# Summer School on Mathematical Crystallography

**3-7 June 2019, Nancy (France)**

**International Union of CrystallographyCommision on Mathematical and Theoretical Crystallography**

IUCr MaThCryst CRM² Cristallographie, Résonance Magnétique et Modélisations AFC C2MP métropole GrandNancy

# CRYSTAL-STRUCTURE DESCRIPTIONS

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# CRYSTAL-STRUCTURE TOOLS

## Crystal structure descriptions

Structure transformations

Equivalent structure descriptions

Comparison between different structure descriptions

# www.cryst.ehu.es

FCT/ZTF

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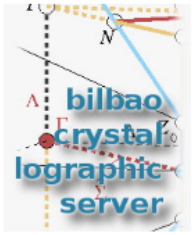


**Bilbao Crystallographic Server in forthcoming schools and workshops**

**News:**

- **New Article in Acta Cryst. A** 05/2019: Gallego *et al.* "Automatic calculation of symmetry-adapted tensors in magnetic and non-magnetic materials: a new tool of the Bilbao Crystallographic Server." *Acta Cryst.* (2019) **A75**, 438-447.
- **New Article in Nature** 03/2019: Vergniory *et al.* "A complete catalogue of high-quality topological materials" *Nature* (2019). **566**, 480-485.
- **Updated versions of TENSOR and MTENSOR** 03/2019: The programs give the general expression of tensor properties for a given point group and magnetic point group, respectively..

- Space-group symmetry
- Magnetic Symmetry and Applications
- Group-Subgroup Relations of Space Groups
- Representations and Applications
- Solid State Theory Applications
- Structure Utilities
- 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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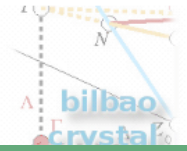



**Space-group symmetry**

**Magnetic Symmetry and Applications**

### 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<br>(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 |

complete catalogue of high-quality topological materials" *Nature* (2019). 566, 480-485.

- Updated versions of TENSOR and MTENSOR 03/2019: The programs give the general expression of tensor properties for a given point group and magnetic point group, respectively..

**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/nancy2019/

You need to download:

- CrystalStructureTools.txt

# STRUCTURE TRANSFORMATION

# Crystal structure descriptions

## What do we need to describe a crystal structure?

Space Group (*IT*A number)

Lattice parameters

Number of independent atoms in the asymmetric unit

Atom type and number

The Wyckoff position

The coordinates x, y, z

```
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**

# *ITA* settings structure descriptions

**Inorganic Crystal Structure Database**

**$CaPbO_3$**

CIF ▾ | Export | Bonds | Pattern | Structure | Jmol

| | |
|---|---|
| **Title** | Crystal structure and its role in electrical properties of the perovskite Ca Pb O3 synthesized at high pressure. |
| **Authors** | Yamamoto, A.;Khasanova, N.R.;Izumi, F.;Wu, X.-J.;Kamiyama, T.;Torii, S.;Tajima, S. |
| **Reference** | Chemistry of Materials (1999) **11**, 747-753<br>**Link XRef SCOPUS SCIRUS Google** |
| **Compound** | **Ca1 O3 Pb1** - Calcium plumbate **[ABX3] [oP20] [d c2 b] []** |
| **Cell** | 5.67102(4), 5.88752(4), 8.14954(6), 90., 90., 90.<br>**PBNM (62)** V=272.1 |
| **Remarks** | R=0.011000 : RVP NDP |

| Atom (site) | Oxid. | | x, y, z, B, Occupancy | | | | |
|---|---|---|---|---|---|---|---|
| Ca1 | (4c) | 2 | 0.9860(3) | 0.0563(2) | 0.25 | 0.84(3) | 1 |
| Pb1 | (4b) | 4 | 0.5 | 0 | 0 | 0.38(2) | 1 |
| O1 | (4c) | -2 | 0.1200(3) | 0.4452(2) | 0.25 | 0.67(3) | 1 |
| O2 | (8d) | -2 | 0.6907(2) | 0.3051(2) | 0.0613(2) | 0.96(2) | 1 |

→ **Non-standard setting**

$(a, b, c)_n = (a, b, c)_s P$

| ITA number | Setting | P | $P^{-1}$ |
|---|---|---|---|
| 62 | *P n m a* | a,b,c | a,b,c |
| 62 | *P m n b* | b,a,-c | b,a,-c |
| 62 | *P b n m* | c,a,b | b,c,a |
| 62 | *P c m n* | -c,b,a | c,b,-a |
| 62 | *P m c n* | b,c,a | c,a,b |
| 62 | *P n a m* | a,-c,b | a,c,-b |

**Initial setting structure description**

$X_f=(P,p)^{-1}X_i$

**Final setting structure description**

# *ITA* settings structure descriptions

**SETSTRU** http://www.cryst.ehu.es/cryst/setstru.html

## Transform a structure to an alternative setting

**$CaPbO_3$**

**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]

Datei auswählen Keine ausgewählt

**CIF file**

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

Structure

```
# Space ITA number
62
# Lattice parameters
5.67102 5.88752 8.14954 90. 90. 90.
# Number of independent atoms in the asymmetric unit
4
# [atom type] [number] [WP] [x] [y] [z]
Ca 1 4c 0.9860 0.0563 0.2500
Pb 1 4b 0.5000 0.0000 0.0000
O  1 4c 0.1200 0.4452 0.2500
O  2 8d 0.6907 0.3051 0.0613
```

**BCS format**

Transform Structure

[ Bilbao Crystallographic Server Main Menu ]

# *ITA* settings structure descriptions

## SETSTRU

**$CaPbO_3$**

### Choose the initial and final space groups symbols

The standard setting (default) of the space group 62 is *Pnma*

| Initial | Final | Setting | P | $P^{-1}$ |
|---|---|---|---|---|
| ◉ | ◉ | *P n m a* | a,b,c | a,b,c |
| ○ | ○ | *P m n b* | b,a,-c | b,a,-c |
| ◉ | ○ | *P b n m* | c,a,b | b,c,a |
| ○ | ○ | *P c m n* | -c,b,a | c,b,-a |
| ○ | ○ | *P m c n* | b,c,a | c,a,b |
| ○ | ○ | *P n a m* | a,-c,b | a,c,-b |

**Note:**

1. The listed transformation matrices **P** describe the transformation from standard to non-conventional setting:

$$(a, b, c)_n = (a, b, c)_s \, P$$

2. The non-zero elements of the transformation matrices **P** are listed by columns, *i.e.* **P = -a,-a-c, -b** means:

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

Transform

### Transformation to standard setting of space group 62

#### Initial structure

**Initial Setting:** *Pbnm* (62)

```
62
5.67102 5.88752 8.14954 90. 90. 90.
4
Ca      1       -       0.986000        0.056300        0.250000
Pb      1       -       0.500000        0.000000        0.000000
O       1       -       0.120000        0.445200        0.250000
O       2       -       0.690700        0.305100        0.061300
```

#### Final structure

**Final Setting:** *Pnma* (62)

```
62
5.8875 8.1495 5.6710 90.00 90.00 90.00
4
Ca      1       4c      0.056300        0.250000        0.986000
Pb      1       4b      0.000000        0.000000        0.500000
O       1       4c      0.445200        0.250000        0.120000
O       2       8d      0.305100        0.061300        0.690700
```

Visualize this structure | CIF File | Cartesian Coordinates

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

Matrix form:

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

# *ITA* settings structure descriptions

## SETSTRU

**$CaPbO_3$**

### Choose the initial and final space groups symbols

The standard setting (default) of the space group 62 is *Pnma*

| Initial | Final | Setting | P | $P^{-1}$ |
|---|---|---|---|---|
| ◉ | ◉ | *P n m a* | a,b,c | a,b,c |
| ○ | ○ | *P m n b* | b,a,-c | b,a,-c |
| ◉ | ○ | *P b n m* | c,a,b | b,c,a |
| ○ | ○ | *P c m n* | -c,b,a | c,b,-a |
| ○ | ○ | *P m c n* | b,c,a | c,a,b |
| ○ | ○ | *P n a m* | a,-c,b | a,c,-b |

**Note:**

1. The listed transformation matrices **P** describe the transformation from standard to non-conventional setting:

$$(a, b, c)_n = (a, b, c)_s \, P$$

2. The non-zero elements of the transformation matrices **P** are listed by columns, *i.e.* **P = -a,-a-c, -b** means:

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

Transform

### Atoms Data:

| AT. | WP | SS | Representative | Atomic orbit |
|---|---|---|---|---|
| Ca1 | 4c (x,1/4,z) | .m. | (0.056300,0.250000,0.986000) | (0.056300,0.250000,0.986000)<br>(0.443700,0.750000,0.486000)<br>(0.943700,0.750000,0.014000)<br>(0.556300,0.250000,0.514000) |
| Pb1 | 4b (0,0,1/2) | -1 | (0.000000,0.000000,0.500000) | (0.000000,0.000000,0.500000)<br>(0.500000,0.000000,0.000000)<br>(0.000000,0.500000,0.500000)<br>(0.500000,0.500000,0.000000) |
| O1 | 4c (x,1/4,z) | .m. | (0.445200,0.250000,0.120000) | (0.445200,0.250000,0.120000)<br>(0.054800,0.750000,0.620000)<br>(0.554800,0.750000,0.880000)<br>(0.945200,0.250000,0.380000) |
| O2 | 8d (x,y,z) | 1 | (0.305100,0.061300,0.690700) | (0.305100,0.061300,0.690700)<br>(0.194900,0.938700,0.190700)<br>(0.694900,0.561300,0.309300)<br>(0.805100,0.438700,0.809300)<br>(0.694900,0.938700,0.309300)<br>(0.805100,0.061300,0.809300)<br>(0.305100,0.438700,0.690700)<br>(0.194900,0.561300,0.190700) |

# Exercise 3.1


Compare the two structure descriptions and check if they belong to the same structure type

**$ZrSiO_4$**

Print **2** entries selected.

CC=Collection Code: [AB2X4]=ANX Form: [cF56]=Pearson: [e d a]=Wyckoff Symbol: [Al2MgO4]=Structure Type:

******Click the ANX, Pearson or Wyckoff Symbol to find structures with that symbol***.***

CC=45520 — Details | Bonds | Pattern | Structure | Jmol

| | |
|---|---|
| **Title** | Redetermination of the oxygen parameters in zircon (Zr Si O4). |
| **Authors** | Krstanovic, I.R. |
| **Reference** | Acta Crystallographica (1958) **11**, 896-897<br>**Link XRef SCOPUS SCIRUS Google** |
| **Compound** | **Zr (Si O4)** - **[Zircon]** Zirconium silicate **[ABX4]** **[tI24]** **[h b a]** **[ZrSiO4]** |
| **Cell** | 6.6164(5), 6.6164, 6.0150(5), 90., 90., 90.<br>**I41/AMDZ (141)** V=263.32 |
| **Remarks** | R=0.070000 : PDC =01-073-6646 : PDF =6-266 : TYP =ZrSiO4 : XDS MIN =Zircon :<br>At least one temperature factor missing in the paper.<br>hk0- and 0kl-data, crystals not metamict |

| Atom (site) | Oxid. | | x, y, z, B, Occupancy | | | | |
|---|---|---|---|---|---|---|---|
| Zr1 | (4a) | 4 | 0 | 0.75 | 0.125 | 0 | 1 |
| Si1 | (4b) | 4 | 0 | 0.75 | 0.625 | 0 | 1 |
| O1 | (16h) | -2 | 0 | 0.067(3) | 0.198(3) | 0 | 1 |

Origin choice 2

CC=31101 — Details | Bonds | Pattern | Structure | Jmol

| | |
|---|---|
| **Title** | Die Kristallstruktur von Zirkon und die Kriterien fuer spezielle Lagen in tetragonalen Raumgruppen.. |
| **Authors** | Wyckoff, R.W.G.;Hendricks, S.B. |
| **Reference** | Zeitschrift fuer Kristallographie, Kristallgeometrie, Kristallphysik, Kristallchemie (1927) **66**, 73-102<br>**Link XRef SCOPUS SCIRUS Google**<br>**Also:** Philosophical Magazine, Serie (1926) **1**, 1151-1151 |
| **Compound** | **Zr (Si O4)** - **[Zircon]** Zirconium silicate **[ABX4]** **[tI24]** **[h b a]** **[ZrSiO4]** |
| **Cell** | 6.61, 6.61, 5.98, 90., 90., 90.<br>**I41/AMDS (141)** V=261.28 |
| **Remarks** | COR MIN =Zircon : PDF =6-266 : TYP =ZrSiO4 : XDS<br>At least one temperature factor missing in the paper.<br>No R value given in the paper.<br>Revised data of 31084 |

| Atom (site) | Oxid. | | x, y, z, B, Occupancy | | | | |
|---|---|---|---|---|---|---|---|
| Zr1 | (4a) | 4 | 0 | 0 | 0 | 0 | 1 |
| Si1 | (4b) | 4 | 0 | 0 | 0.5 | 0 | 1 |
| O1 | (16h) | -2 | 0 | 0.2(1) | 0.34(2) | 0 | 1 |

Origin choice 1

# Exercise 3.1


**Structure 1**

Space group *I4$_1$/amd* (No. 141)
a=6.600 Å  c=5.88 Å  Origin choice 1 at *-4m2*

**Structure 2**

Space group *I4$_1$/amd* (No. 141)
a=6.616 Å  c=6.015 Å  Origin choice 2 at *2/m*

Compare the two structure descriptions and check if they belong to the same structure type

Use the tool of Bilbao Crystallographic Server: **SETSTRU**

**Hint:** In order to compare the different data, the parameters of Structure 1 are to be transformed to 'origin at center 2/m', *i.e.* ORIGIN CHOICE 2

# Structure transformation

**TRANSTRU** http://www.cryst.ehu.es/cryst/transtru.html

Transform Structure

$Pb_3(VO_4)_2$

**Transform Structure**

TRANSTRU can transform a structure in two ways:

- To a lower symmetry space group. The transformed structure is given in the low symmetry space group basis, taking care of all possible splittings of the Wyckoff positions.
- With an arbitrary matrix. The structure, including the cell parameters and the atoms in the unit cell, is transformed with an arbitrary matrix introduced by the user.

Only the default choice for the conventional setting of the space groups is used.

Structure Data
[in CIF format]

Datei auswählen Keine ausgewählt

**CIF file**

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

```
166
5.6739 5.6739 20.3412 90. 90. 120.
6
Pb 1 3a  0.0000 0.0000 0.0000
Pb 2 6c  0.0000 0.0000 0.2073
PV 1 6c  0.0000 0.0000 0.3924
O  1 6c  0.0000 0.0000 0.3247
O  2 18h 0.8433 0.1567 0.4299
```

High Symmetry Structure

**BCS format**

Transform structure to a subgroup basis

Transform structure with an arbitrary matrix

Show

**subgroup basis**

**arbitrary transformation**

# Structure transformation

**Description R-3m (No. 166)**

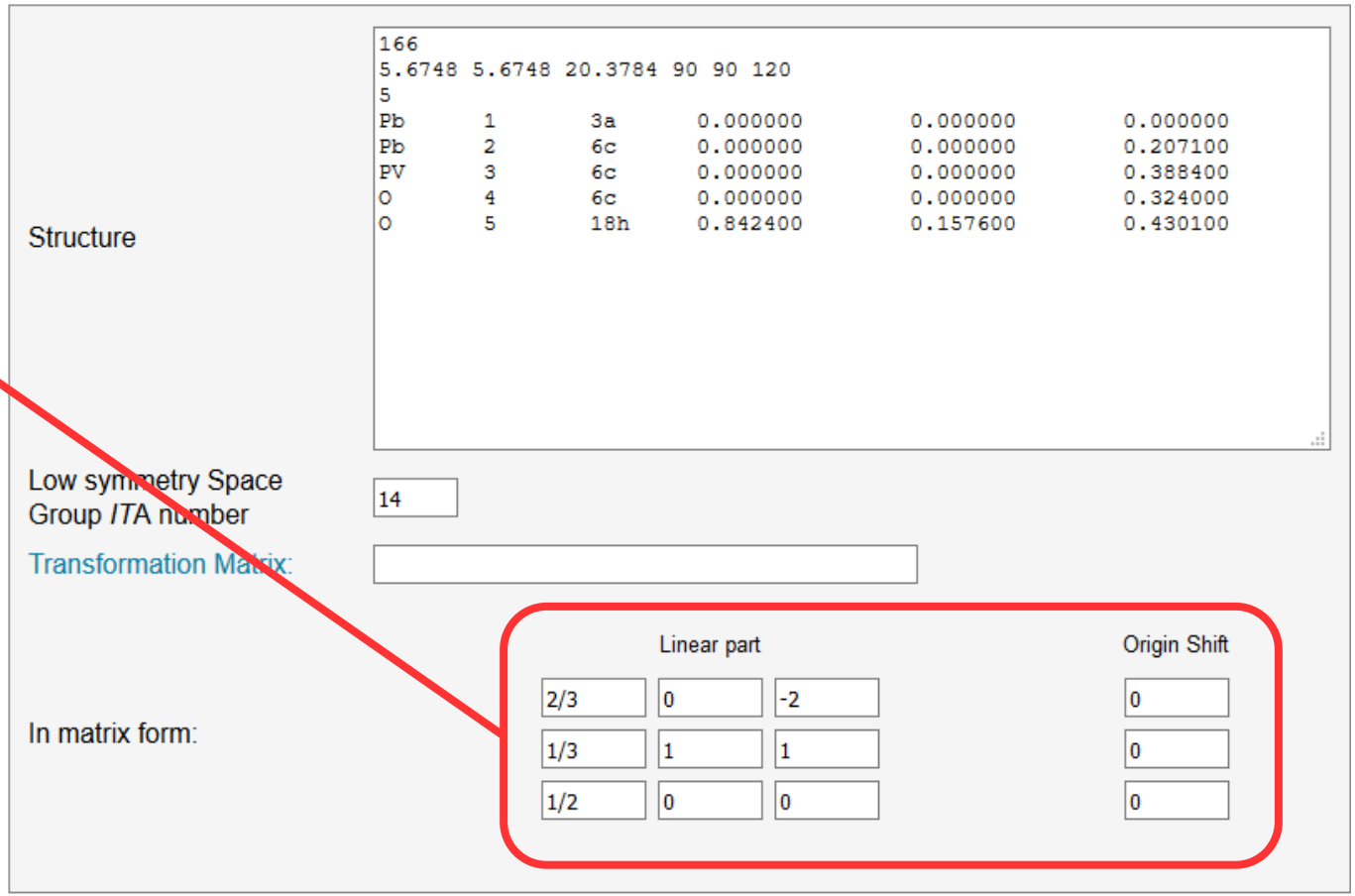
**(P,p)**

**Description $P2_1/c$ (No. 14)**

**Validity (P,p)**

**WP splitting**

**$Pb_3(VO_4)_2$**

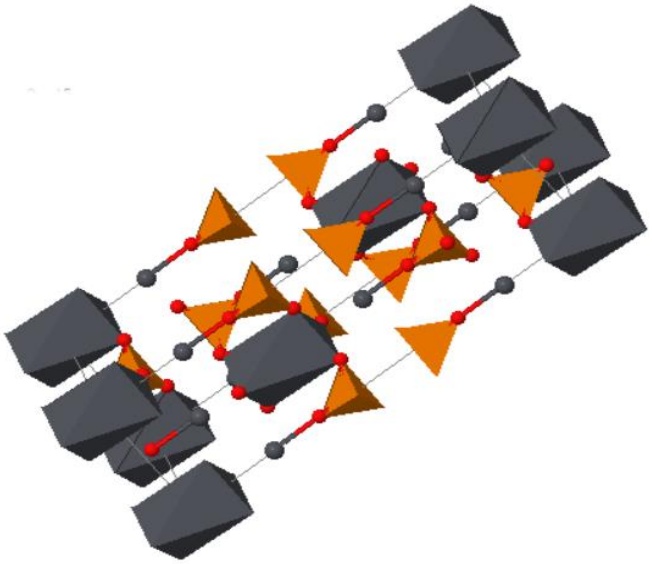


# Structure transformation

## High symmetry structure

166
5.6739 5.6739 20.3412 90. 90. 120.
5

| | | | | | |
|---|---|---|---|---|---|
| Pb | 1 | 3a | 0.000000 | 0.000000 | 0.000000 |
| Pb | 2 | 6c | 0.000000 | 0.000000 | 0.207300 |
| PV | 1 | 6c | 0.000000 | 0.000000 | 0.392400 |
| O | 1 | 6c | 0.000000 | 0.000000 | 0.324700 |
| O | 2 | 18h | 0.843300 | 0.156700 | 0.429900 |

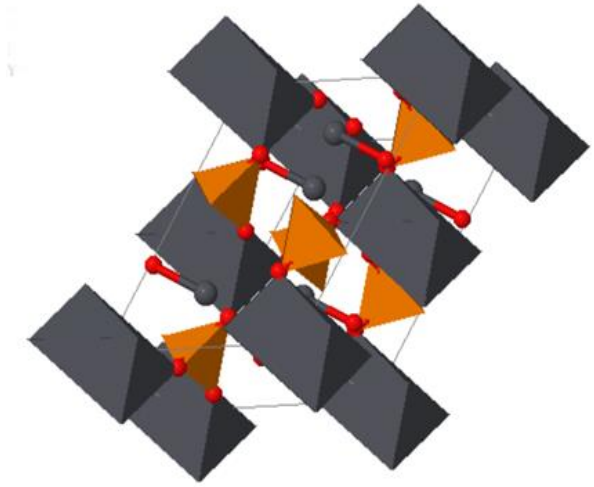


**(P,p)=**2/3**a**+1/3**b**+1/3**c**,**b**,-2**a**-**b**

## Low symmetry structure

014
7.530264 5.673900 9.827483 90.000000 115.786674 90.000000
7

| | | | | | |
|---|---|---|---|---|---|
| Pb | 1 | 2a | 0.000000 | 0.000000 | 0.000000 |
| Pb | 2 | 4e | 0.621900 | 0.000000 | 0.207300 |
| PV | 1 | 4e | 0.177200 | 0.000000 | 0.392400 |
| O | 1 | 4e | 0.974100 | 0.000000 | 0.324700 |
| O | 2 | 4e | 0.289700 | 0.735050 | 0.008250 |
| O | 2_2 | 4e | 0.289700 | 0.500000 | 0.773200 |
| O | 2_3 | 4e | 0.710300 | 0.764950 | 0.491750 |



# Exercise 3.1 (cont.)


Apply the program **TRANSTRU** in order to check if the two structure descriptions belong to the same structure type

**Structure 1**

Space group $I4_1/amd$ (No. 141)
a=6.600 Å  c=5.88 Å  Origin choice 1 at *-4m2*

**Structure 2**

Space group $I4_1/amd$ (No. 141)
a=6.616 Å  c=6.015 Å  Origin choice 2 at *2/m*

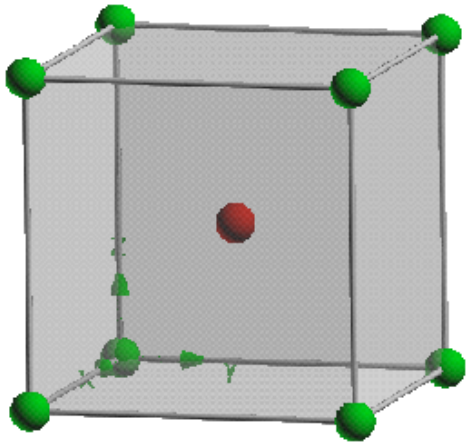
**Coordinate transformation**

Origin choice 2 ⟶ Origin choice 1

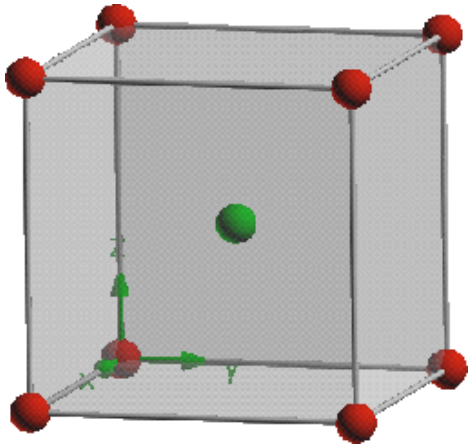
***p***=0,1/4,-1/8

# EQUIVALENT STRUCTURE DESCRIPTIONS

# Equivalent structures descriptions



CsCl
Pm-3m (No. 221)



1a (0,0,0)
1b (1/2,1/2,1/2)

1b (1/2,1/2,1/2)
1a (0,0,0)

How to find all possible equivalent descriptions of a crystal structure?

Number of equivalent descriptions = |N(G)|/|G|

Index of the group in its Euclidean normalizer

# Equivalent structures descriptions

**EQUIVSTRU** http://www.cryst.ehu.es/cryst/equivstru.html

## Equivalent Descriptions of Crystal Structures

**CsCl**

**Equivalent Structures**

Given a space group ITA number, the cell parameters (separated with spaces) and the atom positions, the program EQUIVSTRU transforms the corresponding structure with the elements of the euclidean normalizer of the space group. All the transformed structures are equivalent symmetry descriptions of the given initial structure. The atom positions are identified generating the Wyckoff sets.

Only the default choice for the conventional setting of

Structure Data [in CIF format] Examinar... No se ha seleccionado ningún archivo.

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

**CIF file**

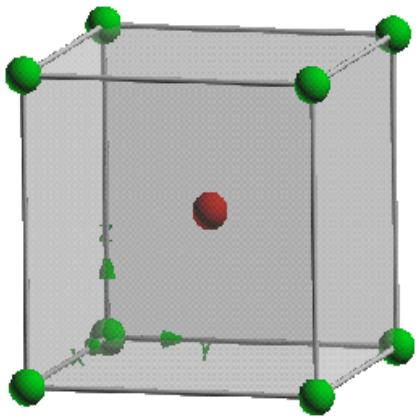
Structure

```
#Exercise 2.4.2a(CsCl)
# Space Group ITA number
221
# Lattice parameters
4.12599 4.12599 4.12599 90.0 90.0 90.0
# Number of independent atoms in the asymmetric unit
2
# [atom type] [number] [WP] [x] [y] [z]
Cl    1   1a    0.000000 0.000000 0.000000
Cs    1   1b    0.500000 0.500000 0.500000
```

**BCS format**

Show

# Equivalent structures descriptions



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

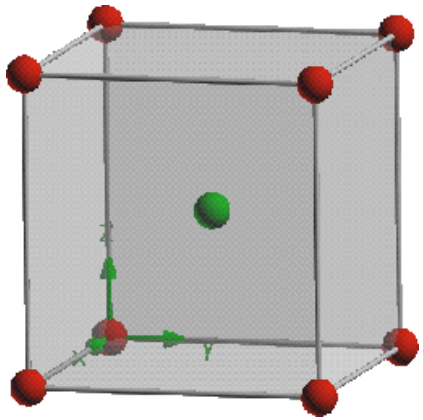
**Normalizer coset representative: x,y,z**

| 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 3.2(b)

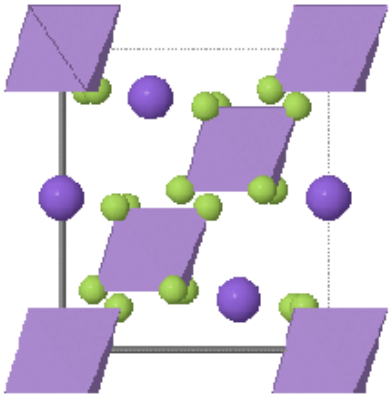
How many equivalent sets of coordinates can be used to describe the structure $P(C_6C_5)_4[MoNCl_4]$? What are their coordinates?

| Atom | Wyckoff position | Coordinate triplets $x$ | $y$ | $z$ |
|---|---|---|---|---|
| P | $2b$ | 0.25 | 0.75 | 0 |
| Mo | $2c$ | 0.25 | 0.25 | 0.121 |
| N | $2c$ | 0.25 | 0.25 | −0.093 |
| C1 | $8g$ | 0.362 | 0.760 | 0.141 |
| C2 | $8g$ | 0.437 | 0.836 | 0.117 |
| Cl | $8g$ | 0.400 | 0.347 | 0.191 |

# Exercise 3.3

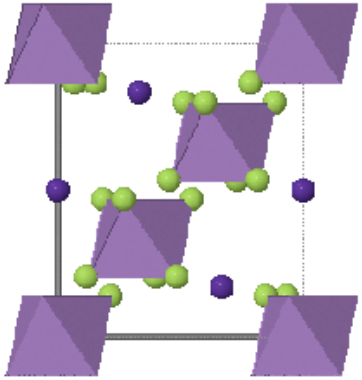

Do the following three structures belong to the same structure type?
Try to find analogous coordinate descriptions for all three crystal structures

$KAsF_6$



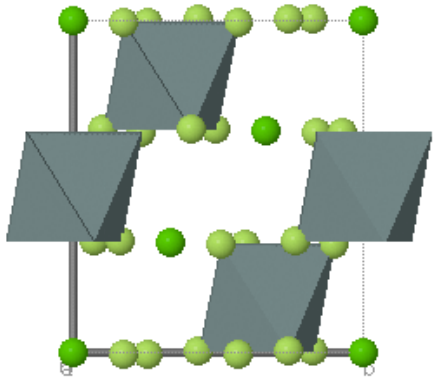
148
7.3480 7.3480 7.2740 90.00 90.00 120.00
3
K 1 3b 0.333333 0.666666 0.166666
As 1 3a 0 0 0
F 1 18f 0.1292 0.2165 0.1381

$BaIrF_6$



148
7.3965 7.3965 7.2826 90.00 90.00 120.00
3
Ba 1 3b 0.333333 0.666666 0.166666
Ir 1 3a 0 0 0
F 1 18f 0.0729 0.2325 0.1640

$BaSnF_6$



148
7.4279 7.4279 7.4180 90.00 90.00 120.00
3
Ba 1 3a 0 0 0
Sn 1 3b 0 0 0.5
F 1 18f 0.2586 0.8262 0.0047

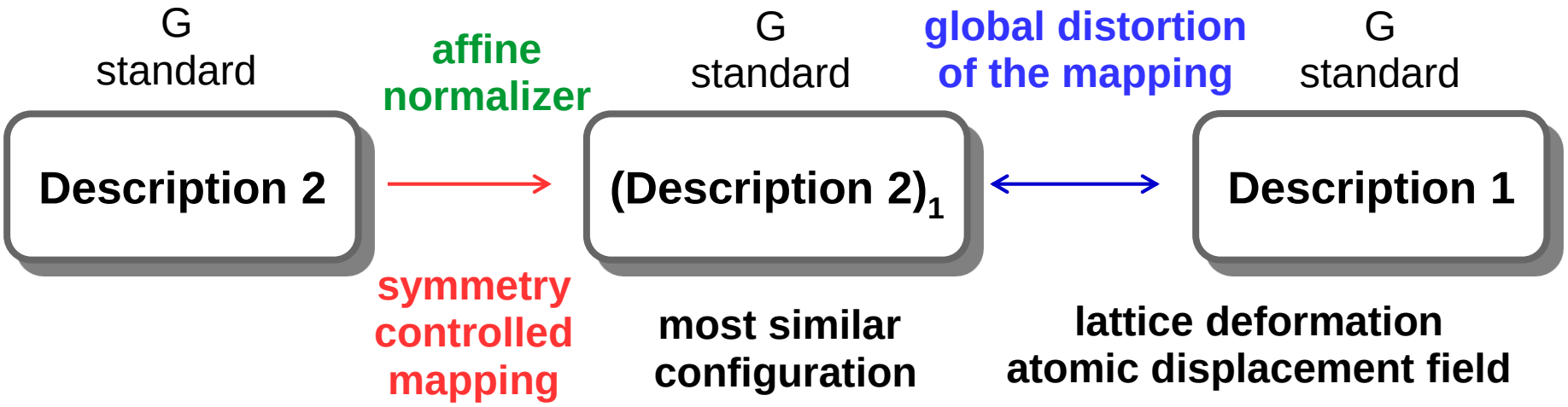
R-3 (No. 148) ➡ 4 equivalent descriptions: x,y,z; x,y,z+1/2; y,x,-z; y,x,-z+1/2

# COMPARISON OF STRUCTURES

# Comparison of structures

The program measures **the similarity between two structures** with the same or different compositions:

- same space-group (or space groups that form an enantiomorphic pair)
- same sequence of the occupied Wyckoff positions
- the same total number of atoms in the unit cells



# Comparison of structures

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

**degree of lattice distortion**

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

$\eta_i$-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

# Comparison of structures

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

**structural descriptor**

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

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

weighted mean difference between atomic coordinates

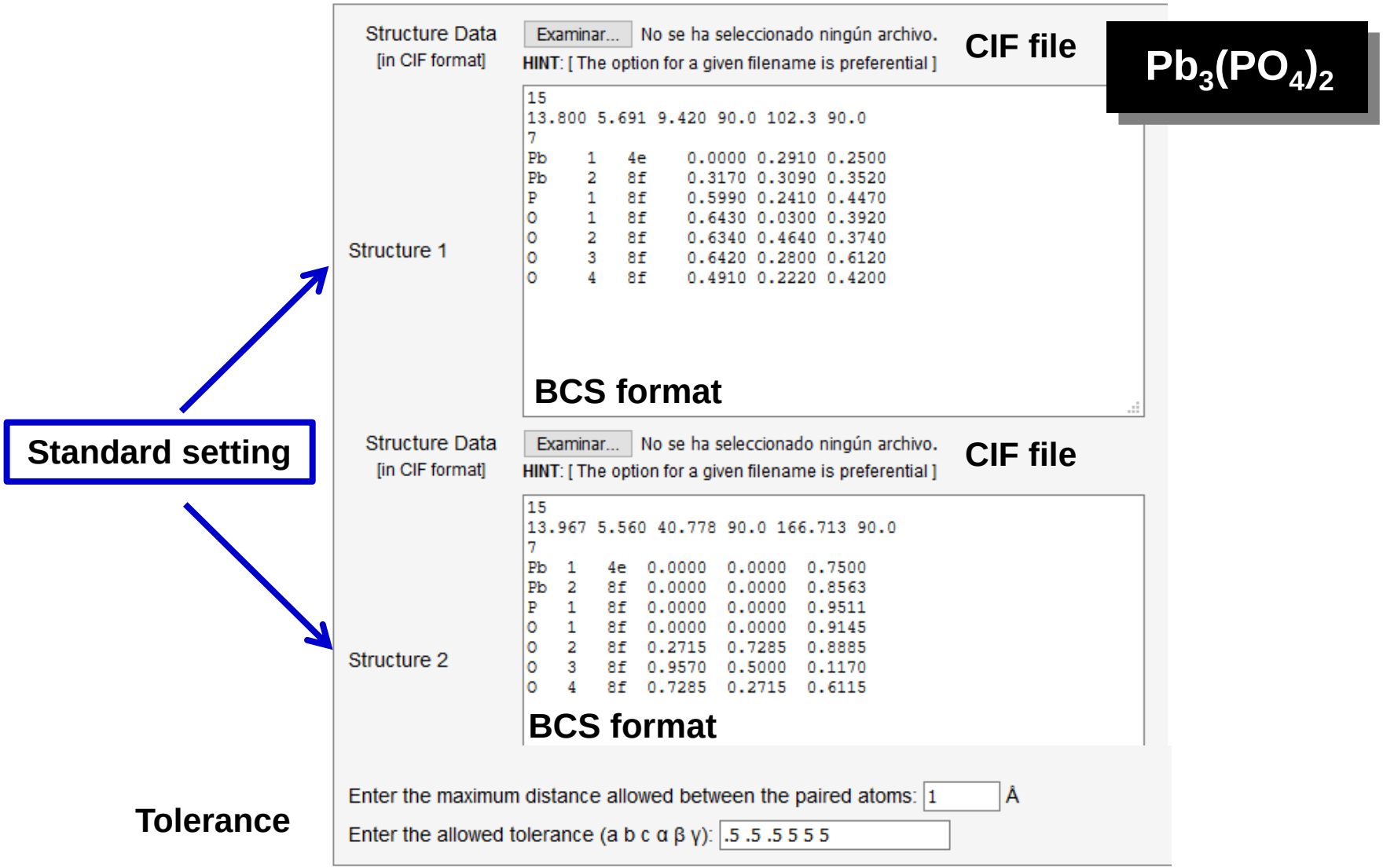
$$\Delta(d) = \frac{[(b_1/a_1)(c_1/a_1)]}{[(b_2/a_2)(c_2/a_2)]}$$

relation between axial ratios

Bergerhoff *et al*. *Acta Cryst*.(1999), **B**55, 147

# Comparison of structures

**COMPSTRU** http://www.cryst.ehu.es/cryst/compstru.html



# Comparison of structures

$Pb_3(PO_4)_2$

### 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
```

**(P, p): -a,-b,3a+c ; 1/4,1/4,0**

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

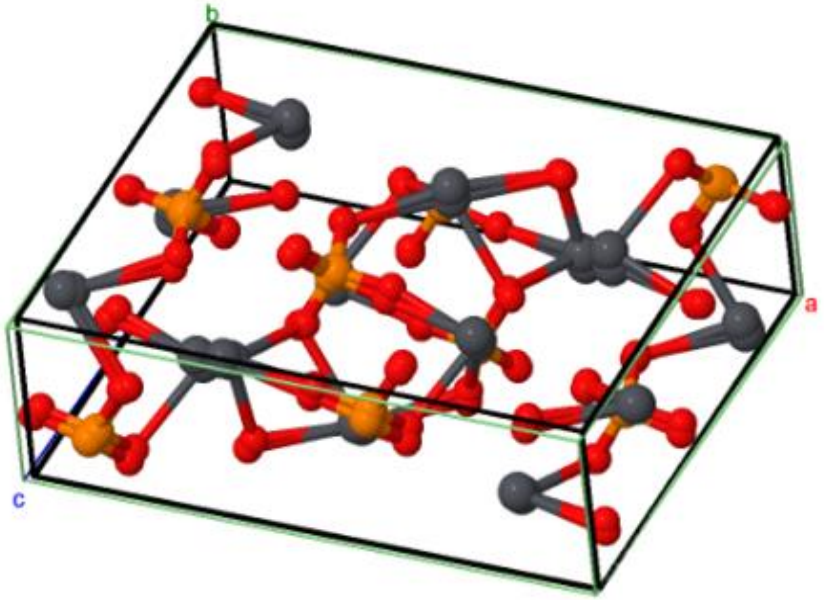
```
015
13.967000 5.560000 9.630055 90.000000 103.295059 90.000000
7
Pb      1       4e      0.500000        0.250000        0.750000
Pb      2       8f      0.818900        0.250000        0.856300
P       1       8f      0.103300        0.250000        0.951100
O       1       8f      0.993500        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
```

# Comparison of structures

## Visualization of the comparison

$Pb_3(PO_4)_2$

-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

NEW

# Exercise 3.4


In ICSD can be found several structure data sets of ε-$Fe_2O_3$, all of them of symmetry $Pna2_1$(No.33). Compare the following two descriptions and check if they belong to the same structure type.

**ICSD for WWW**

**Details of the selected entries**

Print **2** entries selected.

CC=Collection Code: [AB2X4]=ANX Form: [cF56]=Pearson: [e d a]=Wyckoff Symbol: [Al2MgO4]=Structure Type:

******Click the ANX, Pearson or Wyckoff Symbol to find structures with that symbol***.***

| CC=173024 | Details · Bonds · Pattern · Structure · Jmol |
|---|---|
| **Title** | High- and low-temperature crystal and magnetic structure of epsilon-Fe2 O3 and their correlation to its magnetic properties. |
| **Authors** | Gich, M.;Frontera, C.;Roig, A.;Taboada, E.;Molins, E.;Rechenberg, H.R.;Ardisson, J.D.;Macedo, W.A.A.;Ritter, C.;Hardy, V.;Sort, J.;Skumryev, V.;Nogues, J. |
| **Reference** | Chemistry of Materials (2007) **18**, 3889-3897<br>**Link XRef SCOPUS SCIRUS Google** |
| **Compound** | **Fe2 O3** - Iron(III) oxide - epsilon **[A2X3] [oP40] [a10] [AlFeO3]** |
| **Cell** | 5.0885(5), 8.7802(14), 9.4709(13), 90., 90., 90.<br>**PNA21 (33)** V=423.14 |
| **Remarks** | R=0.013300 : NDP RVP SNP TEM =200 : TYP =AlFeO3 : XDP MAG<br>At least one temperature factor missing in the paper. |

| Atom (site) | | Oxid. | x, y, z, B, Occupancy | | | | |
|---|---|---|---|---|---|---|---|
| O1 | (4a) | -2 | 0.978(2) | 0.3282(15) | 0.4314(11) | 0 | 1 |
| O2 | (4a) | -2 | 0.515(2) | 0.4907(17) | 0.4187(16) | 0 | 1 |
| O3 | (4a) | -2 | 0.650(3) | 0.9979(13) | 0.1883(9) | 0 | 1 |
| O4 | (4a) | -2 | 0.160(3) | 0.1537(15) | 0.1956(7) | 0 | 1 |
| O5 | (4a) | -2 | 0.841(3) | 0.1580(15) | 0.6669(7) | 0 | 1 |
| O6 | (4a) | -2 | 0.527(2) | 0.1637(19) | 0.9362(9) | 0 | 1 |
| Fe1 | (4a) | 3 | 0.1928(11) | 0.1505(6) | 0.5807(3) | 0 | 1 |
| Fe2 | (4a) | 3 | 0.6826(6) | 0.0291(3) | 0.7897(5) | 0 | 1 |
| Fe3 | (4a) | 3 | 0.1858(10) | 0.1519(6) | 0 | 0 | 1 |
| Fe4 | (4a) | 3 | 0.8104(7) | 0.1580(4) | 0.3071(3) | 0 | 1 |

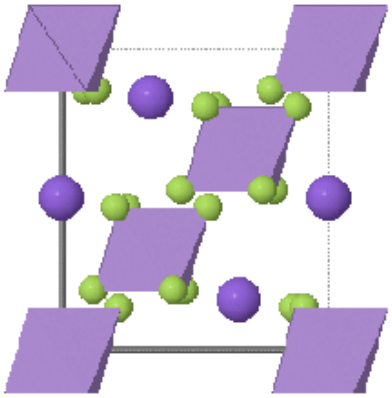
| CC=415250 | Details · Bonds · Pattern · Structure · Jmol |
|---|---|
| **Title** | Synthesis and structural analysis of epsilon-(Fe2 O3). |
| **Authors** | Kelm, K.;Mader, W. |
| **Reference** | Zeitschrift fuer Anorganische und Allgemeine Chemie (2005) **631**, 2363-2369<br>**Link XRef SCOPUS SCIRUS Google** |
| **Compound** | **Fe2 O3** - Diiron(III) oxide - epsilon **[A2X3] [oP40] [a10] [AlFeO3]** |
| **Cell** | 5.0715(2), 8.7359(4), 9.4178(4), 90, 90, 90<br>**PNA21 (33)** V=417.24 |
| **Remarks** | R=0.039000 : TYP =AlFeO3 : XDP RVP |

| Atom (site) | | Oxid. | x, y, z, B, Occupancy | | | | |
|---|---|---|---|---|---|---|---|
| Fe1 | (4a) | 3 | 0.6768(9) | 0.8427(5) | 0.0000000 | 0.050(2) | 1.0000000 |
| Fe2 | (4a) | 3 | 0.204(1) | 0.3509(8) | 0.7726(9) | 0.063(3) | 1.0000000 |
| Fe3 | (4a) | 3 | 0.807(1) | 0.6605(8) | 0.693(1) | 0.069(2) | 1.0000000 |
| Fe4 | (4a) | 3 | 0.6852(9) | 0.4634(5) | 0.983(2) | 0.046(1) | 1.0000000 |
| O1 | (4a) | -2 | 0.337(2) | 0.853(2) | 0.887(1) | 0.0063326 | 1.0000000 |
| O2 | (4a) | -2 | 0.019(3) | 0.474(2) | 0.610(2) | 0.0063326 | 1.0000000 |
| O3 | (4a) | -2 | 0.453(3) | 0.677(2) | 0.651(2) | 0.0063326 | 1.0000000 |
| O4 | (4a) | -2 | 0.527(3) | 0.669(2) | 0.100(1) | 0.0063326 | 1.0000000 |
| O5 | (4a) | -2 | 0.668(3) | 0.334(2) | 0.863(1) | 0.0063326 | 1.0000000 |
| O6 | (4a) | -2 | 0.336(3) | 0.513(1) | 0.891(1) | 0.0063326 | 1.0000000 |

# Exercise 3.3 (cont)

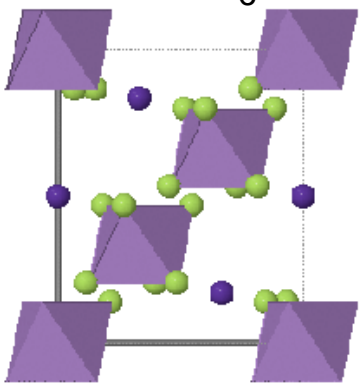

Do these compounds belong to the **same structure type** ?

$KAsF_6$



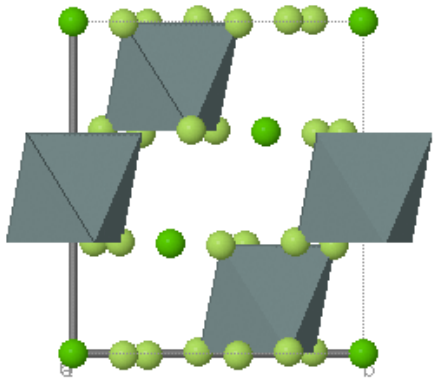
```
148
7.3480 7.3480 7.2740 90.00 90.00 120.00
3
K     1   3b    0.333333 0.666666 0.166666
As    1   3a    0 0 0
F     1   18f   0.1292 0.2165 0.1381
```

$BaIrF_6$



```
148
7.3965 7.3965 7.2826 90.00 90.00 120.00
3
Ba    1   3b    0.333333 0.666666 0.166666
Ir    1   3a    0 0 0
F     1   18f   0.0729 0.2325 0.1640
```

$BaSnF_6$



```
148
7.4279 7.4279 7.4180 90.00 90.00 120.00
3
Sn    1   3b    0 0 0.5
Ba    1   3a    0 0 0
F     1   18f   0.2586 0.8262 0.0047
```

Koch, Fischer. *MathCryst Satell.*, ECM22, Budapest 2004

# Comparison of structures

## STUDY OF THE FAMILY **$ABX_3$**

### R-3 (148);WP sequence: fc2; Pearson: hR10

| | AA1 | AA2 | AA3 | AA4 | AA5 | AA6 | AA7 | AA8 | AA9 | AB1 | AB2 | AB3 | AB4 | AB5 | AB6 | AB7 | AC1 | AC2 | AC3 | AD1 | AD2 | AE1 | AE2 | B1 | C1 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| AA1 | 0 | 0,0 | 0,1 | 0,1 | 0,1 | 0,1 | 0,1 | 0,1 | 0,2 | 0,1 | 0,1 | 0,2 | 0,0 | 0,2 | 0,3 | 0,1 | 0,2 | 0,2 | 0,2 | 0,2 | 0,2 | 1,3 | 1,2 | 0,5 | 0,7 |
| AA2 | 0,0 | 0 | 0,1 | 0,1 | 0,1 | 0,1 | 0,1 | 0,1 | 0,2 | 0,1 | 0,1 | 0,2 | 0,0 | 0,2 | 0,3 | 0,1 | 0,2 | 0,2 | 0,2 | 0,2 | 0,2 | 1,3 | 1,2 | 0,5 | 0,7 |
| AA3 | 0,1 | 0,1 | 0 | 0,2 | 0,2 | 0,2 | 0,1 | 0,1 | 0,3 | 0,0 | 0,1 | 0,1 | 0,1 | 0,1 | 0,1 | 0,1 | 0,1 | 0,1 | 0,1 | 0,1 | 0,1 | 1,4 | 1,3 | 0,4 | 0,7 |
| AA4 | 0,1 | 0,1 | 0,2 | 0 | 0,1 | 0,0 | 0,1 | 0,1 | 0,2 | 0,1 | 0,2 | 0,2 | 0,1 | 0,3 | 0,2 | 0,2 | 0,2 | 0,2 | 0,3 | 0,2 | 0,3 | 1,3 | 1,2 | 0,4 | 0,7 |
| AA5 | 0,1 | 0,1 | 0,2 | 0,1 | 0 | 0,1 | 0,1 | 0,2 | 0,2 | 0,1 | 0,1 | 0,2 | 0,1 | 0,2 | 0,3 | 0,1 | 0,2 | 0,2 | 0,2 | 0,2 | 0,2 | 1,2 | 1,2 | 0,5 | 0,7 |
| AA6 | 0,1 | 0,1 | 0,2 | 0,0 | 0,1 | 0 | 0,1 | 0,2 | 0,2 | 0,1 | 0,2 | 0,2 | 0,1 | 0,3 | 0,2 | 0,2 | 0,2 | 0,2 | 0,3 | 0,2 | 0,3 | 1,2 | 1,2 | 0,4 | 0,8 |
| AA7 | 0,1 | 0,1 | 0,1 | 0,1 | 0,1 | 0,1 | 0 | 0,1 | 0,3 | 0,1 | 0,2 | 0,2 | 0,1 | 0,2 | 0,2 | 0,2 | 0,2 | 0,2 | 0,3 | 0,2 | 0,3 | 1,3 | 1,3 | 0,4 | 0,7 |
| AA8 | 0,1 | 0,1 | 0,1 | 0,1 | 0,2 | 0,2 | 0,1 | 0 | 0,3 | 0,1 | 0,1 | 0,1 | 0,1 | 0,2 | 0,2 | 0,1 | 0,1 | 0,1 | 0,2 | 0,2 | 0,2 | 1,4 | 1,3 | 0,4 | 0,7 |
| AA9 | 0,2 | 0,2 | 0,3 | 0,2 | 0,2 | 0,2 | 0,3 | 0,3 | 0 | 0,3 | 0,3 | 0,4 | 0,2 | 0,4 | 0,3 | 0,3 | 0,3 | 0,3 | 0,4 | 0,3 | 0,4 | 1,5 | 1,4 | 0,6 | 0,7 |
| AB1 | 0,1 | 0,1 | 0,0 | 0,1 | 0,1 | 0,1 | 0,1 | 0,1 | 0,3 | 0 | 0,1 | 0,1 | 0,1 | 0,1 | 0,1 | 0,1 | 0,1 | 0,1 | 0,2 | 0,1 | 0,2 | 2,0 | 1,9 | 0,5 | 0,7 |
| AB2 | 0,1 | 0,1 | 0,1 | 0,2 | 0,1 | 0,2 | 0,2 | 0,1 | 0,3 | 0,1 | 0 | 0,1 | 0,1 | 0,1 | 0,2 | 0,0 | 0,1 | 0,1 | 0,2 | 0,2 | 0,2 | 1,3 | 1,3 | 0,5 | 0,7 |
| AB3 | 0,2 | 0,2 | 0,1 | 0,2 | 0,2 | 0,2 | 0,2 | 0,1 | 0,4 | 0,1 | 0,1 | 0 | 0,2 | 0,1 | 0,2 | 0,2 | 0,0 | 0,1 | 0,1 | 0,1 | 0,1 | 1,4 | 1,3 | 0,5 | 0,7 |
| AB4 | 0,0 | 0,0 | 0,1 | 0,1 | 0,1 | 0,1 | 0,1 | 0,1 | 0,2 | 0,1 | 0,1 | 0,2 | 0 | 0,2 | 0,2 | 0,0 | 0,1 | 0,2 | 0,2 | 0,2 | 0,2 | 1,3 | 1,2 | 0,5 | 0,7 |
| AB5 | 0,2 | 0,2 | 0,1 | 0,3 | 0,2 | 0,3 | 0,2 | 0,2 | 0,4 | 0,1 | 0,1 | 0,1 | 0,2 | 0 | 0,2 | 0,1 | 0,1 | 0,1 | 0,1 | 0,1 | 0,1 | 1,5 | 1,5 | 0,4 | 0,7 |
| AB6 | 0,3 | 0,3 | 0,1 | 0,2 | 0,3 | 0,2 | 0,2 | 0,2 | 0,3 | 0,1 | 0,2 | 0,2 | 0,2 | 0,2 | 0 | 0,3 | 0,2 | 0,1 | 0,2 | 0,1 | 0,2 | 1,9 | 1,8 | 0,5 | 0,7 |
| AB7 | 0,1 | 0,1 | 0,1 | 0,2 | 0,1 | 0,2 | 0,2 | 0,1 | 0,3 | 0,1 | 0,0 | 0,2 | 0,0 | 0,1 | 0,3 | 0 | 0,2 | 0,2 | 0,2 | 0,2 | 0,2 | 1,3 | 1,2 | 0,4 | 0,7 |
| AC1 | 0,2 | 0,2 | 0,1 | 0,2 | 0,2 | 0,2 | 0,2 | 0,1 | 0,3 | 0,1 | 0,1 | 0,0 | 0,1 | 0,1 | 0,2 | 0,2 | 0 | 0,1 | 0,1 | 0,1 | 0,1 | 1,5 | 1,9 | 0,4 | 0,7 |
| AC2 | 0,2 | 0,2 | 0,1 | 0,2 | 0,2 | 0,2 | 0,2 | 0,1 | 0,3 | 0,1 | 0,1 | 0,1 | 0,2 | 0,1 | 0,1 | 0,2 | 0,1 | 0 | 0,1 | 0,1 | 0,1 | 1,4 | 1,3 | 0,3 | 0,7 |
| AC3 | 0,2 | 0,2 | 0,1 | 0,3 | 0,2 | 0,3 | 0,3 | 0,2 | 0,4 | 0,2 | 0,2 | 0,1 | 0,2 | 0,1 | 0,2 | 0,2 | 0,1 | 0,1 | 0 | 0,1 | 0,1 | 1,6 | 1,5 | 0,4 | 0,7 |
| AD1 | 0,2 | 0,2 | 0,1 | 0,2 | 0,2 | 0,2 | 0,2 | 0,2 | 0,3 | 0,1 | 0,2 | 0,1 | 0,2 | 0,1 | 0,1 | 0,2 | 0,1 | 0,1 | 0,1 | 0 | 0,1 | 2,2 | 2,0 | 0,4 | 0,7 |
| AD2 | 0,2 | 0,2 | 0,1 | 0,3 | 0,2 | 0,3 | 0,3 | 0,2 | 0,4 | 0,2 | 0,2 | 0,1 | 0,2 | 0,1 | 0,2 | 0,2 | 0,1 | 0,1 | 0,1 | 0,1 | 0 | 2,2 | 2,0 | 0,4 | 0,7 |
| AE1 | 1,3 | 1,3 | 1,4 | 1,3 | 1,2 | 1,2 | 1,3 | 1,4 | 1,5 | 2,0 | 1,3 | 1,4 | 1,3 | 1,5 | 1,9 | 1,3 | 1,5 | 1,4 | 1,6 | 2,2 | 2,2 | 0 | 0,1 | 1,9 | 1,3 |
| AE2 | 1,2 | 1,2 | 1,3 | 1,2 | 1,2 | 1,2 | 1,3 | 1,3 | 1,4 | 1,9 | 1,3 | 1,3 | 1,2 | 1,5 | 1,8 | 1,2 | 1,9 | 1,3 | 1,5 | 2,0 | 2,0 | 0,1 | 0 | 1,8 | 1,2 |
| B1 | 0,5 | 0,5 | 0,4 | 0,4 | 0,5 | 0,4 | 0,4 | 0,4 | 0,6 | 0,5 | 0,5 | 0,5 | 0,5 | 0,4 | 0,5 | 0,4 | 0,4 | 0,3 | 0,4 | 0,4 | 0,4 | 1,9 | 1,8 | 0 | 0,5 |
| C1 | 0,7 | 0,7 | 0,7 | 0,7 | 0,7 | 0,8 | 0,7 | 0,7 | 0,7 | 0,7 | 0,7 | 0,7 | 0,7 | 0,7 | 0,7 | 0,7 | 0,7 | 0,7 | 0,7 | 0,7 | 0,7 | 1,3 | 1,2 | 0,5 | 0 |

Bergerhoff
(structure descriptor)

Bilbao Server
(global distortion)