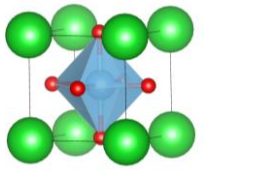
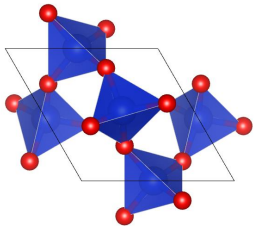
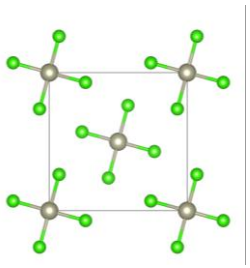
Crystal-Structure Tools

Crystallography Online: Workshop on the use and applications of the structural and magnetic tools of the Bilbao Crystallographic Server

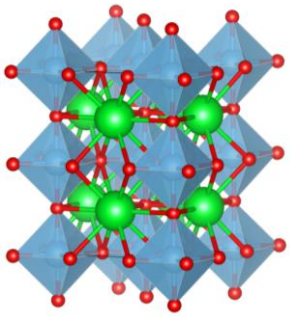




COMPSTRU

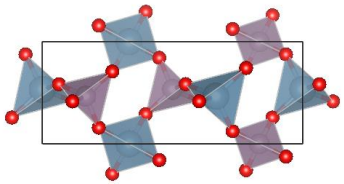


SETSTRU

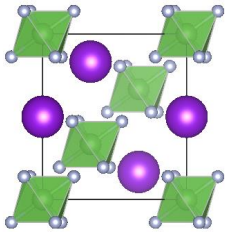


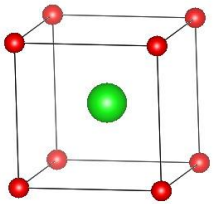
SUBGROUPS

TRANSTRU

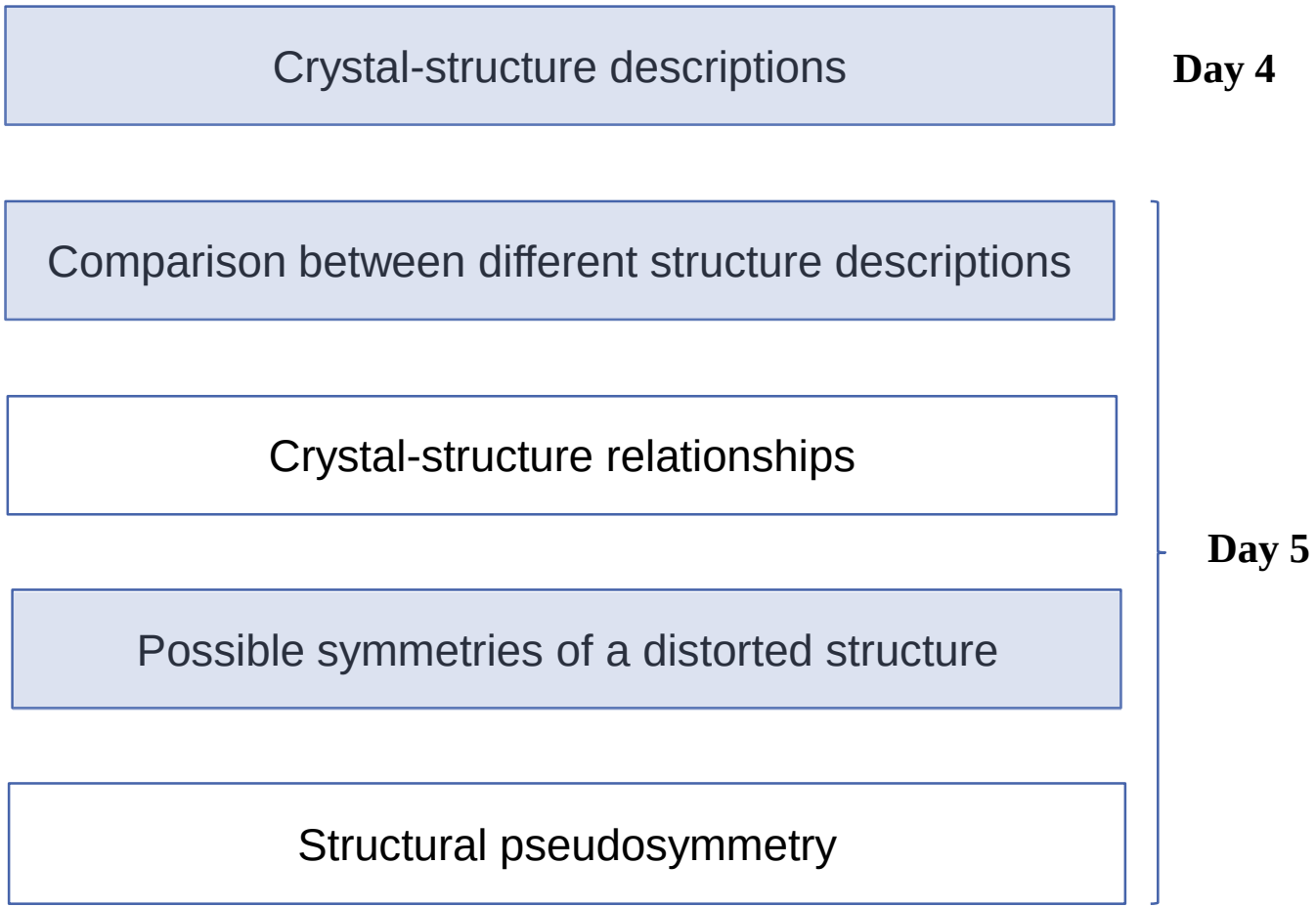


EQUIVSTRU





Crystal-Structure Tools



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bilbao crystallographic server

Crystallography Online: Workshop on the use of the structural and magnetic tools of the Bilbao Crystallographic Server
27 June - 1 July 2022, Leioa (Spain)

Forthcoming schools and workshops

News:

- **Space-group symmetry**
  05/2022: The monoclinic and tetragonal ITA-settings database has been completed.
- **New Article**
  04/2022: Regnault *et al.* "Catalogue of flat-band stoichiometric materials". Nature (2022) **603**, 824-828
- **New version of B-IncStrDB**
  02/2022: New version of the data-base of incommensurate structures.
- **New upload option in MAGNDATA**
  10/2021: New feature that permits anyone to submit to this database any published magnetic structure not yet included in the collection.

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- Space-group symmetry
- Magnetic Symmetry and Applications
- Group-Subgroup Relations of Space Groups
- Representations and Applications
- Solid State Theory Applications
- Structure Utilities
- Topological Quantum Chemistry
- Subperiodic Groups: Layer, Rod and Frieze Groups
- Structure Databases
- Raman and Hyper-Raman scattering
- Point-group symmetry
- Plane-group symmetry
- Double point and space groups

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Space-group symmetry

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
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

(2022) **603**, 824-828

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Raman and Hyper-Raman scattering

Point-group symmetry

Plane-group symmetry

Double point and space groups

Crystal-Structure Tools

You can access to the material of this session:

http://www.cryst.ehu.es/resources/bcs_workshop2022/

You need to download:

- CrystalStructureTools.txt

CRYSTAL STRUCTURE DESCRIPTIONS

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 majority of the programs in the BCS only accepts, as input data, structures described in a standard/default setting of the space group:

  - *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 is $(\boldsymbol{P}, \boldsymbol{p}) = -\boldsymbol{a} - \boldsymbol{c}, \boldsymbol{b}, \boldsymbol{a}; 0,0,0$

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

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

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

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

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

Example – Structure transformation

1) Transform the unit cell parameters

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

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

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

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

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

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

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

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

ITA 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 *ITA*-setting into another *ITA*-setting

*IT*A setting structure description

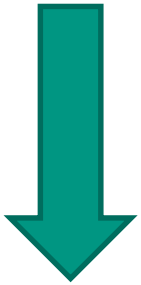
Choose the initial and final space groups symbols

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)

*IT*A 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

Exercise 1

- 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   16f   0.2413  0.1511  0.0861
```

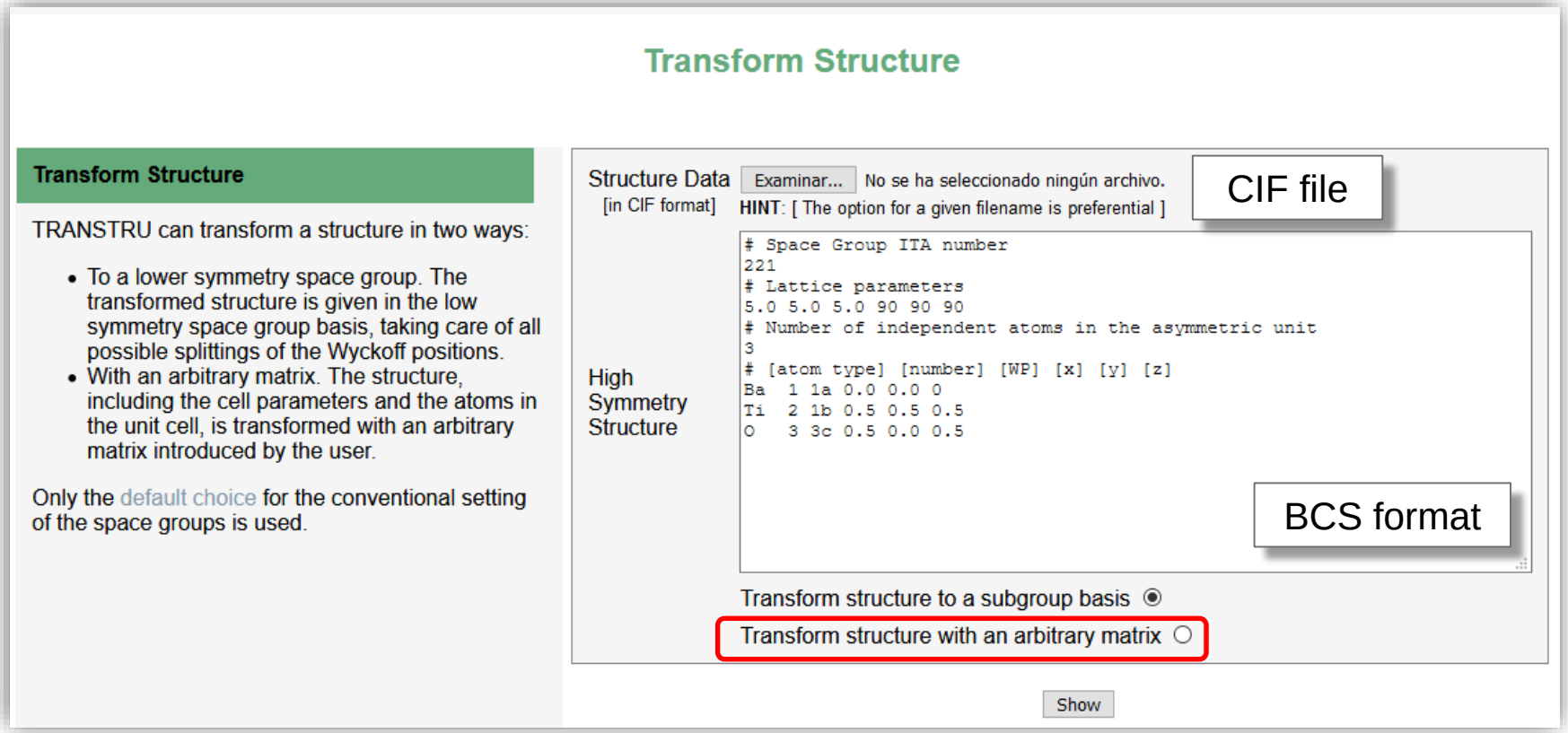
```
# (b) Origin choice 2
# ICSD: 15586
88
5.243  5.243  11.376  90  90  90
3
Ca 1   4b    0.0000  0.2500  0.6250
W  1   4a    0.0000  0.2500  0.1250
O  1   16f   0.1504  0.0085  0.2111
```

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

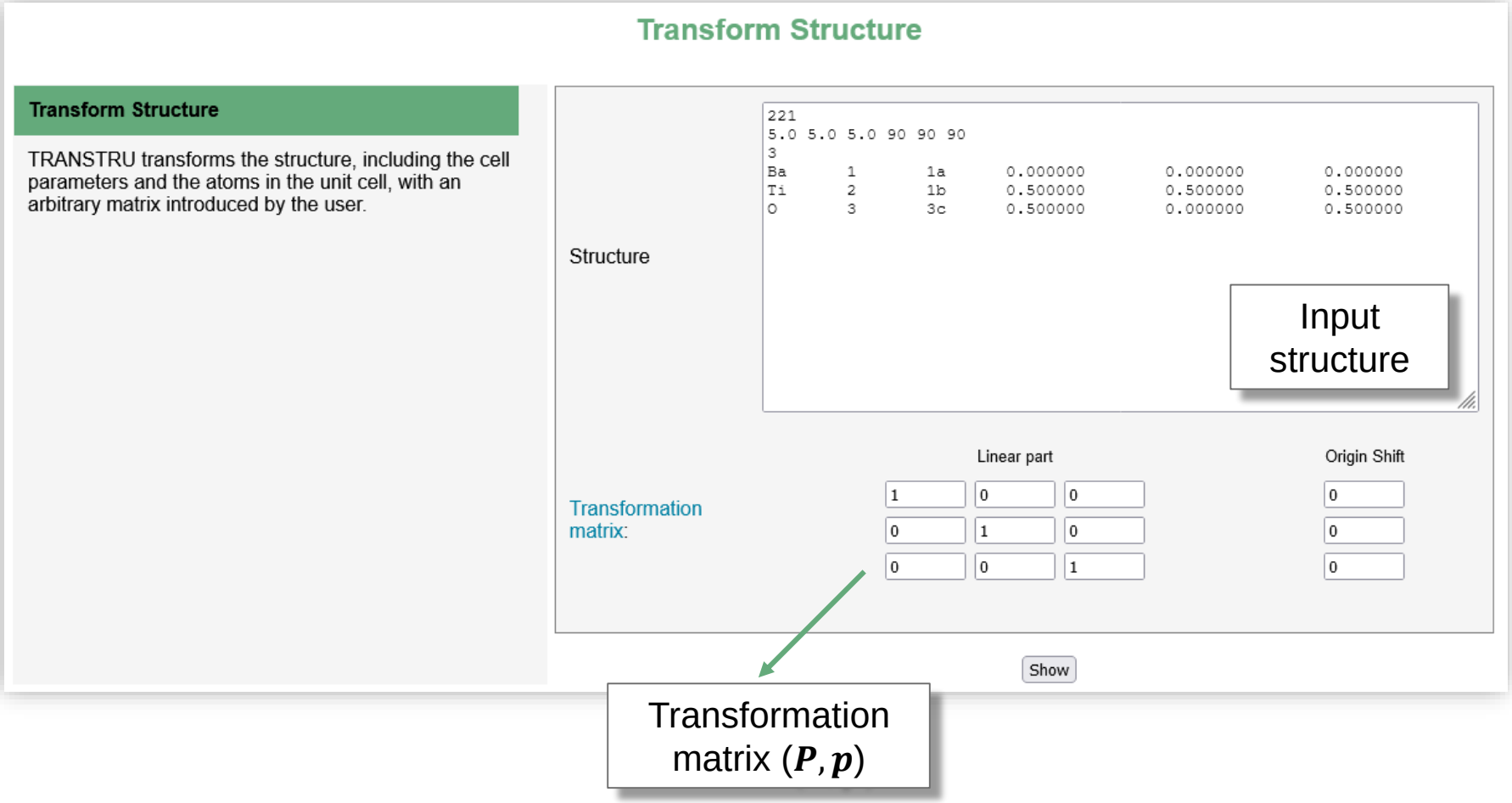
Structure transformation

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



Exercise 1 (cont.)

- Apply the program TRANSTRU in order to compare the two structure descriptions of $CaWO_4$.

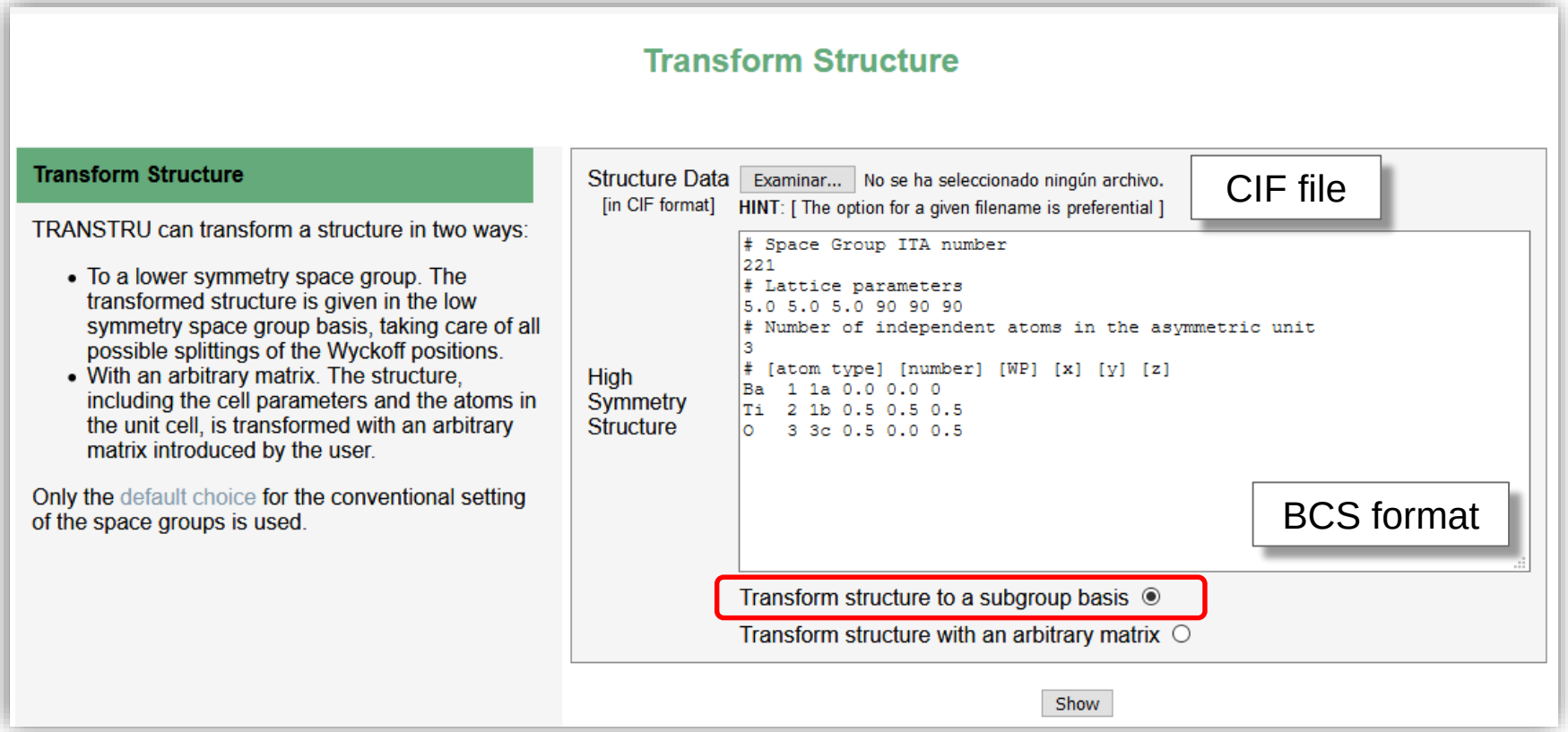
```
# (a) Origin choice 1
# ICSD: 15869
88
5.243  5.243  11.376  90  90  90
3
Ca 1   4b    0.0000  0.0000  0.5000
W  1   4a    0.0000  0.0000  0.0000
O  1   16 f  0.2413  0.1511  0.0861
```

```
# (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
```

Origin choice 1 ⟶ **a,b,c**; 0,1/4,1/8

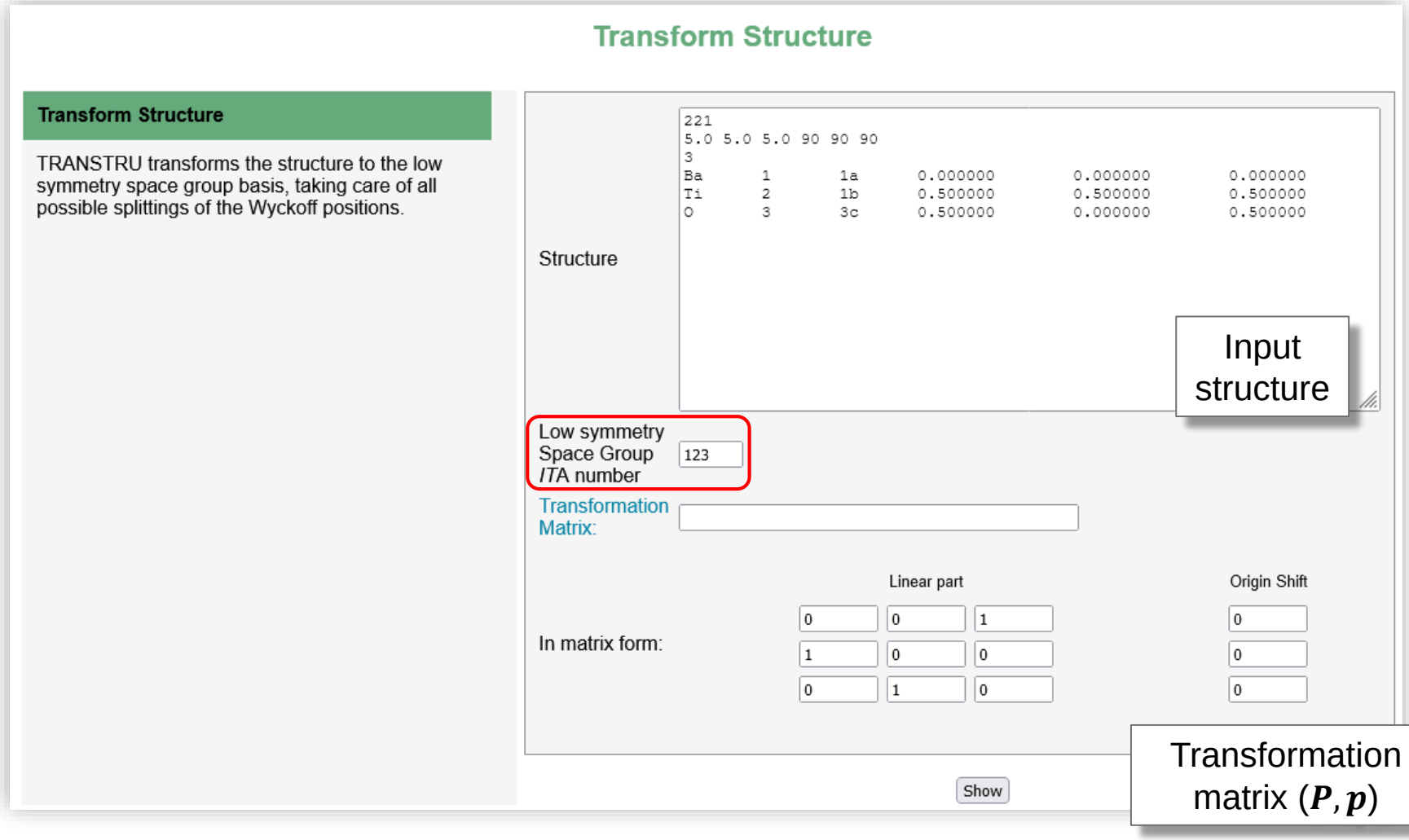
Structure transformation

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.

Exercise 2

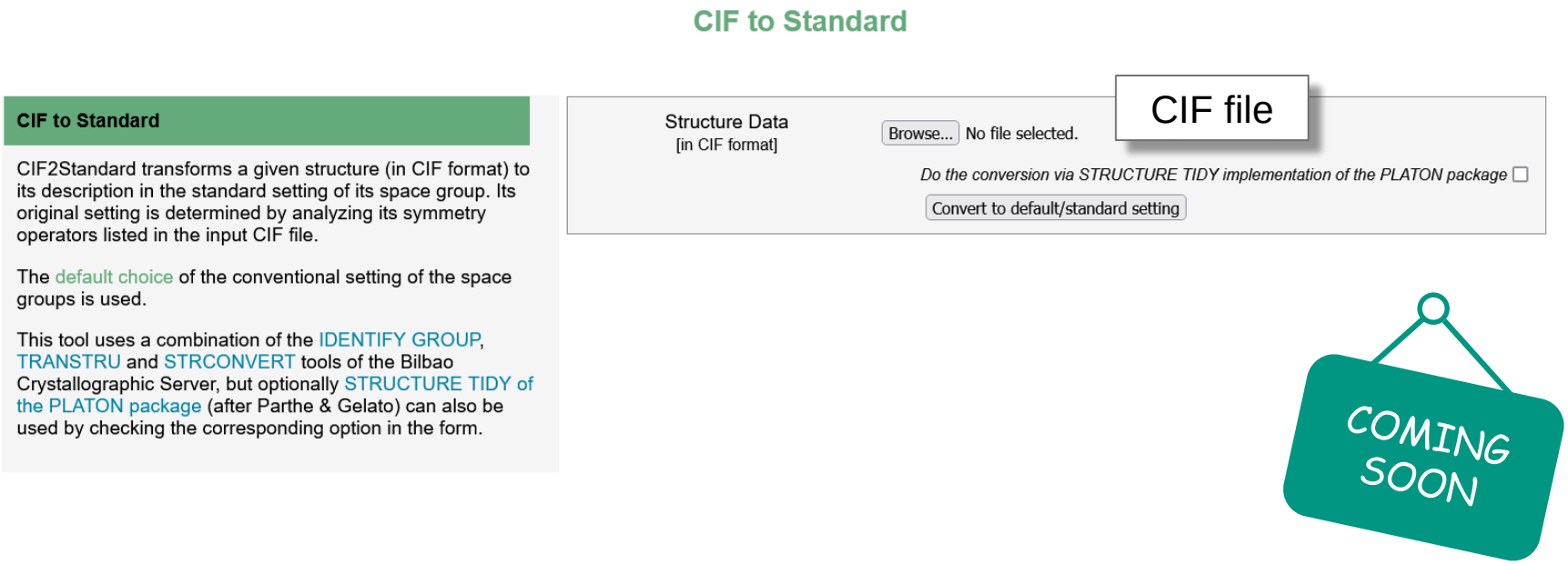
- The high-symmetry phase of AlLi crystallizes in the cubic face-centered space group $Fd\bar{3}m$ (No. 227):

227
6.370 6.370 6.370 90.0 90.0 90.0
2
Li 1 8a 0.375 0.375 0.375
Al 2 8b 0.125 0.125 0.125

Derived the structural model of the tetragonal phase $I4_1/amd$ (No. 141) of AlLi applying the following matrix-column pair $(\boldsymbol{P}, \boldsymbol{p}) = \frac{1}{2}(\boldsymbol{a} - \boldsymbol{b}), \frac{1}{2}(\boldsymbol{a} + \boldsymbol{b}), \boldsymbol{c}; \frac{1}{4}, \frac{1}{4}, 0$

Structure transformation

CIF2Standard Transform a given structure (in CIF format) to its description in the standard setting



Output – 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)

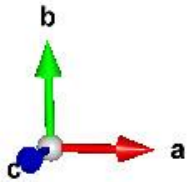
CIF file of the structure in standard setting: cif2std_13517.cif

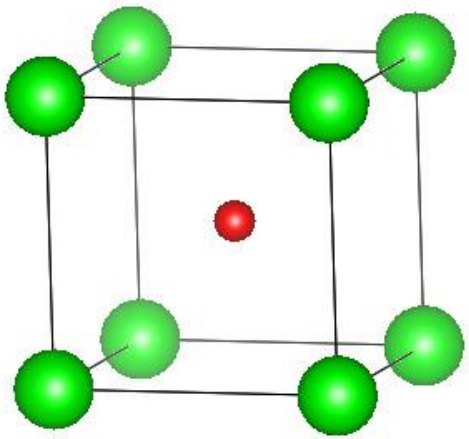
Download CIF file (standard setting)

Equivalent crystal structure descriptions

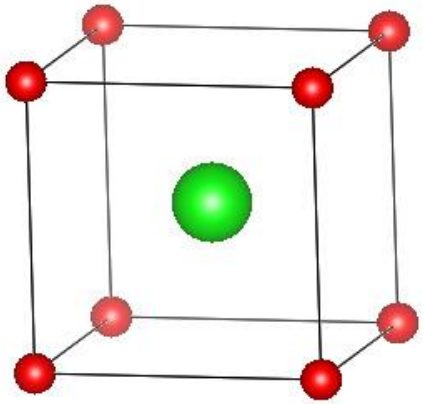
- There are almost always several possible ways to describe the exactly same crystal structure

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 $N_{\mathcal{E}}(G)$

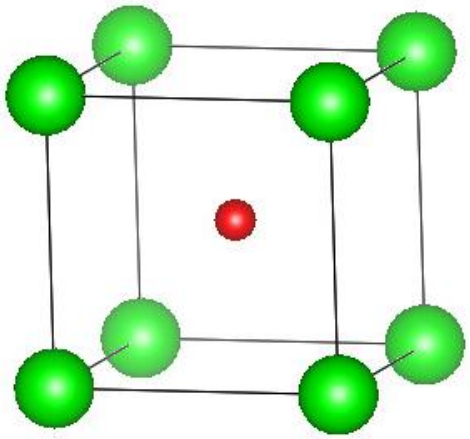
Example – CsCl

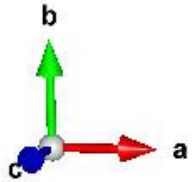
- CsCl crystallizes in space group $Pm\bar{3}m$ (No. 221)

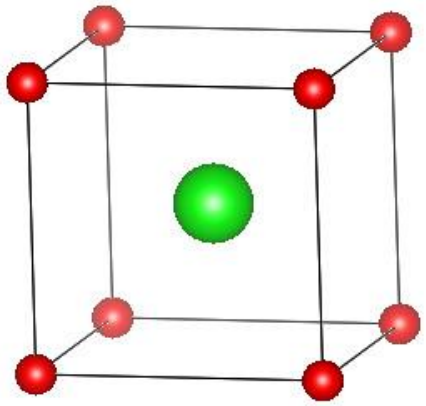
Cs	1a	0	0	0
Cl	1b	0.5	0.5	0.5

$t(1/2,1/2,1/2)$

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







Example – $ReNCl_4$

- $ReNCl_4$ crystallizes in space group $I4$ (No. 79):

```
#ICSD:419181
79
8.267 8.267 4.051 90. 90. 90.
3
Re  1  2a   0.000000   0.000000  -0.008100
Cl  1  8c  -0.070900   0.262700   0.066000
N   1  2a   0.000000   0.000000   0.589000
```

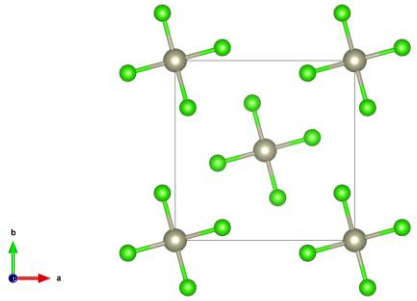
Space group $\mathcal{G}$		Euclidean normalizer $\mathcal{N}_\mathcal{E}(\mathcal{G})$ and chirality-preserving normalizer $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$		Additional generators of $\mathcal{N}_\mathcal{E}(\mathcal{G})$ and $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$			
No.	Hermann–Mauguin symbol	Symbol	Basis vectors	Translations	Inversion through a centre at	Further generators	Index of $\mathcal{G}$ in $\mathcal{N}_\mathcal{E}(\mathcal{G})$ or $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$
75	$P4$	$P^1 4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \varepsilon\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,t$	0, 0, 0	y, x, z	$(2\cdot\infty)\cdot 2\cdot 2$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P^1 422$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \varepsilon\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,t$	/	$y, x, \bar{z}$	$(2\cdot\infty)\cdot 2$
76	$P4_1$	$P^1 422$ [$\equiv \mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$]	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \varepsilon\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,t$	/	$y, x, \bar{z}$	$(2\cdot\infty)\cdot 2$
77	$P4_2$	$P^1 4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \varepsilon\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,t$	0, 0, 0	y, x, z	$(2\cdot\infty)\cdot 2\cdot 2$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P^1 422$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \varepsilon\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,t$	/	$y, x, \bar{z}$	$(2\cdot\infty)\cdot 2$
78	$P4_3$	$P^1 422$ [$\equiv \mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$]	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \varepsilon\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,t$	/	$y, x, \bar{z}$	$(2\cdot\infty)\cdot 2$
79	$I4$	$P^1 4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \varepsilon\mathbf{c}$	$0, 0, t$	0, 0, 0	y, x, z	$\infty\cdot 2\cdot 2$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P^1 422$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \varepsilon\mathbf{c}$	$0, 0, t$	/	$y, x, \bar{z}$	$\infty\cdot 2$

The index of $I4$ in $P^1 4/mmm$ is $\infty\cdot 2\cdot 2 \Rightarrow$ there are infinitely many possibilities

Example – $ReNCl_4$

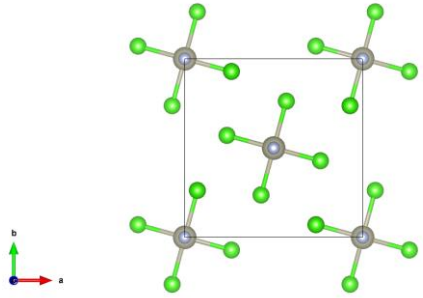
Structure 1 (*x*, *y*, *z*)

Re	0.000000	0.000000	-0.008100
Cl	-0.070900	0.262700	0.066000
N	0.000000	0.000000	0.589000



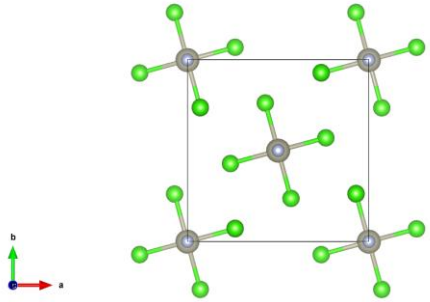
Structure 2 (-*y*, -*x*, -*z*)

Re	0.000000	0.000000	0.008100
Cl	-0.262700	0.070900	-0.066000
N	0.000000	0.000000	-0.589000



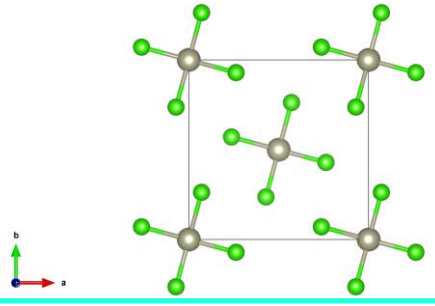
Structure 3 (-*x*, -*y*, -*z*)

Re	0.000000	0.000000	0.008100
Cl	0.070900	-0.262700	-0.066000
N	0.000000	0.000000	-0.589000



Structure 4 (*y*, *x*, *z*)

Re	0.000000	0.000000	-0.008100
Cl	0.262700	-0.070900	0.066000
N	0.000000	0.000000	0.589000



$+ (0\ 0\ t)$

Infinite set of coordinates

Enantiomorphic structure

This transformation does not preserve the chirality

Example – Quartz

- Right quartz crystallizes in the space group $P3_221$ (No. 154)

```
#ICSD:34644
154
4.9138  4.9138  5.4052  90.  90.  120.
2
Si  1  3a  0.469800   0.000000   0.666667
O  1  6c  0.414500   0.266200   0.785600
```

Euclidean normalizer (general metric) of the Group $P3_221$ (No. 154)

Euclidean normalizer of $P3_221$ (a,b,c): $P6_422$ (a+b,-a,1/2c)

Index of $P3_221$ in $P6_422$ (**a+b,-a,1/2c**): 4 with i_L=2 and i_P=2

Additional generators of $P6_422$ (**a+b,-a,1/2c**) with respect to $P3_221$

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)
-x,-y,z	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	2 0,0,z

The index of $P3_221$ in $P6_422$ is 4 ⇒ there are four symmetrically equivalent descriptions

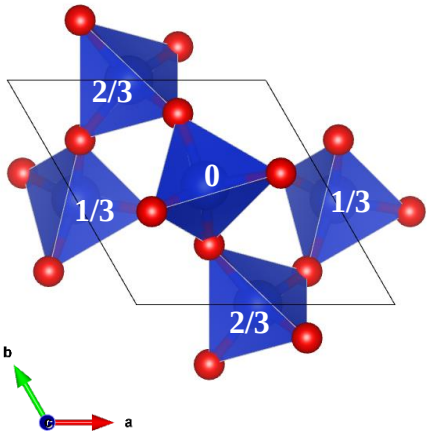
Example – Quartz

#Structure 1 (*x*, *y*, *z*)
Si 0.469800 0.000000 0.666667
O 0.414500 0.266200 0.785600

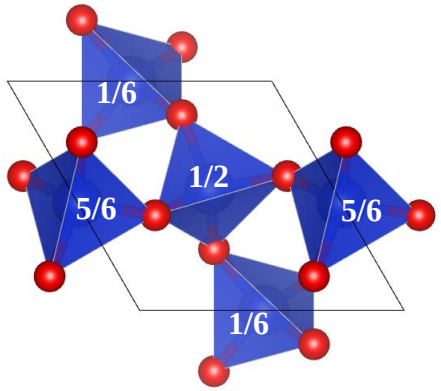
#Structure 2 (*x*, *y*, *z*+1/2)
Si 0.469800 0.000000 0.166667
O 0.414500 0.266200 0.285600

#Structure 3 (-*x*, -*y*, *z*)
Si -0.469800 0.000000 0.666667
O -0.414500 -0.266200 0.785600

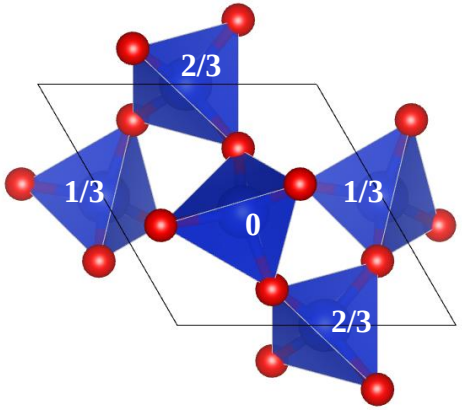
#Structure 4 (-*x*, -*y*, z+1/2)
Si -0.469800 0.000000 0.166667
O -0.414500 -0.266200 0.285600



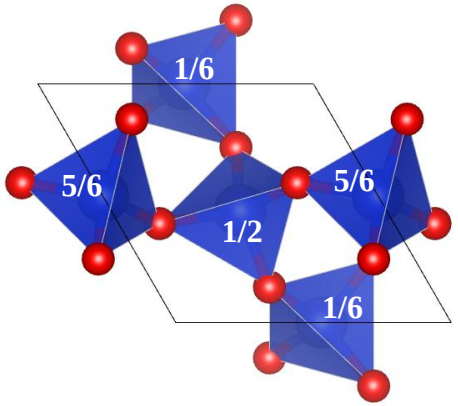
x, y, z



x, y, z+1/2



-x, -y, z



-x, -y, z+1/2

Example – Quartz

- The space group $P3_221$ (No. 154) is an *enantiomorphic* or *chiral space group*
- The space group $P3_221$and$P3_121$ (No. 152) form and *enantiomorphic pair*

Descriptions of enantiomorphic structure with space group $P3_121$ (No. 152)

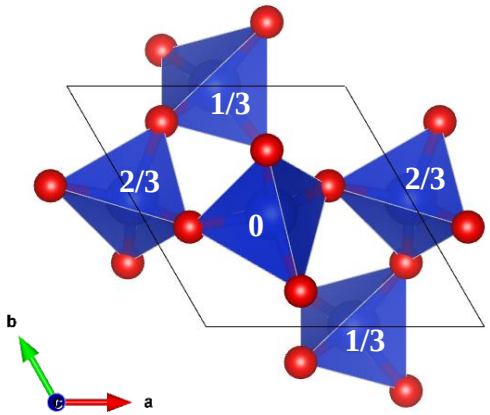
```
# Enantiomorphic structure (-x, -y, -z)
152
4.9138 4.9138 5.4052 90.00 90.00 120.00
2
Si  1  3a  -0.469800   0.000000   -0.666667
O  1  6c  -0.414500  -0.266200   -0.785600
```

```
# Enantiomorphic structure (-x, -y, -z+1/2)
152
4.9138 4.9138 5.4052 90.00 90.00 120.00
2
Si  1  3a  -0.469800   0.000000   -0.166667
O  1  6c  -0.414500  -0.266200   -0.285600
```

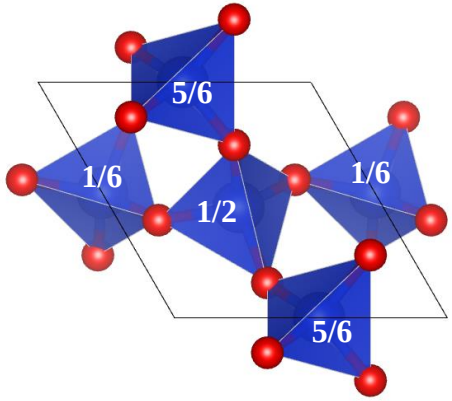
```
# Enantiomorphic structure (x, y, -z)
152
4.9138 4.9138 5.4052 90.00 90.00 120.00
2
Si  1  3a   0.469800   0.000000   -0.666667
O  1  6c   0.414500   0.266200   -0.785600
```

```
# Enantiomorphic structure (x, y, -z+1/2)
152
4.9138 4.9138 5.4052 90.00 90.00 120.00
2
Si  1  3a  0.469800   0.000000   -0.166667
O  1  6c  0.414500   0.266200   -0.285600
```

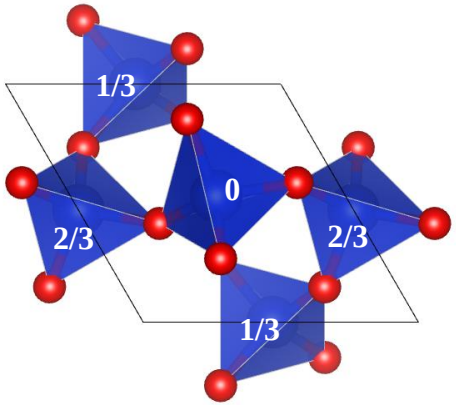
Example – Quartz (enantiomorphic structures)



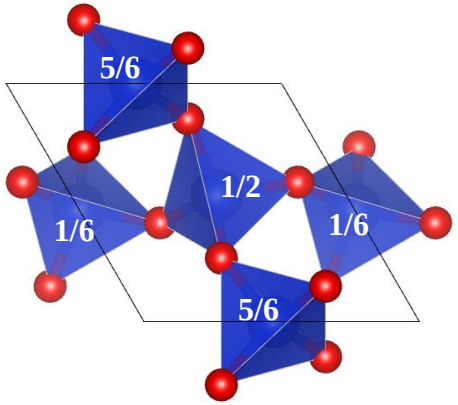
$-x, -y, -z$



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



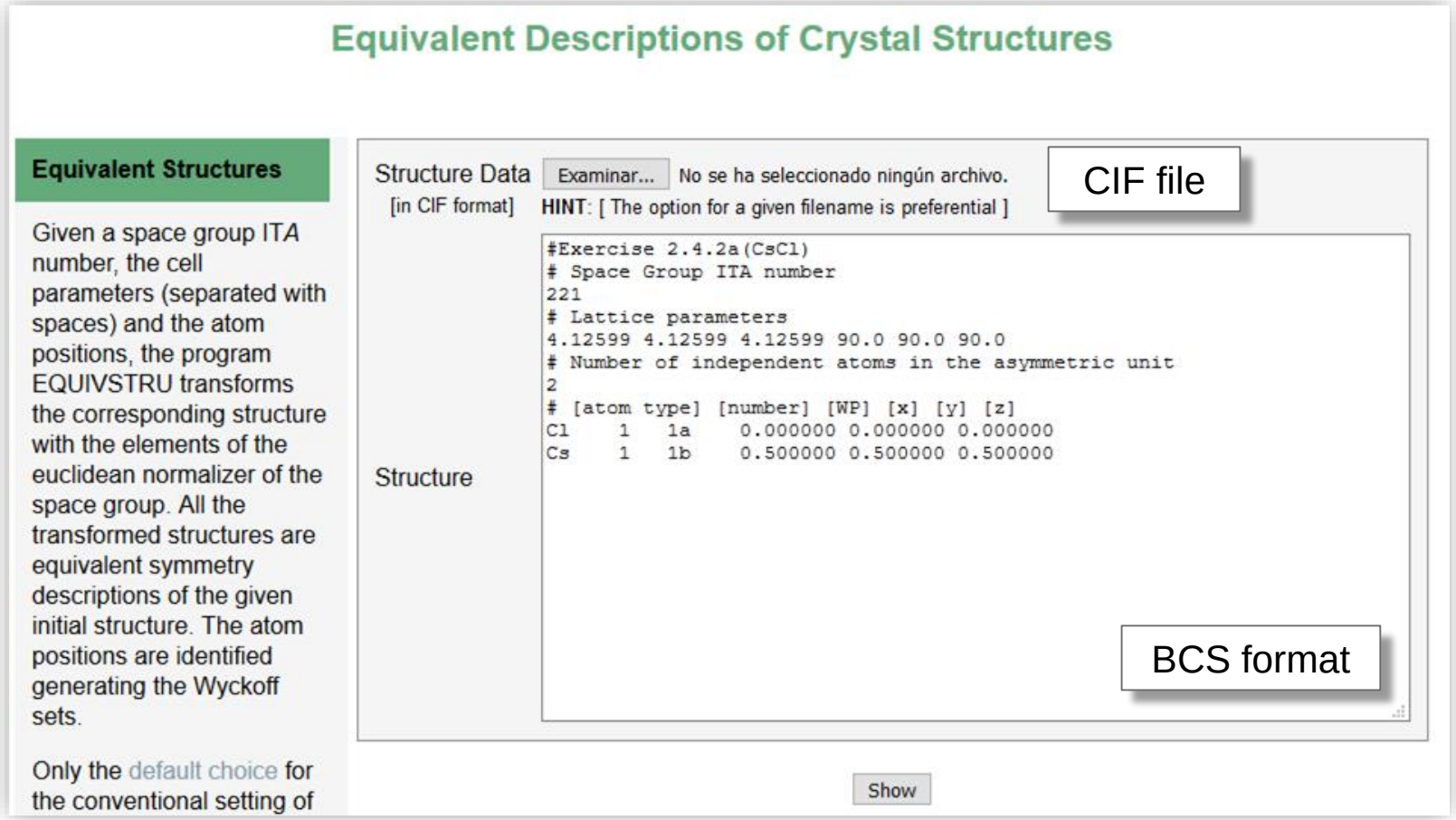
$x, y, -z$



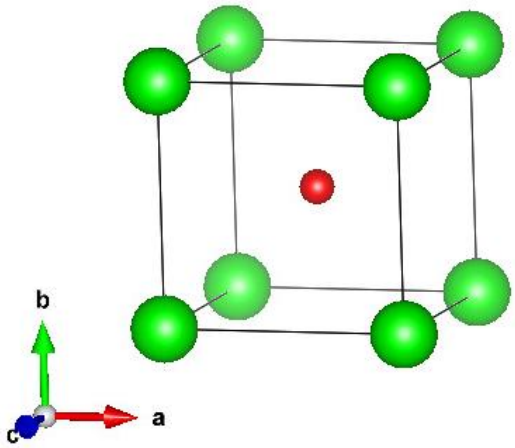
$x, y, -z+1/2$

Equivalent crystal structure descriptions

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



EQUIVSTRU – Output



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

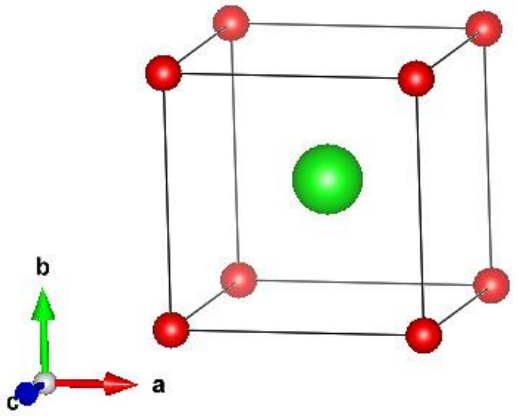
Normalizer coset representative: x,y,z

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**

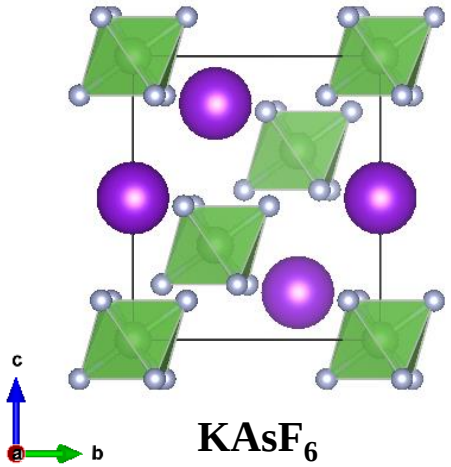
Normalizer coset representative: x+1/2,y+1/2,z+1/2

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)



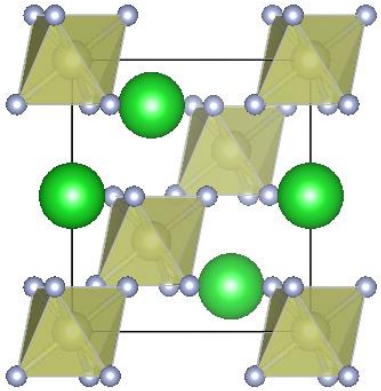
Exercise 3

- Evaluate the similarity between the following three structures. Try to find analogous coordinate descriptions for all three crystal structures



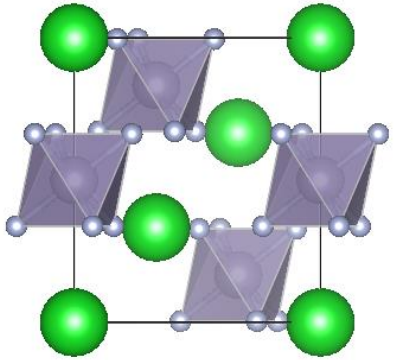
$KAsF_6$

#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



$BaIrF_6$

#ICSD: 240981
148
7.3965 7.3965 7.2826 90. 90. 120.
3
Ir 1 3a 0.000000 0.000000 0.000000
F 1 18f 0.072900 0.232500 0.164000
Ba 1 3b 0.333333 0.666667 0.166700



$BaSnF_6$

#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

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