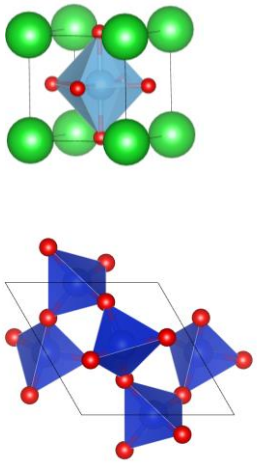
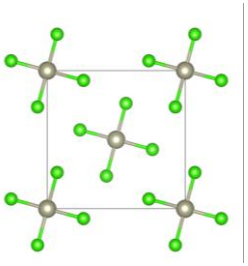
Crystal-Structure Tools

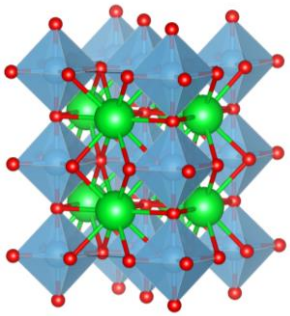
Crystallography Online: Workshop on the use and applications of the structural and magnetic tools of the Bilbao Crystallographic Server



COMPSTRU

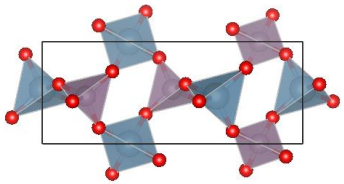


SETSTRU

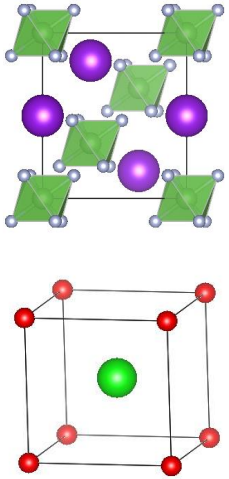


SUBGROUPS

TRANSTRU



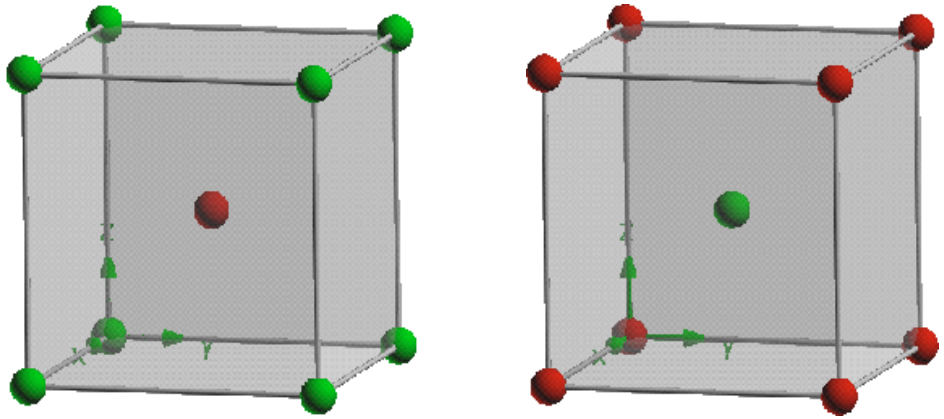
EQUIVSTRU



COMPARISON BETWEEN DIFFERENT STRUCTURE DESCRIPTIONS

Comparison of structures

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



Are these two structures of Cs Cl similar?

Yes

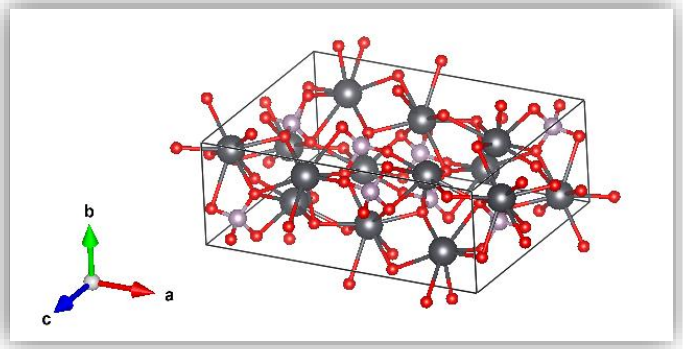
Similarity between two crystal structures

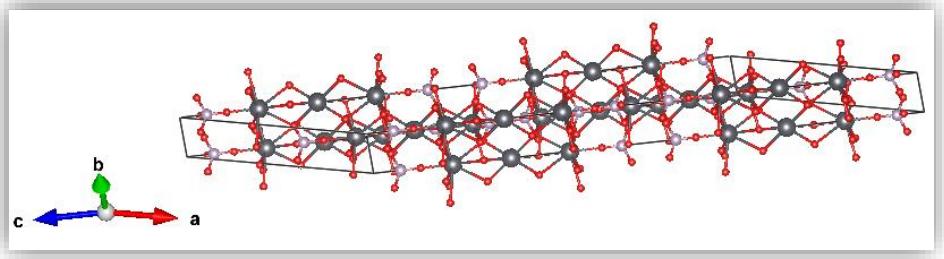
#Structure 1

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

#Structure 2

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





Are these two structures similar?

www.cryst.ehu.es

bilbao crystallographic server

FCT/ZTF

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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

- 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.

Raman and Hyper-Raman scattering

Point-group symmetry

Plane-group symmetry

Double point and space groups

Crystal-Structure Tools

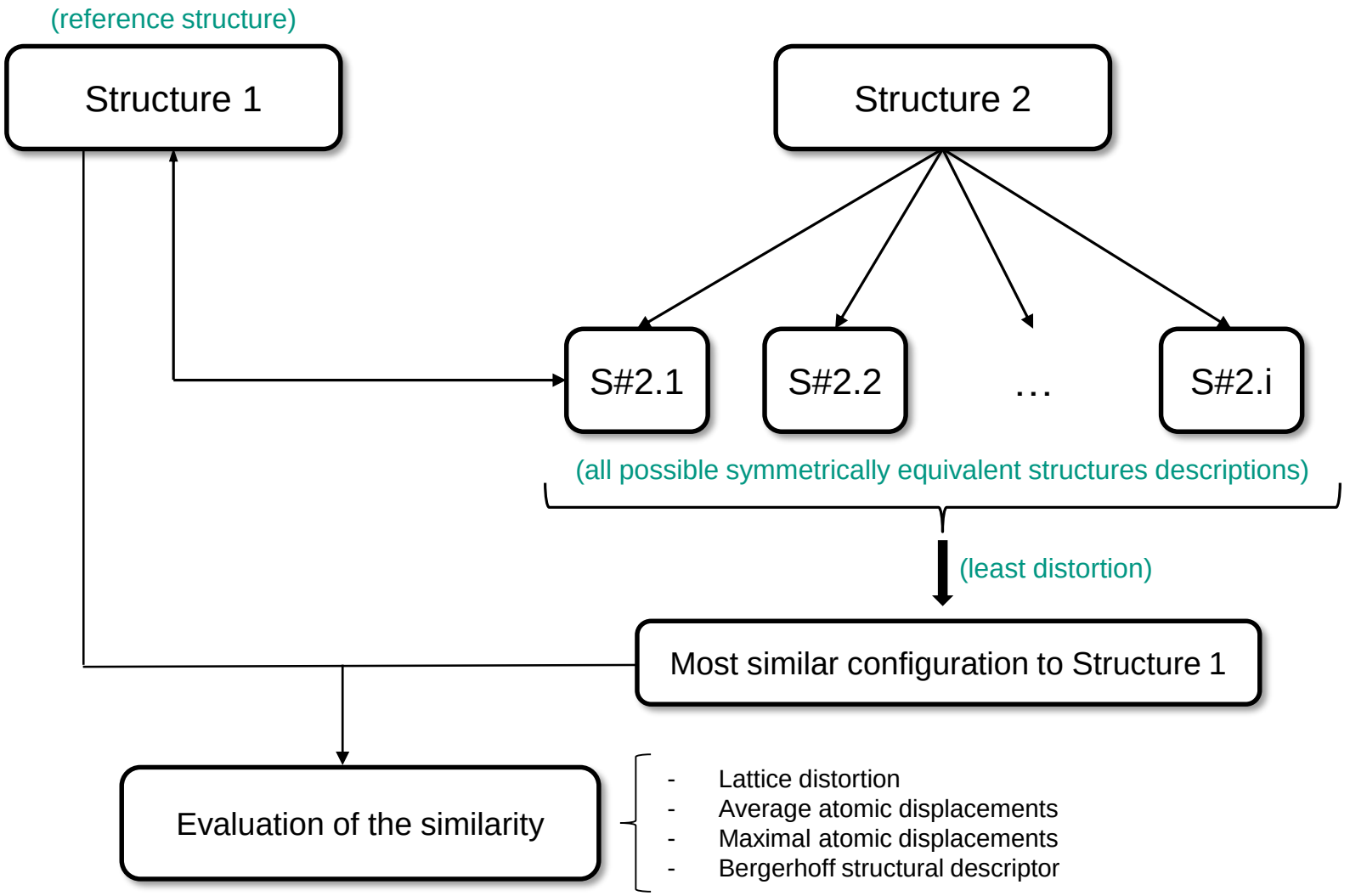
You can access to the material of this session:

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

You need to download:

- CrystalStructureTools.txt

The program COMPSTRU



The program COMPSTRU

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

degree of lattice distortion

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

η_i-eigenvalues of the Lagrangian strain tensor

average atomic displacements

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

u_i atomic displacements

maximal atomic displacements

maximal displacements of the paired atoms

The program COMPSTRU

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

structural descriptor

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

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

weighted mean difference between atomic coordinates

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

relation between axial ratios

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

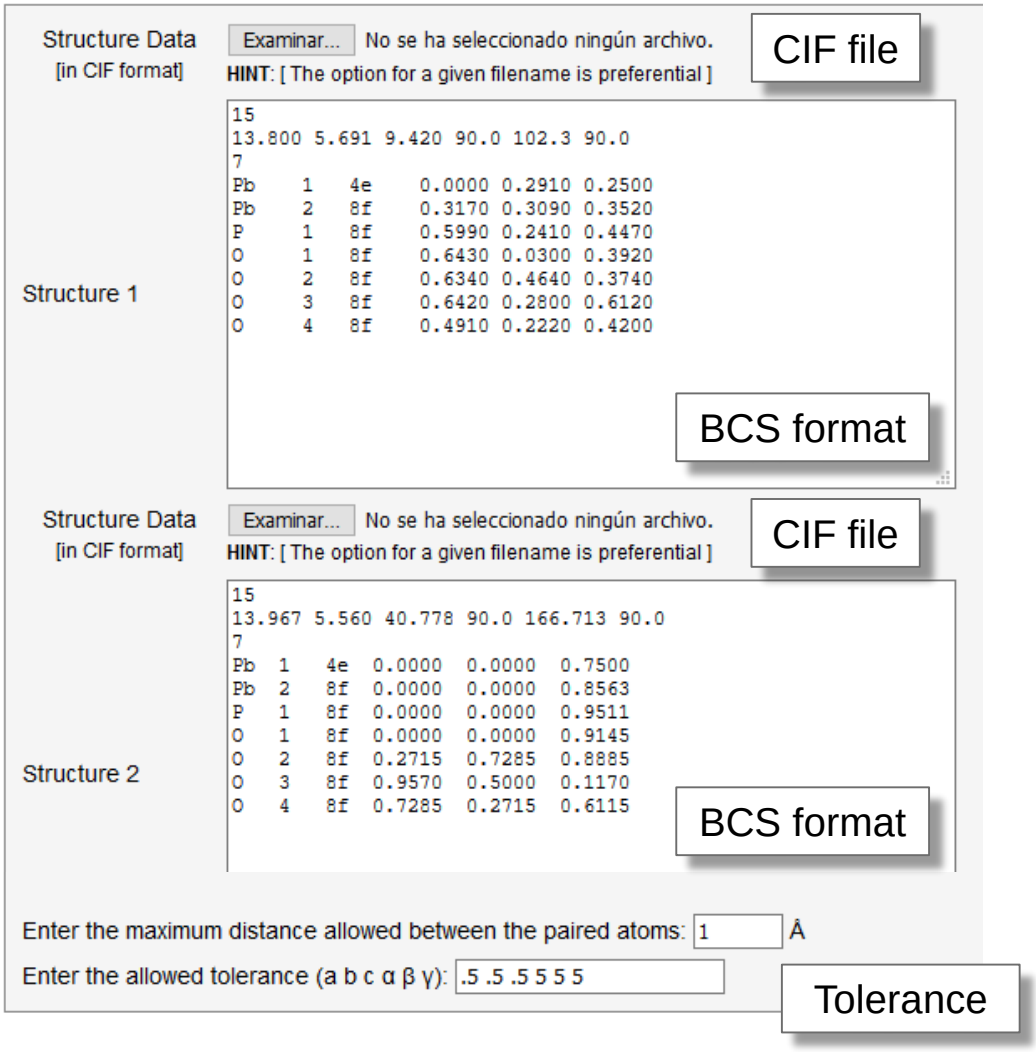
Input – COMPSTRU

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

Input:

Two crystal structures described in the standard setting

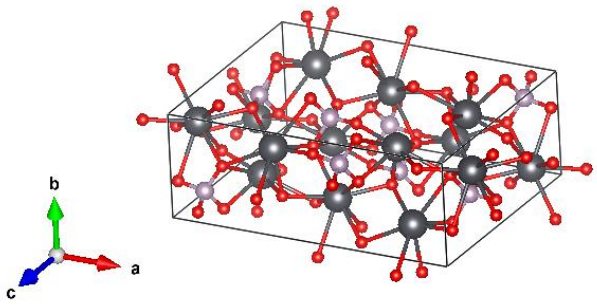
- Isopointal structures with the same/different composition
- Chiral structures



Are these two structures similar?

$Pb_3(PO_4)_2$

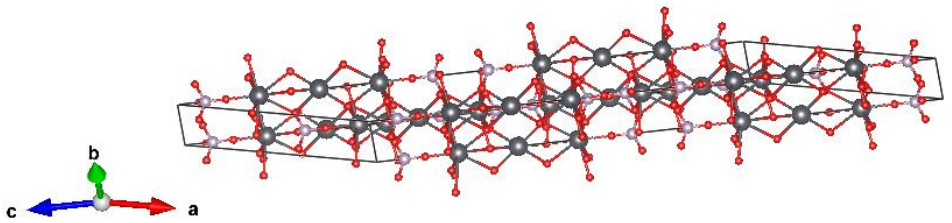
#Structure 1



15
13.800 5.691 9.420 90.0 102.3 90.0
7

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

#Structure 2



15
13.967 5.560 40.778 90.0 166.713
90.0
7

Pb	1	4e	0.0000	0.0000	0.7500
Pb	2	8f	0.0000	0.0000	0.8563
P	1	8f	0.0000	0.0000	0.9511
O	1	8f	0.0000	0.0000	0.9145
O	2	8f	0.2715	0.7285	0.8885
O	3	8f	0.9570	0.5000	0.1170
O	4	8f	0.7285	0.2715	0.6115

Output – COMPSTRU

$Pb_3(PO_4)_2$

Structure #1

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

WP		Atom	Atomic Displacements			
			u_x	u_y	u_z	|u|
4e	(0,y,1/4)	Pb1	0.0000	-0.0410	0.0000	0.2333
8f	(x,y,z)	Pb2	0.0019	-0.0590	0.0043	0.3386
8f	(x,y,z)	P1	0.0043	0.0090	0.0041	0.0816
8f	(x,y,z)	O1	0.0010	-0.0085	-0.0035	0.0617
8f	(x,y,z)	O2	0.0100	0.0145	0.0145	0.1910
8f	(x,y,z)	O3	0.0020	-0.0300	0.0050	0.1777
8f	(x,y,z)	O4	0.0025	0.0280	-0.0055	0.1733

Evaluation of the structure similarity

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

Structure #2

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

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

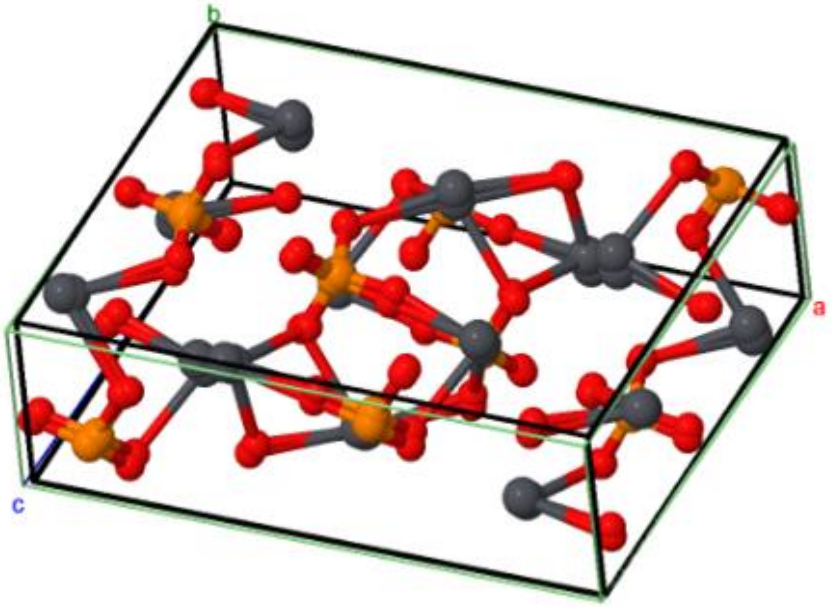
Description of Structure #2 in the most similar configuration to Structure #1

```
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
```

Input – COMPSTRU

$Pb_3(PO_4)_2$

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



Structure #1
Structure #2

Structure #2 (most similar)

Compare Structures
Compare Lattices
Atomic Displacements

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

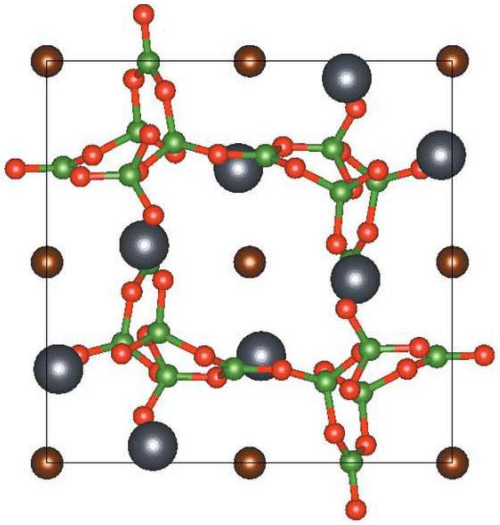
Show Distances
cutoff: 0.5

Save PNG+Jmol

Example: Structures with different composition

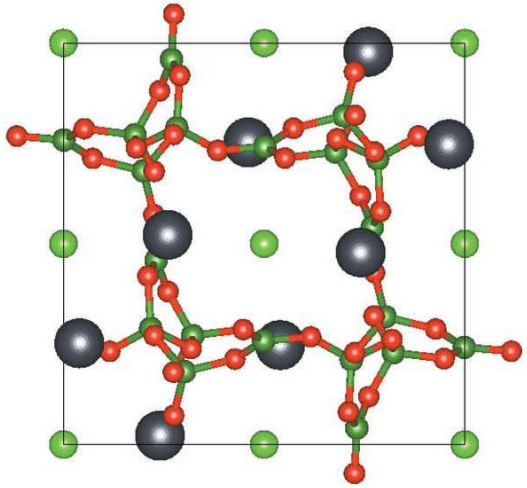
Are these two structures equivalent?

$Pb_2B_5O_9Br$



Belokoneva *et al*., 2003

$Pb_2B_5O_9Cl$



Egorova *et al*., 2008

Comparison of isopointal structures with different composition

Example: Structures with different composition

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

Structure #1

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

Structure #2

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

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

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

Example: Structures with different composition

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

Structure 1

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

Structure 2

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

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

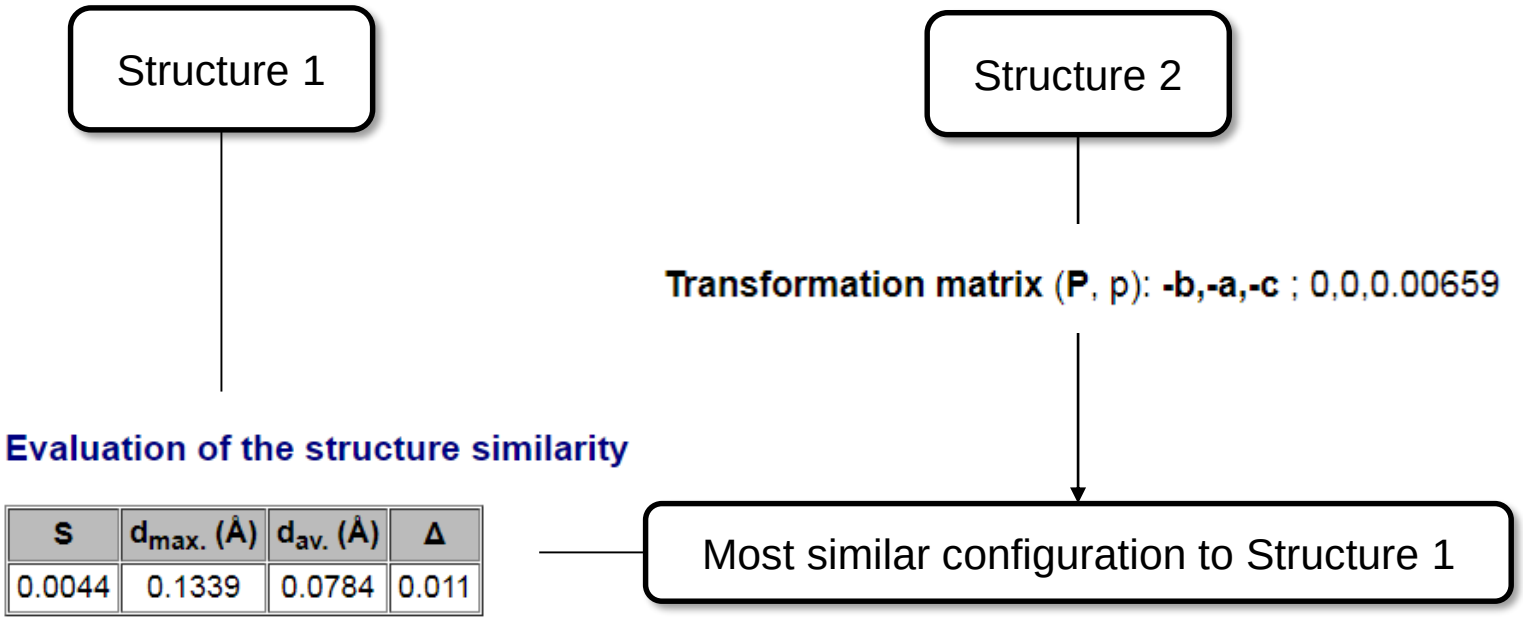
Structure #1	Structure #2
Cl	Br
O	O
Pb	Pb
B	B

Do you agree with the proposed correspondence scheme?

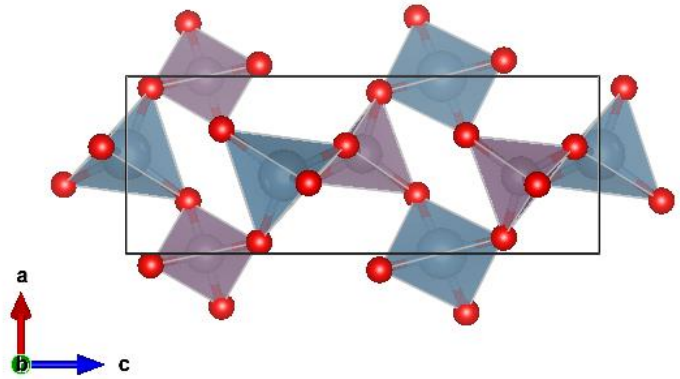
Yes No

DIFFERENT COMPOSITION

Example: Structures with different composition



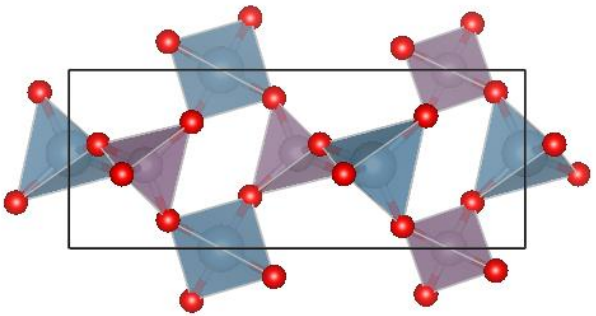
Example: Chiral Structures



$P3_121$ (No. 152)

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

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



$P3_221$ (No. 154)

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

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

Example: Chiral Structures

Structure #1

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

Structure #2

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

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

Atom pairings and distances

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

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

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

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

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

Exercise 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:173024
33
5.0885 8.7802 9.4709 90 90 90
10

O	1	4a	0.978000	0.328200	0.431400
O	2	4a	0.515000	0.490700	0.418700
O	3	4a	0.650000	0.997900	0.188300
O	4	4a	0.160000	0.163700	0.195600
O	5	4a	0.841000	0.168000	0.666900
O	6	4a	0.527000	0.163700	0.936200
Fe	7	4a	0.192800	0.150600	0.580700
Fe	8	4a	0.682600	0.029100	0.789700
Fe	9	4a	0.185800	0.151900	0.000000
Fe	10	4a	0.810400	0.158000	0.307100

#ICSD:415250
33
5.0715 8.7359 9.4178 90 90 90
10

O	1	4a	0.337000	0.853000	0.887000
O	2	4a	0.019000	0.474000	0.610000
O	3	4a	0.453000	0.677000	0.651000
O	4	4a	0.527000	0.669000	0.100000
O	5	4a	0.868000	0.334000	0.863000
O	6	4a	0.336000	0.513000	0.891000
Fe	7	4a	0.204000	0.350900	0.772600
Fe	8	4a	0.807000	0.660500	0.693000
Fe	9	4a	0.676800	0.842700	0.000000
Fe	10	4a	0.685200	0.463400	0.983000

Isopointal and isoconfigurational structures

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

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

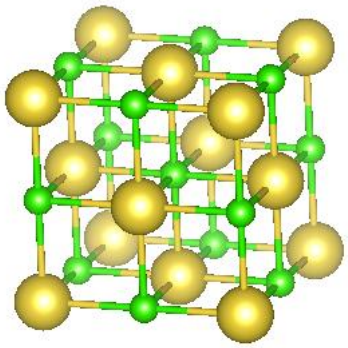
Lima-de Faria *et al. Acta Cryst.* (1990), A**41**, 1

Example I

NaCl

225
5.63347 5.63347 5.63347 90. 90. 90.
2

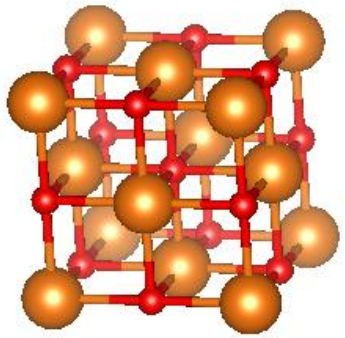
Na	1	4a	0.000000 0.000000 0.000000
Cl	1	4b	0.500000 0.500000 0.500000



MgO

225
4.2052 4.2052 4.2052 90. 90. 90.
2

Mg	1	4a	0.000000 0.000000 0.000000
O	1	4b	0.500000 0.500000 0.500000



NaCl and MgO are *isopointal* structures

NaCl and MgO are *isoconfigurational* structures

Example II

Pyrite: $Pa\bar{3}$

a=5.42 A

Fe 4a 0 0 0

S 8c *x x x*

with *x=0.384*

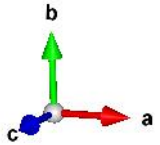
CO_2: $Pa\bar{3}$

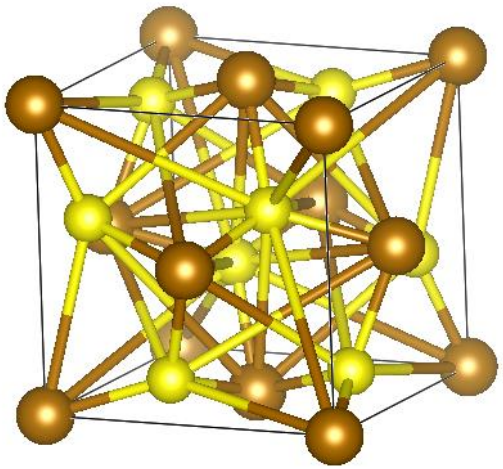
a=5.62 A

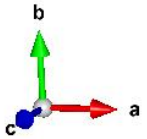
C 4a 0 0 0

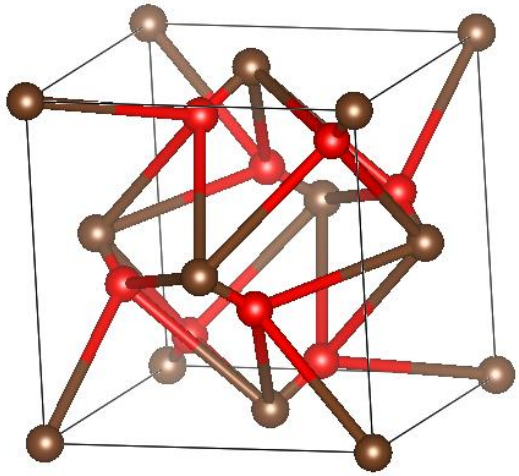
O 8c *x x x*

with *x=0.118*





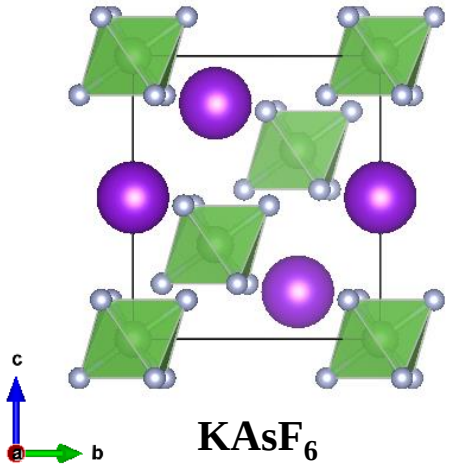




Pyrite and CO_2 are *isopointal* structures

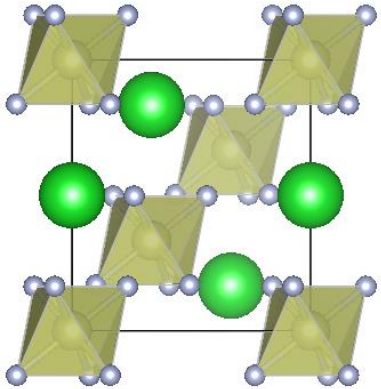
Exercise 5

- Do the following three structures belong to the same structure type?



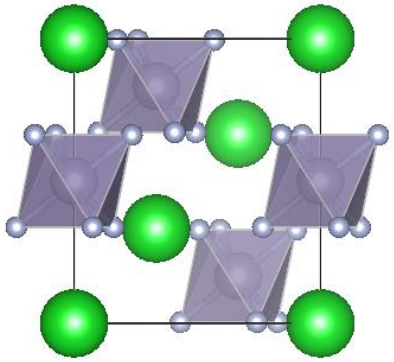
$KAsF_6$

#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

Structure types - COMPSTRU

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

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