Summer School on Mathematical Crystallography

3-7 June 2019, Nancy (France)

International Union of CrystallographyCommision on Mathematical and Theoretical Crystallography

SYMMETRY DATABASES OF THE BILBAO CRYSTALLOGRAPHIC SERVER

Gemma de la Flor Martin
Karlsruhe Institute of Technology

Karlsruher Institut für Technologie

SYMMETRY DATABASES

Symmetry operations – matrix-column representation

Symmetry operations – geometric interpretation

General and special Wyckoff positions and site-symmetry

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Bilbao Crystallographic Server in forthcoming schools and workshops

News:

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

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

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Space-group symmetry

Magnetic Symmetry and Applications

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.

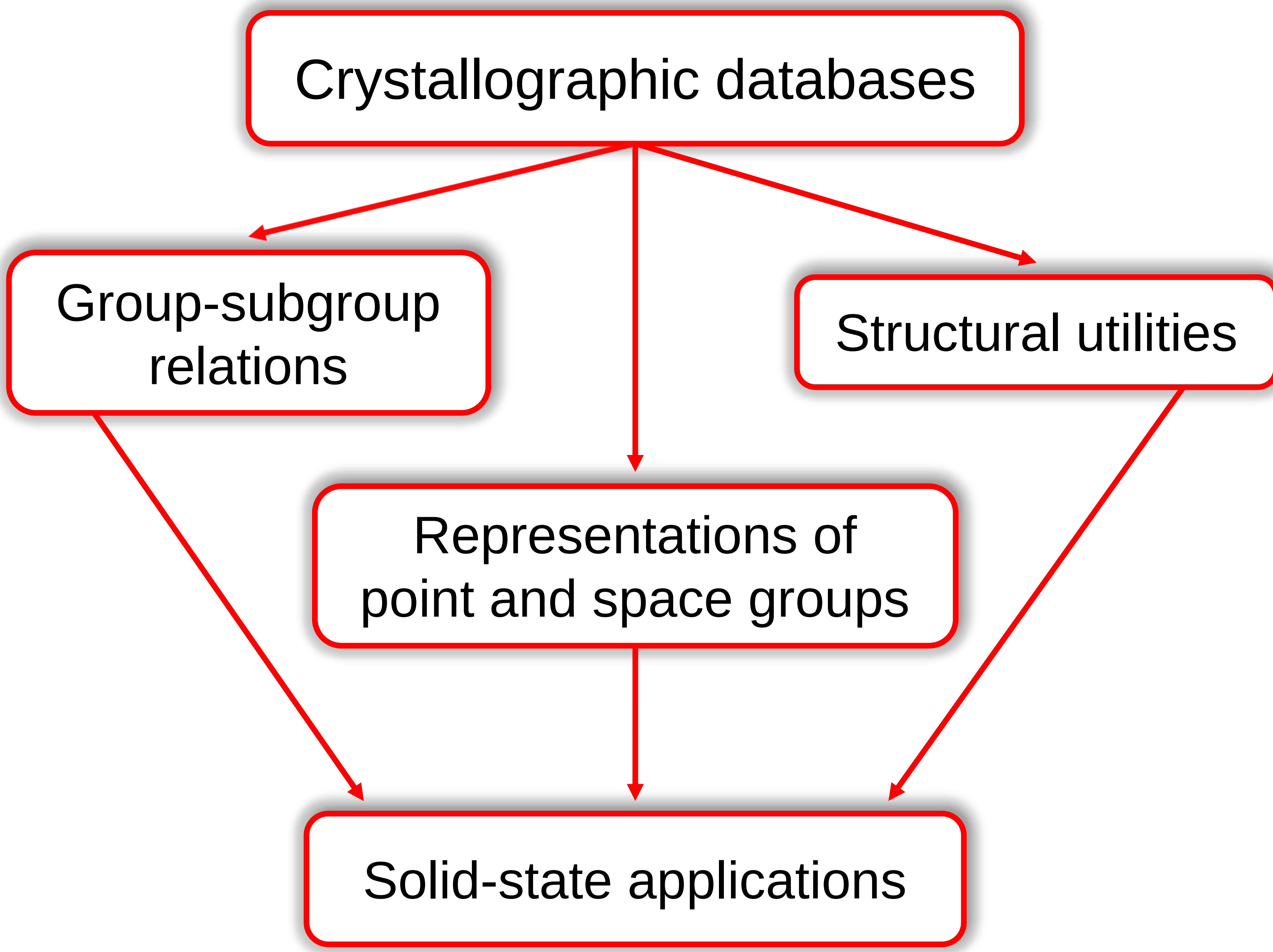
- Updated versions of TENSOR and MTENSOR 03/2019: The programs give the general expression of tensor properties for a given point group and magnetic point group, respectively..

Raman and Hyper-Raman scattering

Point-group symmetry

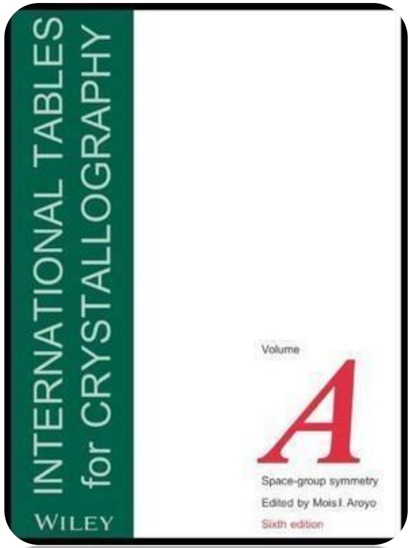
Plane-group symmetry

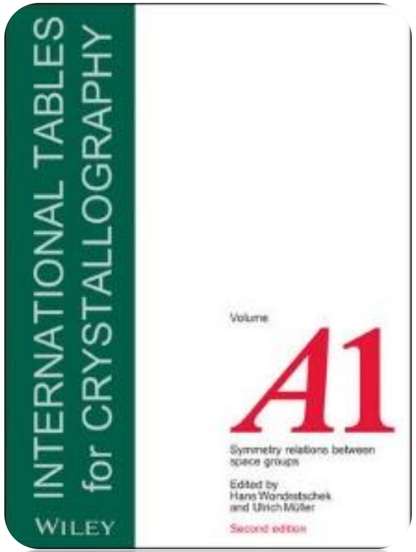
Double point and space groups


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

Crystallographic databases

International Tables for Crystallography

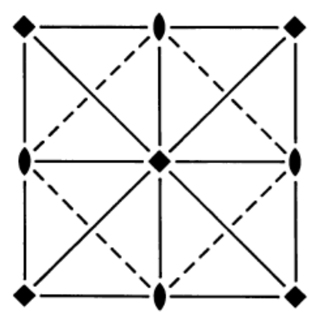


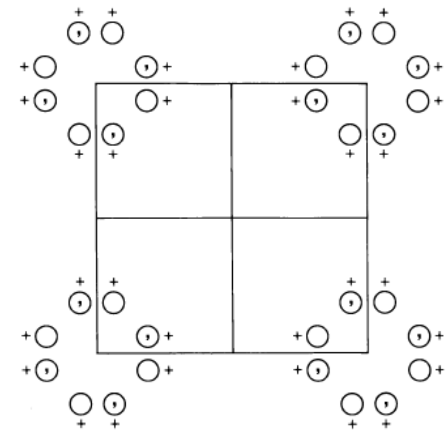


Crystallographic databases

GENERAL LAYOUT: LEFT-HAND PAGE

$P4mm$	C_{4v}^{1}	$4mm$	Tetragonal
No. 99	$P4mm$		Patterson symmetry $P4/mmm$





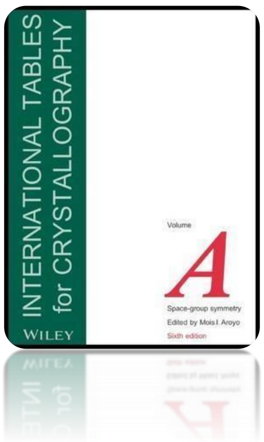
Origin on $4mm$

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

No. 99 $P4mm$

HKLCOND

GENPOS

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

Positions

WYCKPOS

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
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	no conditions
							Special:
4	f	$.m.$	$x,\frac{1}{2},z$	$\bar{x},\frac{1}{2},z$	$\frac{1}{2},x,z$	$\frac{1}{2},\bar{x},z$	no extra conditions
4	e	$.m.$	$x,0,z$	$\bar{x},0,z$	$0,x,z$	$0,\bar{x},z$	no extra conditions
4	d	$..m$	x,x,z	$\bar{x},\bar{x},z$	$\bar{x},x,z$	$x,\bar{x},z$	no extra conditions
2	c	$2mm.$	$\frac{1}{2},0,z$	$0,\frac{1}{2},z$			hkl : $h+k=2n$
1	b	$4mm$	$\frac{1}{2},\frac{1}{2},z$				no extra conditions
1	a	$4mm$	$0,0,z$				no extra conditions

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 $x,x,0$

MAXSUB

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)

SERIES

Maximal isomorphic subgroups of lowest index

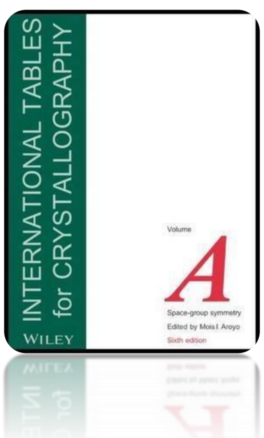
IIc [2] $P4mm$ ($\mathbf{c}'=2\mathbf{c}$) (99); [2] $C4mm$ ($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$) ($P4mm$, 99)

MINSUP

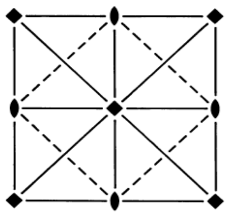
Minimal non-isomorphic supergroups

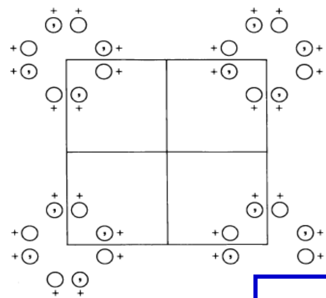
I [2] $P4/mmm$ (123); [2] $P4/nmm$ (129)

II [2] $I4mm$ (107)



$P4mm$	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

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

HKLCOND

Positions

GENPOS

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
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							Special:
4	f	$.m.$	$x,\frac{1}{2},z$	$\bar{x},\frac{1}{2},z$	$\frac{1}{2},x,z$	$\frac{1}{2},\bar{x},z$	no extra conditions
4	e	$.m.$	$x,0,z$	$\bar{x},0,z$	$0,x,z$	$0,\bar{x},z$	no extra conditions
4	d	$..m$	x,x,z	$\bar{x},\bar{x},z$	$\bar{x},x,z$	$x,\bar{x},z$	no extra conditions
2	c	$2mm.$	$\frac{1}{2},0,z$	$0,\frac{1}{2},z$			hkl : $h+k=2n$
1	b	$4mm$	$\frac{1}{2},\frac{1}{2},z$				no extra conditions
1	a	$4mm$	$0,0,z$				no extra conditions

WYCKPOS

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] $p1m1$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
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Maximal non-isomorphic subgroups

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Maximal isomorphic subgroups of lowest index

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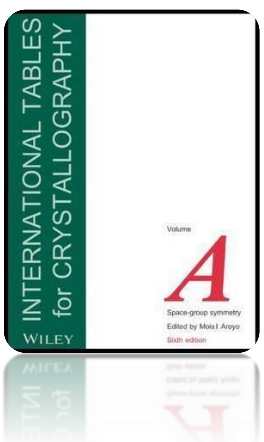
SERIES

Minimal non-isomorphic supergroups

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

II [2] $I4mm$ (107)

MINSUP



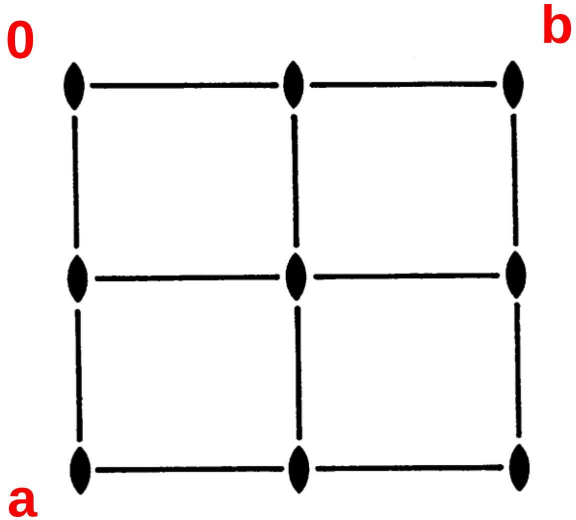
SYMMETRY OPERATIONS

MATRIX-COLUMN REPRESENTATION

Symmetry operations

Example: Pmm2

Diagram of symmetry elements



Coordinates

General positions

4 i 1 (1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $x,\bar{y},z$ (4) $\bar{x},y,z$

T_G	$T_G 2$	$T_G m_y$	$T_G m_x$
$(1,0)$	$(2,0)$	$(m_y,0)$	$(m_x,0)$
$(1,t_1)$	$(2,t_1)$	(m_y,t_1)	(m_x,t_1)
$(1,t_2)$	$(2,t_2)$	(m_y,t_2)	(m_x,t_2)
...	...	...	...
$(1,t_j)$	$(2,t_j)$	(m_y,t_j)	(m_x,t_j)
...	...	...	...

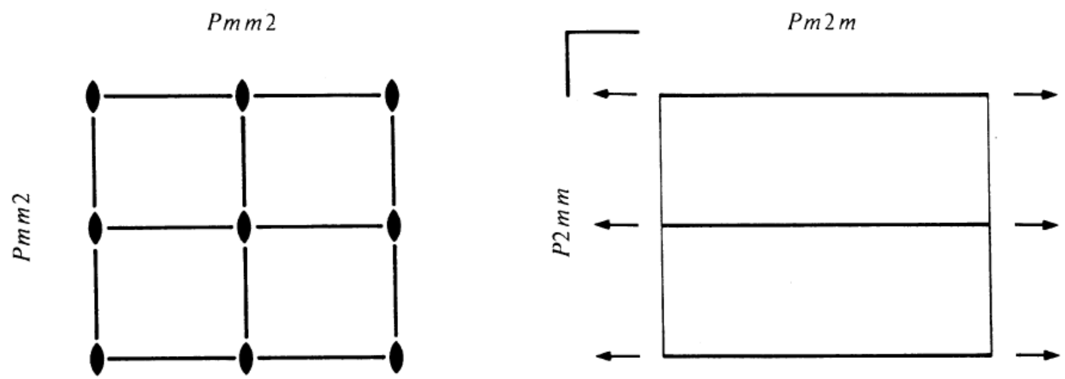
Symmetry operations

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

Symmetry operations

$Pmm2$ | 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

Matrix-column presentation

4 i 1 (1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $x,\bar{y},z$ (4) $\bar{x},y,z$

Geometric interpretation

Symmetry operations

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

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-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

Space group number

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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 ... group.

If you are using this program i... please cite it in the following fo...

Aroyo, et. al. Zeitschrift fuer K... 1, 15-...

If you are interested in other p... Crystallographic Server, click h...

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]

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.

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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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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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]

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.

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

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 *Pba*2 (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 $\frac{1}{4},y,z$

Seitz Symbol for Symmetry Operations

Seitz symbols { **R | t** }

short-hand descriptions of the matrix-column presentations of the symmetry operations of the space groups

- rotation part **R**

specify the type and the order of the symmetry operation

orientation of the symmetry element by the direction of the axis for rotations and rotoinversions, or the direction of the normal to reflection planes

1 and $\bar{1}$	identity and inversion
m	reflections
2, 3, 4 and 6	rotations
$\bar{3}$, $\bar{4}$ and $\bar{6}$	rotoinversions

- translation part t

Translation parts of the coordinate triplets of the *General position* block

Seitz symbols for Symmetry Operations

$P2_1/c$

No. 14

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

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

$$(1)\ x,y,z \quad (2)\ \bar{x},y+\tfrac{1}{2},\bar{z}+\tfrac{1}{2} \quad (3)\ \bar{x},\bar{y},\bar{z} \quad (4)\ x,\bar{y}+\tfrac{1}{2},z+\tfrac{1}{2}$$

The geometric descriptions given in the Symmetry Operations block in ITA are:

$$(1)\ 1 \quad (2)\ 2(0,\tfrac{1}{2},0)\ 0,y,\tfrac{1}{4} \quad (3)\ \bar{1}\ 0,0,0 \quad (4)\ c\ x,\tfrac{1}{4},z$$

The Seitz notation are given as

$$(1)\ \{1|0\} \quad (2)\ \{2_{010}|0,\tfrac{1}{2},\tfrac{1}{2}\} \quad (3)\ \{\bar{1}|0\} \quad (4)\ \{m_{010}|0,\tfrac{1}{2},\tfrac{1}{2}\}$$

Seitz Symbol for Symmetry Operations

Example

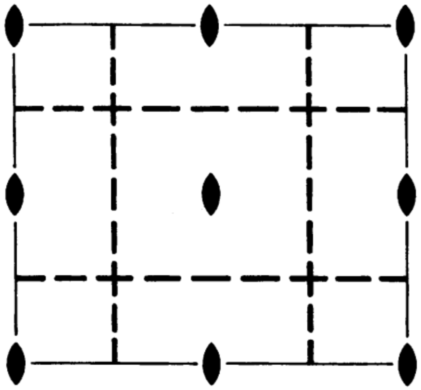
Seitz symbols for symmetry operations of rhombohedral, hexagonal and trigonal crystal systems

ITA description				Seitz symbol
No.	Coordinate triplet	Type	Orientation	
1	x, y, z	1		1
2	z, x, y	3^+	x, x, x	3^+_{111}
3	y, z, x	3^-	x, x, x	3^-_{111}
4	$\bar{z}, \bar{y}, \bar{x}$	2	$\bar{x}, 0, x$	$2_{\bar{1}01}$
5	$\bar{y}, \bar{x}, \bar{z}$	2	$x, \bar{x}, 0$	$2_{1\bar{1}0}$
6	$\bar{x}, \bar{z}, \bar{y}$	2	$0, y, \bar{y}$	$2_{01\bar{1}}$
7	$\bar{x}, \bar{y}, \bar{z}$	$\bar{1}$		$\bar{1}$
8	$\bar{z}, \bar{x}, \bar{y}$	$\bar{3}^+$	x, x, x	$\bar{3}^+_{111}$
9	$\bar{y}, \bar{z}, \bar{x}$	$\bar{3}^-$	x, x, x	$\bar{3}^-_{111}$
10	z, y, x	m	x, y, x	$m_{\bar{1}01}$
11	y, x, z	m	x, x, z	$m_{1\bar{1}0}$
12	x, z, y	m	x, y, y	$m_{01\bar{1}}$

ITA description				Seitz symbol
No.	Coordinate triplet	Type	Orientation	
1	x, y, z	1		1
2	$\bar{y}, x-y, z$	3^+	$0, 0, z$	3^+_{001}
3	$\bar{x}+y, \bar{x}, z$	3^-	$0, 0, z$	3^-_{001}
4	$\bar{x}, \bar{y}, z$	2	$0, 0, z$	2_{001}
5	$y, \bar{x}+y, z$	6^-	$0, 0, z$	6^-_{001}
6	$x-y, x, z$	6^+	$0, 0, z$	6^+_{001}
7	$y, x, \bar{z}$	2	$x, x, 0$	2_{110}
8	$x-y, \bar{y}, \bar{z}$	2	$x, 0, 0$	2_{100}
9	$\bar{x}, \bar{x}+y, \bar{z}$	2	$0, y, 0$	2_{010}
10	$\bar{y}, \bar{x}, \bar{z}$	2	$x, \bar{x}, 0$	$2_{1\bar{1}0}$
11	$\bar{x}+y, y, \bar{z}$	2	$x, 2x, 0$	2_{120}
12	$x, x-y, \bar{z}$	2	$2x, x, 0$	2_{210}
13	$\bar{x}, \bar{y}, \bar{z}$	$\bar{1}$		$\bar{1}$
14	$y, \bar{x}+y, \bar{z}$	$\bar{3}^+$	$0, 0, z$	$\bar{3}^+_{001}$
15	$x-y, x, \bar{z}$	$\bar{3}^-$	$0, 0, z$	$\bar{3}^-_{001}$
16	$x, y, \bar{z}$	m	$x, y, 0$	m_{001}
17	$\bar{y}, x-y, \bar{z}$	$\bar{6}^-$	$0, 0, z$	$\bar{6}^-_{001}$
18	$\bar{x}+y, \bar{x}, \bar{z}$	$\bar{6}^+$	$0, 0, z$	$\bar{6}^+_{001}$
19	$\bar{y}, \bar{x}, z$	m	$x, \bar{x}, z$	m_{110}
20	$\bar{x}+y, y, z$	m	$x, 2x, z$	m_{100}
21	$x, x-y, z$	m	$2x, x, z$	m_{010}
22	y, x, z	m	x, x, z	$m_{1\bar{1}0}$
23	$x-y, \bar{y}, z$	m	$x, 0, z$	m_{120}
24	$\bar{x}, \bar{x}+y, z$	m	$0, y, z$	m_{210}

Glazer *et al.* *Acta Cryst.*(2014). **A**70, 300–302

Example: Space group Pba2 (No. 32)



$Pba2$	C_{2v}^{8}	$mm2$	Orthorhombic
No. 32	$Pba2$		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

Matrix-column presentation

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

Geometric interpretation

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

Seitz symbols

(1) { 1 | 0 } (2) { 2_{001} | 0 } (3) { m_{010} | 1/2 1/2 0 } (4) {m_{100}| 1/2 1/2 0}

SYMMETRY OPERATIONS

GEOMETRIC INTERPRETATION

Geometrical Interpretation of (W,w)

Rotational part (W)

1. Type of isometry

	$\det(\boldsymbol{W})=+1$					$\det(\boldsymbol{W})=-1$				
$\mathrm{tr}(\boldsymbol{W})$	3	2	1	0	-1	-3	-2	-1	0	1
type	1	6	4	3	2	$\bar{1}$	$\bar{6}$	$\bar{4}$	$\bar{3}$	$\bar{2}=m$
order	1	6	4	3	2	2	6	4	6	2

2. Axis or normal direction u $\quad \boldsymbol{W}\boldsymbol{u}=\pm\boldsymbol{u}$

2.1 Rotations $\quad \mathbf{Y}(\mathbf{W})=\mathbf{W}^{n-1}+\mathbf{W}^{n-2}+\cdots+\mathbf{W}+\mathbf{I}$

2.2 Rotoinversions $\quad \mathbf{Y}(-\mathbf{W})$

2.3 Reflections $\quad \mathbf{Y}(-\mathbf{W})=-\mathbf{W}+\mathbf{I}$

3. Sense of rotation $\quad \mathbf{Z}=[\mathbf{u}|\mathbf{x}|\det(\mathbf{W})\mathbf{W}\cdot\mathbf{x}]$

Geometrical Interpretation of (W,w)

Translational part (w)

4. Intrinsic translation

4.1 Screw vector $\mathbf{w}_g = \frac{1}{n}(\mathbf{Y} \cdot \mathbf{w})$

4.2 Reflection plane $\mathbf{w}_g = \frac{1}{2}(\mathbf{W} + \mathbf{I})$

5. Location symmetry element

5.1 $\mathbf{w}_g = 0$ $(\mathbf{W}, \mathbf{w})\mathbf{x}_F = \mathbf{x}_F$

5.2 $\mathbf{w}_g \neq 0$ $(\mathbf{W}, \mathbf{w}_l)\mathbf{x}_F = \mathbf{x}_F$ where $\mathbf{w}_l = \mathbf{w} - \mathbf{w}_g$

Geometrical Interpretation of (W,w)

Ia-3d (No. 230)

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

$$\mathbf{W} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix} ; \quad \mathbf{w} = \begin{pmatrix} 3/4 \\ 1/4 \\ 1/4 \end{pmatrix}$$

Geometrical Interpretation of (W,w)

Ia-3d (No. 230)

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

$$\mathbf{W} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}, \quad \mathbf{w} = \begin{pmatrix} 3/4 \\ 1/4 \\ 1/4 \end{pmatrix}$$

Determine the type of isometry:

$$det(\mathbf{W}) = 1; \quad tr(\mathbf{W}) = -1$$

	det(W) = +1					det(W) = −1				
tr(W)	3	2	1	0	−1	−3	−2	−1	0	1
type	1	6	4	3	2	$\bar{1}$	$\bar{6}$	$\bar{4}$	$\bar{3}$	$\bar{2} = m$
order	1	6	4	3	2	2	6	4	6	2

2-fold rotation

Geometrical Interpretation of (W,w)

Ia-3d (No. 230)

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

2-fold rotation

$$\mathbf{W} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}, \quad \mathbf{w} = \begin{pmatrix} 3/4 \\ 1/4 \\ 1/4 \end{pmatrix}$$

Determine the direction of the rotation axis calculating the matrix Y(W)

$$\mathbf{Y}(\mathbf{W}) = \mathbf{W}^{n-1} + \mathbf{W}^{n-2} + \cdots + \mathbf{W} + \mathbf{I} \quad \xrightarrow{n=2} \quad \mathbf{Y}(\mathbf{W}) = \mathbf{W} + \mathbf{I}$$

$$\mathbf{Y}(\mathbf{W}) = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix} + \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

The direction of the rotation axis with respect to the body centred cubic basis is given by the non-zero columns, **u** = (1,1,0)

Geometrical Interpretation of (W,w)

Ia-3d (No. 230)

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

$$\mathbf{W} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix} ; \quad \mathbf{w} = \begin{pmatrix} 3/4 \\ 1/4 \\ 1/4 \end{pmatrix}$$

2-fold rotation
u=(1,1,0)

The intrinsic part is calculated:

$$\mathbf{w}_g = \frac{1}{n}(\mathbf{Y} \cdot \mathbf{w})$$

n=2 ⇒

$$\mathbf{w}_g = \frac{1}{2} \begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 3/4 \\ 1/4 \\ 1/4 \end{pmatrix} = \begin{pmatrix} 1/2 \\ 1/2 \\ 0 \end{pmatrix}$$

$$\mathbf{w}_g \neq 0$$

the symmetry operation is a **screw rotation**

Geometrical Interpretation of (W,w)

Ia-3d (No. 230)

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

$$\mathbf{W} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}; \quad \mathbf{w} = \begin{pmatrix} 3/4 \\ 1/4 \\ 1/4 \end{pmatrix}$$

2-fold screw rotation
u=(1,1,0)
Screw rotation wg=(1/2,1/2,0)

The location of the screw axis is calculated:

$$\mathbf{w}_g \neq 0 \quad \Rightarrow \quad (\mathbf{W}, \mathbf{w}_l)\,\mathbf{x}_F = \left(\begin{array}{ccc|c} 0 & 1 & 0 & 1/4 \\ 1 & 0 & 0 & -1/4 \\ 0 & 0 & \bar{1} & 1/4 \end{array}\right) \begin{pmatrix} x_F \\ y_F \\ z_F \end{pmatrix} = \begin{pmatrix} x_F \\ y_F \\ z_F \end{pmatrix}$$

$$x_F = y_F + 1/4; \quad y_F = x_F - 1/4; \quad -z_F + 1/4 = z_F \Rightarrow z_F = 1/8$$

Geometrical Interpretation of (W,w)

Ia-3d (No. 230)

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

$$\mathbf{W} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}; \quad \mathbf{w} = \begin{pmatrix} 3/4 \\ 1/4 \\ 1/4 \end{pmatrix}$$

The geometric interpretation of the symmetry operation is:

$$2(1/2,1/2,0) \quad x, x-1/4, 1/8$$

→ Location of the symmetry element

↓ screw component

Geometrical Interpretation of (W,w)

SYMMETY OPERATION http://www.cryst.ehu.es/cryst/matrices.html

Geometric Interpretation of Matrix Column Representation of Symmetry Operation

Symmetry Operation

This program calculates the geometric interpretation of matrix column representation of symmetry operation for a given crystal system or space group.

Input:

i) The crystal system or the space group number.

ii) The matrix column representation of symmetry operation.

The program is able to calculate the geometrical interpretation refer either to the standard/default setting of the chosen space group or to the so-called ITA Settings.

If you want to work on a non conventional setting click on **Non conventional setting**, this will show you a form where you have to introduce the transformation matrix relating the conventional setting of the group you have chosen with the non conventional one you are interested in.

Output:

We obtain the geometric interpretation of the symmetry operation according to the *International Tables for Crystallography*, Vol. A. criteria and in Seitz notation.

Introduce the crystal system

Or enter the sequential number of group as given in the *International Tables for Crystallography*, Vol. A [choose it] 230

Introduce the matrix-column representation of the symmetry operation in:

- Coordinate triplets: y+3/4,x+1/4,-z+1/4
- Or in matrix form

Rotational part			Translational part
1	0	0	0
0	1	0	0
0	0	1	0

[Standard/Default Setting] [Non Conventional Setting] [ITA Settings]

Geometrical Interpretation of (W,w)

SYMMETY OPERATION http://www.cryst.ehu.es/cryst/matrices.html

Geometric Interpretation of Matrix Column Representation of Symmetry Operation

Symmetry Operation

This program calculates the geometric interpretation of matrix column representation of symmetry operation for a given crystal system or space group.

Input:

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Output:

We obtain the geometric interpretation of the symmetry operation according to the *International Tables for Crystallography*, Vol. A. criteria and in Seitz notation.

Introduce the crystal system

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

choose it 230

Introduce the matrix-column representation of the symmetry operation in:

- Coordinate triplets: y+3/4,x+1/4,-z+1/4
- Or in matrix form

Rotational part			Translational part
1	0	0	0
0	1	0	0
0	0	1	0

(x,y,z) form	Matrix form	Symmetry Operation: ITA	Symmetry Operation: Seitz
y+3/4,x+1/4,-z+1/4	$\begin{pmatrix} 0 & 1 & 0 & 3/4 \\ 1 & 0 & 0 & 1/4 \\ 0 & 0 & -1 & 1/4 \end{pmatrix}$	2 (1/2,1/2,0) x,x-1/4,1/8	$\{ 2_{110} \mid 3/4\ 1/4\ 1/4 \}$

Exercise 2.15

(a) Construct the matrix-column pairs (**W**,**w**) of the following coordinate triplets:

(1) x, y, z | (2) -x, y+1/2, -z+1/2
(3) -x,-y,-z | (4) x, -y+1/2, z+1/2

(b) Characterize geometrically these matrix-column pairs taking into account that they refer to a monoclinic basis with unique axis b (type of operation, glide/screw component, location of the symmetry operation).

(c) Use the program SYMMETRY OPERATIONS for the geometric interpretation of the matrix-column pairs of the symmetry operations.

Exercise 2.16

(a) Characterize geometrically the matrix-column pairs listed under *General position* of the space group *P4mm* in *ITA*.

(b) Consider the diagram of the symmetry elements of *P4mm*. Try to determine the matrix-column pairs of the symmetry operations whose symmetry elements are indicated on the unit-cell diagram.

(c) Compare your results with the results of the program SYMMETRY OPERATIONS

GENERAL AND SPECIAL WYCKOFF POSITONS SITE-SYMMETRY

General and special positions

Orbit of a point X_0 under G

$G(X_0) = \{(\mathbf{W},\mathbf{w})X_0, (\mathbf{W},\mathbf{w}) \in G\}$

Site-symmetry group

$S = \{(\mathbf{W},\mathbf{w})\}$ of a point X_0

$$(\mathbf{W},\mathbf{w})X_0 = X_0 \Rightarrow \begin{pmatrix} W_{11} & W_{12} & W_{13} & w_1 \\ W_{21} & W_{22} & W_{23} & w_2 \\ W_{31} & W_{32} & W_{33} & w_3 \end{pmatrix} \begin{pmatrix} x_0 \\ y_0 \\ z_0 \end{pmatrix} = \begin{pmatrix} x_0 \\ y_0 \\ z_0 \end{pmatrix}$$

Multiplicity: $|P|/|S_o|$

General position X_o

$S = \{(1,0)\} \simeq 1$

Multiplicity: $|P|$

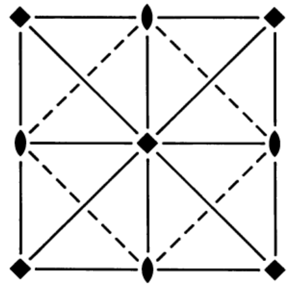
Special position X_o

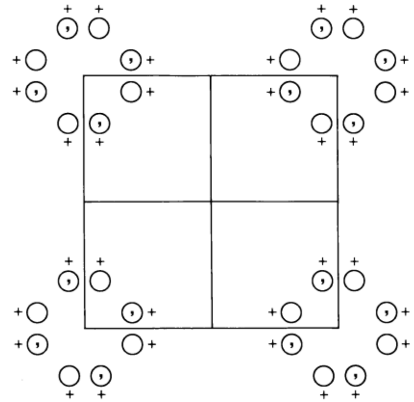
$S > 1 = \{(1,0),...,\}$

Multiplicity: $|P|/|S_o|$

Site-symmetry groups: oriented symbols

Example: 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

Multiplicity

Wyckoff letter

Site-symmetry

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*	$0,0,z$			

Site-symmetry group

Determine the site-symmetry group for the WP 2i (x,0,0)

General Positions of the Group *P*222 (No. 16)

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,y,-z	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{pmatrix}$	2 0,y,0	{ 2_{010} | 0 }
4	x,-y,-z	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{pmatrix}$	2 x,0,0	{ 2_{100} | 0 }

Wyckoff Positions of Group *P*222 (No. 16)

Multiplicity	Wyckoff letter	Site symmetry	Coordinates
4	u	1	(x,y,z) (-x,-y,z) (-x,y,-z) (x,-y,-z)
2	t	..2	(1/2,1/2,z) (1/2,1/2,-z)
2	s	..2	(0,1/2,z) (0,1/2,-z)
2	r	..2	(1/2,0,z) (1/2,0,-z)
2	q	..2	(0,0,z) (0,0,-z)
2	p	.2.	(1/2,y,1/2) (1/2,-y,1/2)
2	o	.2.	(1/2,y,0) (1/2,-y,0)
2	n	.2.	(0,y,1/2) (0,-y,1/2)
2	m	.2.	(0,y,0) (0,-y,0)
2	l	2..	(x,1/2,1/2) (-x,1/2,1/2)
2	k	2..	(x,1/2,0) (-x,1/2,0)
2	j	2..	(x,0,1/2) (-x,0,1/2)
2	i	2..	(x,0,0) (-x,0,0)
1	h	222	(1/2,1/2,1/2)
1	g	222	(0,1/2,1/2)
1	f	222	(1/2,0,1/2)
1	e	222	(1/2,1/2,0)
1	d	222	(0,0,1/2)
1	c	222	(0,1/2,0)
1	b	222	(1/2,0,0)
1	a	222	(0,0,0)

Site-symmetry group

Determine the site-symmetry group for the WP 2i (x,0,0)

$$(\mathbf{W},\mathbf{w})X_0 = X_0$$

x,y,z $\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}\begin{pmatrix}x\\0\\0\end{pmatrix}=\begin{pmatrix}x\\0\\0\end{pmatrix}$ ✔

-x,-y,z $\begin{pmatrix}\bar{1}&0&0\\0&\bar{1}&0\\0&0&1\end{pmatrix}\begin{pmatrix}x\\0\\0\end{pmatrix}=\begin{pmatrix}-x\\0\\0\end{pmatrix}$ ✘

-x,y,-z $\begin{pmatrix}\bar{1}&0&0\\0&1&0\\0&0&\bar{1}\end{pmatrix}\begin{pmatrix}x\\0\\0\end{pmatrix}=\begin{pmatrix}-x\\0\\0\end{pmatrix}$ ✘

x,-y,-z $\begin{pmatrix}1&0&0\\0&\bar{1}&0\\0&0&\bar{1}\end{pmatrix}\begin{pmatrix}x\\0\\0\end{pmatrix}=\begin{pmatrix}x\\0\\0\end{pmatrix}$ ✔

S_0 = {(x,y,z);(x,-y,-z)}

Site-symmetry

2..

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

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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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/def
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**.

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

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.

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

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

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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

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

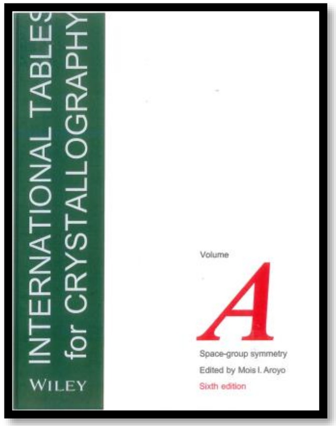
Please, enter the transformation:

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 (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x}+\frac{1}{2},\bar{y},z$ (6) $x+\frac{1}{2},y,\bar{z}$	(3) $\bar{x},y,\bar{z}+\frac{1}{2}$ (7) $x,\bar{y},z+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y},\bar{z}+\frac{1}{2}$ (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

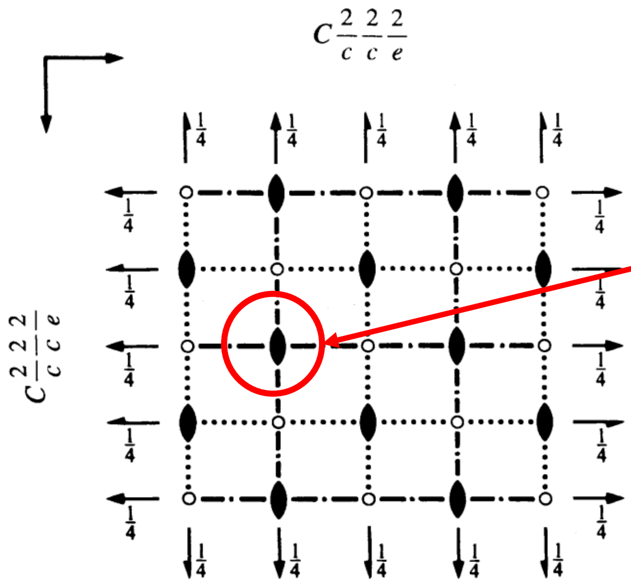
Site Symmetry Group 222

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 2.17

Consider the special Wyckoff positions of the the space group P4mm (No. 99)

1. Determine the site-symmetry groups of Wyckoff positions 1a and 1b. Compare the results with the listed *ITA* data.

2. The coordinate triplets (x,1/2,z) and (1/2,x,z), belong to Wyckoff position 4f. Compare their site-symmetry groups.

3. Compare your results with the results of theprogram WYCKPOS.

Exercise 2.18

Consider the Wyckoff-positions data of the space group *I41/amd (No.141), origin choice 2*.

a) Determine the site-symmetry groups of Wyckoff positions *4a*, *4c, 8d and 8e*. Compare the results with the listed ITA data. Compare your results with the results of the program WYCKPOS.

b) Characterize geometrically the isometries (3), (7), (12), (13) and (16) as listed under General Position. Compare the results with the corresponding geometric descriptions listed under Symmetry operations block in ITA. Comment on the differences between the corresponding symmetry operations listed under the sub-blocks (0, 0, 0) and (1/2, 1/2, 1/2).

c) Compare your results with the results of the program SYMMETRY OPERATIONS.

d) How do the above results change if *origin choice 1* setting of $I4_1$/amd is considered?

Exercise 2.23

ITA-conventional setting of space groups

Consider the space group *P21/c* (No. 14). Show that the relation between the *General* and *Special* position data of *P*11*21/a* (setting *unique axis c*) can be obtained from the data *P*1*21/c*1(setting *unique axis b*) applying the transformation $(\mathbf{a}',\mathbf{b}',\mathbf{c}')_{\mathbf{c}} = (\mathbf{a},\mathbf{b},\mathbf{c})_{\mathbf{b}}\boldsymbol{P}$, with $\boldsymbol{P}$= $\boldsymbol{c},\boldsymbol{a},\boldsymbol{b}$.

Use the retrieval tools GENPOS (generators and general positions) and WYCKPOS (Wyckoff positions) for accessing the space-group data. 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*.

Exercise 2.24

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.

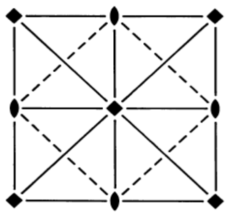
Consider the General position data of the space group *Im-3m* (No. 229). Using the option *Non-conventional setting* obtain the matrix-column pairs of the symmetry operations with respect to a primitive basis, applying the transformation (**a**',**b**',**c**') = 1/2(-**a**+**b**+**c**,**a**-**b**+**c**,**a**+**b**-**c**)

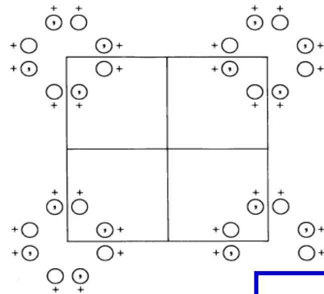
$P4mm$ | C^1_{4v} | $4mm$ | Tetragonal

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

Bilbao Crystallographic Server

Space-group symmetry





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

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

GENPOS

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			

WYCKPOS

HKLCOND

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

Symmetry of special projections

Along [001] $p4mm$
a′ = a b′ = b
Origin at 0,0,z

Along [100] $p1m1$
a′ = b b′ = c
Origin at x,0,0

Along [110] $p1m1$
a′ = $\frac{1}{2}$(−a+b) b′ = 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] $P4_2mc$ (c′ = 2c) (105); [2] $P4cc$ (c′ = 2c) (103); [2] $P4_2cm$ (c′ = 2c) (101); [2] $C4md$ (a′ = 2a, b′ = 2b) ($P4bm$, 100); [2] $F4mc$ (a′ = 2a, b′ = 2b, c′ = 2c) ($I4cm$, 108); [2] $F4mm$ (a′ = 2a, b′ = 2b, c′ = 2c) ($I4mm$, 107)

MAXSUB

Maximal isomorphic subgroups of lowest index

IIc [2] $P4mm$ (c′ = 2c) (99); [2] $C4mm$ (a′ = 2a, b′ = 2b) ($P4mm$, 99)

SERIES

Minimal non-isomorphic supergroups

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

II [2] $I4mm$ (107)

MINSUP