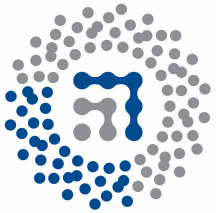

ZTF-FCT
Zientzia eta Teknologia Fakultatea
Facultad de Ciencia y Tecnología

Universidad del País Vasco
Euskal Herriko Unibertsitatea

Use of the structural programs of the Bilbao Crystallographic Server. Structure Utilities.

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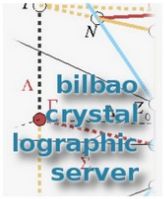
Universidad del País Vasco, UPV-EHU
BILBAO, SPAIN

www.cryst.ehu.es

FCT/ZTF

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.
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EQUIVSTRU	Equivalent Descriptions for a given Crystal Structure
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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

magnetic structure not yet included in the collection.

Double point and space groups

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

General Position of the Group $I4_1/amd$ (No. 141) [origin choice 2]

from GENPOS

Click here to get the general position in text format

No.	(x,y,z) form	Matrix form	Symmetry operation	
			ITA	Seitz ℹ
(0,0,0) + set				
1	x,y,z	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	1	{ 1 | 0 }
2	-x+1/2,-y,z+1/2	$\begin{pmatrix} -1 & 0 & 0 & 1/2 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 1/2 \end{pmatrix}$	2 (0,0,1/2) 1/4,0,z	{ 2_{001} | 1/2 0 1/2 }
3	-y+1/4,x+3/4,z+1/4	$\begin{pmatrix} 0 & -1 & 0 & 1/4 \\ 1 & 0 & 0 & 3/4 \\ 0 & 0 & 1 & 1/4 \end{pmatrix}$	4^+ (0,0,1/4) -1/4,1/2,z	{ 4^+_{001} | 1/4 3/4 1/4 }
4	y+1/4,-x+1/4,z+3/4	$\begin{pmatrix} 0 & 1 & 0 & 1/4 \\ -1 & 0 & 0 & 1/4 \\ 0 & 0 & 1 & 3/4 \end{pmatrix}$	4^- (0,0,3/4) 1/4,0,z	{ 4^-_{001} | 1/4 1/4 3/4 }
5	-x+1/2,y,-z+1/2	$\begin{pmatrix} -1 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1/2 \end{pmatrix}$	2 1/4,y,1/4	{ 2_{010} | 1/2 0 1/2 }
6	x,-y,-z	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{pmatrix}$	2 x,0,0	{ 2_{100} | 0 }
7	y+1/4,x+3/4,-z+1/4	$\begin{pmatrix} 0 & 1 & 0 & 1/4 \\ 1 & 0 & 0 & 3/4 \\ 0 & 0 & -1 & 1/4 \end{pmatrix}$	2 (1/2,1/2,0) x,x+1/4,1/8	{ 2_{110} | 1/4 3/4 1/4 }

1 x,y,z
2 x+1/2,y+1/2,z+1/2
3 x,-y,-z
4 x+1/2,-y+1/2,-z+1/2
5 -x,y+1/2,-z
6 -x+1/2,y,-z+1/2
7 -x,-y+1/2,z
8 -x+1/2,-y,z+1/2
9 -y+1/4,-x+1/4,-z+3/4
10 -y+3/4,-x+3/4,-z+1/4
11 -y+1/4,x+3/4,z+1/4
12 -y+3/4,x+1/4,z+3/4
13 y+3/4,-x+3/4,z+1/4
14 y+1/4,-x+1/4,z+3/4
15 y+3/4,x+1/4,-z+3/4
16 y+1/4,x+3/4,-z+1/4
17 -x,-y,-z
18 -x+1/2,-y+1/2,-z+1/2
19 -x,y,z
20 -x+1/2,y+1/2,z+1/2
21 x,-y+1/2,z
22 x+1/2,-y,z+1/2
23 x,y+1/2,-z
24 x+1/2,y,-z+1/2
25 y+3/4,x+3/4,z+1/4
26 y+1/4,x+1/4,z+3/4
27 y+3/4,-x+1/4,-z+3/4
28 y+1/4,-x+3/4,-z+1/4
29 -y+1/4,x+1/4,-z+3/4
30 -y+3/4,x+3/4,-z+1/4
31 -y+1/4,-x+3/4,z+1/4
32 -y+3/4,-x+1/4,z+3/4

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 inversion center for centrosymmetric space groups listed with two origin choices)

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

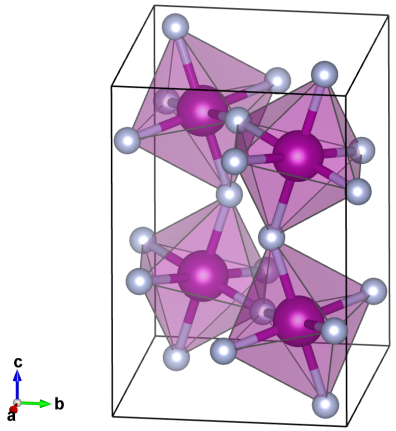
Example – Transformation to Standard using SETSTRU

Transform the crystal structure of manganese trifluoride MnF_3, described in the space group $I12/a1$ (No. 15), to its standard setting $C12/c1$

Initial Setting: $I12/a1$ (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



MnF_3

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

-a -c ,b ,a ; 0,0,0

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

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

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
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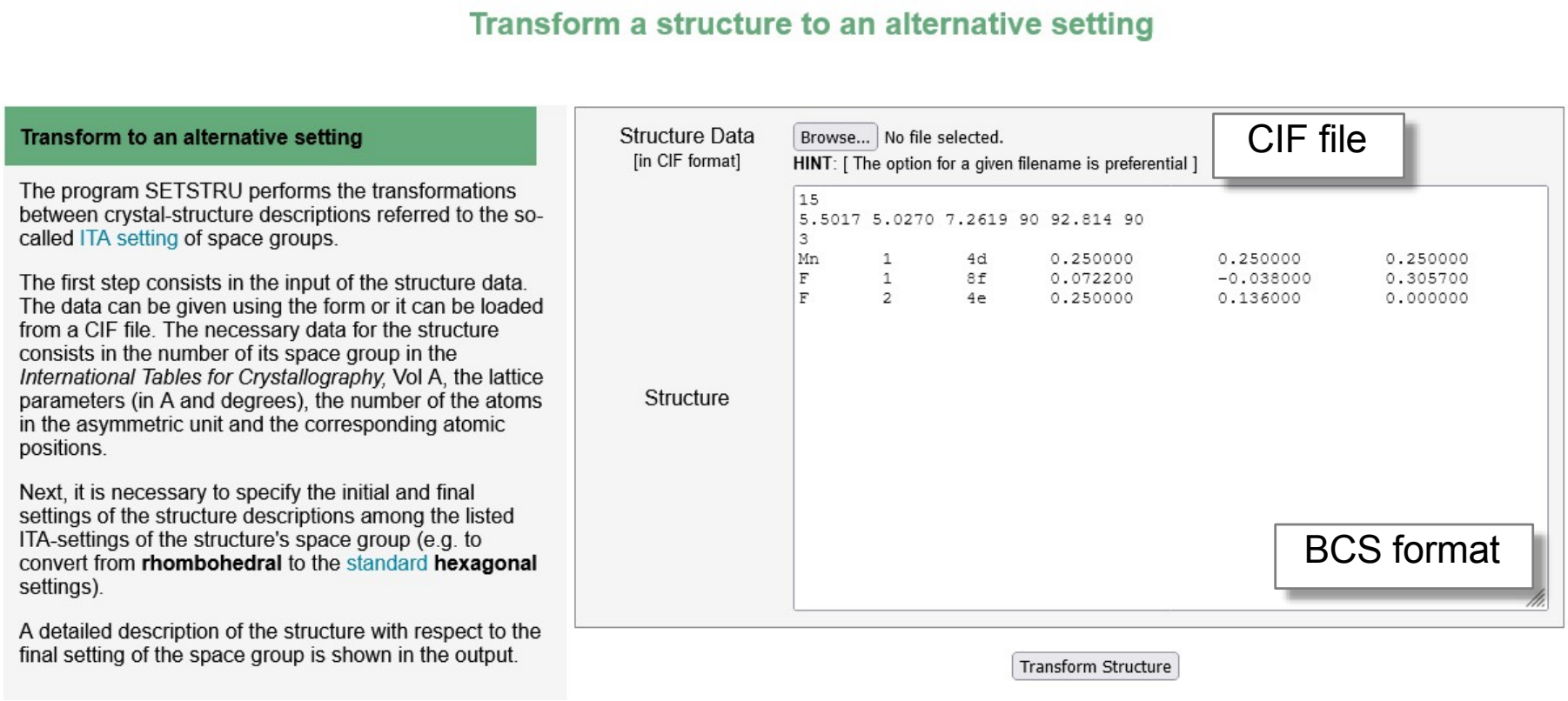
STRUCTURE RELATIONS	Evaluation of structure relationships [transformation matrix] between group-subgroup related phases
PSEUDOLATTICE	Pseudosymmetry of a lattice and compatible supergroups

*IT*A settings structure descriptions

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



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

*IT*A setting structure description

Choose the initial and final space groups symbols

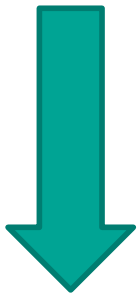
The standard setting (default) of the space group 15 is *C*12/*c*1 [*cell choice 1*]

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: $I12/a1$ (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: $C12/1$ (No. 15)

SETSTRU

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: C12/*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
```

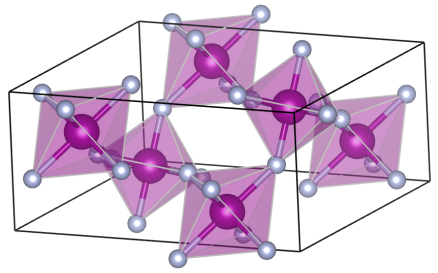
CIF File

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

Matrix form:

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

new CIF file in the chosen setting is provided



MnF_3

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

ITA 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

SETSTRU

you can also change from any initial ITA setting to any other ITA setting

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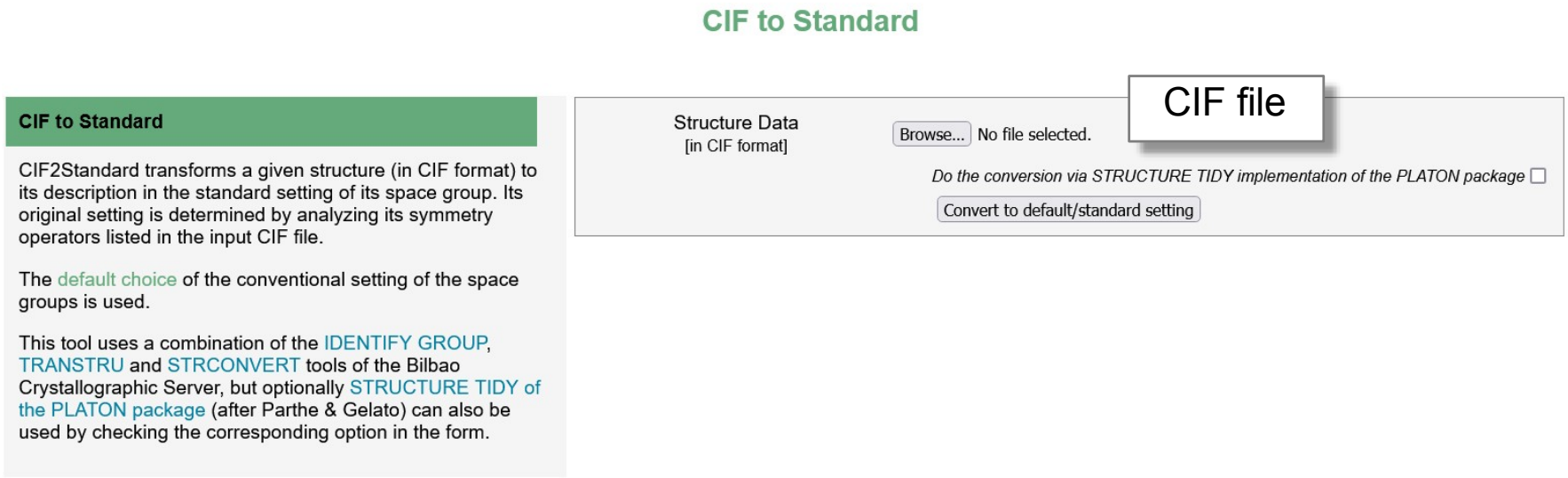
PSEUDOLATTICE	Pseudosymmetry of a lattice and compatible supergroups

Structure transformation

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



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
8.8928 5.0270 7.2619 90.00 38.17 90.00
3

Mn	1	4a	0.000000	0.000000	0.000000
F	1	8f	-0.177800	-0.288000	0.233500
F	2	4e	0.000000	-0.114000	-0.250000

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

Download CIF file (standard setting)

Transform structure (standard setting)

transformation different that used by SETSTRU:
-a -c ,b ,a ; 0,0,0

Output – CIF2Standard

CIF to Standard Setting

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

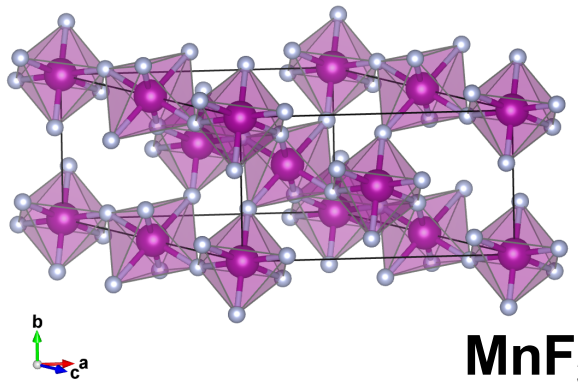
It has been transformed to the standard setting *C*2/*c* via the transformation matrix: a+c+1/4,b+1/4,c+1/4

15
8.8928 5.0270 7.2619 90.00 38.17 90.00
3

Mn	1	4a	0.000000	0.000000	0.000000
F	1	8f	-0.177800	-0.288000	0.233500
F	2	4e	0.000000	-0.114000	-0.250000

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

Download CIF file (standard setting)



MnF_3

Transform structure (standard setting)

transformation different that used by SETSTRU:
-a -c ,b ,a ; 0,0,0

Space-group symmetry	
GENPOS	Generators and General Positions of Space Groups
WYCKPOS	Wyckoff Positions of Space Groups
HKLCOND	Reflection conditions of Space Groups
MAXSUB	Maximal Subgroups of Space Groups
SERIES	Series of Maximal Isomorphic Subgroups of Space Groups
WYCKSETS	Equivalent Sets of Wyckoff Positions
NORMALIZER	Normalizers of Space Groups
KVEC	The k-vector types and Brillouin zones of Space Groups
SYMMETRY OPERATIONS	Geometric interpretation of matrix column representations of symmetry operations
IDENTIFY GROUP	Identification of a Space Group from a set of generators in an arbitrary setting

1 'x,y,z'
2 '-x+1/2,y,-z'
3 '-x,-y,-z'
4 'x+1/2,-y,z'
5 'x+1/2,y+1/2,z+1/2'
6 '-x,y+1/2,-z+1/2'
7 '-x+1/2,-y+1/2,-z+1/2'
8 'x,-y+1/2,z+1/2'

Space group operations in the CIF file using I12/a1 setting

IDENTIFY GROUP: Identification of a Space Group from a set of generators in an arbitrary setting.

IDENTIFY GROUP: Identifies a Space Group given a set of generators

IDENTIFY GROUP identifies a Space Group given a set of generators and shows the transformation matrix to a standard or reference (default) description of the Space Group.

Help

Enter the generators of the Space Group in the box below, given in any basis of the lattice, as in the example:
x+1/2,y+1/2,z
-y+1/3,x+1/4,z+1/4

Assumed lattice translations:
x + 1 , y , z
x , y + 1 , z
x , y , z + 1

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

Submit

The Space Group has been identified as *C*2/*c* (No. 15)

Transformation Matrix to the standard/default setting

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

Your Transformation Matrix is also valid.

Check an alternative Transformation Matrix

-1	0	1	0
0	1	0	0
-1	0	0	0

Submit

Input generators

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

General positions of the Space Group *C*2/*c* in the given setting

(0,0,0),(1/2,1/2,1/2)+

1 x,y,z
2 -x+1/2,y,-z
3 -x+1/2,-y+1/2,-z+1/2
4 x,-y+1/2,z+1/2

[Get general positions in matrix form]

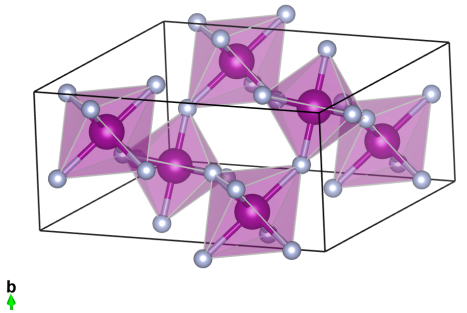
[Get general positions in plain text format]

Very similar (in this example equal) structures can be de described very differently even under the same standard setting of the space group

MnF_3

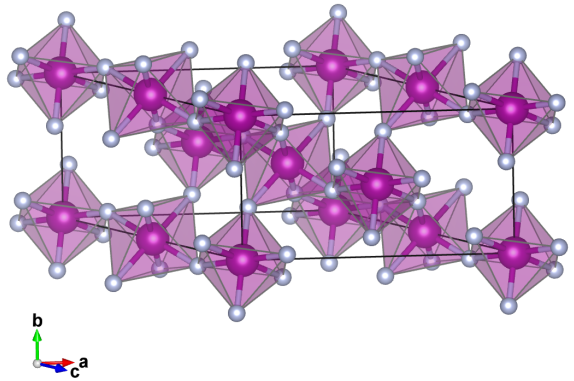
15
8.8928 5.0270 5.5017 90.00 125.35 90.00
3

Mn	1	4d	0.750000	0.250000	0.000000
F	1	8f	0.694300	0.962000	0.766500
F	2	4e	0.000000	0.136000	0.250000



15
8.8928 5.0270 7.2619 90.00 38.17 90.00
3

Mn	1	4a	0.000000	0.000000	0.000000
F	1	8f	-0.177800	-0.288000	0.233500
F	2	4e	0.000000	-0.114000	-0.250000



Structure Utilities	
CELLTRAN	Transform Unit Cells
STRAIN	Strain Tensor Calculation
WPASSIGN	Assignment of Wyckoff Positions
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Comparison of crystal structure descriptions

Compare Structure Descriptions

Often a quantitative comparison of two structure descriptions of the same phase, coming from different sources, is difficult because the descriptions, although postulating the same space group symmetry, are described using different sets of atoms in the asymmetric unit, or different equivalent choices of origin or cell orientations. The program COMPSTRU compares two structure descriptions of the same or different composition using the following algorithm:

First, the program transforms the description of Structure 2 to the most similar configuration of the descripion of Structure 1. After that the description of Structure 2 in the most similar configuration to the description of Structure 1 is chosen so that the maximal difference d_{max} of the atomic positions of the matching atoms has a minimal value. The difference between the two descriptions is quantified by evaluation of the global distortion decomposed into a spontaneous strain (lattice deformation) and atomic displacement field representing the differences in the positions of the matching atoms of the two structure descriptions. In addition, for the chosen solution the program calculates two additional descriptors of the similarity.

The program COMPSTRU can also be used for the recognition of similar atomic arrangement of different compounds that is essential for the classification of crystal structures into structure types.

NOTE: The program only accepts, as input data, structural data described in a **standard/default setting** of the space group. If the original structural data is described with respect to an **ITA setting**, the program **SETSTRU** can be used to transform it to the standard setting. In the case of more arbitrary non-conventional settings, the tool **TRANSTRU** can be of some help, if the **transformation** to the standard setting is known.

If you are using this program in the preparation of a paper, please cite it in the following form:

G. de la Flor, D. Orobengoa, E. Tasci, J. M. Perez-Mato and M. I. Aroyo. "Comparison of structures applying the tools available at the Bilbao Crystallographic Server". J. Appl. Cryst. (2016). 49, 653-664.

Structural Data
[in CIF format]

Examinar... No se ha seleccionado ningún archivo.

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

Description of Structure 1

```
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
```

Structural Data
[in CIF format]

Examinar... No se ha seleccionado ningún archivo.

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

Description of Structure 2

```
15
8.8928 5.0270 7.2619 90.00 38.17 90.00
3
Mn      1       4a      0.000000        0.000000        0.000000
F       1       8f      -0.177800       -0.288000       0.233500
F       2       4e      0.000000        -0.114000       -0.250000
```

Enter the tolerance for the maximum difference in the positions of matching atoms: 1 Å

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

Show

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

Description of Structure #1

```
15
8.8928 5.0270 5.5017 90.00 125.35 90.00
3
Mn      1       4d      0.750000        0.250000        0.000000
F       1       8f      0.694300        0.962000        0.766500
F       2       4e      0.000000        0.136000        0.250000
```

Description of Structure #2

```
15
8.8928 5.0270 7.2619 90.00 38.17 90.00
3
Mn      1       4a      0.000000        0.000000        0.000000
F       1       8f      0.822200        0.712000        0.233500
F       2       4e      0.000000        0.886000        0.750000
```

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

Select	Transformation (P,p)	Cell parameters of the description of Structure #1 Cell parameters of the description of Structure #2 applying the transformation matrix	Strain
◉	a,b,-a+c	8.8928 5.0270 5.5017 90.0000 125.3500 90.0000 8.8928 5.0270 5.5024 90.0000 125.3516 90.0000	0.0000
○	-a+2c,-b,a-c	8.8928 5.0270 5.5017 90.0000 125.3500 90.0000 9.3242 5.0270 5.5024 90.0000 128.9331 90.0000	0.0232

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

Description of Structure #1 (Reference description)

```
15
8.8928 5.0270 5.5017 90.00 125.35 90.00
3
Mn      1       4d      0.750000        0.250000        0.000000
F       1       8f      0.694300        0.962000        0.766500
F       2       4e      0.000000        0.136000        0.250000
```

Visualized this structure description | CIF File | Cartesian Coordinates

Description of Structure #2

```
15
8.8928 5.0270 7.2619 90.00 38.17 90.00
3
Mn      1       4a      0.000000        0.000000        0.000000
F       1       8f      0.822200        0.712000        0.233500
F       2       4e      0.000000        0.886000        0.750000
```

Visualized this structure description | CIF File | Cartesian Coordinates

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

The description of Structure #2 in the most similar configuration to the reference description is chosen so that the maximal difference d_{max} of the atomic positions of the matching atoms has a minimal value.

```
015
8.892800 5.027000 5.502377 90.000000 125.351616 90.000000
3
Mn      1       4d      0.750000        0.250000        0.000000
F       1       8f      0.694300        0.962000        0.766500
F       2       4e      0.000000        0.136000        0.250000
```

Visualized this structure description | CIF File | Cartesian Coordinates

Transformation matrix (**P**, p): **a,b,-a+c** ; -1/4,1/4,1/2

Matrix form:

$$(\mathbf{P}, p) = \begin{pmatrix} 1 & 0 & -1 & -1/4 \\ 0 & 1 & 0 & 1/4 \\ 0 & 0 & 1 & 1/2 \end{pmatrix}$$

Program finds the most appropiate transformation among those keeping the standard setting

Matching atoms and differences in the atomic positions

Matching atoms					
WP		Atom	Coordinates in S_1	Atom	Coordinates in S_2
4d	(1/4,1/4,1/2)	Mn1	(0.750000,0.250000,0.000000)	Mn1	(0.750000,0.250000,0.000000)
8f	(x,y,z)	F1	(0.694300,0.962000,0.766500)	F1	(0.694300,0.962000,0.766500)
4e	(0,y,1/4)	F2	(0.000000,0.136000,0.250000)	F2	(0.000000,0.136000,0.250000)

WP		Atom	Differences in the Atomic Positions			
			u_x	u_y	u_z	|u|
4d	(1/4,1/4,1/2)	Mn1	0.0000	0.0000	0.0000	0.0000
8f	(x,y,z)	F1	0.0000	0.0000	0.0000	0.0000
4e	(0,y,1/4)	F2	0.0000	0.0000	0.0000	0.0000

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

Evaluation of the similarity of the two descriptions

S	$d_{max.}$ (Å)
0.0000	0

- Lattice and atomic position criteria:
  - The degree of lattice distortion (**S**) is related to the spontaneous strain (it is the square root of the sum of the squared eigenvalues of the strain tensor divided by 3). For the given two structure descriptions, the **degree of lattice distortion (S)** is **0.0000**.
  - The parameter $\mathbf{d_{max.}}$ corresponds to the maximum difference between the atomic positions of the matching atoms. In this case, the maximum difference between the atomic positions of the matching atoms ($\mathbf{d_{max.}}$) is: **0.0000 Å**
- For the chosen description of Structure #2, the following additional descriptiors of the similarity have been calculated:

$d_{av.}$ (Å)	δ
0.0000	0.000

How many different descriptions of the same structure exist? (in the standard setting of its space group)

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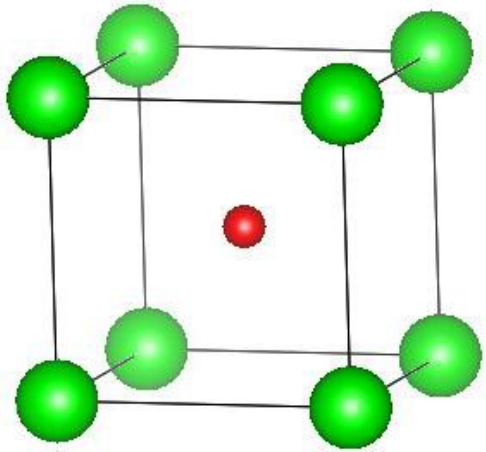
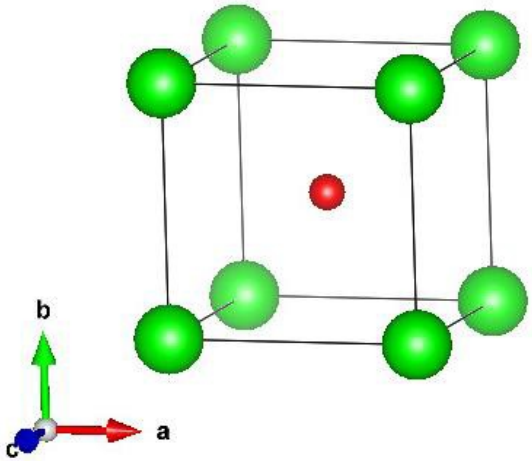
Example – CsCl

- space group Pm-3m (No. 221)

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



EQUIVSTRU – Output



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

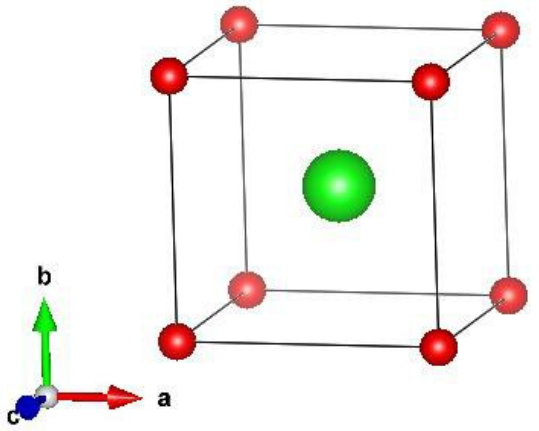
Normalizer coset representative: x,y,z

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)



- **Equivalent description 2**

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

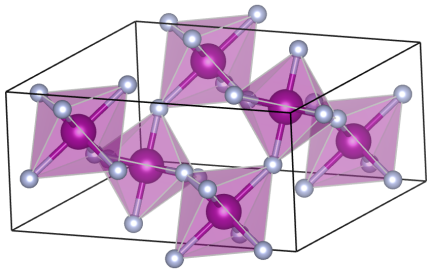
  Click here to get more information about the transformation: show hide

```
15
8.8928 5.0270 5.5017 90.00 125.35 90.00
3
Mn     1     -    0.250000 0.250000 0.000000
F      1     -    0.194300 0.962000 0.766500
F      2     -    -0.500000 0.136000 0.250000
```

  Note: You can save the CIF file and visualize it with an application as Jmol

  View Structure with Jmol

MnF_3



- **Equivalent description 3**

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

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

```
15
8.8928 5.0270 5.5017 90.00 125.35 90.00
3
Mn     1     -    0.750000 0.250000 -0.500000
F      1     -    0.694300 0.962000 0.266500
F      2     -    0.000000 0.136000 -0.250000
```

  Note: You can save the CIF file and visualize it with an application as Jmol

  View Structure with Jmol

- **Equivalent description 4**

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