Workshop Symmetriebeziehungen in der Kristallchemie

Max Planck Institute for Chemical Physics of Solids

30.09. - 02.10.2019 Dresden

Deutsche Gesellschaft für Kristallographie

GDCh Gesellschaft Deutscher Chemiker

NETZSCH

BILBAO CRYSTALLOGRAPHIC SERVER

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Summary

Symmetry databases of the Bilbao Crystallographic Server

Symmetry relations of space groups

Crystal-structure descriptions

Crystal-structure relations

SYMMETRY DATABASES OF THE BILBAO CRYSTALLOGRAPHIC SERVER

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FCT/ZTF

bilbao crystallographic server

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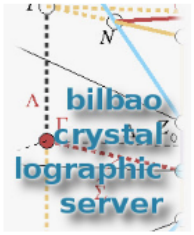
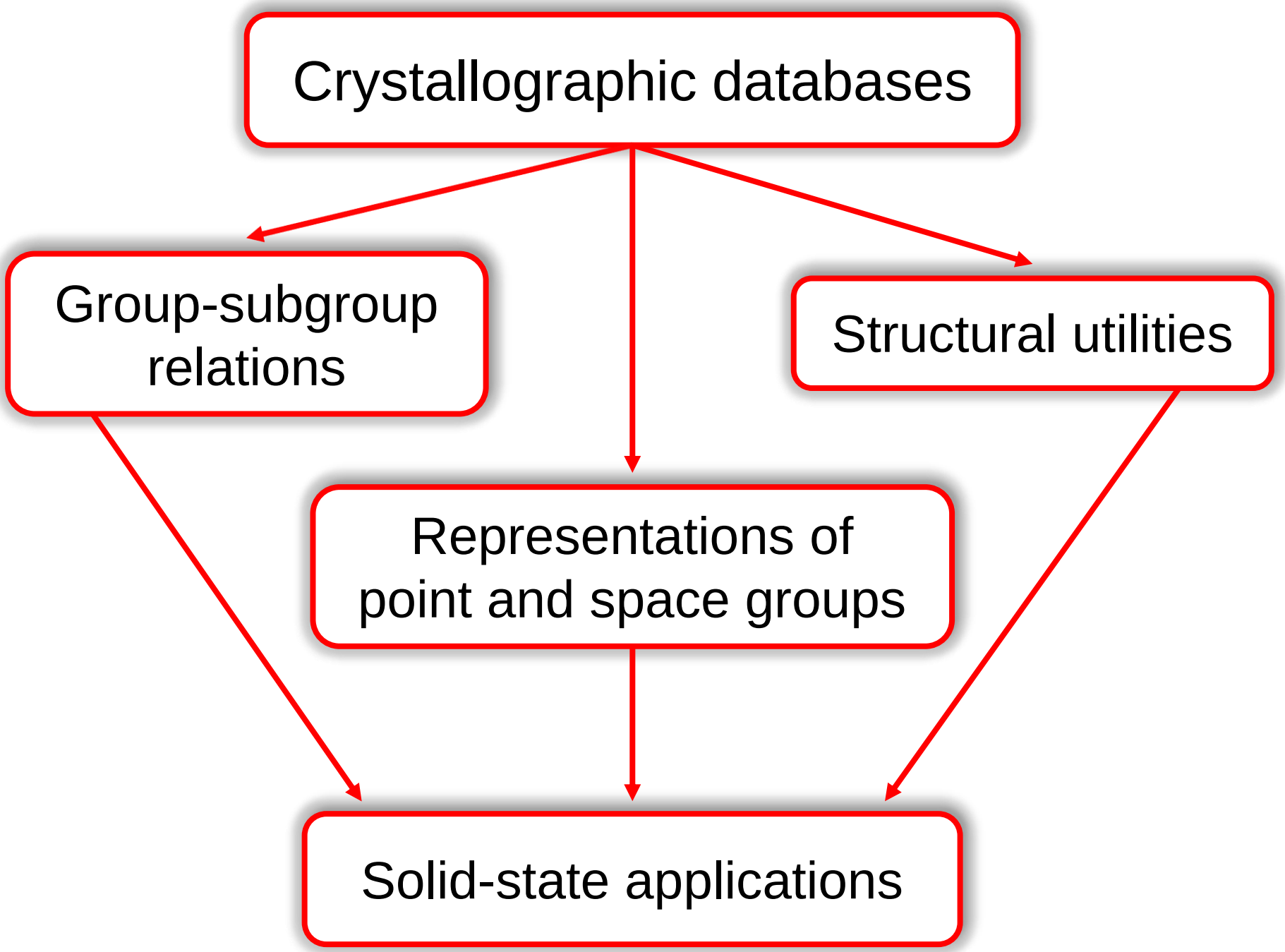


Bilbao Crystallographic Server in forthcoming schools and workshops

News:

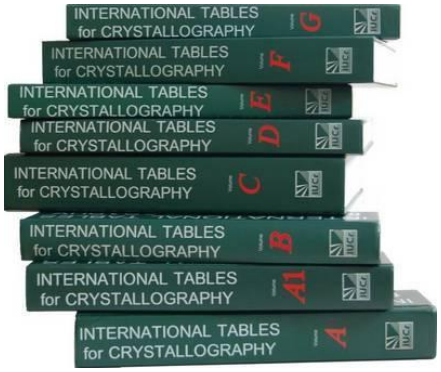
- **New Article in Acta Cryst. A** 05/2019: Gallego *et al.* "Automatic calculation of symmetry-adapted tensors in magnetic and non-magnetic materials: a new tool of the Bilbao Crystallographic Server." *Acta Cryst.* (2019) **A75**, 438-447.
- **New Article in Nature** 03/2019: Vergniory *et al.* "A 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..

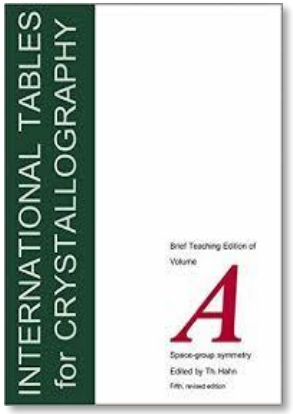
- Space-group symmetry
- Magnetic Symmetry and Applications
- Group-Subgroup Relations of Space Groups
- Representations and Applications
- Solid State Theory Applications
- Structure Utilities
- Subperiodic Groups: Layer, Rod and Frieze Groups
- Structure Databases
- Raman and Hyper-Raman scattering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


Crystallographic databases
Group-subgroup relations
Structural utilities
Representations of point and space groups
Solid-state applications

Crystallographic databases

International Tables for Crystallography



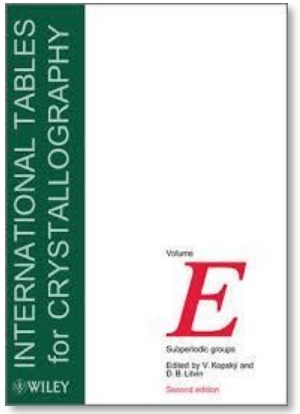


Plane groups

Point groups

Space groups

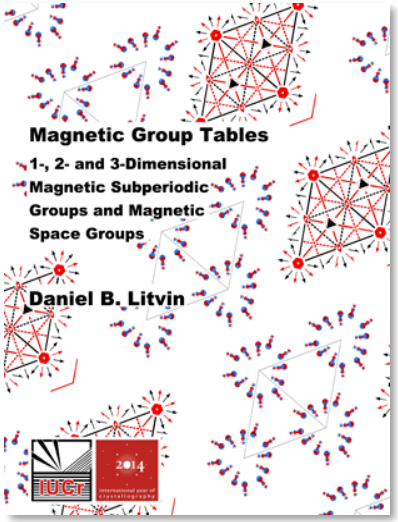
Space groups



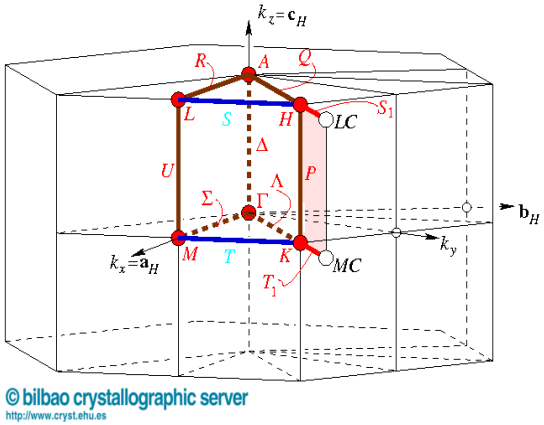
Subperiodic groups:

- Frieze groups
- Rod groups
- Layer groups

Crystallographic databases

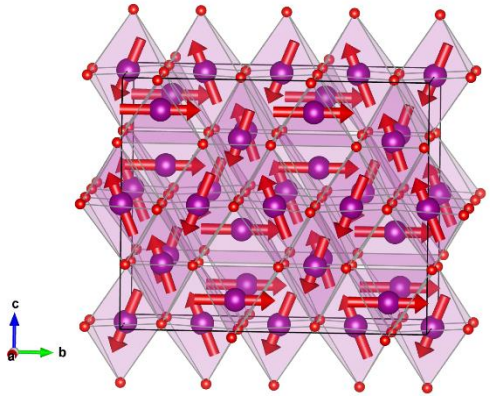


Magnetic groups



Brillouin zone database:

- Space groups
- Layer groups



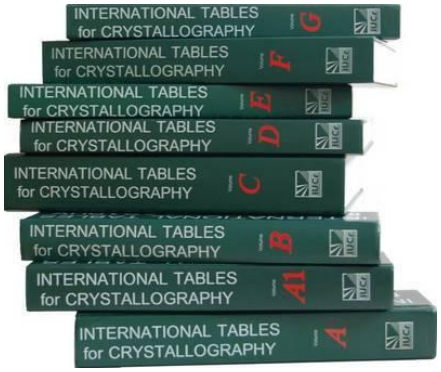
MAGNDATA
Magnetic Structure
Database

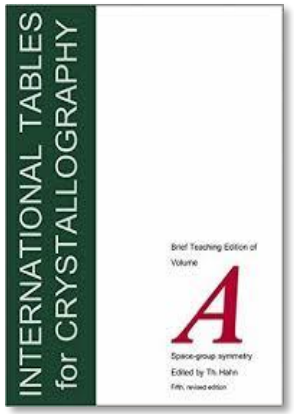
Double space
groups

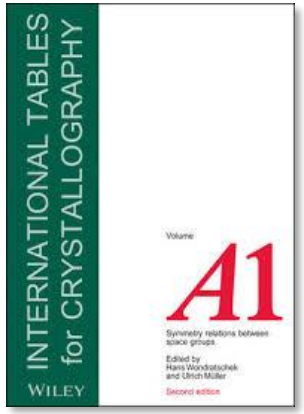
Bilbao Incommensurate Structures Database
B-IncStrDB

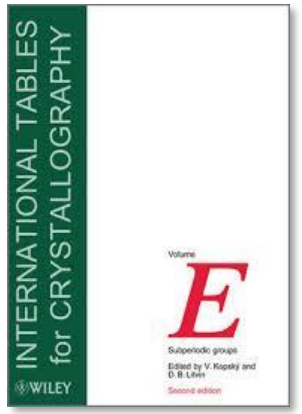
Crystallographic databases

International Tables for Crystallography









Plane groups

Point groups

Space groups

Space groups

Subperiodic groups:

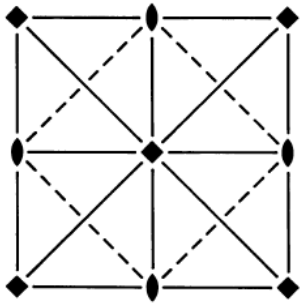
- Frieze groups
- Rod groups
- Layer groups

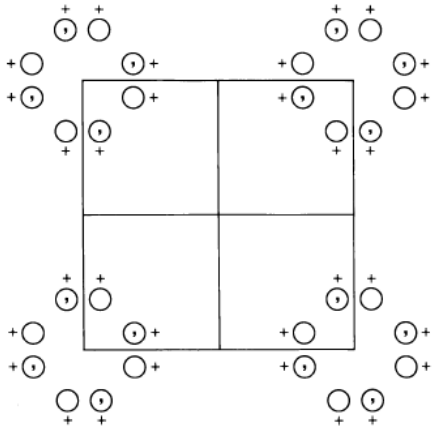
Crystallographic databases

GENERAL LAYOUT: LEFT-HAND PAGE

$P4mm$ C_{4v}^{1} $4mm$ Tetragonal

No. 99 $P4mm$ Patterson symmetry $P4/mmm$





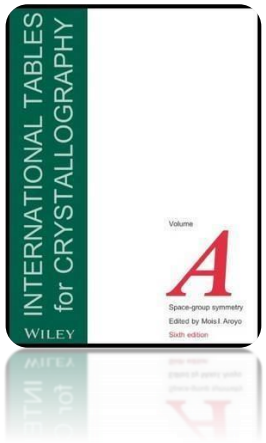
Origin on $4mm$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le 1$; $x \le y$

Symmetry operations

(1) 1	(2) 2 0,0,z	(3) 4^+ 0,0,z	(4) 4^- 0,0,z
(5) m x,0,z	(6) m 0,y,z	(7) m x,$\bar{x}$,z	(8) m x,x,z

SYMMETRY OPERATIONS



GENERAL LAYOUT: RIGHT-HAND PAGE

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	g	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$
			(5) $x,\bar{y},z$	(6) $\bar{x},y,z$	(7) $\bar{y},\bar{x},z$	(8) y,x,z
4	f	$.m.$	$x,\frac{1}{2},z$	$\bar{x},\frac{1}{2},z$	$\frac{1}{2},x,z$	$\frac{1}{2},\bar{x},z$
4	e	$.m.$	$x,0,z$	$\bar{x},0,z$	$0,x,z$	$0,\bar{x},z$
4	d	$..m$	x,x,z	$\bar{x},\bar{x},z$	$\bar{x},x,z$	$x,\bar{x},z$
2	c	$2mm.$	$\frac{1}{2},0,z$	$0,\frac{1}{2},z$		
1	b	$4mm$	$\frac{1}{2},\frac{1}{2},z$			
1	a	$4mm$	$0,0,z$			

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [110] $p1m1$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2] $P411$ ($P4$, 75) 1; 2; 3; 4
[2] $P21m$ ($Cmm2$, 35) 1; 2; 7; 8
[2] $P2m1$ ($Pmm2$, 25) 1; 2; 5; 6

IIa none

IIb [2] $P4_2mc$ ($\mathbf{c}' = 2\mathbf{c}$) (105); [2] $P4cc$ ($\mathbf{c}' = 2\mathbf{c}$) (103); [2] $P4_2cm$ ($\mathbf{c}' = 2\mathbf{c}$) (101); [2] $C4md$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P4bm$, 100); [2] $F4mc$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($I4cm$, 108); [2] $F4mm$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($I4mm$, 107)

Maximal isomorphic subgroups of lowest index

IIc [2] $P4mm$ ($\mathbf{c}' = 2\mathbf{c}$) (99); [2] $C4mm$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P4mm$, 99)

Minimal non-isomorphic supergroups

I [2] $P4/mmm$ (123); [2] $P4/nmm$ (129)

II [2] $I4mm$ (107)

Reflection conditions

General:

no conditions

Special:

no extra conditions

no extra conditions

no extra conditions

hkl : $h+k=2n$

no extra conditions

no extra conditions

HKLCOND

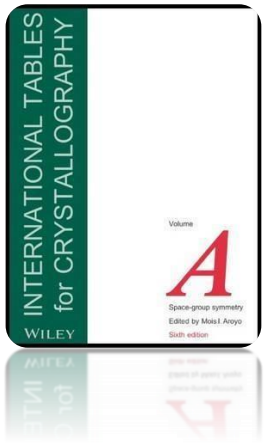
GENPOS

WYCKPOS

MAXSUB

SERIES

MINSUP



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Space-group symmetry

Magnetic Symmetry and Applications

Space-group symmetry

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

03/2019: Vergniory *et al.* "A complete catalogue of high-quality topological materials" *Nature* (2019). 566, 480-485.

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Raman and Hyper-Raman scattering

Point-group symmetry

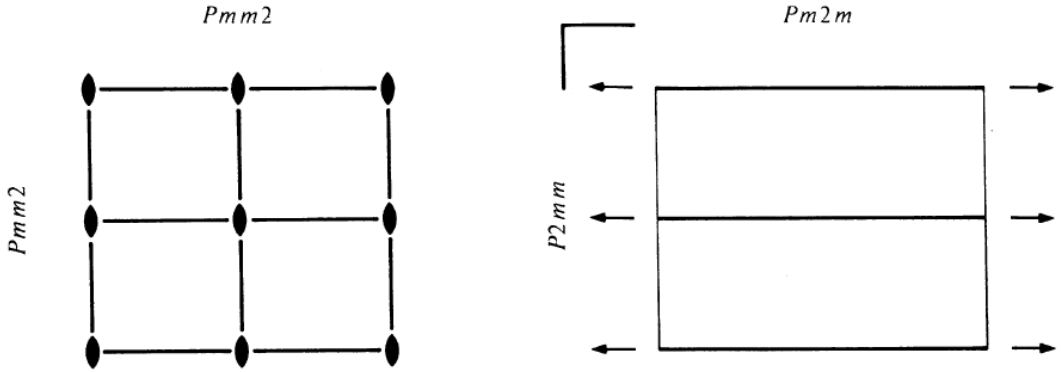
Plane-group symmetry

Double point and space groups

Generators and General positions

$Pmm2$ C_{2v}^{1} $mm2$ Orthorhombic

No. 25 $Pmm2$ Patterson symmetry $Pmmm$



Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			
4 i 1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x,\bar{y},z$	(4) $\bar{x},y,z$

Matrix-column resentation

Symmetry operations

(1) 1	(2) 2 0,0,z	(3) m x,0,z	(4) m 0,y,z

Geometric interpretation

Generators and General positions

GENPOS http://www.cryst.ehu.es/cryst/get_gen.html

Generators and General Positions

Space group number

How to select the group

The space groups are specified by their sequential number as given in the *International Tables for Crystallography*, Vol. A. You can give this number, if you know it, or you can choose it from the table with the space group numbers and symbols if you click on the button [**choose it**].

The available crystallographic data refer either to the standard/default setting of the chosen space group or to the so-called ITA Settings.

To get the data in any Non-conventional setting it is necessary to specify the corresponding transformation that relates the non-conventional to the standard/default setting of the space group.

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

Aroyo, *et. al. Zeitschrift fuer Kristallographie* (2006), **221**, 1, 15-27.

If you are interested in other publications related to Bilbao Crystallographic Server, click here

Please, enter the sequential number of group as given in the *International Tables for Crystallography*, Vol. A

choose it 32

Show:

Generators only ○

All General Positions ◉

Standard/Default Setting | Non Conventional Setting | ITA Settings

Generators and General positions

Table of Space Group Symbols

No space group has been selected by now.

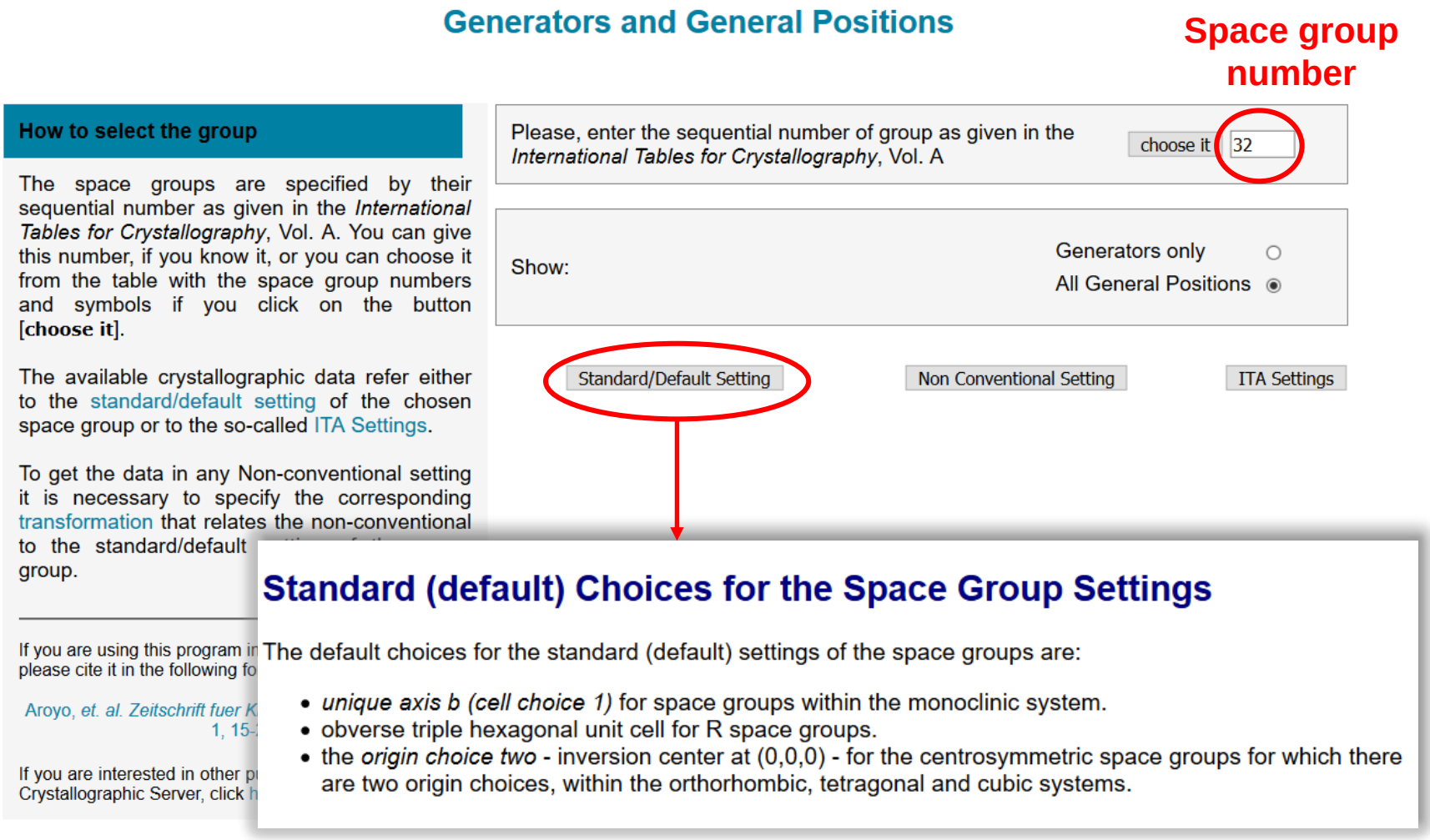
Click over the group name to see the group generators/general positions

The program you want to use works ONLY with the default choice for the group setting

1	$P1$	2	$P\text{-}1$	3	$P2$	4	$P2_1$	5	$C2$
6	Pm	7	Pc	8	Cm	9	Cc	10	$P2/m$
11	$P2_1/m$	12	$C2/m$	13	$P2/c$	14	$P2_1/c$	15	$C2/c$
16	$P222$	17	$P222_1$	18	$P2_12_12$	19	$P2_12_12_1$	20	$C222_1$
21	$C222$	22	$F222$	23	$I222$	24	$I2_12_12_1$	25	$Pmm2$
26	$Pmc2_1$	27	$Pcc2$	28	$Pma2$	29	$Pca2_1$	30	$Pnc2$
31	$Pmn2_1$	32	$Pba2$	33	$Pna2_1$	34	$Pnn2$	35	$Cmm2$
36	$Cmc2_1$	37	$Ccc2$	38	$Amm2$	39	$Aem2$	40	$Ama2$
41	$Aea2$	42	$Fmm2$	43	$Fdd2$	44	$Imm2$	45	$Iba2$
46	$Ima2$	47	$Pmmm$	48	$Pnnn$	49	$Pccm$	50	$Pban$
51	$Pmma$	52	$Pnna$	53	$Pmna$	54	$Pcca$	55	$Pbam$
56	$Pccn$	57	$Pbcm$	58	$Pnnm$	59	$Pmmn$	60	$Pbcn$

Generators and General positions

GENPOS http://www.cryst.ehu.es/cryst/get_gen.html



Generators and General positions

GENPOS http://www.cryst.ehu.es/cryst/get_gen.html

Generators and General Positions

Space group number

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If you are interested in other publications related to Bilbao Crystallographic Server, click here

Please, enter the sequential number of group as given in the *International Tables for Crystallography*, Vol. A choose it 32

Show: Generators only All General Positions

Standard/Default Setting Non Conventional Setting ITA Settings

General Positions of the Group *Pba*2 (No. 32) in Non Conventional Setting

Please, enter the transformation:

	Linear part			Origin shift
1	0	0		0
0	1	0		0
0	0	1		0

Change the basis

Generators and General positions

GENPOS http://www.cryst.ehu.es/cryst/get_gen.html

Generators and General Positions

Space group number

How to select the group

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Please, enter the sequential number of group as given in the *International Tables for Crystallography*, Vol. A choose it [32]

Show: Generators only ○ All General Positions ◉

Standard/Default Setting | Non Conventional Setting | ITA Settings

ITA-Settings for the Space Group 32

Note: The transformation matrices must be read by columns. **P** is the transformation from standard to the ITA-setting.

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

ITA number	Setting	P	P^{-1}
32	*P b a 2*	a,b,c	a,b,c
32	*P 2 c b*	c,a,b	b,c,a
32	*P c 2 a*	b,c,a	c,a,b

Example GENPOS: Space group Pba2 (No. 32)

Space-group symmetry operations

short hand notation

matrix-column representation $\begin{pmatrix} W_{11} W_{12} W_{13} \\ W_{21} W_{22} W_{23} \\ W_{31} W_{32} W_{33} \end{pmatrix} \begin{pmatrix} w_1 \\ w_2 \\ w_3 \end{pmatrix}$

Geometric interpretation

Seitz symbols

General Positions of the Group *Pba2* (No. 32)

Click here to get the general positions in text format

No.	(x,y,z) form	Matrix form	Symmetry operation	
			ITA	Seitz
1	x,y,z	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	1	{ 1 | 0 }
2	-x,-y,z	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	2 0,0,z	{ 2_{001} | 0 }
3	x+1/2,-y+1/2,z	$\begin{pmatrix} 1 & 0 & 0 & 1/2 \\ 0 & -1 & 0 & 1/2 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	a x,1/4,z	{ m_{010} | 1/2 1/2 0 }
4	-x+1/2,y+1/2,z	$\begin{pmatrix} -1 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 1/2 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	b 1/4,y,z	{ m_{100} | 1/2 1/2 0 }

ITA data

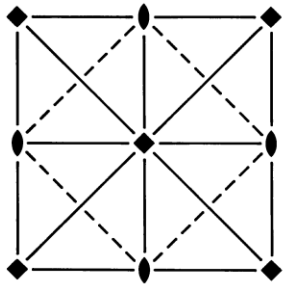
General positions

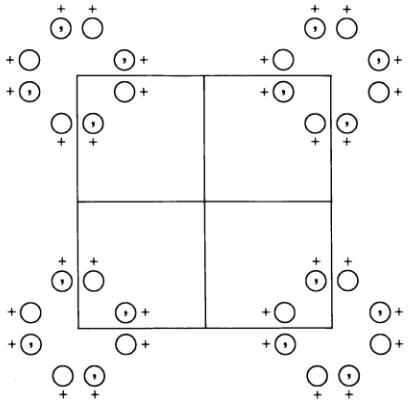
4 *c* 1 (1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$ (4) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$

Symmetry operations

(1) 1 (2) 2 0,0,z (3) a $x,\frac{1}{4},z$ (4) b $\frac{1}{4},y,z$

Wyckoff Position P4mm (No. 99)





Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	g	1	(1) x,y,z (5) $x,\bar{y},z$	(2) $\bar{x},\bar{y},z$ (6) $\bar{x},y,z$	(3) $\bar{y},x,z$ (7) $\bar{y},\bar{x},z$	(4) $y,\bar{x},z$ (8) y,x,z
4	f	. m .	$x,\frac{1}{2},z$	$\bar{x},\frac{1}{2},z$	$\frac{1}{2},x,z$	$\frac{1}{2},\bar{x},z$
4	e	. m .	$x,0,z$	$\bar{x},0,z$	$0,x,z$	$0,\bar{x},z$
4	d	. . m	x,x,z	$\bar{x},\bar{x},z$	$\bar{x},x,z$	$x,\bar{x},z$
2	c	2 m m.	$\frac{1}{2},0,z$	$0,\frac{1}{2},z$		
1	b	4 m m	$\frac{1}{2},\frac{1}{2},z$			
1	a	4 m m	$0,0,z$			

Multiplicity

Wyckoff letter

Site-symmetry

General positions

Special positions

Wyckoff Positions

WYCKPOS http://www.cryst.ehu.es/cryst/get_wp.html

Wyckoff Positions

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The available crystallographic data refer either to the standard/default setting of the chosen space group or to the so-called ITA Settings.

To get the data in any Non-conventional setting it is necessary to specify the corresponding transformation that relates the non-conventional to the standard/default setting of the space group.

Please, enter the sequential number of group as given in *International Tables for Crystallography*, Vol. A or choose it: 68

Standard/Default Setting | Non Conventional Setting | ITA Settings

Wyckoff Positions

WYCKPOS http://www.cryst.ehu.es/cryst/get_wp.html

Wyckoff Positions

How to select the group

The space groups are specified by their number as given in the *International Tables for Crystallography*, Vol. A. You can give this number, if you know it, or you can choose it from the table with the space group numbers and symbols if you click on the link **choose it**.

The available crystallographic data refer either to the standard/default setting of the chosen space group or to the so-called ITA Settings.

To get the data in any Non-conventional setting it is necessary to specify the corr
transformation that relates the nc
conventional to the standard/defa
the space group.

Please, enter the sequential number of group as given in *International Tables for Crystallography*, Vol. A or choose it: 68

Standard/Default Setting | Non Conventional Setting | ITA Settings

Standard (default) Choices for the Space Group Settings

The default choices for the standard (default) settings of the space groups are:

- *unique axis b (cell choice 1)* for space groups within the monoclinic system.
- obverse triple hexagonal unit cell for R space groups.
- the *origin choice two* - inversion center at (0,0,0) - for the centrosymmetric space groups for which there are two origin choices, within the orthorhombic, tetragonal and cubic systems.

Wyckoff Positions

WYCKPOS http://www.cryst.ehu.es/cryst/get_wp.html

Wyckoff Positions

How to select the group

The space groups are specified by their number as given in the *International Tables for Crystallography*, Vol. A. You can give this number, if you know it, or you can choose it from the table with the space group numbers and symbols if you click on the link **choose it**.

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Please, enter the sequential number of group as given in *International Tables for Crystallography*, Vol. A or choose it: 68

Standard/Default Setting | Non Conventional Setting | ITA Settings

ITA-Settings for the Space Group 68

Note: The transformation matrices must be read by columns. **P** is the transformation from standard to the ITA-setting.

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

ITA number	Setting	P	P^{-1}
68	*C c c* e [origin 1]	a,b+1/4,c+1/4	a,b-1/4,c-1/4
68	*A* e *a a* [origin 1]	c,a+1/4,b+1/4	b-1/4,c,a-1/4
68	*B b* e *b* [origin 1]	b,c+1/4,a+1/4	c-1/4,a-1/4,b
68	*C c c* e [origin 2]	a,b,c	a,b,c
68	*A* e *a a* [origin 2]	c,a,b	b,c,a
68	*B b* e *b* [origin 2]	b,c,a	c,a,b

Wyckoff Positions

WYCKPOS http://www.cryst.ehu.es/cryst/get_wp.html

Wyckoff Positions

How to select the group

The space groups are specified by their number as given in the *International Tables for Crystallography*, Vol. A. You can give this number, if you know it, or you can choose it from the table with the space group numbers and symbols if you click on the link **choose it**.

The available crystallographic data refer either to the standard/default setting of the chosen space group or to the so-called ITA Settings.

To get the data in any Non-conventional setting it is necessary to specify the corresponding transformation that relates the non-conventional to the standard/default setting of the space group.

Please, enter the sequential number of group as given in *International Tables for Crystallography*, Vol. A or choose it: 68

Standard/Default Setting | Non Conventional Setting | ITA Settings

Wyckoff Positions of Group *Ccce* (No. 68) [origin choice 2] in Non Conventional Setting

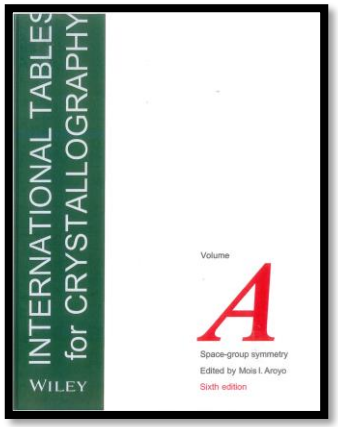
Please, enter the transformation:

Linear part			Origin shift
1	0	0	0
0	1	0	0
0	0	1	0

Change the basis

Wyckoff Positions

16	*i*	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z$	(3) $\bar{x},y,\bar{z}+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y},\bar{z}+\frac{1}{2}$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x+\frac{1}{2},y,\bar{z}$	(7) $x,\bar{y},z+\frac{1}{2}$	(8) $\bar{x}+\frac{1}{2},y,z+\frac{1}{2}$
8	*h*	. . 2	$\frac{1}{4},0,z$	$\frac{3}{4},0,\bar{z}+\frac{1}{2}$	$\frac{3}{4},0,\bar{z}$	$\frac{1}{4},0,z+\frac{1}{2}$
8	*g*	. . 2	$0,\frac{1}{4},z$	$0,\frac{1}{4},\bar{z}+\frac{1}{2}$	$0,\frac{3}{4},\bar{z}$	$0,\frac{3}{4},z+\frac{1}{2}$
8	*f*	. 2 .	$0,y,\frac{1}{4}$	$\frac{1}{2},\bar{y},\frac{1}{4}$	$0,\bar{y},\frac{3}{4}$	$\frac{1}{2},y,\frac{3}{4}$
8	*e*	2 . .	$x,\frac{1}{4},\frac{1}{4}$	$\bar{x}+\frac{1}{2},\frac{3}{4},\frac{1}{4}$	$\bar{x},\frac{3}{4},\frac{3}{4}$	$x+\frac{1}{2},\frac{1}{4},\frac{3}{4}$
8	*d*	$\bar{1}$	$0,0,0$	$\frac{1}{2},0,0$	$0,0,\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$
8	*c*	$\bar{1}$	$\frac{1}{4},\frac{3}{4},0$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{3}{4},\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$
4	*b*	2 2 2	$0,\frac{1}{4},\frac{3}{4}$	$0,\frac{3}{4},\frac{1}{4}$		
4	*a*	2 2 2	$0,\frac{1}{4},\frac{1}{4}$	$0,\frac{3}{4},\frac{3}{4}$		



Space Group : *Ccce* (No. 68) [origin choice 2]
Point : (0,1/4,1/4)
Wyckoff Position : 4a

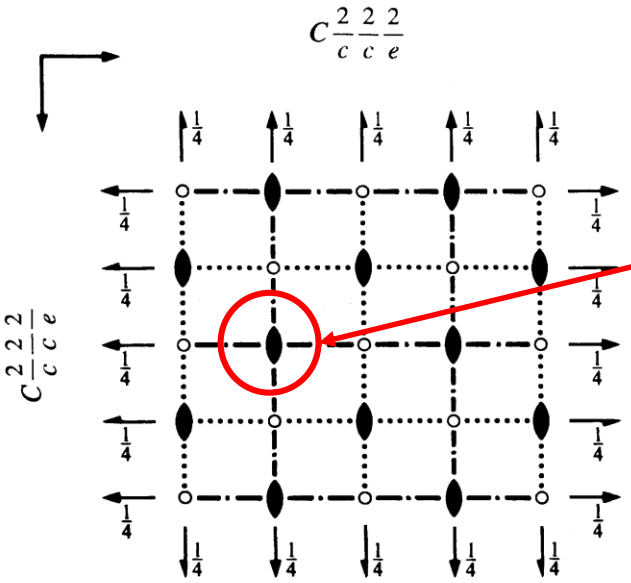
Site Symmetry Group 222

x,y,z	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	1
-x,y,-z+1/2	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1/2 \end{pmatrix}$	2 0,y,1/4
-x,-y+1/2,z	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 1/2 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	2 0,1/4,z
x,-y+1/2,-z+1/2	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 1/2 \\ 0 & 0 & -1 & 1/2 \end{pmatrix}$	2 x,1/4,1/4

Wyckoff Positions of Group *Ccce* (No. 68) [origin choice 2]

Multiplicity	Wyckoff letter	Site symmetry	Coordinates
			(0,0,0) + (1/2,1/2,0) +
16	i	1	(x,y,z) (-x+1/2,-y,z) (-x,y,-z+1/2) (x+1/2,-y,-z+1/2) (-x,-y,-z) (x+1/2,y,-z) (x,-y,z+1/2) (-x+1/2,y,z+1/2)
8	h	..2	(1/4,0,z) (3/4,0,-z+1/2) (3/4,0,-z) (1/4,0,z+1/2)
8	g	..2	(0,1/4,z) (0,1/4,-z+1/2) (0,3/4,-z) (0,3/4,z+1/2)
8	f	.2.	(0,y,1/4) (1/2,-y,1/4) (0,-y,3/4) (1/2,y,3/4)
8	e	2..	(x,1/4,1/4) (-x+1/2,3/4,1/4) (-x,3/4,3/4) (x+1/2,1/4,3/4)
8	d	-1	(0,0,0) (1/2,0,0) (0,0,1/2) (1/2,0,1/2)
8	c	-1	(1/4,3/4,0) (1/4,1/4,0) (3/4,3/4,1/2) (3/4,1/4,1/2)
4	b	222	(0,1/4,3/4) (0,3/4,1/4)
4	a	222	(0,1/4,1/4) (0,3/4,3/4)

Wyckoff Positions



1/2,y,1/4

2 x,1/4,1/4

Wyckoff position and site symmetry group of a specific point

Specify the point by its relative coordinates (in fractions or decimals)
Variable parameters (x,y,z) are also accepted

x = 1/2 y = 1/4 z = 1/4

Show

Space Group : *Ccce* (No. 68) [origin choice 2]
Point : (1/2,1/4,1/4)
Wyckoff Position : 4b

Site Symmetry Group 222

x,y,z	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	1
-x+1,y,-z+1/2	$\begin{pmatrix} -1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1/2 \end{pmatrix}$	2 1/2,y,1/4
-x+1,-y+1/2,z	$\begin{pmatrix} -1 & 0 & 0 & 1 \\ 0 & -1 & 0 & 1/2 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	2 1/2,1/4,z
x,-y+1/2,-z+1/2	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 1/2 \\ 0 & 0 & -1 & 1/2 \end{pmatrix}$	2 x,1/4,1/4

Exercise 1.1

ITA-conventional setting of space groups

Consider the space group $P2_1/c$ (No. 14). The relation between the *General* and *Special* position data of $P112_1/a$ (setting *unique axis c*) can be obtained from the data $P12_1/c1$(setting *unique axis b*) applying the transformation $(\mathbf{a'},\mathbf{b'},\mathbf{c'})_{\mathbf{c}} = (\mathbf{a},\mathbf{b},\mathbf{c})_{\mathbf{b}}\mathbf{P}$, with $\mathbf{P}= \mathbf{c},\mathbf{a},\mathbf{b}$.

Use the retrieval tools GENPOS (generators and general positions) and WYCKPOS (Wyckoff positions) for accessing the *IT*A data. Get the data on general and special positions in different settings either by specifying transformation matrices to new bases (Non-conventional Setting option), or by selecting one of the settings of the monoclinic groups listed in *IT*A (*IT*A Setting option).

Exercise 1.2

Non-conventional setting of space groups

Use the retrieval tools GENPOS or *Generators* and *General positions*, WYCKPOS (or *Wyckoff positions*) for accessing the space-group data on the *Bilbao Crystallographic Server*. Get the data on general and special positions in different settings either by specifying transformation matrices to new bases, or by selecting one of the 530 settings of the monoclinic and orthorhombic groups listed in ITA.

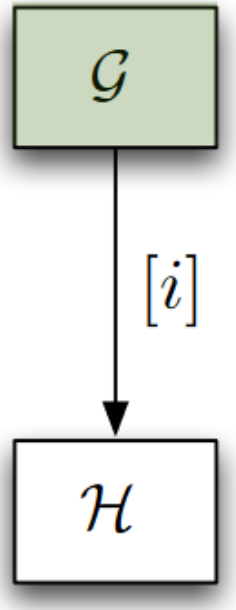
Consider the General position data of the space group *Im-3m* (No. 229). Using the option *Non-conventional setting* obtain the matrix-column pairs of the symmetry operations with respect to a primitive basis, applying the transformation (**a**',**b**',**c**') = 1/2(-**a**+**b**+**c**,**a**-**b**+**c**,**a**+**b**-**c**)

SYMMETRY RELATIONS OF SPACE GROUPS

Group-subgroup relations

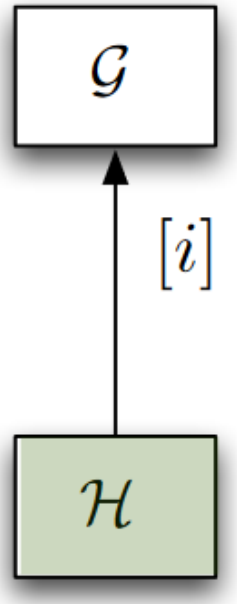
Applications

Group-subgroup relations



- Possible low symmetry structures
- Domain structure analysis
- Prediction of new structures

Group-supergroup relations



- Possible high-symmetry structures
- Prediction of phase transitions
- Determination of prototype structures

Subgroups types

Subgroup $H < G$ if $H = \{e, h_1, h_2, ..., h_k\} \subset G$ and H satisfies the group axioms.

There are three subgroup types:

$H < G$ is called a *translationengleiche subgroup* if G and H have the same group of translations, $T_H = T_G$ and H belongs to a crystal class of lower symmetry than G, $P_H < P_G$

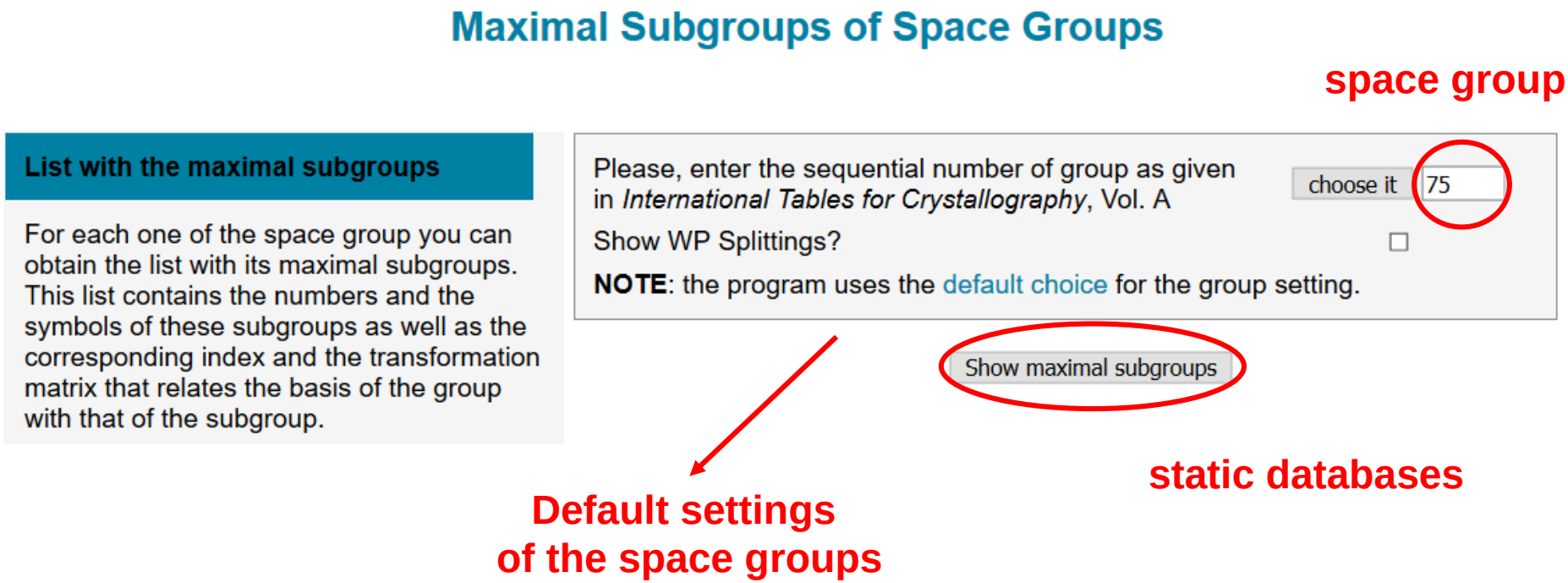
$H < G$ is called a *klassengleiche subgroup*, if G and H belong to the same crystal class, $P_H = P_G$; therefore, H has fewer translations than G, $T_H < T_G$

H is called *general subgroup* of G, if $T_H < T_G$ and $P_H < P_G$

H is a maximal subgroup of G if **NO** intermediate subgroup Z exist such that: $H < Z < G$

Maximal subgroups of space groups

MAXSUB http://www.cryst.ehu.es/cryst/maxsub.html



Maximal subgroups of space groups

Maximal subgroups of group *P*4 (No. 75)

Note: The program uses the default choice for the group settings.

In the following table the list of maximal subgroups is given. Click over "setting..." to see the possible setting(s) for the given subgroup.

N	IT number	HM symbol	Index	Transformations
1	3	*P*2	2	show..
2	75	*P*4	2	show..
3	75	*P*4	3	show..
4	75	*P*4	5	show..
5	75	*P*4	7	show..
6	75	*P*4	9	show..
7	77	$P4_2$	2	show..
8	79	*I*4	2	show..

Maximal subgroups of space groups

Maximal subgroups of group *P*4 (No. 75)

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1	3	*P*2	2	show..
2	75	*P*4	2	show..
3	75	*P*4	3	show..
4	75	*P*4	5	show..
5	75	*P*4	7	show..
6	75	*P*4	9	show..
7	77	$P4_2$	2	show..
8	79	*I*4	2	show..

Maximal subgroup(s) of type $P4_2$ (No. 77) of index 2

for Space Group *P*4 (No. 75)

Click over **[ChBasis]** to view the general positions of the subgroup in the basis of the supergroup.

Conjugacy class a

Subgroup(s)	Transformation Matrix	More...
group No 1	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	ChBasis

Maximal subgroups of space groups

International Tables for Crystallography, Vol. A1

ed. H. Wondratschek, U. Mueller

$P4$ No. 75 $P4$ C_4^1

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
4	*d*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},\bar{z}$

I Maximal *translationengleiche* subgroups

[2] $P2$ (3, $P112$) 1; 2

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}' = 2\mathbf{c}$			
$P4_2$ (77)	$\langle 2;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P4$ (75)	$\langle 2;\ 3\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
[2] $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$			
$C4$ (75, $P4$)	$\langle 2;\ 3\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
$C4$ (75, $P4$)	$\langle 2+(1,1,0);\ 3+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,1/2,0$
[2] $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$, $\mathbf{c}' = 2\mathbf{c}$			
$F4$ (79, $I4$)	$\langle 2;\ 3\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	
$F4$ (79, $I4$)	$\langle 2;\ 3+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$1/2,1/2,0$
[3] $\mathbf{c}' = 3\mathbf{c}$			
$P4$ (75)	$\langle 2;\ 3\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	

N	IT number	HM symbol	Index	Transformations
1	3	$P2$	2	show..
2	75	$P4$	2	show..
3	75	$P4$	3	show..
4	75	$P4$	5	show..
5	75	$P4$	7	show..
6	75	$P4$	9	show..
7	77	$P4_2$	2	show..
8	79	$I4$	2	show..

Subgroup(s)	Transformation Matrix	More...
group No 1	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	ChBasis

Exercise 2.1

(a) The retrieval tool MAXSUB gives an access to the database on maximal subgroups of space groups as listed in *IT*A1. Determine the maximal subgroups of the group *P*4*mm* (No. 99) using the program MAXSUB.

(b) Use the program SERIES and determine the isomorphic subgroups of the group *P4mm* (No. 99).

Maximal isomorphic subgroups

SERIES http://www.cryst.ehu.es/cryst/series.html

Series of Maximal Isomorphic Subgroups

space group

Series of maximal isomorphic subgroups

For each space group you can obtain the list with its maximal isomorphic subgroups. The list contains the numbers and the symbols of the maximal subgroups as well as, the corresponding index and the transformation matrix that relates the basis of the group with that of the subgroup. It is worth to take account of:

- the program uses the default choice for the group setting.
- only maximal isomorphic subgroups with index less or equal to 27 are displayed (125, in the case of cubic groups)

Please, enter the sequential number of group as given in *International Tables for Crystallography*, Vol. A

choose it 75

NOTE: Other possibility is to define a maximum index for the parametric series of maximal isomorphic subgroups.

Show series

static databases

Maximal isomorphic subgroups

Series of maximal isomorphic subgroups of group *P*4 (No. 75)

Note: Only series with an index less or equal to 27 are displayed

Series 1

Parametric form of the series 1 of maximal isomorphic subgroups of space group *P*4 (No. 75)

Subgroup	Index	Transformation	Conditions
*P*4 (75)	p	[1 0 0 0] [0 1 0 0] [0 0 p 0]	p prime

Number of conjugate subgroups: no conjugate subgroups

Click over **[show..]** to view a specific transformation for a given index

N	IT number	HM symbol	Index	Transformations
1	75	*P*4	2	show..
2	75	*P*4	3	show..
3	75	*P*4	5	show..
4	75	*P*4	7	show..
5	75	*P*4	11	show..
6	75	*P*4	13	show..
7	75	*P*4	17	show..
8	75	*P*4	19	show..
9	75	*P*4	23	show..

Static Databases

Maximal isomorphic subgroups

Series of maximal isomorphic subgroups of group *P*4 (No. 75)

Series 2

Parametric form of the series 2 of maximal isomorphic subgroups of space group *P*4 (No. 75)

Subgroup	Index	Transformation	Conditions
*P*4 (75)	p^2	[p 0 0 u] [0 p 0 v] [0 0 1 0]	prime p > 2 0 <= u < p 0 <= v < p

Number of conjugate subgroups: p^2 conjugate subgroups for p=4n-1

Click over **[show..]** to view a specific transformation for a given index

N	IT number	HM symbol	Index	Transformations
1	75	*P*4	9	show..

Maximal isomorphic subgroups

Series of maximal isomorphic subgroups of group *P*4 (No. 75)

Series 3

Parametric form of the series 3 of maximal isomorphic subgroups of space group *P*4 (No. 75)

Subgroup	Index	Transformation	Conditions
*P*4 (75)	$p=q^2+r^2$	[q r 0 u] [-r q 0 0] [0 0 1 0]	prime p > 4 q > 0 r > 0 0 <= u < p

Number of conjugate subgroups: p conjugate subgroups for p=4n+1

Click over **[show..]** to view a specific transformation for a given index

N	IT number	HM symbol	Index	Transformations
1	75	*P*4	5	show..
2	75	*P*4	13	show..
3	75	*P*4	17	show..

Maximal isomorphic subgroups

International Tables for Crystallography, Vol. A1
ed. H. Wondratschek, U. Mueller

$P4$ No. 75 $P4$ C_4^1

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{c}' = p\mathbf{c}$

$P4$ (75)	$\langle 2;\ 3\rangle$ $p > 1$ no conjugate subgroups	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	

$[p^2]$ $\mathbf{a}' = p\mathbf{a},\ \mathbf{b}' = p\mathbf{b}$

$P4$ (75)	$\langle 2+(2u,2v,0);\ 3+(u+v,-u+v,0)\rangle$ $p > 2;\ 0 \le u < p;\ 0 \le v < p$ p^2 conjugate subgroups for prime $p \equiv 3\ (\mathrm{mod}\ 4)$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$u, v, 0$

$[p = q^2 + r^2]$ $\mathbf{a}' = q\mathbf{a} - r\mathbf{b},\ \mathbf{b}' = r\mathbf{a} + q\mathbf{b}$

$P4$ (75)	$\langle 2+(2u,0,0);\ 3+(u,-u,0)\rangle$ $q > 0;\ r > 0;\ p > 4;\ 0 \le u < p$ p conjugate subgroups for prime $p \equiv 1\ (\mathrm{mod}\ 4)$	$q\mathbf{a} - r\mathbf{b}, r\mathbf{a} + q\mathbf{b}, \mathbf{c}$	$u, 0, 0$

Output SERIES

Subgroup	Index	Transformation	Conditions
*P*4 (75)	p	[1 0 0 0] [0 1 0 0] [0 0 p 0]	p prime

Subgroup	Index	Transformation	Conditions
*P*4 (75)	$p=q^2+r^2$	[q r 0 u] [-r q 0 0] [0 0 1 0]	prime p > 4 q > 0 r > 0 0 <= u < p

Subgroup	Index	Transformation	Conditions
*P*4 (75)	p^2	[p 0 0 u] [0 p 0 v] [0 0 1 0]	prime p > 2 0 <= u < p 0 <= v < p

Exercise 2.1

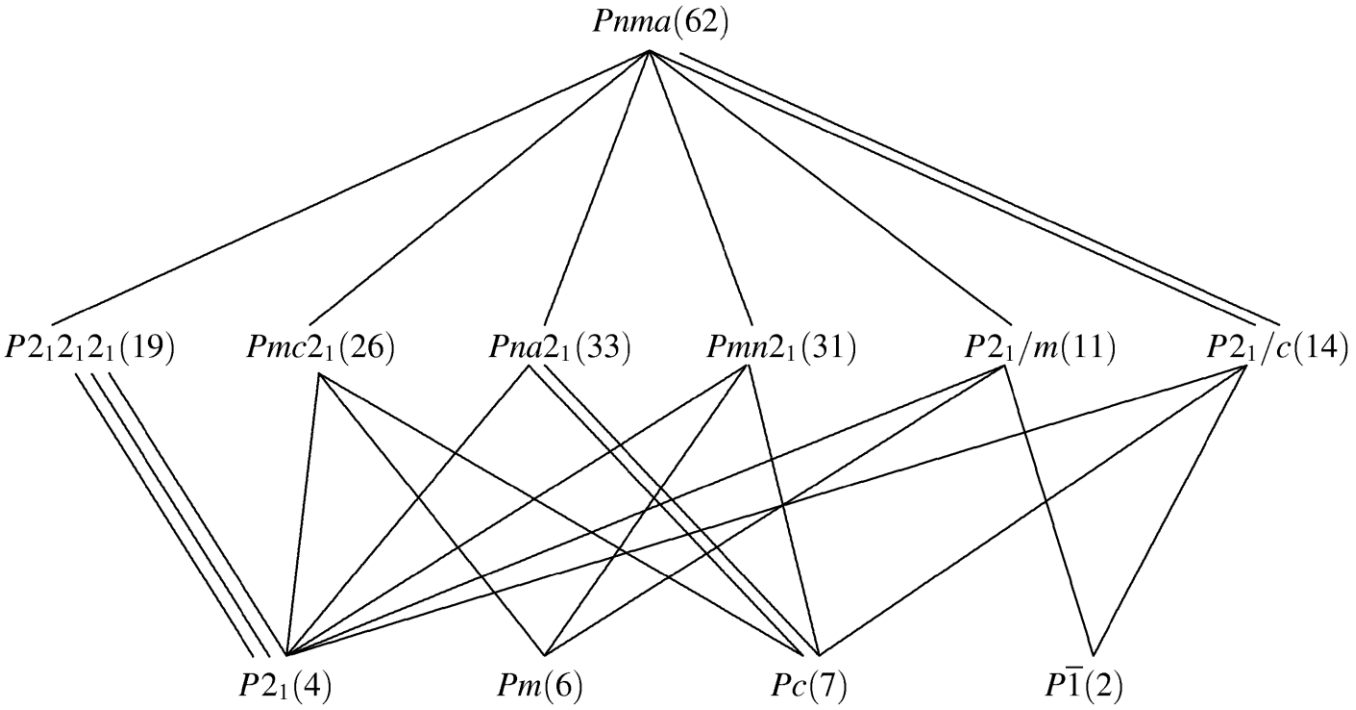
(a) The retrieval tool MAXSUB gives an access to the database on maximal subgroups of space groups as listed in *IT*A1. Determine the maximal subgroups of the group *P*4*mm* (No. 99) using the program MAXSUB.

(b) Use the program SERIES and determine the isomorphic subgroups of the group *P4mm* (No. 99).

Subgroups of Space Groups

International Tables for Crystallography, Vol. A1

ed. H. Wondratschek, U. Mueller



Graph of the *translationengleiche* subgroups of the space group *Pnma*

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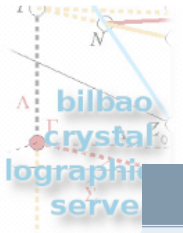

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workshops

News:

- New Article in Cryst. A 05/2019 *al.* "Automatic calc symmetry-adapted magnetic and non-r materials: a new to Bilbao Crystallogra *Acta Cryst.* (2019) 438-447.
- New Article in 03/2019: Vergniory 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

SUBGROUPGRAPH	Lattice of Maximal Subgroups
HERMANN	Distribution of subgroups in conjugated classes
COSETS	Coset decomposition for a group-subgroup pair
WYCKSPLIT	The splitting of the Wyckoff Positions
MINSUP	Minimal Supergroups of Space Groups
SUPERGROUPS	Supergroups of Space Groups
CELLSUB	List of subgroups for a given k-index.
CELLSUPER	List of supergroups for a given k-index.
NONCHAR	Non Characteristic orbits.
COMMONSUBS	Common Subgroups of Space Groups
COMMONSUPER	Common Supergroups of Two Space Groups
INDEX	Index of a group subgroup pair
SUBGROUPS ⚠	Subgroups of a space group consistent with some given supercell, propagation vector(s) or irreducible representation(s)

Point-group symmetry

Plane-group symmetry

Double point and space groups

Subgroups of Space Groups

SUBGROUPGRAPH http://www.cryst.ehu.es/cryst/subgroupgraph.html

Group-Subgroup Lattice and Chains of Maximal Subgroups

Lattice and chains ...

For a given group and supergroup the program SUBGROUPGRAPH will give the lattice of maximal subgroups that relates these two groups and, in the case that the index is specified, all of the possible chains of maximal subgroup that relate the two groups. In the latter case, also there is a possibility to obtain all of the different subgroups of the same type.

Please, enter the sequential numbers of group and subgroup as given in International Tables for Crystallography, Vol. A:

Enter supergroup number (G) or choose it:	10
Enter subgroup number (H) or choose it:	1
Enter the index [G:H] (optional):	4

Construct the lattice

Input:

- Group number (G)
- Subgroup number (H)
- The index [i] (optional)

Subgroups of Space Groups

Chains of maximal subgroups from *P2/m* (No. 10) [unique axis b] to *P*1 (No. 1) with index 4

Chains of subgroups ...

For each chain of maximal subgroups relating G = *P2/m* and H = *P*1 with index 4, there is a set of transformation matrices (P_j, p_j), where each matrix corresponds to a subgroup H_j isomorphic to H.

Click over "transformation" to see the list with the transformation matrices, obtained following the corresponding chain of maximal subgroups.

To see the contracted graph representing the chains, click on **[Show contracted graph]**.

To view the list with different subgroups of a given type and its distribution into the classes of conjugate subgroups click over **[Classify]** buttons.

The program distributes the subgroups into classes by comparing directly their elements in the group basis.

N	Chain [indices]	Chain with HM symbols	Number of subgroup chains	More info ...
1	010 003 001 [2 2]	*P2/m* > *P*2 > *P*1	4	transformation...
2	010 006 001 [2 2]	*P2/m* > *Pm* > *P*1	2	transformation...
3	010 002 001 [2 2]	*P2/m* > *P*-1 > *P*1	2	transformation...

Print this table.

Show contracted graph

Classify (with a complete graph of all subgroups)

Classify (with complete graphs for individual subgroups)

Subgroups of Space Groups

Chains of maximal subgroups from *P2/m* (No. 10) [unique axis b] to *P*1 (No. 1) with index 4

Chains of subgroups ...

For each chain of maximal subgroups relating G = *P2/m* and H = *P*1 with index 4, there is a set of transformation matrices (P_j, p_j), where each matrix corresponds to a subgroup H_j isomorphic to H.

Click over "transformation" to see the list with the transformation matrices, obtained following the corresponding chain of maximal subgroups.

To see the contracted graph representing the chains, click on **[Show contracted graph]**.

To view the list with different subgroups of a given type and its distribution into the classes of conjugate subgroups click over **[Classify]** buttons.

The program distributes the subgroups into classes by comparing directly their elements in the group basis.

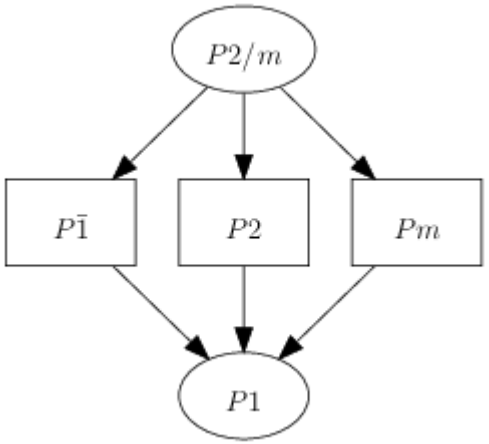
N	Chain [indices]	Chain with HM symbols	Number of subgroup chains	More info ...
1	010 003 001 [2 2]	*P2/m* > *P*2 > *P*1	4	transformation...
2	010 006 001 [2 2]	*P2/m* > *Pm* > *P*1	2	transformation...
3	010 002 001 [2 2]	*P2/m* > *P*-1 > *P*1	2	transformation...

Print this table.

Show contracted graph

Classify (with a complete graph c

Classify (with complete graphs for in



Exercise 2.2

With the help of the program SUBGROUPGRAPH obtain the graph of the *t*-subgroups of *P4mm* (No. 99). Explain the difference between the *contracted* and *complete* graphs of the *t*-subgroups of *P4mm* (No. 99).

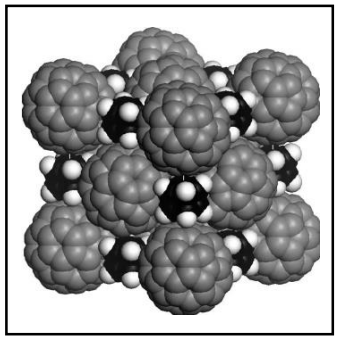
Exercise 2.3

Study the group-subgroup relations between the groups G=$P4_12_12$ (No. 92), and H=$P2_1$ (No. 4), using the program SUBGROUPGRAPH. Consider the cases with specified index *e.g*. [i]=4, and not specified index of the group-subgroup pair.

Group-subgroup phase transition

Possible symmetries of the low temperature phase of a fullerene-cubane crystal

Crystals that include both molecules of fullerene and cubane are known to crystallize at high temperatures in the Fm-3m space group, with the disordered fullerenes centred at the site 4a (0 0 0) and the disordered cubane molecules at 4b (1/2 1/2 1/2) (Nature Mat. 4, 764 (2005)). At low temperature, as the molecules become ordered, the system exhibits a couple of phase transitions. From powder diffraction experiments, the symmetry of the final phase has been reported to be an orthorhombic structure, with the lattice parameters of its primitive orthorhombic unit cell satisfying the approximate relations: $a \approx b \approx a_c/\sqrt{2}$, while $c \approx 2a_c$. However, the phase space group, and therefore its structure, could not be determined (J. Phys. Chem. B 113 2042 (2009)). Obviously, if we could restrict the symmetry of this phase to a minimal set of possible or most probable space groups, we could have a better chance of succeeding in the interpretation and analysis of its diffraction diagram.



Fm-3m

Unkown

structure data:
P orthorhombic
$a_o \approx b_o \approx a_c/\sqrt{2}$, $c_o \approx 2a_c$

Group-subgroup phase transition

SUBGROUP: http://www.cryst.ehu.es/cgi-bin/cryst/programs/subgrmag1_cell.pl

Subgroups: Subgroups compatible with a given supercell or some propagation vector(s).

Enter the serial number of the space group: choose it 225

Alternatively give the operations of the space group in a non-standard setting

The parent space group

Introduce the supercell

Alternatively give the modulation wave-vectors

a_S=	b_S=	c_S=
1/2 a	1/2 a	0 a
+	+	+
-1/2 b	1/2 b	0 b
+	+	+
0 c	0 c	2 c

The supercell is centred: P

primitive

The lattice supercell

. . .

Possible limitations of the subgroup list.

(Check only one option on the left and the specific value on the right)

(Check only one option on the left and the specific value on the right)

- ○ Lowest space group to consider — choose it 1
- ○ Lowest point group to consider — -------
- ◉ Lowest crystal system to consider — Orthorhombic
- ○ Only maximal subgroups

Group-subgroup phase transition

Possible solutions for point group mmm

35	*Pnma* (No. 62)	$\begin{pmatrix} 0 & -1/2 & -1/2 & 0 \\ 0 & 1/2 & -1/2 & 1/4 \\ 2 & 0 & 0 & -1/4 \end{pmatrix}$	24=4x6	Conjugacy Class	Get irreps
36	*Pmmn* (No. 59)	$\begin{pmatrix} 1/2 & -1/2 & 0 & 0 \\ 1/2 & 1/2 & 0 & 1/4 \\ 0 & 0 & 2 & -1/4 \end{pmatrix}$	24=4x6	Conjugacy Class	Get irreps
37	*Pccn* (No. 56)	$\begin{pmatrix} 1/2 & -1/2 & 0 & 0 \\ 1/2 & 1/2 & 0 & 1/4 \\ 0 & 0 & 2 & 1/4 \end{pmatrix}$	24=4x6	Conjugacy Class	Get irreps
38	*Pmma* (No. 51)	$\begin{pmatrix} 0 & -1/2 & -1/2 & 0 \\ 0 & 1/2 & -1/2 & 0 \\ 2 & 0 & 0 & 1/2 \end{pmatrix}$	24=4x6	Conjugacy Class	Get irreps
39	*Pccm* (No. 49)	$\begin{pmatrix} 1/2 & -1/2 & 0 & 0 \\ 1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	24=4x6	Conjugacy Class	Get irreps
40	*Pmmm* (No. 47)	$\begin{pmatrix} 1/2 & -1/2 & 0 & 0 \\ 1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	24=4x6	Conjugacy Class	Get irreps

Group-subgroup phase transition

Possible solutions for point group mm2

48	*Pna*2_1 (No. 33)	$\begin{pmatrix} 0 & -1/2 & 1/2 & -1/8 \\ 0 & 1/2 & 1/2 & 1/8 \\ -2 & 0 & 0 & -1/4 \end{pmatrix}$	48=4x12	Conjugacy Class	Get irreps
49	*Pmn*2_1 (No. 31)	$\begin{pmatrix} 1/2 & 0 & -1/2 & 0 \\ -1/2 & 0 & -1/2 & 0 \\ 0 & 2 & 0 & 1/4 \end{pmatrix}$	48=4x12	Conjugacy Class	Get irreps
50	*Pma*2 (No. 28)	$\begin{pmatrix} 0 & -1/2 & 1/2 & 0 \\ 0 & 1/2 & 1/2 & 0 \\ -2 & 0 & 0 & 0 \end{pmatrix}$	48=4x12	Conjugacy Class	Get irreps
51	*Pcc*2 (No. 27)	$\begin{pmatrix} 1/2 & -1/2 & 0 & 0 \\ 1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	48=4x12	Conjugacy Class	Get irreps
52	*Pmc*2_1 (No. 26)	$\begin{pmatrix} 1/2 & -1/2 & 0 & 0 \\ 1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	48=4x12	Conjugacy Class	Get irreps
53	*Pmm*2 (No. 25)	$\begin{pmatrix} 0 & -1/2 & 1/2 & 0 \\ 0 & 1/2 & 1/2 & 0 \\ -2 & 0 & 0 & 1/2 \end{pmatrix}$	48=4x12	Conjugacy Class	Get irreps
54	*Pmm*2 (No. 25)	$\begin{pmatrix} 1/2 & -1/2 & 0 & 0 \\ 1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix}$	48=4x12	Conjugacy Class	Get irreps

Group-subgroup phase transition

Possible solutions for point group 222

59	$P2_12_12_1$ (No. 19)	$\begin{pmatrix} 1/2 & -1/2 & 0 & 1/8 \\ 1/2 & 1/2 & 0 & 1/8 \\ 0 & 0 & 2 & 1/4 \end{pmatrix}$	48=4x12	Conjugacy Class	Get irreps
60	$P2_12_12$ (No. 18)	$\begin{pmatrix} 1/2 & 1/2 & 0 & 0 \\ -1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & -1/4 \end{pmatrix}$	48=4x12	Conjugacy Class	Get irreps
61	$P222_1$ (No. 17)	$\begin{pmatrix} 1/2 & 1/2 & 0 & 0 \\ -1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	48=4x12	Conjugacy Class	Get irreps
62	$P222$ (No. 16)	$\begin{pmatrix} 1/2 & -1/2 & 0 & 0 \\ 1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 2 & 1/2 \end{pmatrix}$	48=4x12	Conjugacy Class	Get irreps

CRYSTAL-STRUCTURE DESCRIPTIONS

www.cryst.ehu.es

FCT/ZTF

bilbao crystallographic server

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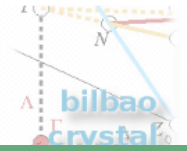


Space-group symmetry

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

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/dresden2019/

You need to download:

- StructuresExercises.txt

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 **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

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) (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)

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)

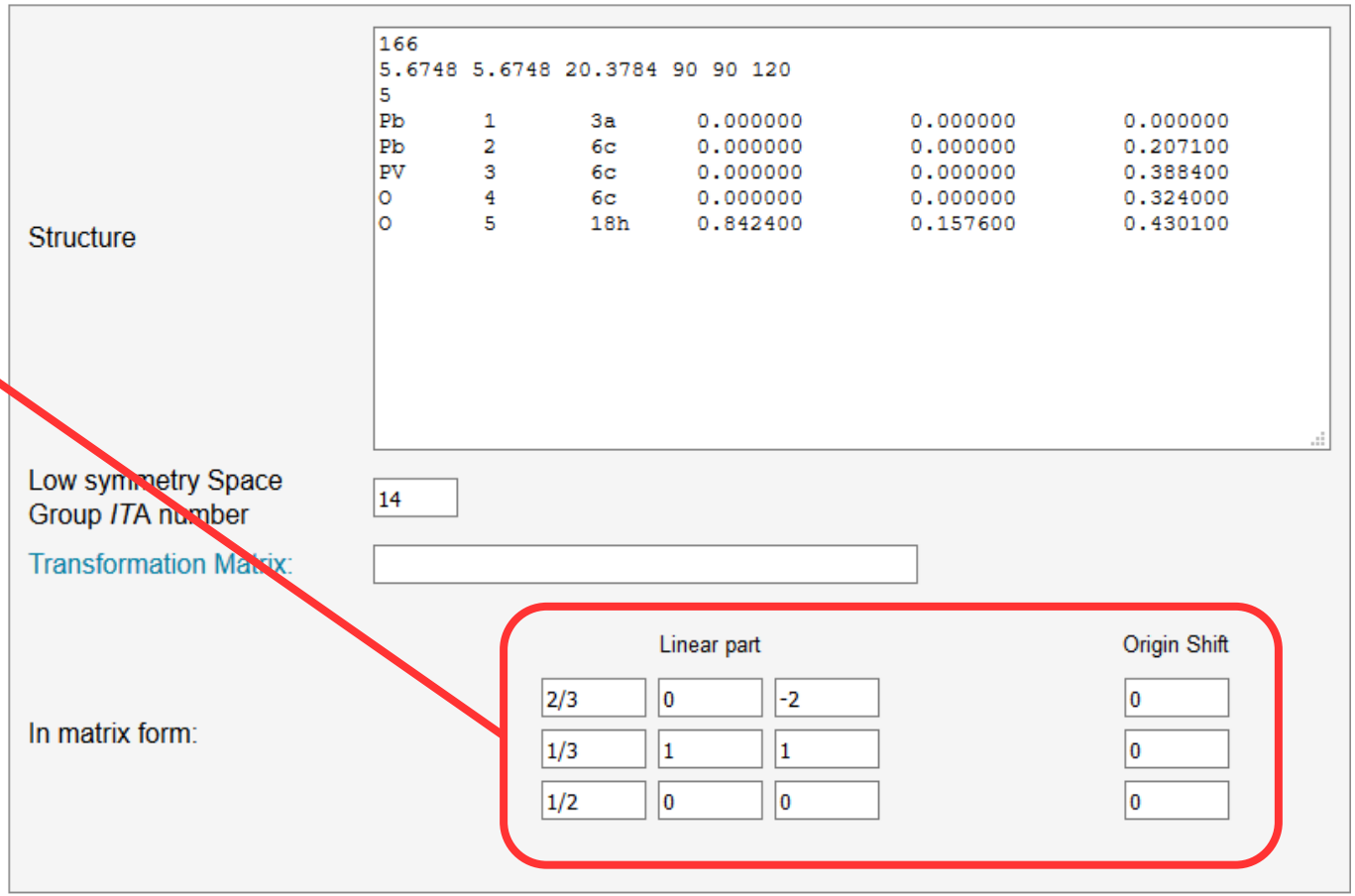
(P,p)

Description $P2_1/c$ (No. 14)

Validity (P,p)

WP splitting

$Pb_3(VO_4)_2$

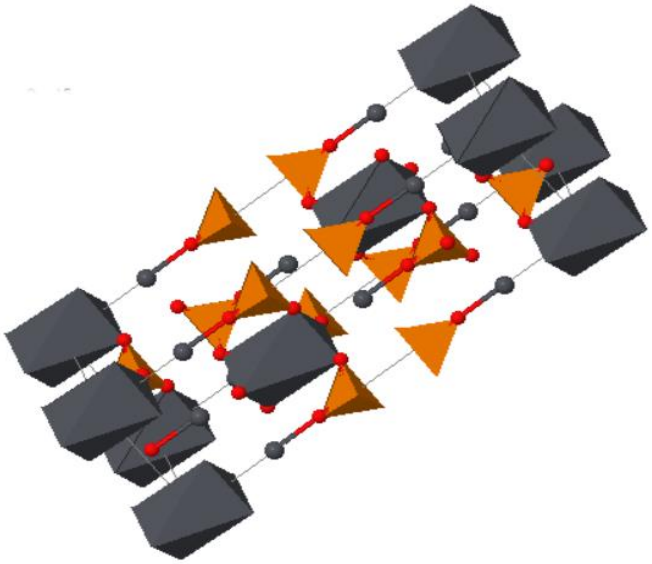


Structure transformation

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

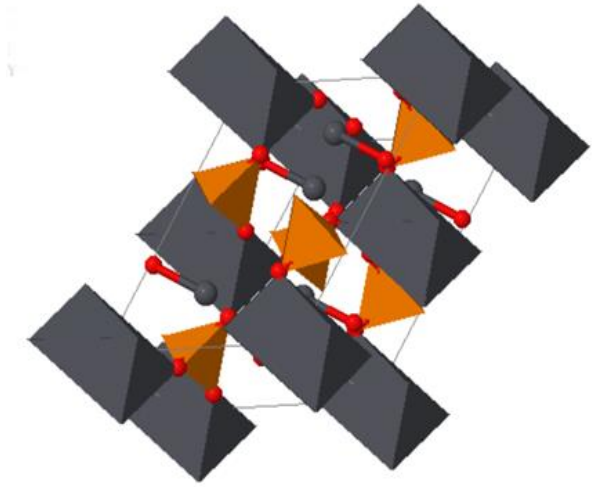


(P,p)=2/3**a**+1/3**b**+1/3**c**,**b**,-2**a**-**b**

Low symmetry structure

014
7.530264 5.673900 9.827483 90.000000 115.786674 90.000000
7

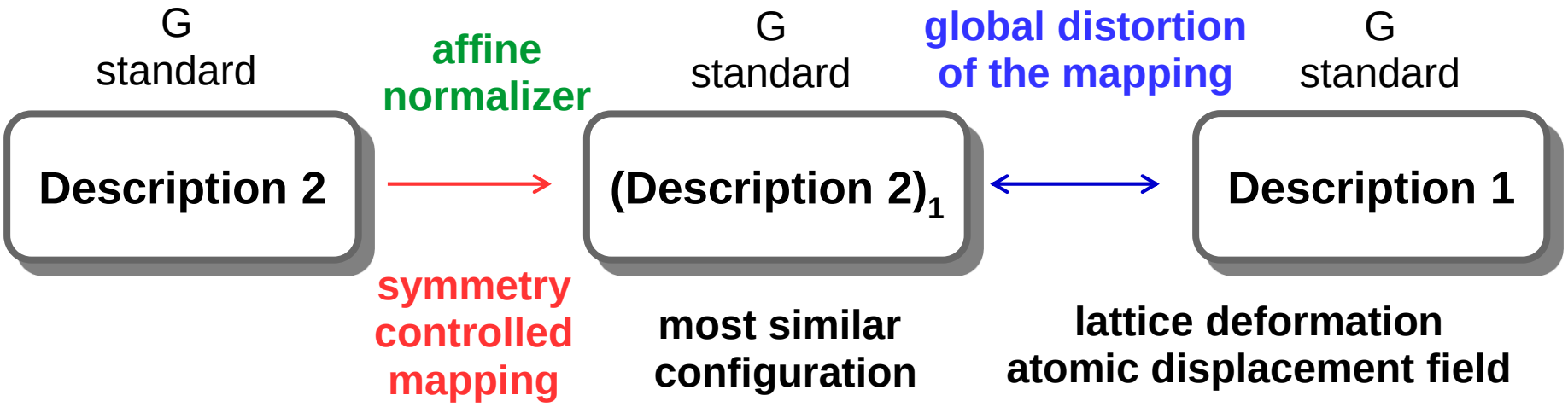
Pb	1	2a	0.000000	0.000000	0.000000
Pb	2	4e	0.621900	0.000000	0.207300
PV	1	4e	0.177200	0.000000	0.392400
O	1	4e	0.974100	0.000000	0.324700
O	2	4e	0.289700	0.735050	0.008250
O	2_2	4e	0.289700	0.500000	0.773200
O	2_3	4e	0.710300	0.764950	0.491750



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

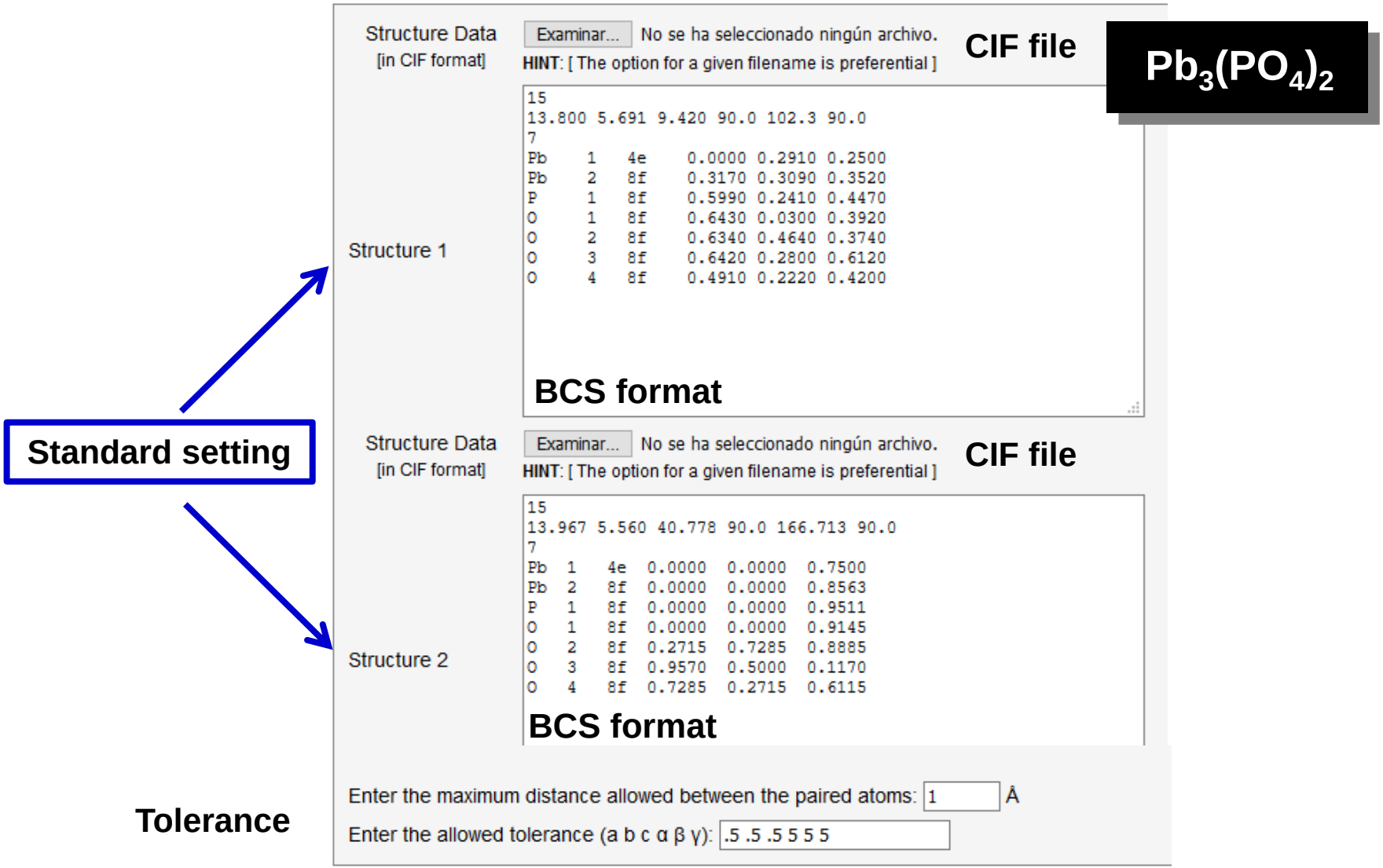
$$\Delta(d) = \frac{[(b_1/a_1)(c_1/a_1)]}{[(b_2/a_2)(c_2/a_2)]}$$

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



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

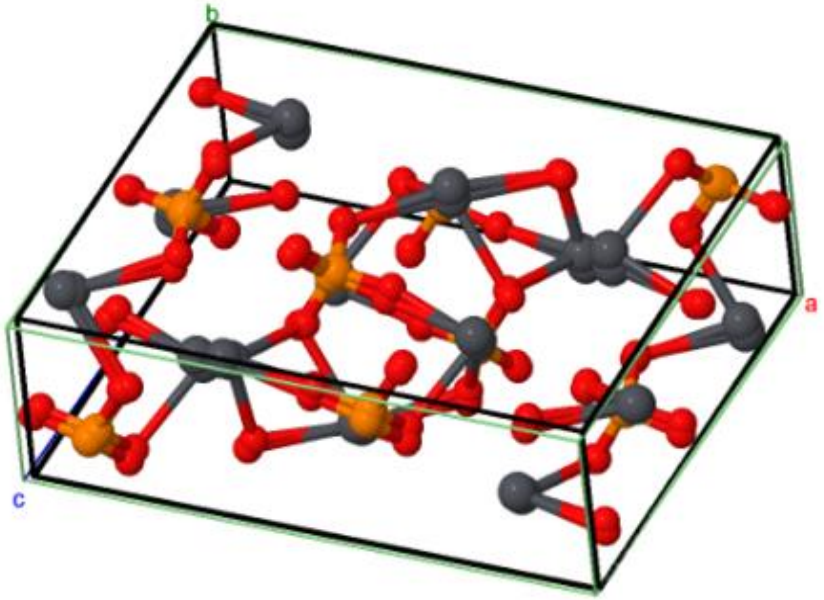
```
015
13.967000 5.560000 9.630055 90.000000 103.295059 90.000000
7
Pb      1       4e      0.500000        0.250000        0.750000
Pb      2       8f      0.818900        0.250000        0.856300
P       1       8f      0.103300        0.250000        0.951100
O       1       8f      0.993500        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 3.1

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)	0.1580(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)	0.1506(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

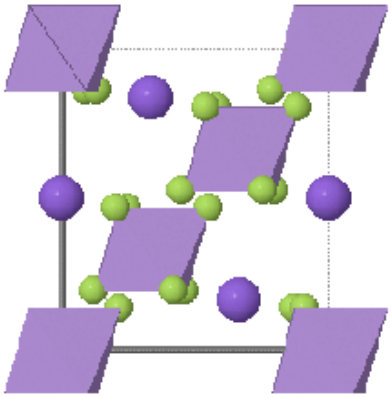
CC=415250	Details Bonds Pattern Structure Jmol
Title	Synthesis and structural analysis of epsilon-(Fe2 O3).
Authors	Kelm, K.;Mader, W.
Reference	Zeitschrift fuer Anorganische und Allgemeine Chemie (2005) **631**, 2363-2369 **Link XRef SCOPUS SCIRUS Google**
Compound	**Fe2 O3** - Diiron(III) oxide - epsilon **[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	0.668(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 3.2

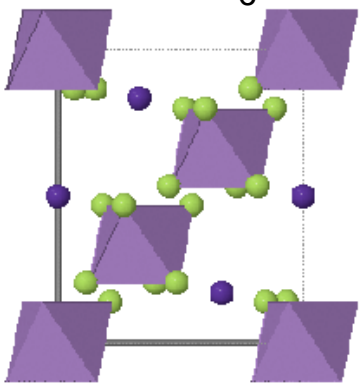
Do these compounds belong to the **same structure type** ?

$KAsF_6$



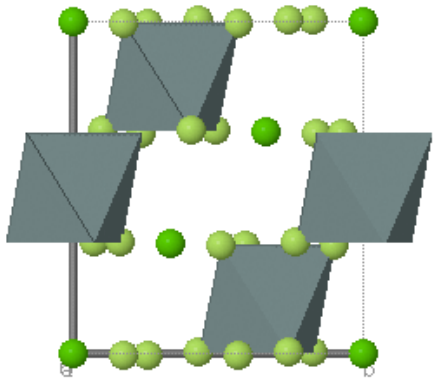
```
148
7.3480 7.3480 7.2740 90.00 90.00 120.00
3
K     1   3b    0.333333 0.666666 0.166666
As    1   3a    0 0 0
F     1   18f   0.1292 0.2165 0.1381
```

$BaIrF_6$



```
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

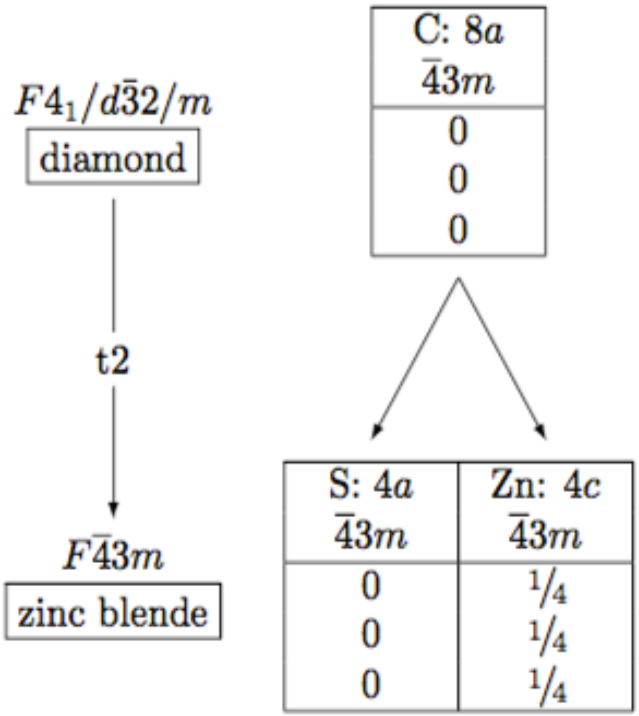
CRYSTAL-STRUCTURE RELATIONS

Structure relations

Symmetry relations using crystallographic group-subgroup relations is a vaulable tool in crystal chemistry and physics.

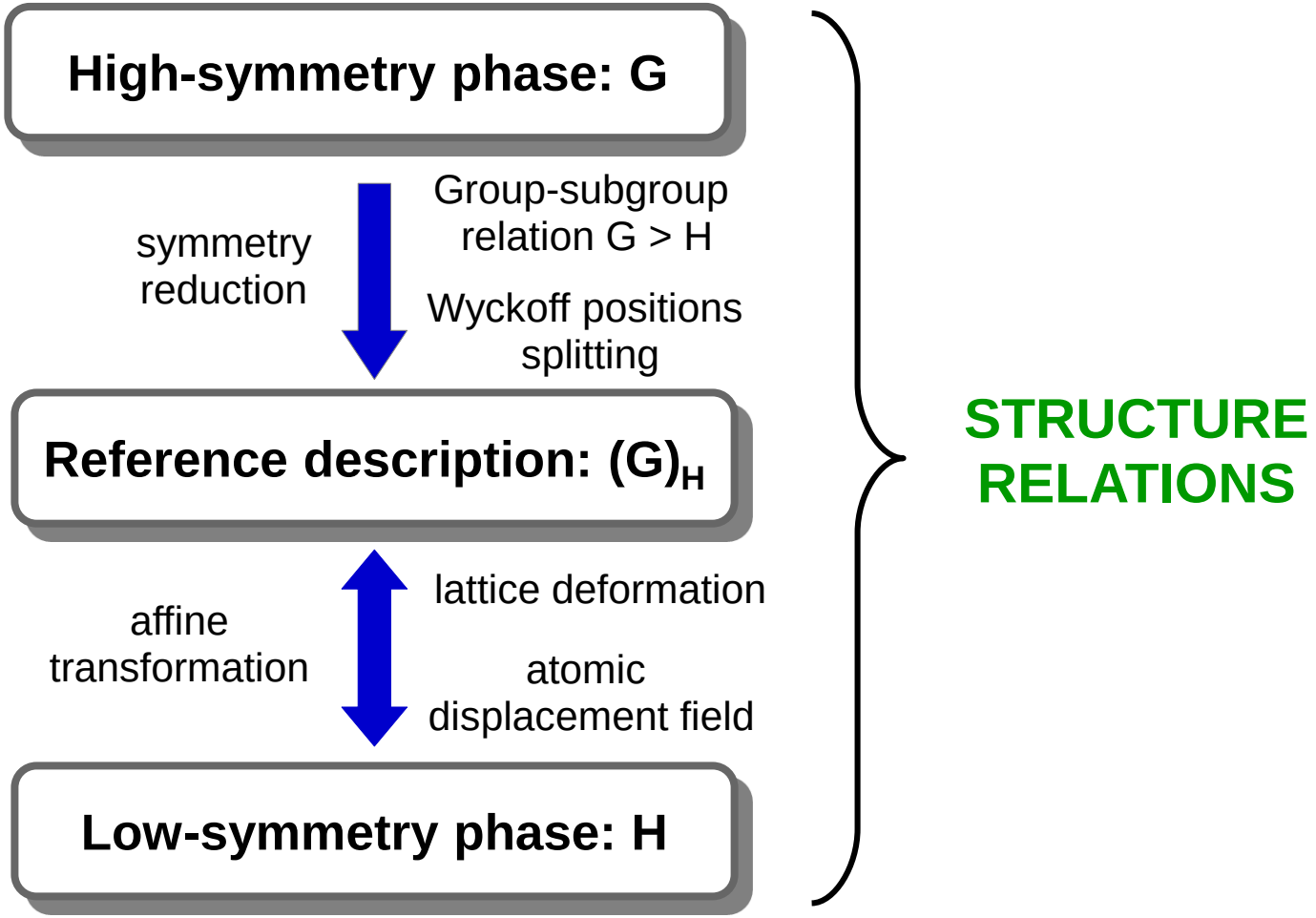
Applications

- Family trees of group-subgroup relations (Bärnighausen tree)
- Twinned crystals and antiphase domains
- Phase transitions
- Prediction of crystal-structure types



Structure relations

Structural Relationship between two structures with group-subgroup related symmetry groups **G > H**



Structure relations

High symmetry structure

Enter the formula units in the **high symmetry structure**
(Leave blank for auto-detection via the volume information)

Structure Data
[CIF format]

Examinar... No se ha seleccionado ningún archivo.

BCS Format

```
# Space Group ITA number
221
# Lattice parameters
4.006 4.006 4.006 90 90 90
# Number of independent atoms in the asymmetric unit
3
# [atom type] [number] [WP] [x] [y] [z]
Ba   1 1a 0.0 0.0 0.0
Ti   1 1b 0.5 0.5 0.5
O    1 3c 0.5 0.0 0.5
```

Low symmetry structure:

Enter the formula units in the **low symmetry structure**
(Leave blank for auto-detection via the volume information)

Structure Data
[CIF format]

Examinar... No se ha seleccionado ningún archivo.

BCS Format

```
# Space Group ITA number
38
# Lattice parameters
3.9828 5.6745 5.6916 90 90 90
# Number of independent atoms in the asymmetric unit
4
# [atom type] [number] [WP] [x] [y] [z]
Ba   1 2a 0.0 0.0 0
Ti   1 2b 0.5 0.0 0.5170
O    1 2a 0.0 0.0 0.4890
O    2 4e 0.5 0.2561 0.2343
```

Calculation parameters:

Enter the allowed tolerance (a b c α β γ): .2 .2 .3 2 2 2

Enter the maximum distance allowed between the paired atoms: 1.5 Å

One or both of the structures are given in a non-standard setting? ◉ No | ○ Yes

Calculation method:

◉ The group-subgroup transformation matrices are automatically fetched from the database.

○ User defined group-subgroup transformation matrix : a,b,c;0,0,0

STRUCTURE RELATIONS

http://www.cryst.ehu.es/cryst/rel.html

$BaTiO_3$

Structure relations

Pm-3m high-symmetry phase

$$(\mathbf{P},p)=\begin{pmatrix} 0 & 1 & 1 & 0.00510 \\ 0 & -1 & 1 & 0.00510 \\ 1 & 0 & 0 & 0 \end{pmatrix}$$

Symmetry controlled mapping

(High-symmetry phase)$_{Amm2}$

Global distortion

Lattice deformation
Atomic displacement field

Amm2 low-symmetry phase

High Symmetry Structure

```
221
4.006 4.006 4.006 90 90 90
3
Ba      1    1a     0.000000 0.000000 0.000000
Ti      1    1b     0.500000 0.500000 0.500000
O       1    3c     0.500000 0.000000 0.500000
```

```
038
4.006000 5.665339 5.665339 90.000000 90.000000 90.000000
4
Ba      1       2a      0.000000        0.000000        0.994920
Ti      1       2b      0.500000        0.000000        0.494920
O       1       4e      0.500000        0.250000        0.244920
O       12      2a      0.000000        0.000000        0.494920
```

Low Symmetry Structure

```
38
3.9828 5.6745 5.6916 90 90 90
4
Ba      1    2a     0.000000 0.000000 0.000000
Ti      1    2b     0.500000 0.000000 0.517000
O       1    2a     0.000000 0.000000 0.489000
O       2    4e     0.500000 0.256100 0.234300
```

Structure relations

WP		Atom	Atomic Displacements			
			u_x	u_y	u_z	|u|
2a	(0,0,z)	Ba1	0.0000	0.0000	-0.0051	0.0289
2b	(1/2,0,z)	Ti1	0.0000	0.0000	-0.0221	0.1257
2a	(0,0,z)	O12	0.0000	0.0000	0.0059	0.0337
4e	(1/2,y,z)	O1	0.0000	-0.0061	0.0106	0.0697

High Symmetry Structure

```
221
4.006 4.006 4.006 90 90 90
3
Ba      1    1a     0.000000 0.000000 0.000000
Ti      1    1b     0.500000 0.500000 0.500000
O       1    3c     0.500000 0.000000 0.500000
```

```
038
4.006000 5.665339 5.665339 90.000000 90.000000 90.000000
4
Ba      1       2a      0.000000        0.000000        0.994920
Ti      1       2b      0.500000        0.000000        0.494920
O       1       4e      0.500000        0.250000        0.244920
O       12      2a      0.000000        0.000000        0.494920
```

Evaluation of the Global Distortion

S	$d_{max.}$ (Å)	$d_{av.}$ (Å)	Δ
0.0025	0.1257	0.0655	0.035

Low Symmetry Structure

```
38
3.9828 5.6745 5.6916 90 90 90
4
Ba      1    2a     0.000000 0.000000 0.000000
Ti      1    2b     0.500000 0.000000 0.517000
O       1    2a     0.000000 0.000000 0.489000
O       2    4e     0.500000 0.256100 0.234300
```

Exercise 4.1

Cristobalite phase transitions

At low temperatures, the space-group symmetry of cristobalite is given by the space group is $P4_12_12$ (92) with lattice parameters $a = 4.9586\mathring{A}$, $c = 6.9074\mathring{A}$. The four silicon atoms are located in Wyckoff position $4(a)..2$ with the coordinates $x, x, 0; -x, -x, 1/2; 1/2 - x, 1/2 + x, 1/4; 1/2 + x, 1/2 - x, 3/4$, $x = 0.3028$. During the phase transition, the tetragonal structure is transformed into a cubic one with space group $Fd\bar{3}m(227)$, $a = 7.147A$. It is listed in the space-group tables with two different origins.

1. If Origin choice 2 setting is used (with point symmetry $\bar{3}m$ at the origin), then the silicon atoms occupy the position $8(a)$ $\bar{4}3m$ with the coordinates 1/8, 1/8, 1/8; 7/8, 3/8, 3/8 and those related by the face - centring translations. Describe the structural distortion from the cubic to the tetragonal phase by the determination of (i) the displacements if the Si atoms in relative and absolute units, and (ii) the lattice distortion accompanying the transition.
2. Repeat the calculations for the characterization of the phase transition using the *Origin-choice 1* description of the high-symmetry phase (*cf. Exercise Data* file for the structure data).

Exercise 4.2 (a)

Lead phosphate phase transition

(a) Lead phosphate $Pb_3(PO_4)_2$ shows a phase transition from a paraelastic high-temperature phase with symmetry $R\bar{3}m$ (No.166) to a ferroelastic phase of symmetry $C2/c$ (No.15). Using the structure data given in the *ExerciseData* file and the tools of the *Bilbao Crystallographic Server*:

(a) characterize the symmetry reduction between the high- and low-symmetry phases (index and transformation matrix);

(b) describe the structural distortion from the rhombohedral to the monoclinic phase by the evaluation of the lattice strain and the atomic displacements accompanying the phase transition.

Exercise 4.2 (b)

Lead vanadate phase transition

(b) Lead phosphate-vanadate $Pb_3(PVO_4)_2$ shows a phase transition from a paraelastic high-temperature phase with symmetry $R\bar{3}m$ (No.166) to a ferroelastic phase of symmetry $P2_1/c$ (No.14). Using the structure data given in the *ExerciseData* file and the tools of the *Bilbao Crystallographic Server* describe the structural distortion from the rhombohedral to the monoclinic phase by the evaluation of the lattice strain and the atomic displacements accompanying the phase transition.

Bärnighausen Trees

Pyrite Structural Family

Aristotype

Basic structure

$P\,2_1/a\,\bar{3}$

FeS_2

Fe:4*a* $\bar{3}$	S: 8*c* 3
0	0.384 [0.616]
0	0.384 [0.616]
0	0.384 [0.616]

t2

t3

$P\,2_1\,3$

NiAsS

Ni: 4*a* 3	S: 4*a* 3	As: 4*a* 3
−0.006	0.385	0.618
−0.006	0.385	0.618
−0.006	0.385	0.618

Hettotypes

Derivatie structures

$P\,2_1/b\,2_1/c\,2_1/a$

PdS_2

Pd:4*a* $\bar{1}$	S:8*c* 1
0	0.393 [0.607]
0	0.388 [0.612]
0	0.425 [0.575]

t2

$-\frac{1}{4}, 0, 0$

$x+\frac{1}{4}, y, z$

$P\,b\,c\,2_1$

CoAsS

Co:4*a* 1	S:4*a* 1	As:4*a* 1
0.259	0.631	0.869
–0.005	0.383	0.619
0	0.380	0.617

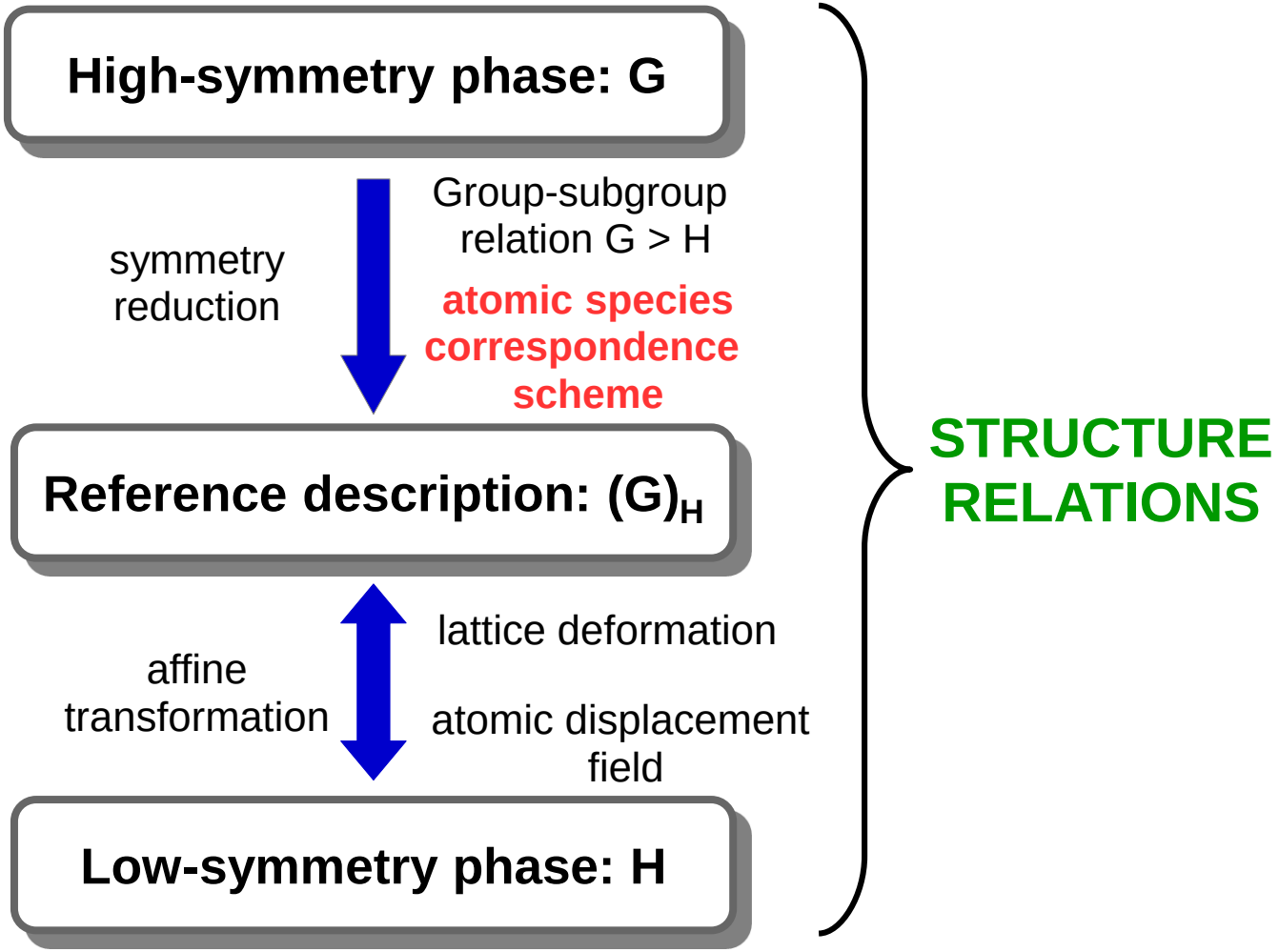
lattice parameters in pm:

	a	*b*	*c*	references
FeS_2	541.8	541.8	541.8	[80]
NiAsS	568.9	568.9	568.9	[107]
PdS_2	546.0	554.1	753.1	[108]
CoAsS	558.9	558.3	558.1	[109]

U. Mueller, Gargnano 2008

Symmetry relations between crystal structures

Structural Relationship between two structures with group-subgroup related symmetry groups **G > H**



Symmetry relations between crystal structures

High symmetry structure

Enter the formula units in the **high symmetry structure**
(Leave blank for auto-detection via the volume information)

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

BCS Format

```
221
3.007 3.007 3.007 90. 90. 90.
3
Al   1    48n 0.170000     0.290000     0.470000
```

Low symmetry structure:

Enter the formula units in the **low symmetry structure**
(Leave blank for auto-detection via the volume information)

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

BCS Format

```
099
4.252540 4.252540 3.00700          000 90.000000 90.
15
Fe   1    8g   0.910000     0.380000     0.170000
Fe   1_2  8g   0.620000     0.090000     0.830000
Fe   1_3  8g   0.440000     0.730000     0.470000
Fe   1_4  8g   0.270000     0.560000     0.530000
Fe   1_5  8g   0.650000     0.820000     0.290000
Fe   1_6  8g   0.820000     0.650000     0.710000
Fe   1_7  8g   0.410000     0.880000     0.170000
Fe   1_8  8g   0.120000     0.590000     0.830000
Fe   1_9  8g   0.940000     0.230000     0.470000
Fe   1_10    8g   0.770000     0.060000     0.530000
Fe   1_11    8g   0.150000     0.320000     0.290000
Fe   1_12    8g   0.320000     0.150000     0.710000
```

Different atomic species

Calculation parameters:

Enter the allowed tolerance (a b c α β γ): 2 2 2 2 2 2

Enter the maximum distance allowed between the paired atoms: 1.5 Å

One or both of the structures are given in a non-standard setting? ◉ No | ○ Yes

Calculation method:

◉ The group-subgroup transformation matrices are automatically fetched from the database.

○ User defined group-subgroup transformation matrix : a,b,c;0,0,0

Species Matching:

☐ Force a species match even if the two structures contain the same types of elements

Exercise 4.3

Hettotype of CsCl structure

Show that the crystal structure of CoU maybe interpreted as a slightly distorted CsCl (or b-brass, CuZn)-type structure. Using the structural data in the Exercise Data file, characterize the structural relationship between the CuZn structure and CoU structure.

#CuZn (CsCl type): Pm-3m
221
2.959 2.959 2.959 90. 90. 90.
2
Cu 1 1a 0.0 0.0 0.0
Zn 1 1b 0.5 0.5 0.5

#CoU type:$I2_13$
199
6.3557 6.3557 6.3557 90. 90. 90.
2
Co 1 8a 0.2940 0.2940 0.2940
U 1 8a 0.0347 0.0347 0.0347

Exercise 4.4

HT-quartz and LT-quartz

(a) Upon heating above 573 ºC the LT-quartz transforms to its HT form. Set up the corresponding Bärnighausen tree that describes the symmetry relations between the two quartz forms. Which additional degree of freedom are present in the lower symmetry form? (The crystal structures of HT-quartz and LT-quartz can be found in the ExerciseData file.)

(b) Consider the structure data of $AlPO_4$ listed in the ExerciseData file. Describe its structural relationship to quartz and construct the corresponding Bärnighausen tree.

Hint:

In order to find the structural relationship between quartz and $AlPO_4$ consider the splitting of Si positions into two: one for Al and one for P.