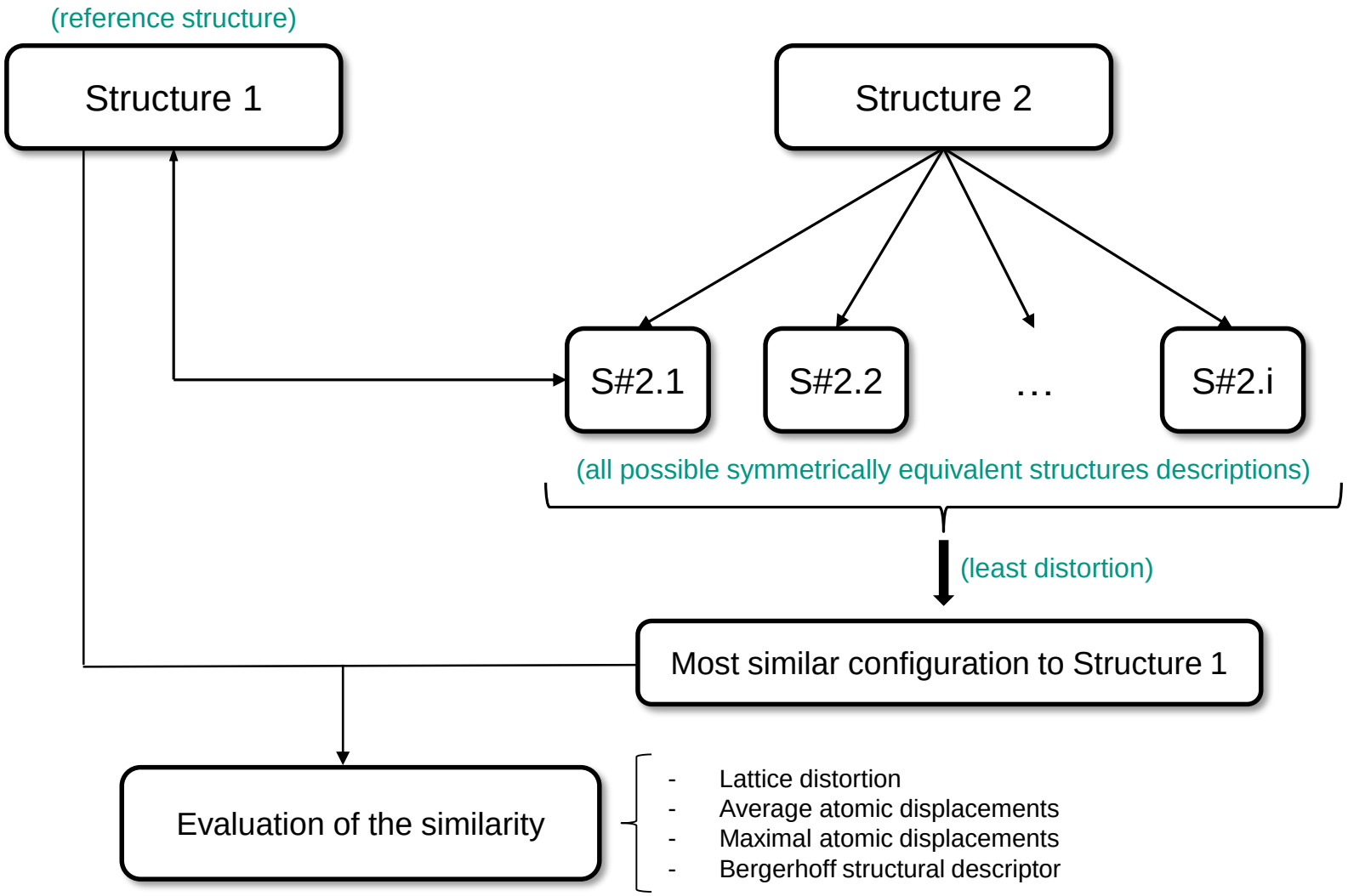


Are these two structures similar?

Crystal Structure Relationships

Structure Utilities	
CELLTRAN	Transform Unit Cells
STRAIN	Strain Tensor Calculation
WPASSIGN	Assignment of Wyckoff Positions
TRANSTRU	Transform structures.
SETSTRU	Alternative Settings for a given Crystal Structure
EQUIVSTRU	Equivalent Descriptions for a given Crystal Structure
CIF2STANDARD	Transforms a given CIF (in any setting) to that of standard setting
STRCONVERT	Convert & Edit Structure Data (supports the CIF, mCIF, VESTA, VASP formats -- with magnetic information where available)
VISUALIZE	Visualize structures using Jmol
COMPSTRU	Comparison of Crystal Structures with the same Symmetry
STRUCTURE RELATIONS	Evaluation of structure relationships [transformation matrix] between group-subgroup related phases
PSEUDOLATTICE	Pseudosymmetry of a lattice and compatible supergroups

The program COMPSTRU



The program COMPSTRU

- How to measure the **similarity** between two descriptions ?

degree of lattice distortion

$$S = \frac{1}{3}\sqrt{\sum_i \eta_i^2}$$

η_i-eigenvalues of the Lagrangian strain tensor

average atomic displacements

$$d_{av} = \frac{1}{n}\sum_i m_i u_i$$

u_i atomic displacements

maximal atomic displacements

maximal displacements of the paired atoms

The program COMPSTRU

- How to measure the **similarity** between two descriptions ?

structural descriptor

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

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

weighted mean difference between atomic coordinates

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

relation between axial ratios

Bergerhoff *et al.*, Acta Cryst B**55** (1998)

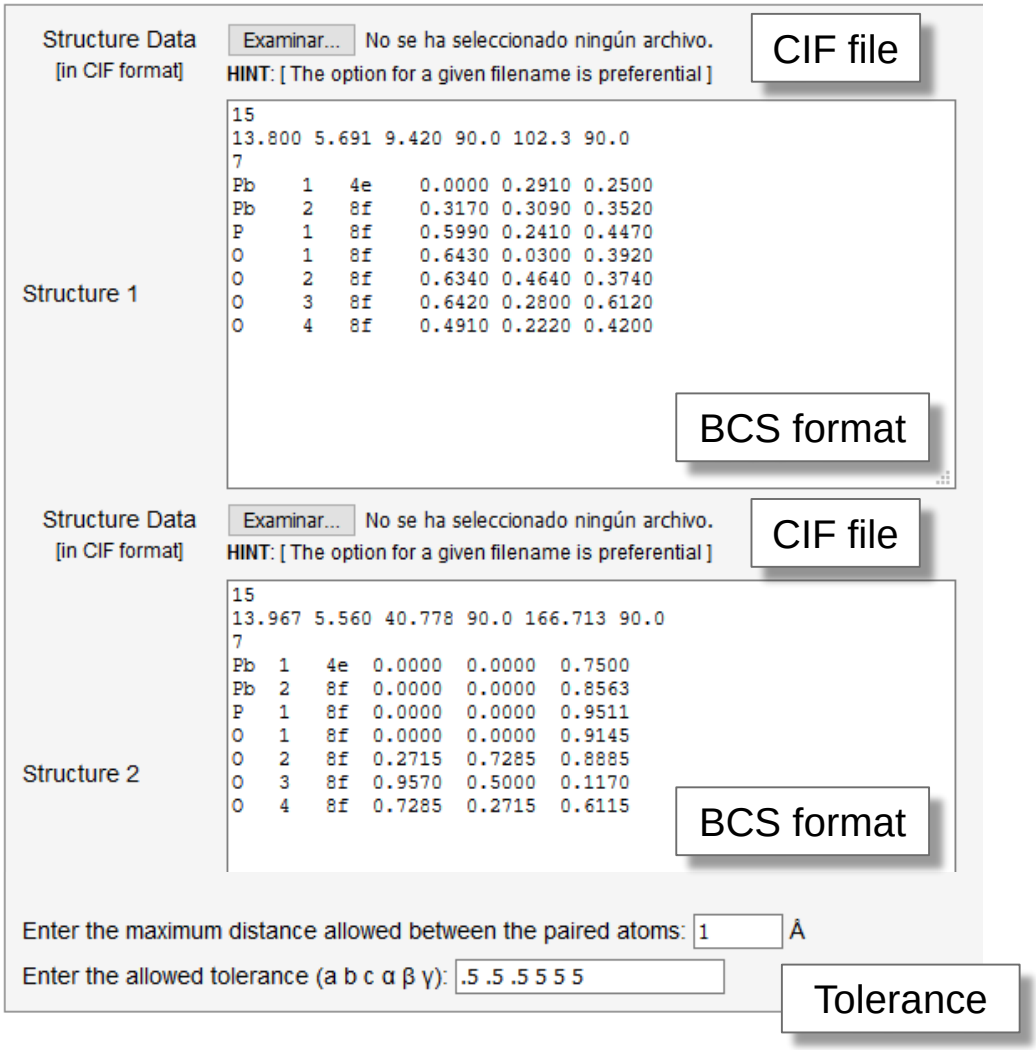
Input – COMPSTRU

COMPSTRU:
https://www.cryst.ehu.es/cryst/compstru.html

Input:

Two crystal structures described in the standard setting

- Isopointal structures with the same/different composition
- Chiral structures

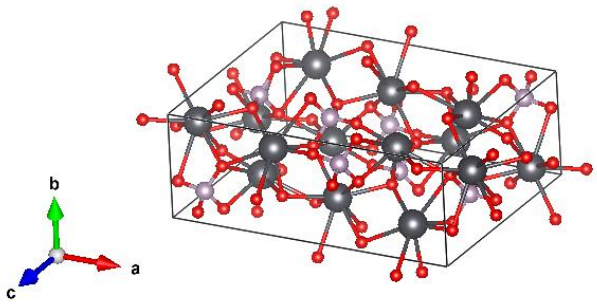


de la Flor *et al. J. Appl. Cryst* **49** (2016)

Are these two structures similar?

$Pb_3(PO_4)_2$

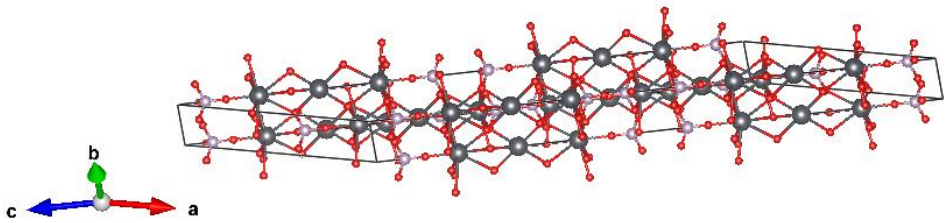
#Structure 1



15
13.800 5.691 9.420 90.0 102.3 90.0
7

Pb	1	4e	0.0000	0.2910	0.2500
Pb	2	8f	0.3170	0.3090	0.3520
P	1	8f	0.5990	0.2410	0.4470
O	1	8f	0.6430	0.0300	0.3920
O	2	8f	0.6340	0.4640	0.3740
O	3	8f	0.6420	0.2800	0.6120
O	4	8f	0.4910	0.2220	0.4200

#Structure 2



15
13.967 5.560 40.778 90.0 166.713
90.0
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	0.2715	0.7285	0.8885
O	3	8f	0.9570	0.5000	0.1170
O	4	8f	0.7285	0.2715	0.6115

COMPSTRU

Karlsruhe Institute of Technology

$Pb_3(PO_4)_2$

Comparison of crystal structures of the same symmetry *C2/c* (No. 15) [unique axis b]

Structure #1

```
15
13.800 5.691 9.420 90.0 102.3 90.0
7
Pb      1       4e      0.000000        0.291000        0.250000
Pb      2       8f      0.317000        0.309000        0.352000
P       1       8f      0.599000        0.241000        0.447000
O       1       8f      0.643000        0.030000        0.392000
O       2       8f      0.634000        0.464000        0.374000
O       3       8f      0.642000        0.280000        0.612000
O       4       8f      0.491000        0.222000        0.420000
```

Structure #2

```
15
13.967 5.560 40.778 90.0 166.713 90.0
7
Pb      1       4e      0.000000        0.000000        0.750000
Pb      2       8f      0.000000        0.000000        0.856300
P       1       8f      0.000000        0.000000        0.951100
O       1       8f      0.000000        0.000000        0.914500
O       2       8f      0.271500        0.728500        0.888500
O       3       8f      0.957000        0.500000        0.117000
O       4       8f      0.728500        0.271500        0.611500
```

The next step is to select a transformation that best matches the lattice parameters of the structures for the chosen tolerance (a b c α β γ) = (.5 .5 .5 5 5 5):

Select	Transformation (P,p)	Cell parameters of the Structure #1 Cell parameters of the Structure #2 applying the transformation matrix	Strain
◉	-a,-b,3a+c	13.8000 5.6910 9.4200 90.0000 102.3000 90.0000 13.9670 5.5600 9.6301 90.0000 103.2951 90.0000	0.0116

Continue

COMPSTRU

$Pb_3(PO_4)_2$

Structure #1

```
15
13.800 5.691 9.420 90.0 102.3 90.0
7
Pb      1       4e      0.000000        0.291000        0.250000
Pb      2       8f      0.317000        0.309000        0.352000
P       1       8f      0.599000        0.241000        0.447000
O       1       8f      0.643000        0.030000        0.392000
O       2       8f      0.634000        0.464000        0.374000
O       3       8f      0.642000        0.280000        0.612000
O       4       8f      0.491000        0.222000        0.420000
```

WP		Atom	Atomic Displacements			
			u_x	u_y	u_z	|u|
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
8f	(x,y,z)	P1	0.0043	0.0090	0.0041	0.0816
8f	(x,y,z)	O1	0.0010	-0.0085	-0.0035	0.0617
8f	(x,y,z)	O2	0.0100	0.0145	0.0145	0.1910
8f	(x,y,z)	O3	0.0020	-0.0300	0.0050	0.1777
8f	(x,y,z)	O4	0.0025	0.0280	-0.0055	0.1733

Evaluation of the structure similarity

S	$d_{max.}$ (Å)	$d_{av.}$ (Å)	Δ
0.0116	0.3386	0.1755	0.066

Structure #2

```
15
13.967 5.560 40.778 90.0 166.713 90.0
7
Pb      1       4e      0.000000        0.000000        0.750000
Pb      2       8f      0.000000        0.000000        0.856300
P       1       8f      0.000000        0.000000        0.951100
O       1       8f      0.000000        0.000000        0.914500
O       2       8f      0.271500        0.728500        0.888500
O       3       8f      0.957000        0.500000        0.117000
O       4       8f      0.728500        0.271500        0.611500
```

$$(\boldsymbol{P},\boldsymbol{p}) = -\boldsymbol{a},-\boldsymbol{b},3\boldsymbol{a}+\boldsymbol{c}\,;\ \mathbf{1/4},\mathbf{1/4},\mathbf{0}$$

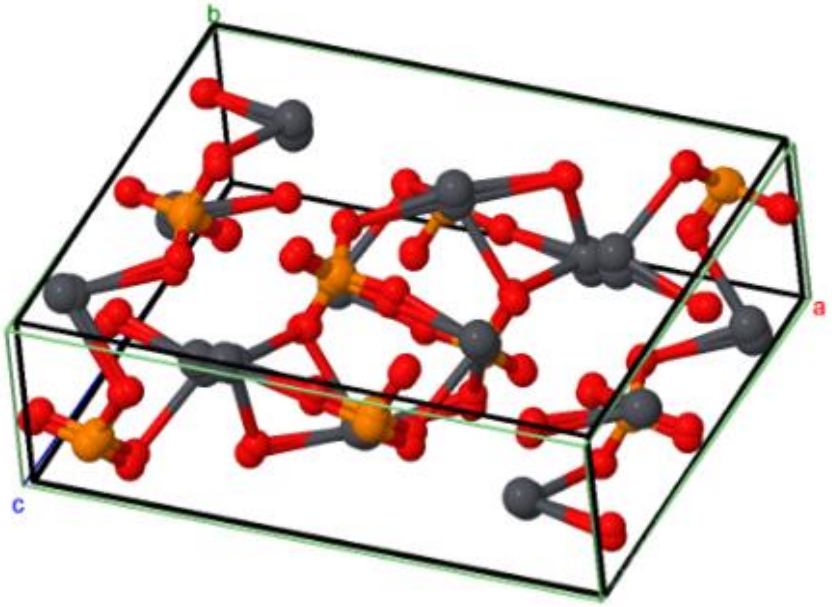
Description of Structure #2 in the most similar configuration to Structure #1

```
015
13.967000 5.560000 9.630055 90.000000 103.295059 90.000000
7
Pb      1       4e      0.500000        0.250000        0.750000
Pb      2       8f      0.818900        0.250000        0.856300
P       1       8f      0.103300        0.250000        0.951100
O       1       8f      0.993500        0.250000        0.914500
O       2       8f      0.644000        0.521500        0.888500
O       3       8f      0.644000        0.750000        0.117000
O       4       8f      0.356000        0.978500        0.611500
```

Input – COMPSTRU

$Pb_3(PO_4)_2$

-C 2yc [C 1 2/c 1] #15
a=13.967Å
b=5.560Å
c=9.630Å
α=90.000°
β=103.295°
γ=90.000°



Structure #1
Structure #2

Structure #2 (most similar)

Compare Structures
Compare Lattices
Atomic Displacements

Structure 1: ☑ opaque
◉ ball&stick ○ stick ○ cross
Structure 2: ☑ opaque
◉ ball&stick ○ stick ○ cross

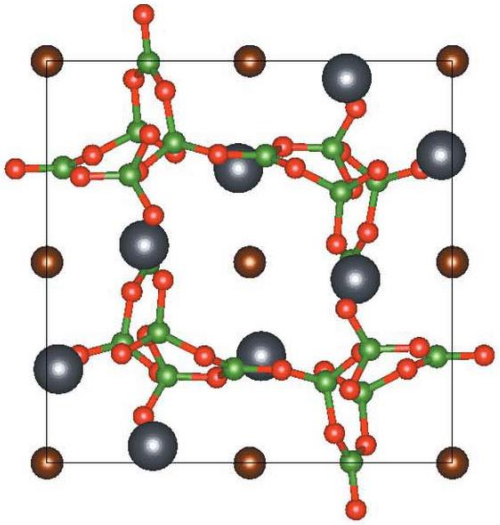
Show Distances
cutoff: 0.5

Save PNG+Jmol

Example: Structures with different composition

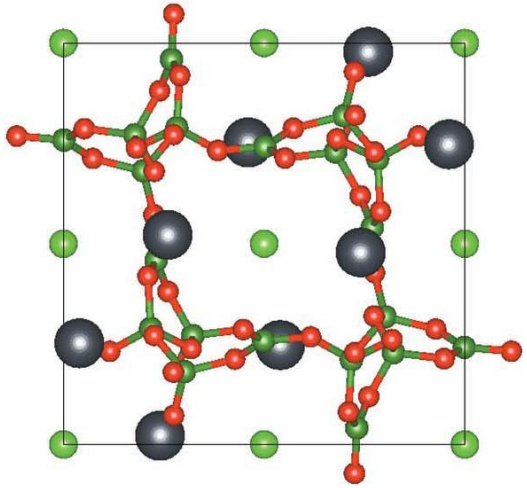
Are these two structures equivalent?

$Pb_2B_5O_9Br$



Belokoneva *et al*., 2003

$Pb_2B_5O_9Cl$



Egorova *et al*., 2008

Comparison of isopointal structures with different composition

Example: Structures with different composition

Comparison of crystal structures of the same symmetry *Pnn*2 (No. 34)

Structure #1

```
34
11.524 11.431 6.5399 90. 90. 90.
18
Pb      1       4c      0.260700        0.042500        0.000000
Pb      2       4c      0.028000        0.233700        0.663000
Br      1       2a      0.000000        0.000000        0.893000
Br      2       2b      0.000000        0.500000        0.626000
O       1       4c      0.247000        0.317000        0.590000
O       2       4c      0.209000        0.426000        0.179000
O       3       4c      0.276000        0.226000        0.253000
O       4       4c      0.078000        0.268000        0.241000
O       5       4c      0.286000        0.455000        0.853000
O       6       4c      0.388000        0.266000        0.842000
O       7       4c      0.184000        0.272000        0.939000
O       8       4c      0.418000        0.213000        0.500000
O       9       4c      0.238000        0.116000        0.570000
B       1       4c      0.275000        0.325000        0.800000
B       2       4c      0.187000        0.298000        0.160000
B       3       4c      0.296000        0.217000        0.480000
B       4       4c      0.461000        0.235000        0.700000
B       5       4c      0.250000        0.497000        0.030000
```

Structure #2

```
34
11.3810 11.3840 6.56335 90. 90. 90.
18
Pb      1       4c      0.039700        0.252300        0.000100
Pb      2       4c      0.240500        0.021900        0.332600
Cl      1       2a      0.000000        0.000000        0.121800
Cl      2       2b      0.500000        0.000000        0.381300
O       1       4c      0.318400        0.238700        0.418600
O       2       4c      0.427100        0.212600        0.826900
O       3       4c      0.225600        0.271700        0.753700
O       4       4c      0.274800        0.072000        0.752600
O       5       4c      0.448100        0.286300        0.160800
O       6       4c      0.260500        0.380800        0.162500
O       7       4c      0.273900        0.180300        0.069800
O       8       4c      0.210400        0.419200        0.506500
O       9       4c      0.115700        0.232100        0.438700
B       1       4c      0.322100        0.271200        0.203400
B       2       4c      0.301500        0.181600        0.854700
B       3       4c      0.217300        0.288900        0.534400
B       4       4c      0.230700        0.458800        0.308800
B       5       4c      0.498800        0.258300        0.976800
```

Select	Transformation (P,p)	Cell parameters of the Structure #1 Cell parameters of the Structure #2 applying the transformation matrix	Strain
○	a,b,c	11.5240 11.4310 6.5399 90.0000 90.0000 90.0000 11.3810 11.3840 6.5633 90.0000 90.0000 90.0000	0.0046
◉	-b,-a,-c	11.5240 11.4310 6.5399 90.0000 90.0000 90.0000 11.3840 11.3810 6.5633 90.0000 90.0000 90.0000	0.0045

All equivalent unit-cell parameters are calculated and compared with the unit-cell parameters of structure 1

Example: Structures with different composition

Comparison of crystal structures of the same symmetry *Pnn*2 (No. 34)

Structure 1

```
34
11.3810 11.3840 6.56335 90. 90. 90.
18
Pb    1   4c    0.039700 0.252300 0.000100
Pb    2   4c    0.240500 0.021900 0.332600
Cl    1   2a    0.000000 0.000000 0.121800
Cl    2   2b    0.500000 0.000000 0.381300
O     1   4c    0.318400 0.238700 0.418600
O     2   4c    0.427100 0.212600 0.826900
O     3   4c    0.225600 0.271700 0.753700
O     4   4c    0.274800 0.072000 0.752600
O     5   4c    0.448100 0.286300 0.160800
O     6   4c    0.260500 0.380800 0.162500
O     7   4c    0.273900 0.180300 0.069800
O     8   4c    0.210400 0.419200 0.506500
O     9   4c    0.115700 0.232100 0.438700
B     1   4c    0.322100 0.271200 0.203400
B     2   4c    0.301500 0.181600 0.854700
B     3   4c    0.217300 0.288900 0.534400
B     4   4c    0.230700 0.458800 0.308800
B     5   4c    0.498800 0.258300 0.976800
```

Structure 2

```
34
11.524 11.431 6.5399 90. 90. 90.
18
Pb    1   4c    0.260700 0.042500 0.000000
Pb    2   4c    0.028000 0.233700 0.663000
Br    1   2a    0.000000 0.000000 0.893000
Br    2   2b    0.000000 0.500000 0.626000
O     1   4c    0.247000 0.317000 0.590000
O     2   4c    0.209000 0.426000 0.179000
O     3   4c    0.276000 0.226000 0.253000
O     4   4c    0.078000 0.268000 0.241000
O     5   4c    0.286000 0.455000 0.853000
O     6   4c    0.388000 0.266000 0.842000
O     7   4c    0.184000 0.272000 0.939000
O     8   4c    0.418000 0.213000 0.500000
O     9   4c    0.238000 0.116000 0.570000
B     1   4c    0.275000 0.325000 0.800000
B     2   4c    0.187000 0.298000 0.160000
B     3   4c    0.296000 0.217000 0.480000
B     4   4c    0.461000 0.235000 0.700000
B     5   4c    0.250000 0.497000 0.030000
```

The similarity of the two structures will be evaluated taking into account the following correspondence between the atomic species:

Structure #1	Structure #2
Cl	Br
O	O
Pb	Pb
B	B

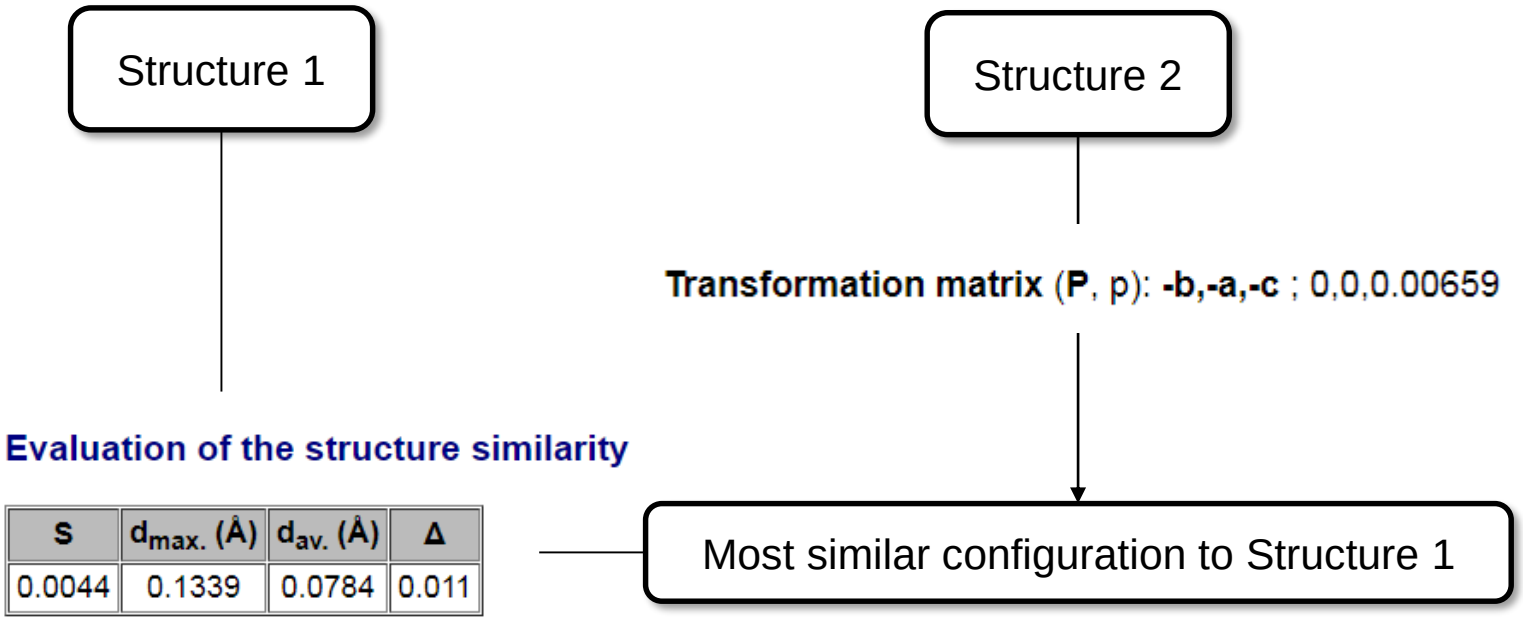
Do you agree with the proposed correspondence scheme?

Yes No

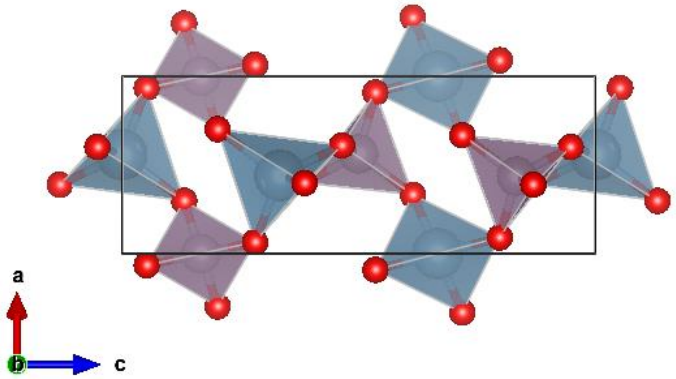
DIFFERENT COMPOSITION

Institute of Applied Geoscience
Division Technical Petrophysics

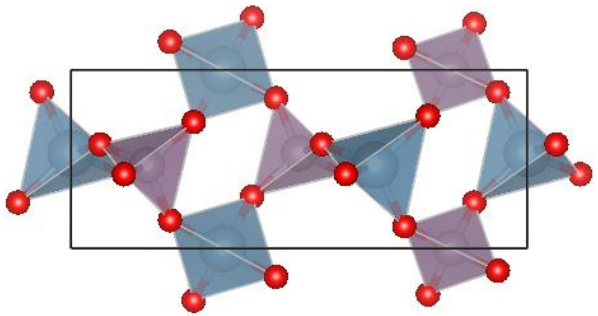
Example: Structures with different composition



Example: Chiral Structures



$P3_121$ (No. 152)



$P3_221$ (No. 154)

#ICSD: 158620
152
4.5191 4.5191 10.471 90. 90. 120.
4

Al	1	3a	0.441200	0.000000	0.333333
P	1	3b	0.437300	0.000000	0.833300
O	1	6c	0.398200	0.332600	0.385500
O	2	6c	0.389200	0.297900	0.868700

#ICSD: 50100
154
4.9438 4.9438 10.9498 90. 90. 120.
4

Al	1	3a	0.466460	0.000000	0.666667
P	1	3b	0.466900	0.000000	0.166700
O	1	6c	0.416400	0.291900	0.602540
O	2	6c	0.415500	0.257400	0.116180

Example: Chiral Structures

Structure #1

```
152
4.5191 4.5191 10.471 90. 90. 120.
4
Al      1       3a      0.441200        0.000000        0.333333
P       1       3b      0.437300        0.000000        0.833300
O       1       6c      0.398200        0.332600        0.385500
O       2       6c      0.389200        0.297900        0.868700
```

Structure #2

```
154
4.9438 4.9438 10.9498 90. 90. 120.
4
Al    1   3a    0.466460 0.000000 0.666667
P     1   3b    0.466900 0.000000 0.166700
O     1   6c    0.416400 0.291900 0.602540
O     2   6c    0.415500 0.257400 0.116180
```

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

Atom pairings and distances

Atom Mappings					
WP		**Atom**	**Coordinates in S_1**	**Atom**	**Coordinates in S_2**
3a	(x,0,1/3)	Al1	(0.441200,0.000000,0.333333)	Al1	(0.466460,0.000000,0.333333)
3b	(x,0,5/6)	P1	(0.437300,0.000000,0.833300)	P1	(0.466900,0.000000,0.833300)
6c	(x,y,z)	O1	(0.398200,0.332600,0.385500)	O1	(0.416400,0.291900,0.397460)
6c	(x,y,z)	O2	(0.389200,0.297900,0.868700)	O2	(0.415500,0.257400,0.883820)

WP		**Atom**	**Atomic Displacements**			
			u_x	u_y	u_z	|u|
3a	(x,0,1/3)	Al1	0.0253	0.0000	0.0000	0.1142
3b	(x,0,5/6)	P1	0.0296	0.0000	0.0000	0.1338
6c	(x,y,z)	O1	0.0182	-0.0407	0.0120	0.2672
6c	(x,y,z)	O2	0.0263	-0.0405	0.0151	0.3073

The enantiomorphic description of Structure #2 in the most similar configuration to Structure #1

```
152
4.943800 4.943800 10.949800 90.000000 90.000000 120.000000
4
Al      1       3a      0.466460        0.000000        0.333333
P       1       3b      0.466900        0.000000        0.833300
O       1       6c      0.416400        0.291900        0.397460
O       2       6c      0.415500        0.257400        0.883820
```

S	$d_{max.}$ (Å)	$d_{av.}$ (Å)	Δ
0.0413	0.3073	0.2328	0.107

Isopointal and isoconfigurational structures

- Two structures are defined as *isopointal* if:
  (1) they have the same space-group type or belong to a pair of enantiomorphic space groups, and
  (2) the atomic positions are the same in both structures

- Two structures are defined as *isoconfigurational* (or belonging to the same structure type) if
  (1) they are isopointal, and
  (2) for all corresponding Wyckoff positions, both, the crystallographic configurations (crystallographic orbits) and their geometric interrelationships, are similar.

Lima-de Faria *et al. Acta Cryst.* (1990), A**41**, 1

Structure types - COMPSTRU

ABX6 family R-3 (148);WP sequence: fba; Pearson: hR8

$KCrF_6$	$LiNbF_6$	$VNbF_6$	$HgRhF_6$	$MgPbF_6$	$InAsF_6$
$RbCrF_6$	$LiRuF_6$	$CoZrF_6$	$NiRhF_6$	$ZnPbF_6$	$CsNbF_6$
$KAsF_6$	$LiRhF_6$	$PdPtF_6$	$CaCrF_6$	$NiPbF_6$	$HgCrF_6$
$RuAsF_6$	$LiTaF_6$	$FeNbF_6$	$MgCrF_6$	$MgPdF_6$	$CoSnF_6$
$CsAsF_6$	$LiOsF_6$	$CaSnF_6$	$CdCrF_6$	$CaPdF_6$	$CsNbF_6$
$RbSbF_6$	$LiIrF_6$	$FeZrF_6$	$MnSnF_6$	$ZnPdF_6$	$MnPtF_6$
$BaSnF_6$	$LiPtF_6$	$CuZrF_6$	$FeSnF_6$	$CdPdF_6$	$CdRhF_6$
$CsBrF_6$	$LiAuF_6$	$CaPtF_6$	$ZnSnF_6$	$LiSbF_6$	$NaBiF_6$
$CsSbF_6$	$NiPtF_6$	$ZnPtF_6$	$NiSnF_6$	$BaIrF_6$	$TlAsF_6$
$CsBiF_6$	$CdPtF_6$	$CoPtF_6$	$CuSnF_6$	$RbBiF_6$	
$CsUF_6$	$LiPF_6$	$MgRhF_6$	$CdSnF_6$	$KRhF_6$	
$KOsF_6$	$LiAsF_6$	$CaRhF_6$	$CdTiF_6$	$CsReF_6$	
$NaCrF_6$	$PdZrF_6$	$ZnRhF_6$	$LiBiF_6$	KPF_6