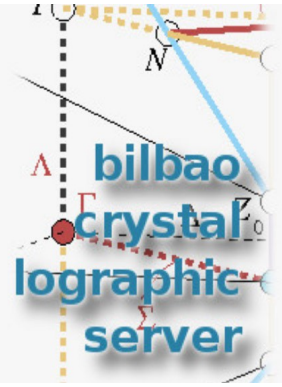
Crystallography Online: Workshop on the use and applications of the structural tools of the Bilbao Crystallographic Server

20-21 August 2018

ECM31
31st European Crystallographic Meeting

Satellite Meeting
31st European Crystallographic Meeting
Oviedo



CRYSTAL-STRUCTURE TOOLS
BILBAO CRYSTALLOGRAPHYC SERVER

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CRYSTAL-STRUCTURE TOOLS

Crystal structure descriptions

Conventional and ITA settings of space groups

Transform structure to a subgroup basis

Equivalent structure descriptions

Comparison between different structure descriptions

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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
- Subperiodic Groups: Layer, Rod and Frieze Groups
- Structure Databases
- Raman and Hyper-Raman scattering
- Point-group symmetry
- Plane-group symmetry

ECM31-Oviedo Satellite

Crystallography online: workshop on the use and applications of the structural tools of the Bilbao Crystallographic Server

20-21 August 2018

News:

- **New program: mCIF2PCR**
  01/2018: Transformation from mCIF to PCR format. The PCR file can be used as input for FullProf.
- **New Article**
  11/2017: Elcoro *et al.* "Double crystallographic groups and their representations on the Bilbao Crystallographic Server" *J. App. Crys.* (2017). **50**, 1457-1477.
- **New Article in Nature**
  07/2017: Bradlyn *et al.* "Topological quantum chemistry" *Nature* (2017).

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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 (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

Point-group symmetry

Plane-group symmetry

News:

- New Article in Nature 07/2017: Bradlyn *et al.* "Topological quantum chemistry" *Nature* (2017).

Crystal structure descriptions

What do we need to describe a crystal structure?

Space Group *ITA* 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 **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. **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

SESTRU http://www.cryst.ehu.es/cryst/setstru.html

$CaPbO_3$

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]

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

SESTRU

$CaPbO_3$

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:

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

ITA settings structure descriptions

SESTRU

$CaPbO_3$

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

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) (0.443700,0.750000,0.486000) (0.943700,0.750000,0.014000) (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) (0.500000,0.000000,0.000000) (0.000000,0.500000,0.500000) (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) (0.054800,0.750000,0.620000) (0.554800,0.750000,0.880000) (0.945200,0.250000,0.380000)
O2	8d (x,y,z)	1	(0.305100,0.061300,0.690700)	(0.305100,0.061300,0.690700) (0.194900,0.938700,0.190700) (0.694900,0.561300,0.309300) (0.805100,0.438700,0.809300) (0.694900,0.938700,0.309300) (0.805100,0.061300,0.809300) (0.305100,0.438700,0.690700) (0.194900,0.561300,0.190700)

Exercise 1.1

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 **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. **I41/AMDZ (141)** V=263.32
Remarks	R=0.070000 : PDC =01-073-6646 : PDF =6-266 : TYP =ZrSiO4 : XDS MIN =Zircon : At least one temperature factor missing in the paper. 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 **Link XRef SCOPUS SCIRUS Google** **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. **I41/AMDS (141)** V=261.28
Remarks	COR MIN =Zircon : PDF =6-266 : TYP =ZrSiO4 : XDS At least one temperature factor missing in the paper. No R value given in the paper. 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 1.1

Structure 1 Space group $I4_1/amd$ (No. 141) a=6.60 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

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

CIF file

```
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)

$Pb_3(VO_4)_2$

(P,p)

Description
$P2_1/c$ (No. 14)

Structure

```
166
5.6748 5.6748 20.3784 90 90 120
5
Pb      1       3a      0.000000        0.000000        0.000000
Pb      2       6c      0.000000        0.000000        0.207100
PV      3       6c      0.000000        0.000000        0.388400
O       4       6c      0.000000        0.000000        0.324000
O       5       18h     0.842400        0.157600        0.430100
```

Low symmetry Space Group *ITA* number: 14

Transformation Matrix:

In matrix form:

Linear part			Origin Shift
2/3	0	-2	0
1/3	1	1	0
1/2	0	0	0

Validity (P,p)

WP splitting

Structure transformation

High symmetry structure

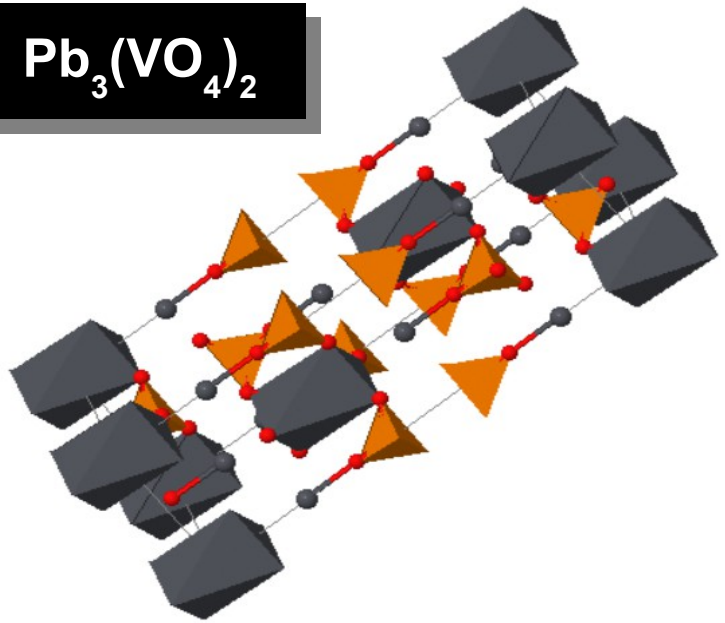
```
166
5.6739 5.6739 20.3412 90. 90. 120.
5
Pb      1       3a      0.000000        0.000000        0.000000
Pb      2       6c      0.000000        0.000000        0.207300
PV      1       6c      0.000000        0.000000        0.392400
O       1       6c      0.000000        0.000000        0.324700
O       2       18h     0.843300        0.156700        0.429900
```

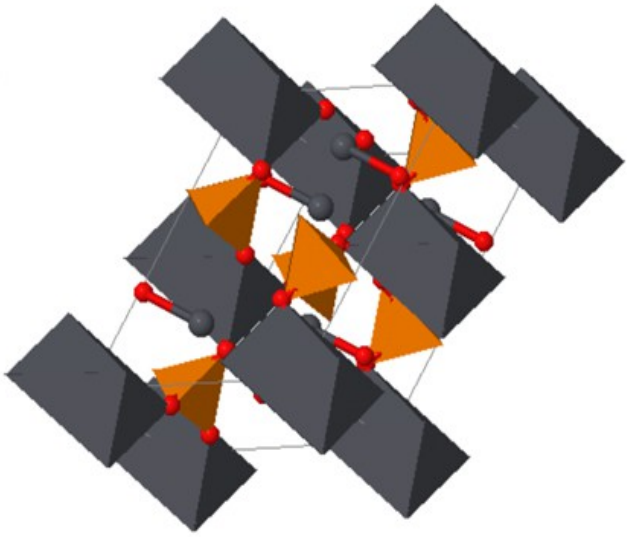
(P,p)=2/3a+1/3b+1/3c,b,-2a-b

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
```

$Pb_3(VO_4)_2$





Exercise 1.1 (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=6.60 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

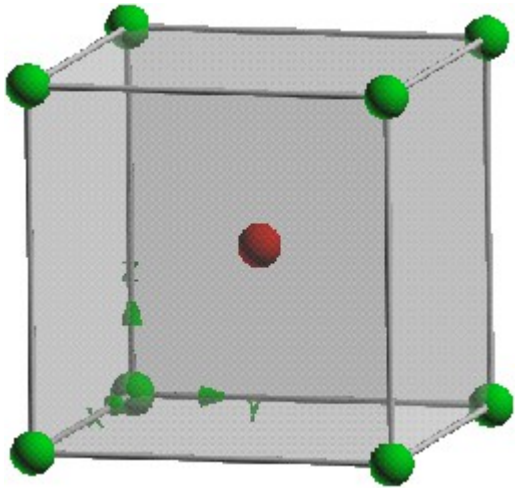
Origin choice 2 at *2/m*

Coordinate transformation

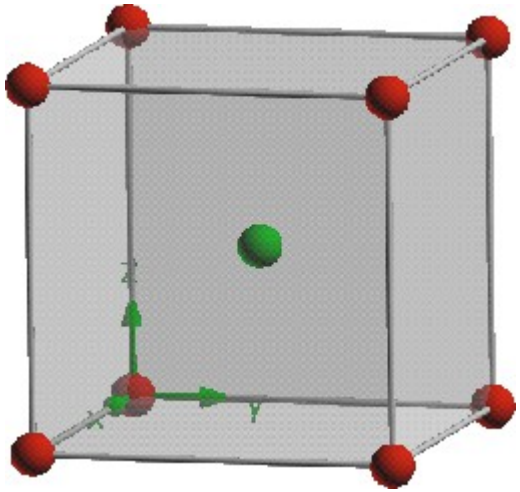
Origin choice 2 ⟶ Origin choice 1

$\boldsymbol{p}$=0,1/4,-1/8

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

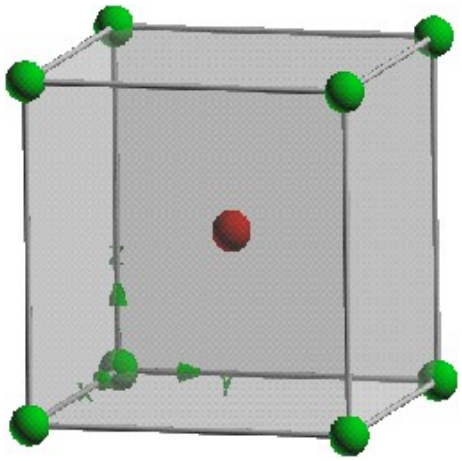
Structure

```
#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)**

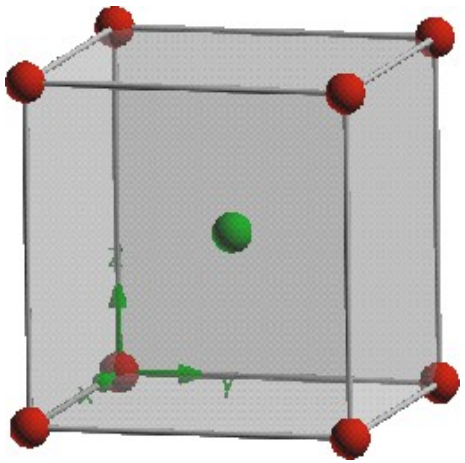
Normalizer coset representative: x,y,z

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 1.2

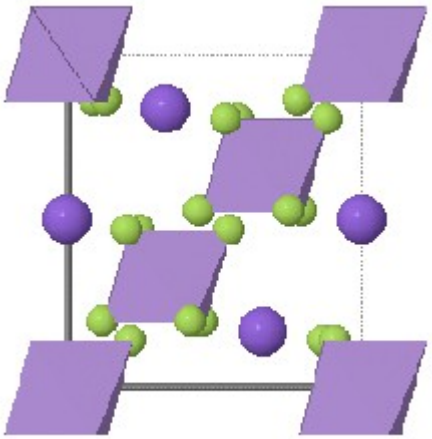
How many equivalent sets of coordinates can be used to describe the structure $P(C_6C_5)_4[MoNCl_4]$? What are their coordinates?

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 1.3

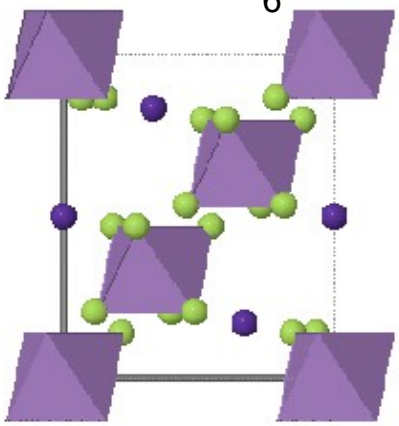
Do the following three structures belong to the same structure type? Try to find analogous coordinate descriptions for all three crystal structures.

$KAsF_6$



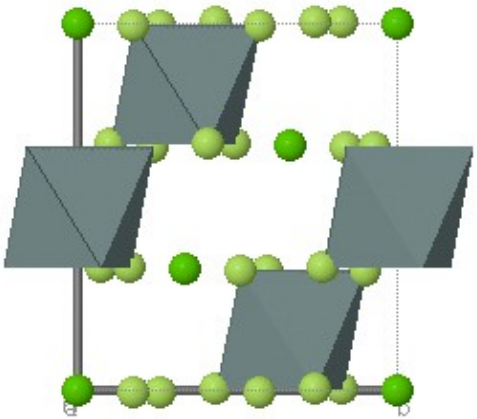
```
148
7.3480 7.3480 7.2740 90.00 90.00 120.00
3
K     1   3b    0.333333 0.666666 0.166666
As    1   3a    0 0 0
F     1   18f   0.1292 0.2165 0.1381
```

$BaIrF_6$



```
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
```

$BaSnF_6$



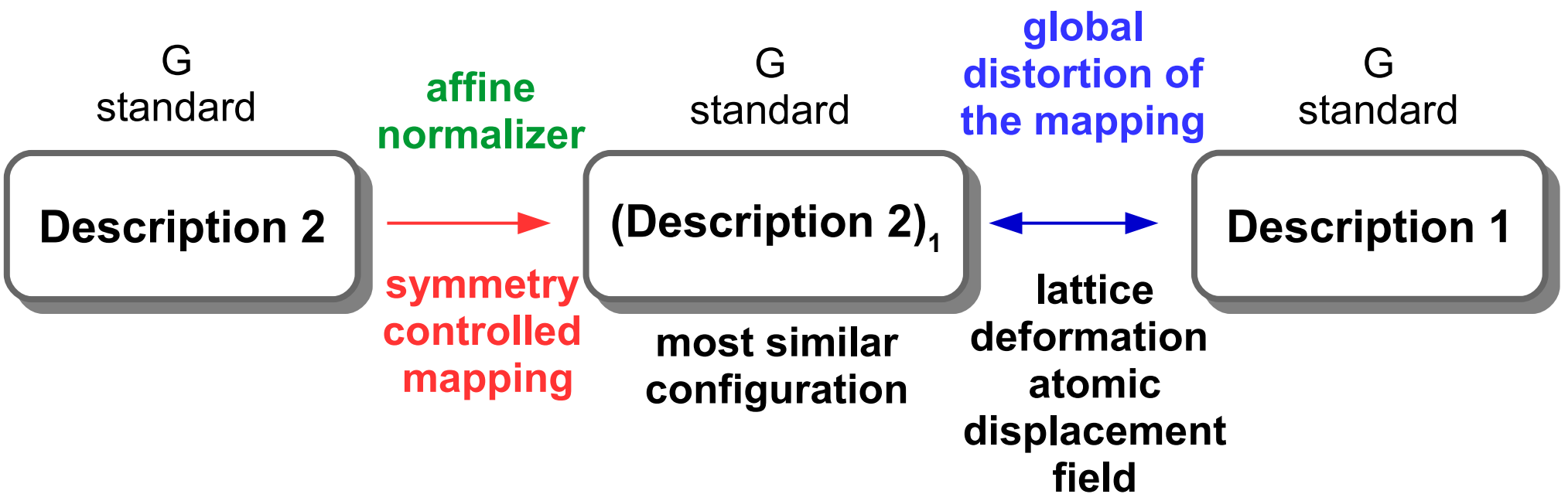
```
148
7.4279 7.4279 7.4180 90.00 90.00 120.00
3
Sn    1   3b    0 0 0.5
Ba    1   3a    0 0 0
F     1   18f   0.2586 0.8262 0.0047
```

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

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

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

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

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

$Pb_3(PO_4)_2$

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

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

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
```

BCS format

Standard setting

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

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

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
```

BCS format

Tolerance

Enter the maximum distance allowed between the paired atoms: 1 Å

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

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
```

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

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

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
```

Evaluation of the structure similarity

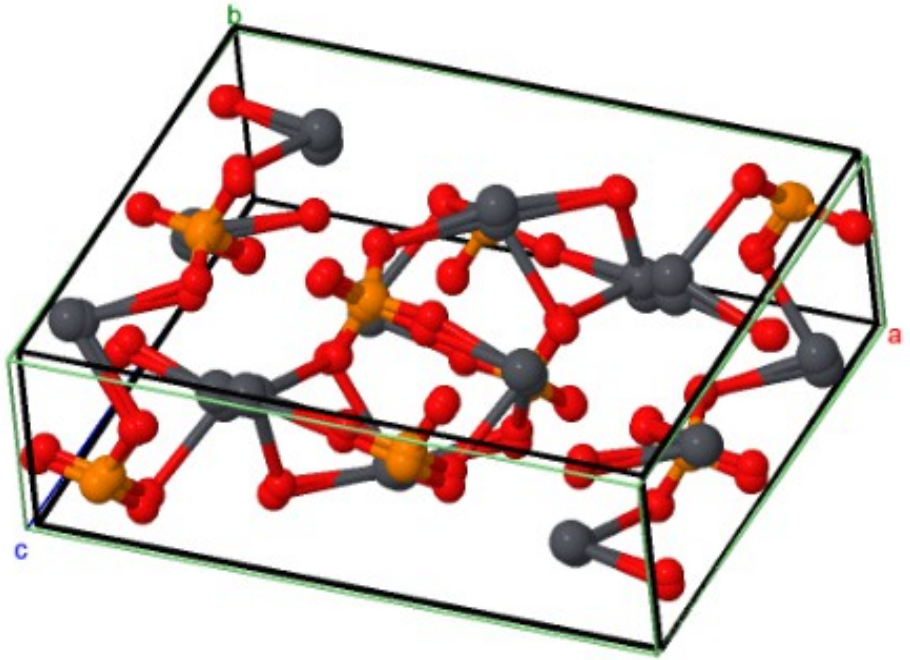
S	$d_{max.}$ (Å)	$d_{av.}$ (Å)	Δ
0.0116	0.3386	0.1755	0.066

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 1.4

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 **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. **PNA21 (33)** V=423.14
Remarks	R=0.013300 : NDP RVP SNP TEM =200 : TYP =AlFeO3 : XDP MAG 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)	0.1680(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)

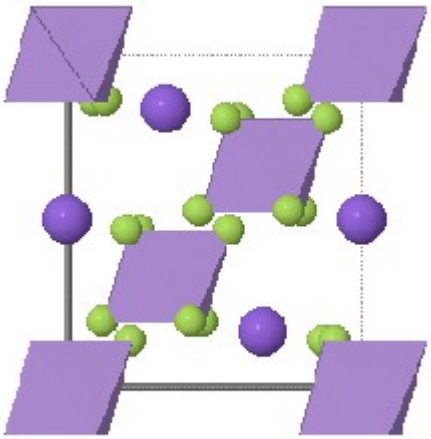
Title	Synthesis and structural analysis of epsilon-(Fe2 O3).
Authors	Kelm, K.;Mader, W.
Reference	Zeitschrift fuer Anorganische und Allgemeine Chemie (2005) **631**, 2383-2389 **Link XRef SCOPUS SCIRUS Google**
Compound	**Fe2 O3** - Diiron(III) oxide - epsilon **[A2X3] [oP40] [a10] [AlFeO3]**
Cell	5.0715(2), 8.7359(4), 9.4178(4), 90, 90, 90 **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	0.868(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 1.3 (cont)

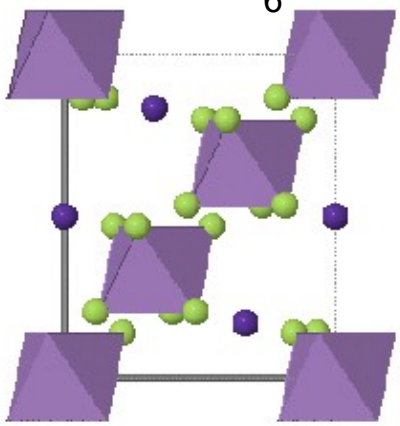
Do these compounds belong to the ***same structure type*** *?*

$KAsF_6$



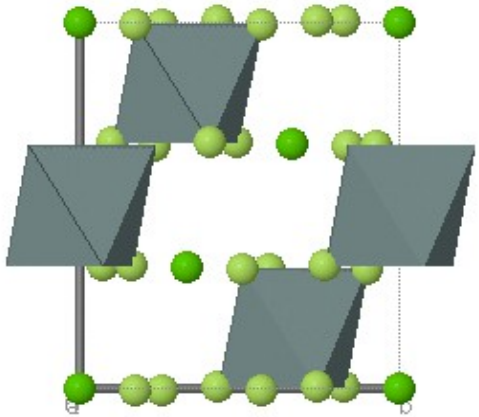
```
148
7.3480 7.3480 7.2740 90.00 90.00 120.00
3
K     1   3b    0.333333 0.666666 0.166666
As    1   3a    0 0 0
F     1   18f   0.1292 0.2165 0.1381
```

$BaIrF_6$



```
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)