CRYSTALLOGRAPHY ONLINE Workshop

on the use and applications of the structural and magnetic tools of the

BILBAO CRYSTALLOGRAPHIC SERVER

Leioa, 27 June -1 July 2022

SPACE-GROUP SYMMETRY

SYMMETRY DATABASES OF BILBAO CRYSTALLOGRAPHIC SERVER

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Crystal Symmetry

Real crystal

Real crystals are finite objects in physical space which due to static (impurities and structural imperfections like disorder, dislocations, etc) or dynamic (phonons) defects are not perfectly symmetric.

↓

Ideal crystal (ideal crystal structures)

Infinite periodic spatial arrangement of the atoms (ions, molecules) with no static or dynamic defects

↓

Crystal pattern:

A model of the ideal crystal (crystal structure) in point space consisting of a strictly 3-dimensional periodic set of points

An abstraction of the atomic nature of the ideal structure, perfectly periodic

SPACE GROUPS

Space group G:

The set of all symmetry operations (isometries) of a crystal pattern

Translation subgroup T:
$T \lhd G$

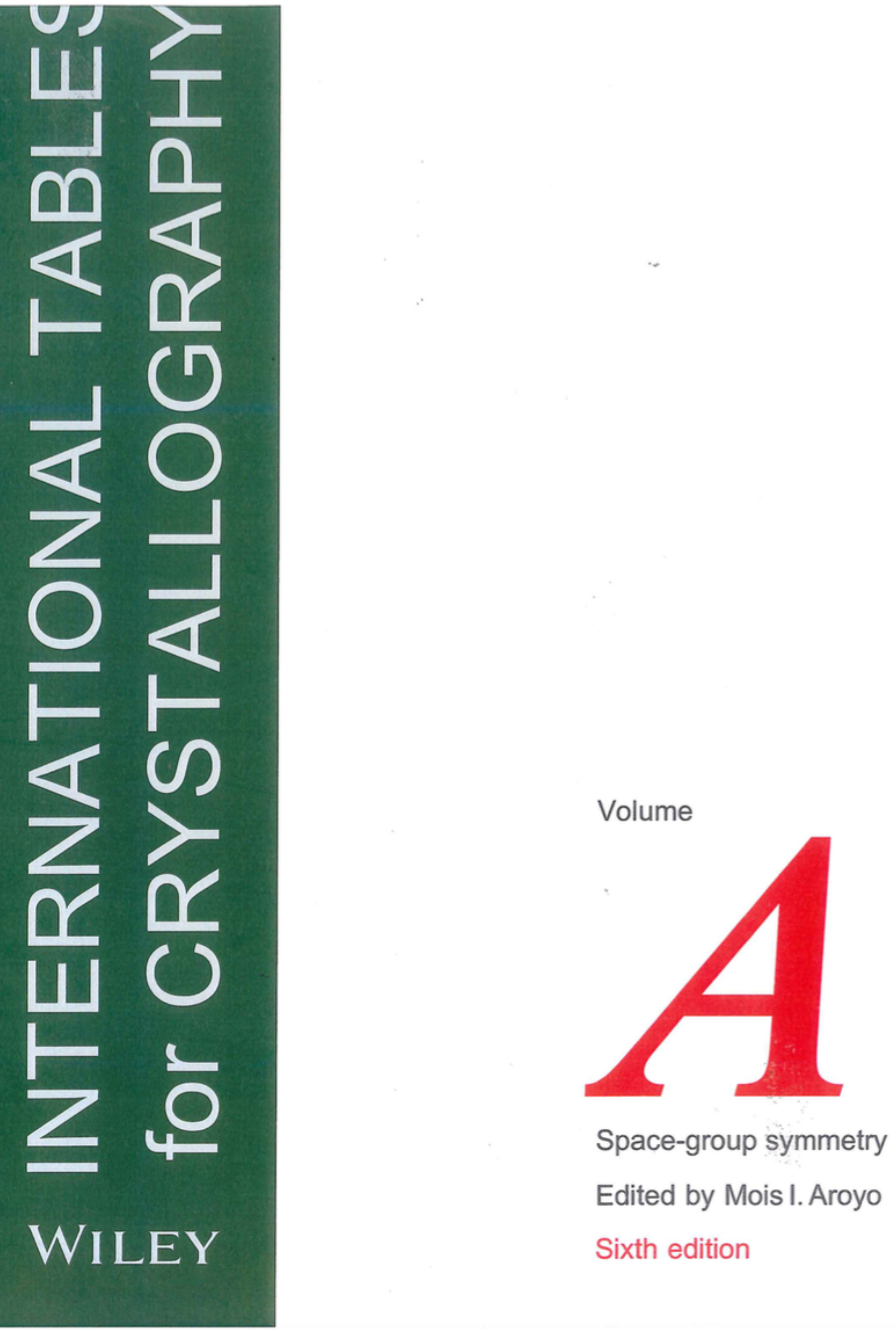
The infinite set of all translations that are symmetry operations of the crystal pattern

Point group of the space groups P_G:

The factor group of the space group G with respect to the translation subgroup T: $P_G \cong G/H$

$$(\boldsymbol{W},\boldsymbol{w}) \longrightarrow \boldsymbol{W} \quad P_G=\{\boldsymbol{W}|(\boldsymbol{W},\boldsymbol{w})\in G\}$$

INTERNATIONAL TABLES FOR CRYSTALLOGRAPHY
VOLUME A: SPACE-GROUP SYMMETRY



Extensive tabulations and illustrations of the 17 plane groups and of the 230 space groups

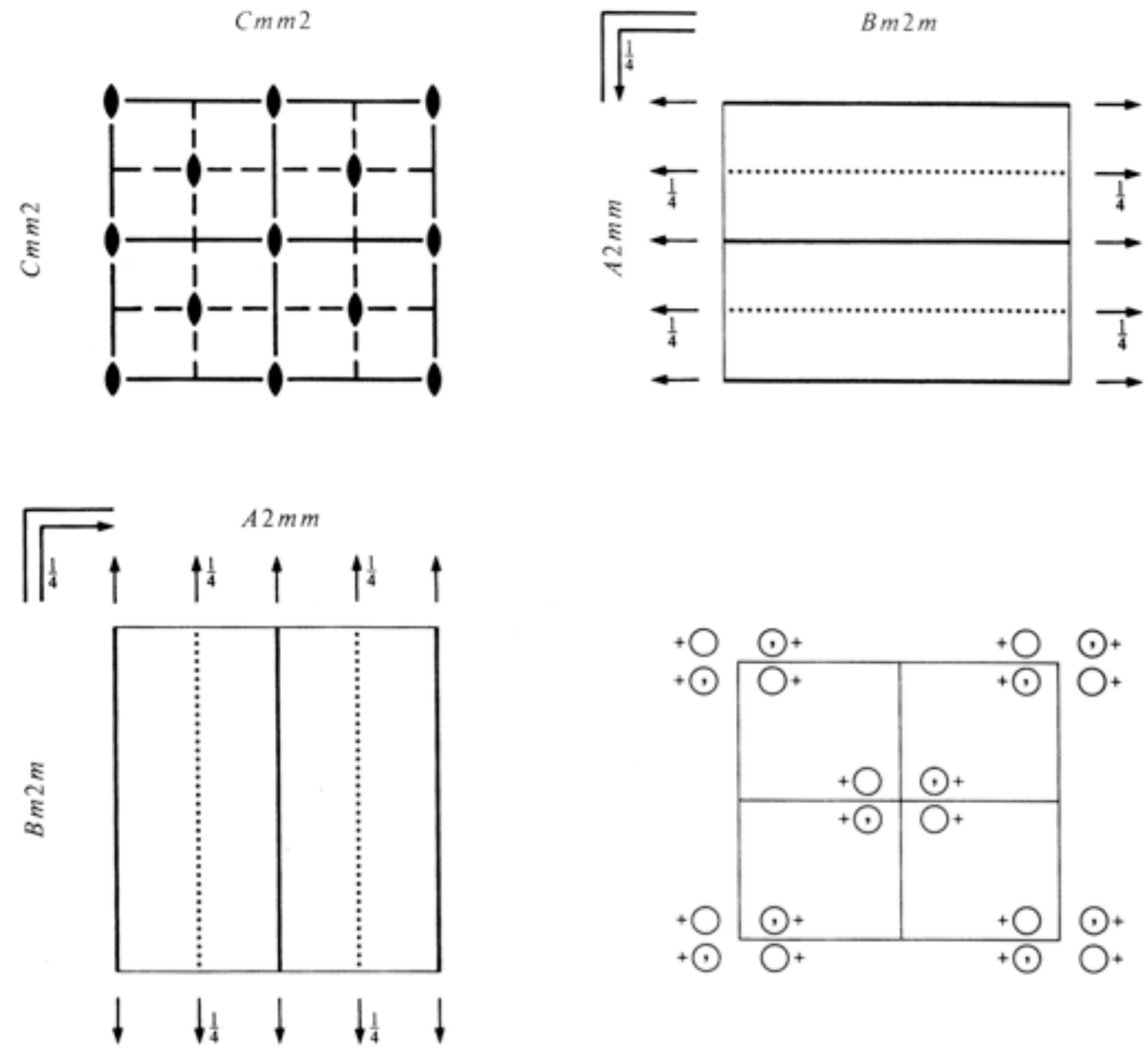
- headline with the relevant group symbols;
- diagrams of the symmetry elements and of the general position;
- specification of the origin and the asymmetric unit;
- list of symmetry operations;
- generators;
- general and special positions with multiplicities, site symmetries, coordinates and reflection conditions;
- symmetries of special projections;

GENERAL LAYOUT: LEFT-HAND PAGE

① *Cmm*2 C_{2v}^{11} *mm*2 Orthorhombic

② No. 35 *Cmm*2 Patterson symmetry *Cmmm*

③



④ **Origin** on *mm*2

⑤ **Asymmetric unit** $0 \le x \le \frac{1}{4}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le 1$

⑥ **Symmetry operations**

For (0,0,0)+ set

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

General Layout: Right-hand page

② Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3)

③ Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},0)+$				General:
8	f	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x,\bar{y},z$	(4) $\bar{x},y,z$	hkl: $h+k=2n$ $0kl$: $k=2n$ $h0l$: $h=2n$ $hk0$: $h+k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$
							Special: as above, plus
4	e	$m..$	$0,y,z$	$0,\bar{y},z$			no extra conditions
4	d	$.m.$	$x,0,z$	$\bar{x},0,z$			no extra conditions
4	c	$..2$	$\frac{1}{4},\frac{1}{4},z$	$\frac{1}{4},\frac{3}{4},z$			hkl: $h=2n$
2	b	$mm2$	$0,\frac{1}{2},z$				no extra conditions
2	a	$mm2$	$0,0,z$				no extra conditions

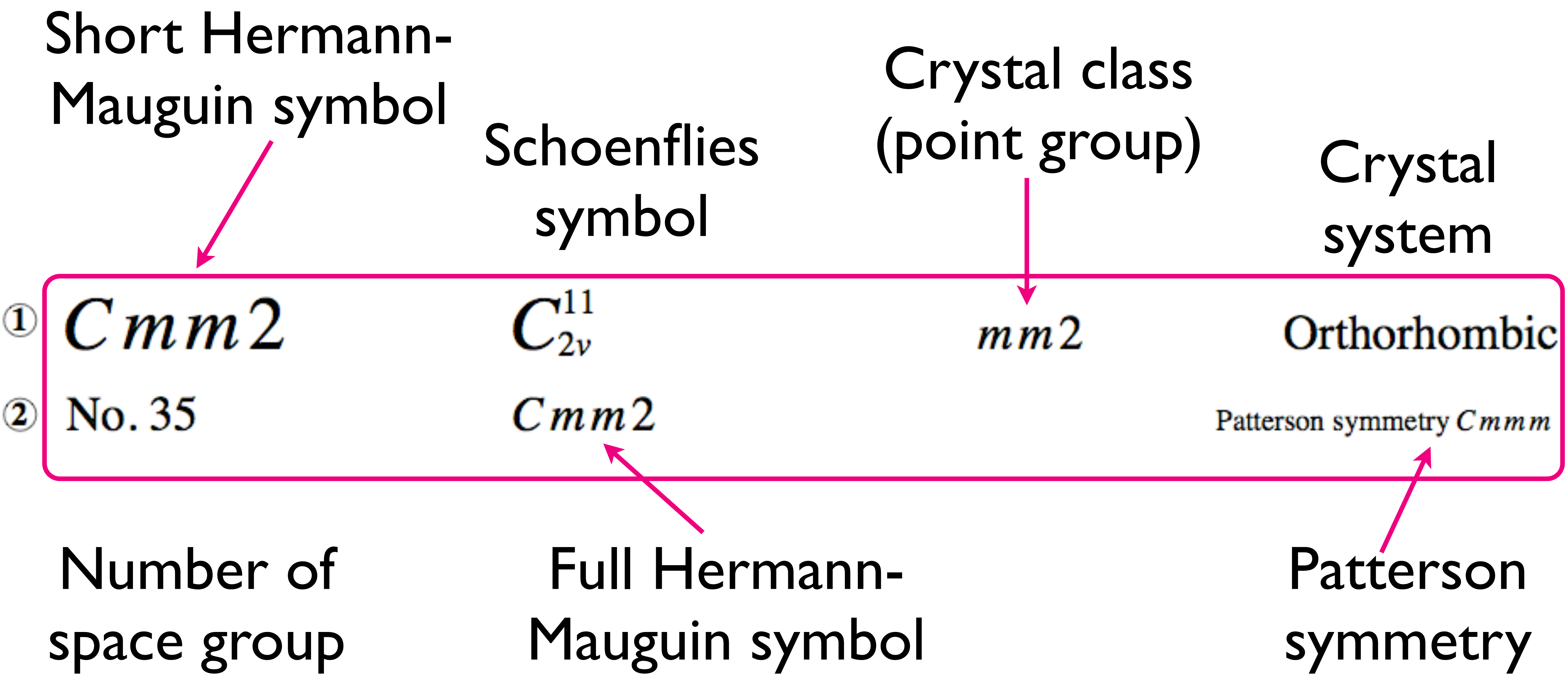
④ Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p11m$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

HEADLINE BLOCK


Short Hermann-Mauguin symbol
Schoenflies symbol
Crystal class (point group)
Crystal system
① $Cmm2$
C_{2v}^{11}
$mm2$
Orthorhombic
② No. 35
$Cmm2$
Patterson symmetry $Cmmm$
Number of space group
Full Hermann-Mauguin symbol
Patterson symmetry

HERMANN-MAUGUIN SYMBOLISM

Hermann-Mauguin symbols for space groups

The Hermann–Mauguin symbol for a space group consists of a sequence of letters and numbers, here called the constituents of the HM symbol.

(i) The first constituent is always a symbol for the conventional cell of the translation lattice of the space group

(ii) The second part of the full HM symbol of a space group consists of one position for each of up to three representative symmetry directions. To each position belong the generating symmetry operations of their representative symmetry direction. The position is thus occupied either by a rotation, screw rotation or rotoinversion and/or by a reflection or glide reflection.

(iii) Simplest-operation rule:

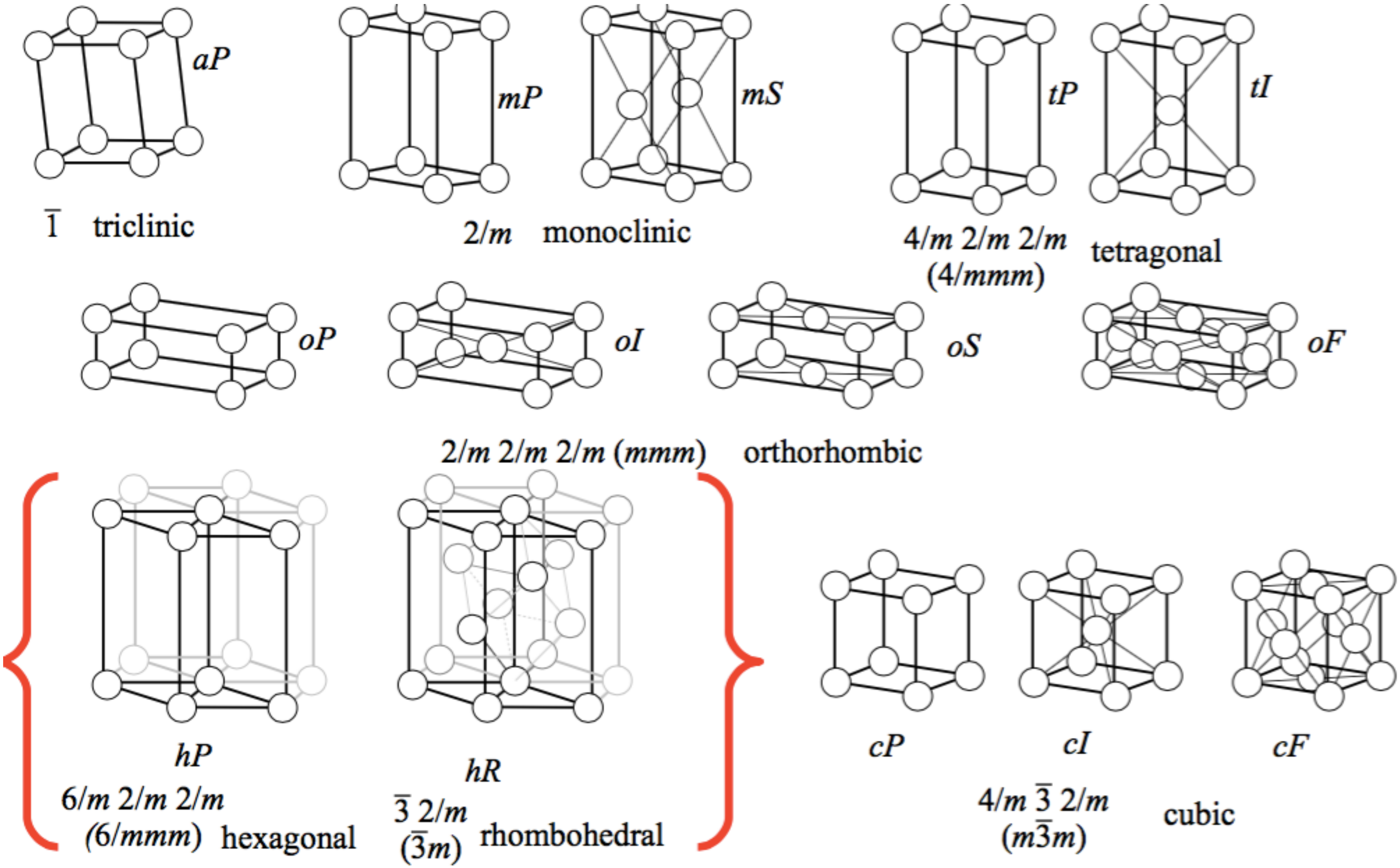
pure rotations > screw rotations;

pure rotations > rotoinversions

reflection m > a; b; c > n

'>' means 'has priority'

Lattice systems: classification based on the symmetry of the lattice



Symmetry directions

A direction is called a ***symmetry direction*** of a crystal structure if it is parallel to an axis of rotation, screw rotation or rotoinversion or if it is parallel to the normal of a reflection or glide-reflection plane. A symmetry direction is thus the direction of the geometric element of a symmetry operation, when the normal of a symmetry plane is used for the description of its orientation.

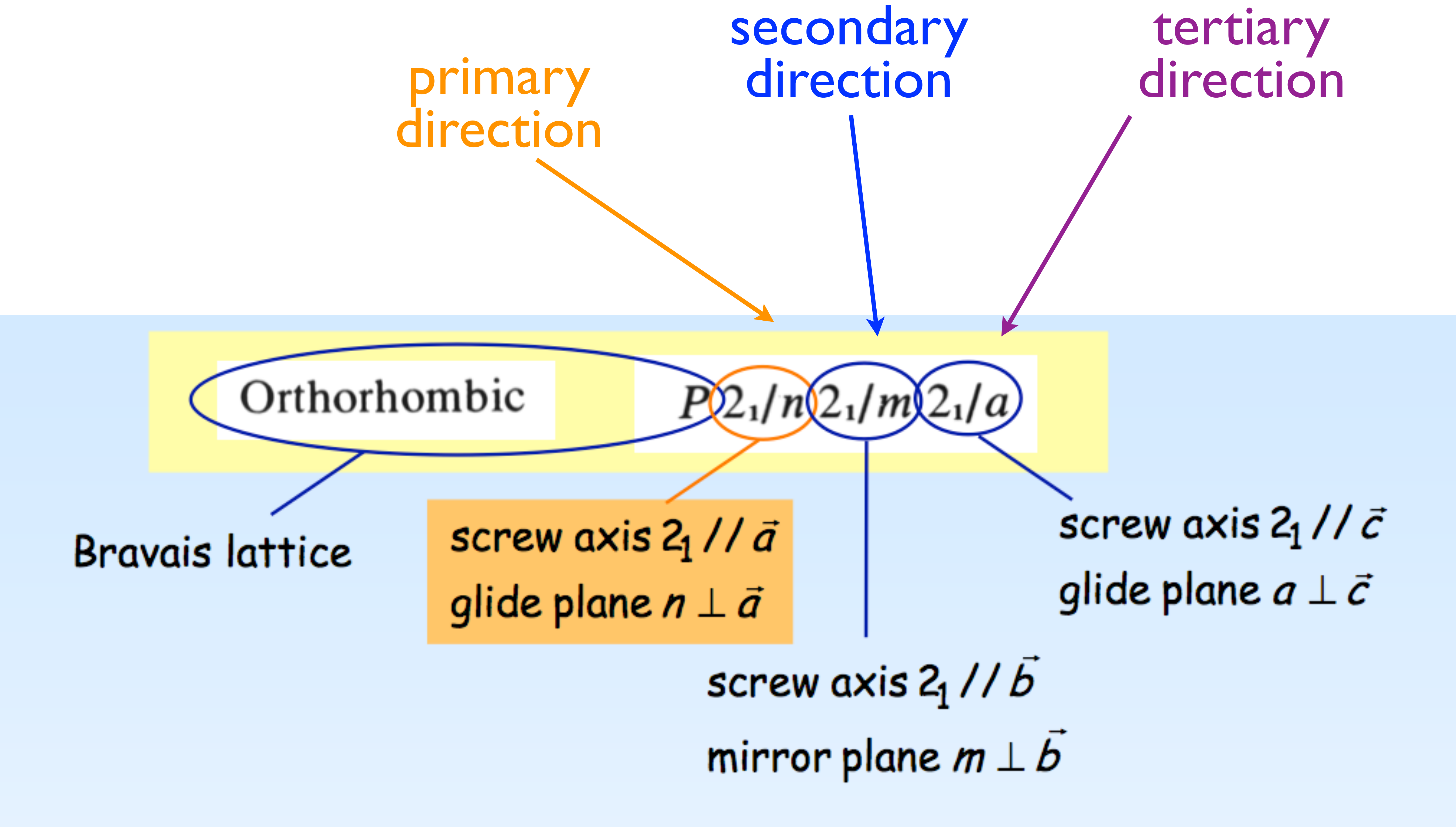
Hermann-Mauguin symbols for space groups

Directions that belong to the same set of equivalent symmetry directions are collected between braces. The first entry in each set is taken as the representative of that set.

Lattice	Symmetry direction (position in Hermann–Mauguin symbol)		
	Primary	Secondary	Tertiary
Triclinic	None		
Monoclinic*	[010] ('unique axis *b*') [001] ('unique axis *c*')		
Orthorhombic	[100]	[010]	[001]
Tetragonal	[001]	$\left\{ \begin{matrix} [100] \\ [010] \end{matrix} \right\}$	$\left\{ \begin{matrix} [1\bar{1}0] \\ [110] \end{matrix} \right\}$
Hexagonal	[001]	$\left\{ \begin{matrix} [100] \\ [010] \\ [\bar{1}\bar{1}0] \end{matrix} \right\}$	$\left\{ \begin{matrix} [1\bar{1}0] \\ [120] \\ [\bar{2}\bar{1}0] \end{matrix} \right\}$
Rhombohedral (hexagonal axes)	[001]	$\left\{ \begin{matrix} [100] \\ [010] \\ [\bar{1}\bar{1}0] \end{matrix} \right\}$	
Rhombohedral (rhombohedral axes)	[111]	$\left\{ \begin{matrix} [1\bar{1}0] \\ [01\bar{1}] \\ [\bar{1}01] \end{matrix} \right\}$	
Cubic	$\left\{ \begin{matrix} [100] \\ [010] \\ [001] \end{matrix} \right\}$	$\left\{ \begin{matrix} [111] \\ [1\bar{1}\bar{1}] \\ [\bar{1}1\bar{1}] \\ [\bar{1}\bar{1}1] \end{matrix} \right\}$	$\left\{ \begin{matrix} [1\bar{1}0] & [110] \\ [01\bar{1}] & [011] \\ [\bar{1}01] & [101] \end{matrix} \right\}$

Example:

Hermann-Mauguin symbols for space groups



SPACE-GROUP SYMMETRY OPERATIONS

Symmetry Operations Characteristics

TYPE of the symmetry operation

preserve or not ***handedness***

SCREW/GLIDE component

GEOMETRIC ELEMENT

ORIENTATION of the geometric element

LOCATION of the geometric element

Crystallographic symmetry operations

characteristics:

fixed points of isometries $(W,w)X_f=X_f$

geometric elements

Types of isometries

preserve handedness

identity: the whole space fixed

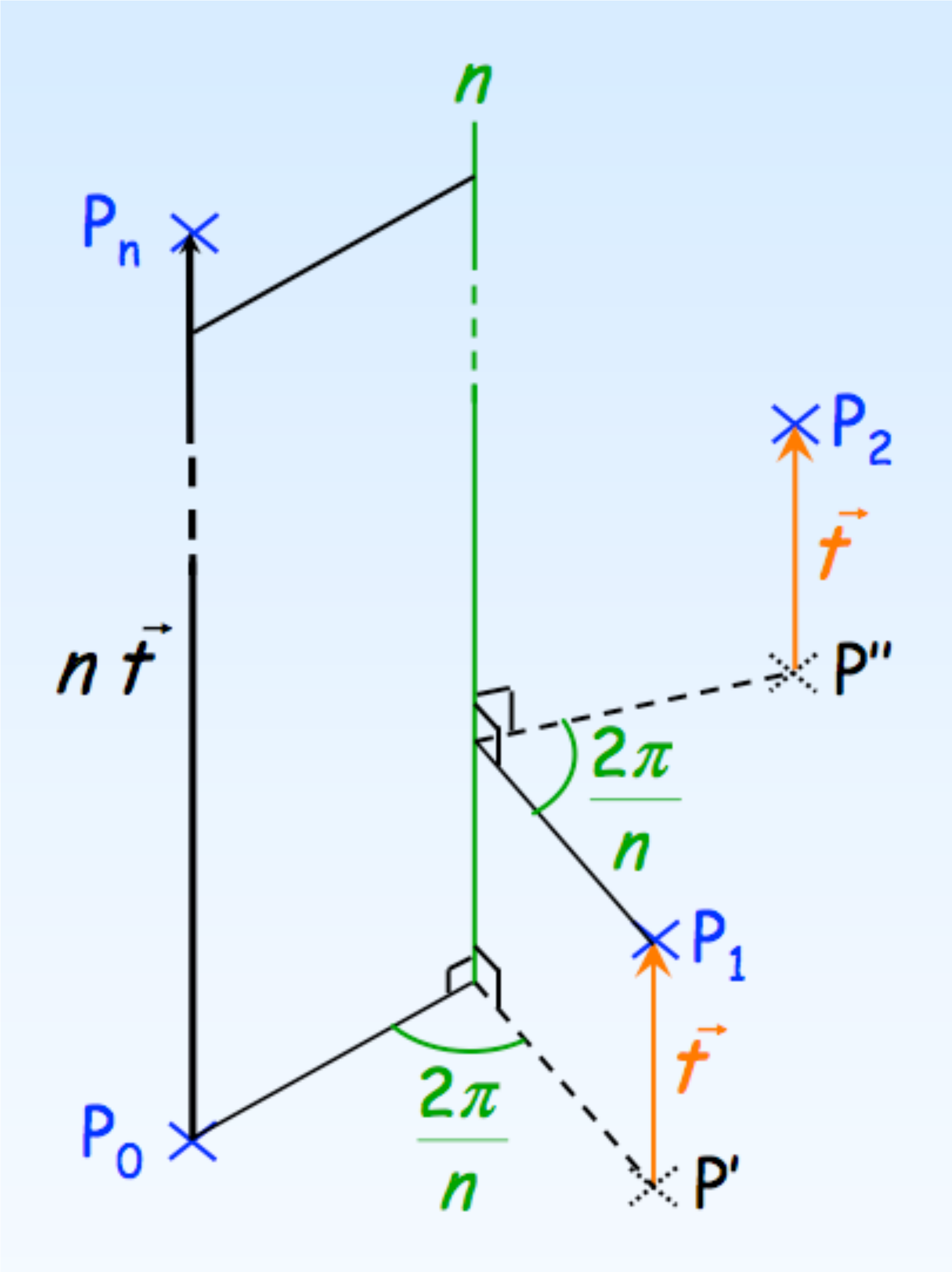
translation t: no fixed point $\tilde{\mathbf{x}} = \mathbf{x} + \mathbf{t}$

rotation: one line fixed
rotation axis $\phi = k \times 360^\circ / N$

screw rotation: no fixed point
screw axis

screw vector

Screw rotation



n-fold rotation followed by a fractional translation $\frac{p}{n}\mathbf{t}$ parallel to the rotation axis

Its application *n* times results in a translation parallel to the rotation axis

Types of isometries do not preserve handedness

characteristics: fixed points of isometries $(W,w)X_f=X_f$
geometric elements

roto-inversion: centre of roto-inversion fixed
roto-inversion axis

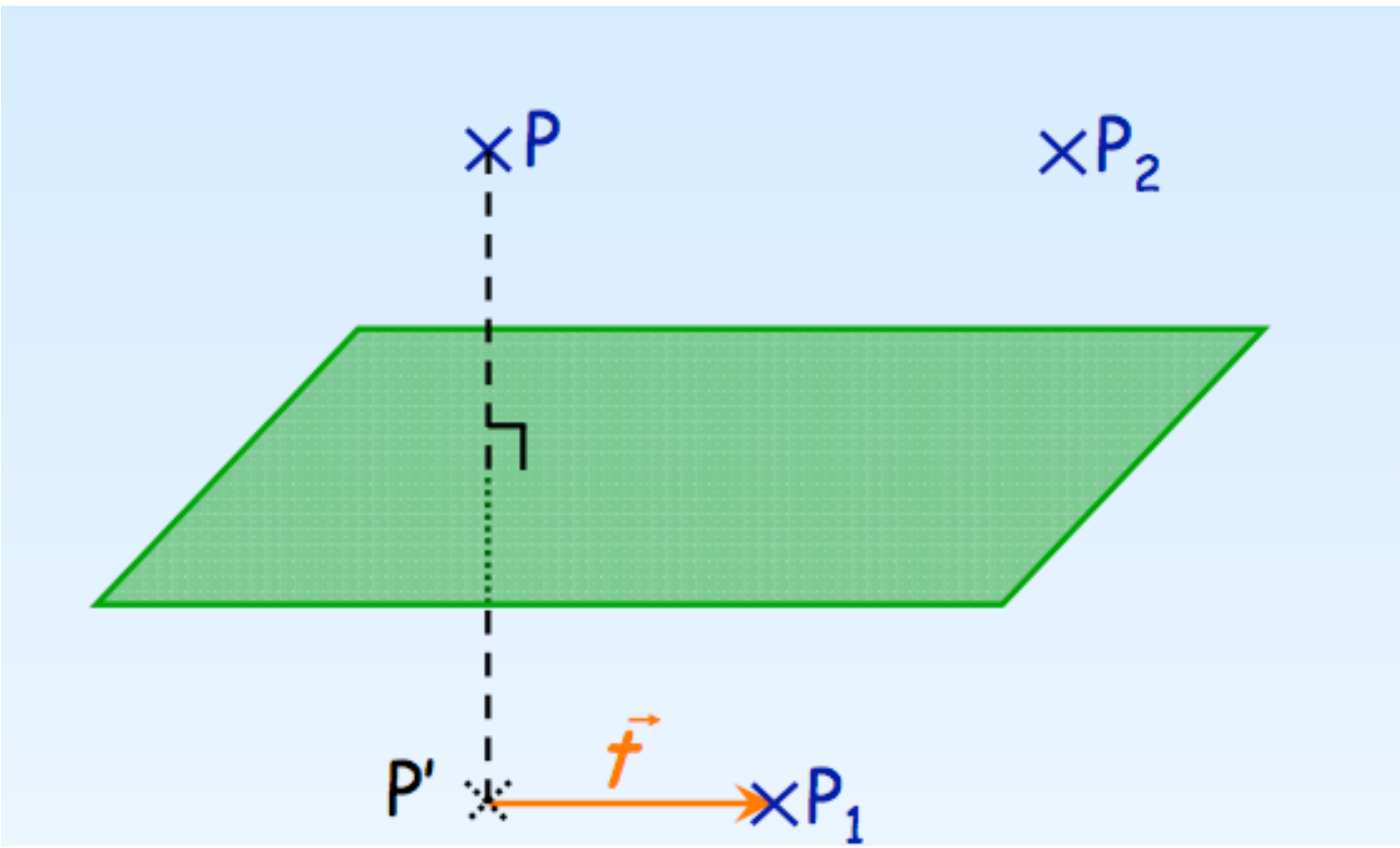
inversion: centre of inversion fixed

reflection: plane fixed
reflection/mirror plane

glide reflection: no fixed point
glide plane glide vector

Crystallographic symmetry operations

Glide plane



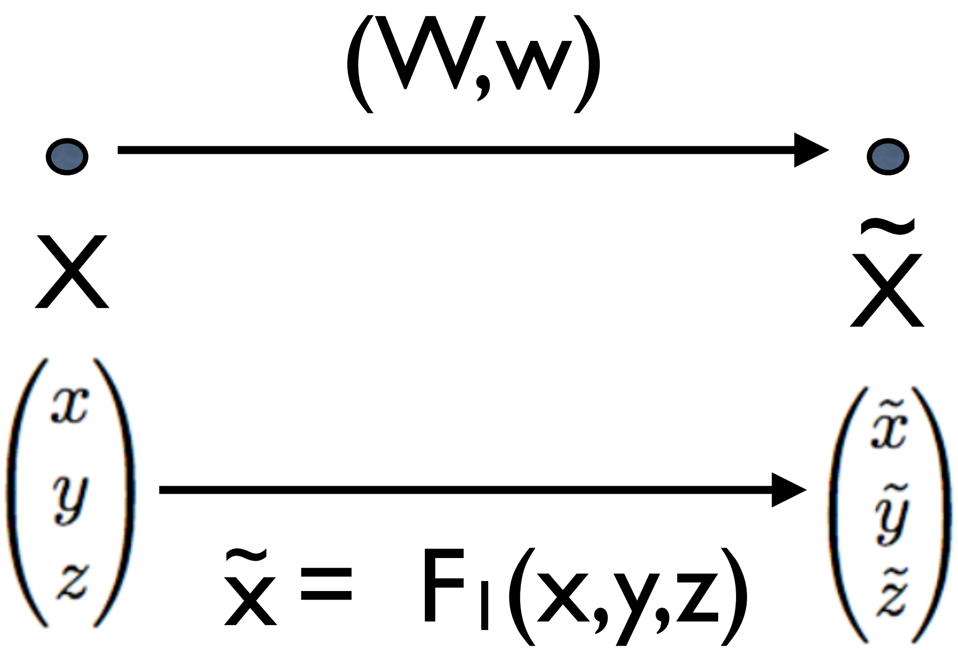
reflection followed by a fractional translation $\frac{1}{2}\mathbf{t}$ parallel to the plane

Its application 2 times results in a translation parallel to the plane

Description of isometries: 3D

coordinate system: $\{O, \mathbf{a}, \mathbf{b}, \mathbf{c}\}$

isometry:



$$\left|\begin{array}{lcl} \tilde{x} & = & W_{11}\,x + W_{12}\,y + W_{13}\,z + w_1 \\ \tilde{y} & = & W_{21}\,x + W_{22}\,y + W_{23}\,z + w_2 \\ \tilde{z} & = & W_{31}\,x + W_{32}\,y + W_{33}\,z + w_3 \end{array}\right.$$

Matrix formalism

$$\begin{pmatrix}\tilde{x}\\ \tilde{y}\\ \tilde{z}\end{pmatrix} = \begin{pmatrix}W_{11} W_{12} W_{13}\\ W_{21} W_{22} W_{23}\\ W_{31} W_{32} W_{33}\end{pmatrix}\begin{pmatrix}x\\ y\\ z\end{pmatrix} + \begin{pmatrix}w_1\\ w_2\\ w_3\end{pmatrix}$$

linear/matrix part

translation column part

$$\tilde{\boldsymbol{x}} = \boldsymbol{W}\,\boldsymbol{x} + \boldsymbol{w}$$

$$\tilde{\boldsymbol{x}} = (\boldsymbol{W}, \boldsymbol{w})\,\boldsymbol{x} \quad \text{or} \quad \tilde{\boldsymbol{x}} = \{\boldsymbol{W} \,|\, \boldsymbol{w}\}\,\boldsymbol{x}$$

matrix-column pair

Seitz symbol

EXERCISES

Problem 1.6.2.1

Referred to an 'orthorhombic' coordinated system (a≠b≠c; α=β=γ=90) two symmetry operations are represented by the following matrix-column pairs:

$$(W_1,w_1)=\left(\begin{array}{ccc|c} -1 & & & 0 \\ & 1 & & 0 \\ & & -1 & 0 \end{array}\right) \qquad (W_2,w_2)=\left(\begin{array}{ccc|c} -1 & & & 1/2 \\ & 1 & & 0 \\ & & -1 & 1/2 \end{array}\right)$$

Determine the images X_i of a point X under the symmetry operations (W_i,w_i) where

$$X=\begin{pmatrix} 0{,}70 \\ 0{,}31 \\ 0{,}95 \end{pmatrix}$$

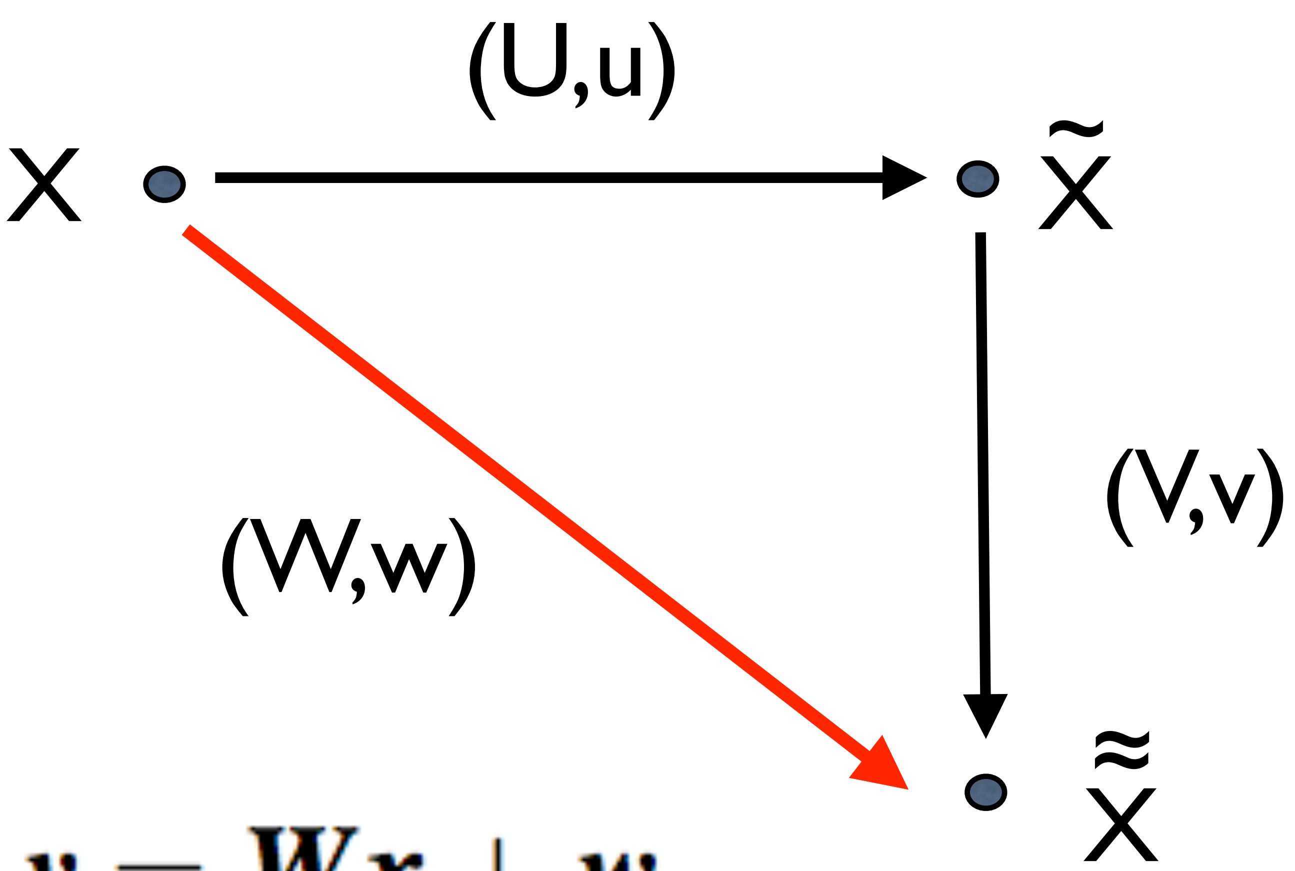
Can you guess what is the geometric 'nature' of (W_1,w_1)?

And of (W_2,w_2)?

Hint:

A drawing could be rather helpful

Combination of isometries



$$\tilde{\boldsymbol{x}} = \boldsymbol{U}\boldsymbol{x} + \boldsymbol{u};$$

$$\tilde{\tilde{\boldsymbol{x}}} = \boldsymbol{V}\tilde{\boldsymbol{x}} + \boldsymbol{v};$$

$$\tilde{\tilde{\boldsymbol{x}}} = \boldsymbol{V}(\boldsymbol{U}\boldsymbol{x} + \boldsymbol{u}) + \boldsymbol{v};$$

$$\tilde{\tilde{\boldsymbol{x}}} = \boldsymbol{V}\boldsymbol{U}\boldsymbol{x} + \boldsymbol{V}\boldsymbol{u} + \boldsymbol{v} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{w}.$$

$$\tilde{\tilde{\boldsymbol{x}}} = (\boldsymbol{V},\, \boldsymbol{v})\,\tilde{\boldsymbol{x}} = (\boldsymbol{V},\, \boldsymbol{v})(\boldsymbol{U},\, \boldsymbol{u})\boldsymbol{x} = (\boldsymbol{W},\, \boldsymbol{w})\boldsymbol{x}.$$

$$(\boldsymbol{W},\, \boldsymbol{w}) = (\boldsymbol{V},\, \boldsymbol{v})(\boldsymbol{U},\, \boldsymbol{u}) = (\boldsymbol{V}\boldsymbol{U},\, \boldsymbol{V}\boldsymbol{u} + \boldsymbol{v}).$$

EXERCISES

Problem 1.6.2.1

Consider the matrix-column pairs of the two symmetry operations:

$$(W_1,w_1)=\left(\begin{array}{ccc|c} 0 & -1 & & 0 \\ 1 & 0 & & 0 \\ & & -1 & 0 \end{array}\right) \qquad (W_2,w_2)=\left(\begin{array}{ccc|c} -1 & & & 1/2 \\ & 1 & & 0 \\ & & -1 & 1/2 \end{array}\right)$$

Determine and compare the matrix-column pairs of the combined symmetry operations:

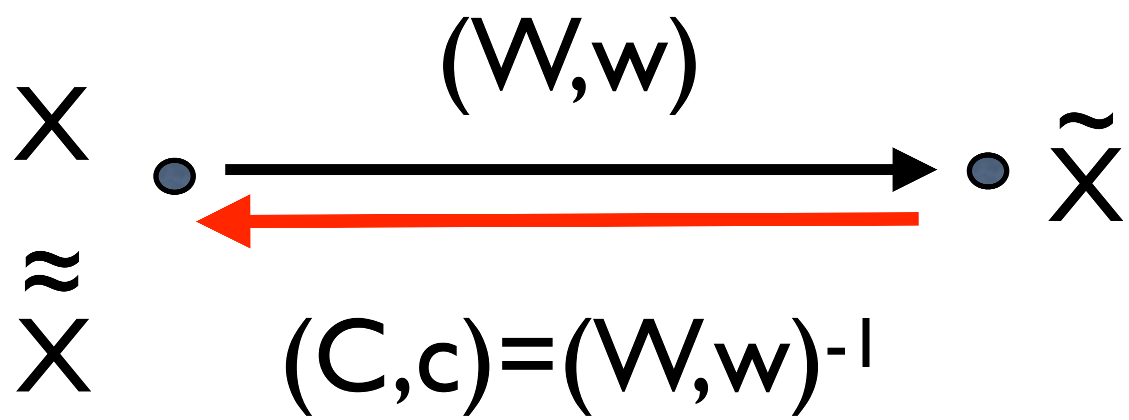
$$(W,w)=(W_1,w_1)(W_2,w_2)$$

$$(W,w)'=(W_2,w_2)(W_1,w_1)$$

combination of isometries:

$$(\boldsymbol{W}_2,\ \boldsymbol{w}_2)\,(\boldsymbol{W}_1,\ \boldsymbol{w}_1) = (\boldsymbol{W}_2\,\boldsymbol{W}_1,\ \boldsymbol{W}_2\,\boldsymbol{w}_1 + \boldsymbol{w}_2)$$

Inverse isometries



$\boldsymbol{I}$ = 3x3 identity matrix

$\boldsymbol{o}$ = zero translation column

$$(C,c)(W,w) = (\boldsymbol{I},\boldsymbol{o})$$

$$(C,c)(W,w) = (CW, Cw+c)$$

$CW=\boldsymbol{I}$ → $C=W^{-1}$

$Cw+c=\boldsymbol{o}$ → $c=-Cw=-W^{-1}w$

EXERCISES

Problem 1.6.2.1

Determine the inverse symmetry operations $(W_1,w_1)^{-1}$ and $(W_2,w_2)^{-1}$ where

$$(W_1,w_1)=\left(\begin{array}{ccc|c} 0 & -1 & & 0 \\ 1 & 0 & & 0 \\ & & -1 & 0 \end{array}\right) \qquad (W_2,w_2)=\left(\begin{array}{ccc|c} -1 & & & 1/2 \\ & 1 & & 0 \\ & & -1 & 1/2 \end{array}\right)$$

Determine the inverse symmetry operation $(W,w)^{-1}$

$$(W,w)=(W_1,w_1)(W_2,w_2)$$

inverse of isometries:

$$(\boldsymbol{W},\, \boldsymbol{w})^{-1} = (\boldsymbol{W}^{-1},\, -\boldsymbol{W}^{-1}\,\boldsymbol{w})$$

Short-hand notation for the description of isometries

isometry:

$$X \bullet \xrightarrow{(W,w)} \bullet \tilde{X}$$

$$\left| \begin{array}{lcl} \tilde{x} & = & W_{11}\,x + W_{12}\,y + W_{13}\,z + w_1 \\ \tilde{y} & = & W_{21}\,x + W_{22}\,y + W_{23}\,z + w_2 \\ \tilde{z} & = & W_{31}\,x + W_{32}\,y + W_{33}\,z + w_3, \end{array} \right.$$

notation rules:

-left-hand side: omitted
-coefficients 0, +1, -1
-different rows in one line

examples:

-1			1/2
	1		0
		-1	1/2

$\longrightarrow$ $\left\{ \begin{array}{l} -x+1/2,\ y,\ -z+1/2 \\ \bar{x}+1/2,\ y,\ \bar{z}+1/2 \end{array} \right.$

EXERCISES

Problem 1.6.2.3

Construct the matrix-column pair (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

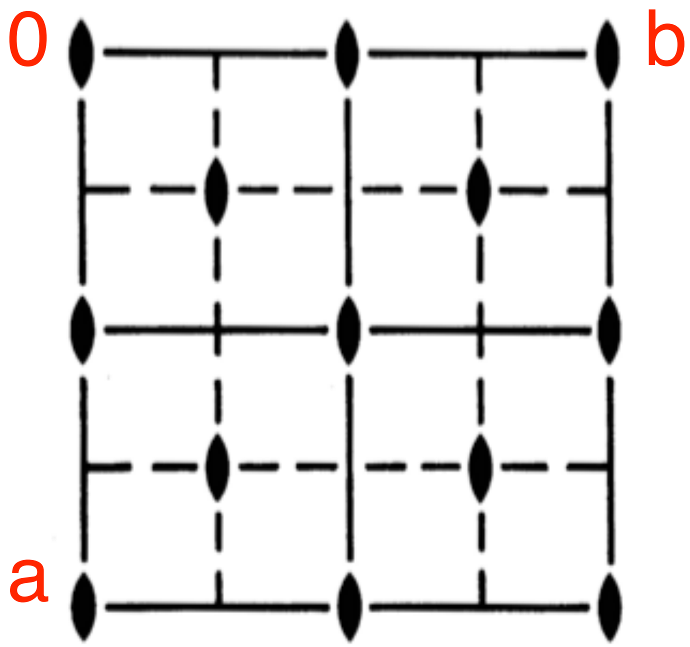
PRESENTATION OF SPACE-GROUP SYMMETRY OPERATIONS

IN INTERNATIONAL TABLES FOR CRYSTALLOGRAPHY, VOL. A

Space group *Cmm*2 (No. 35)

How are the symmetry operations represented in ITA ?

Diagram of symmetry elements



Symmetry operations

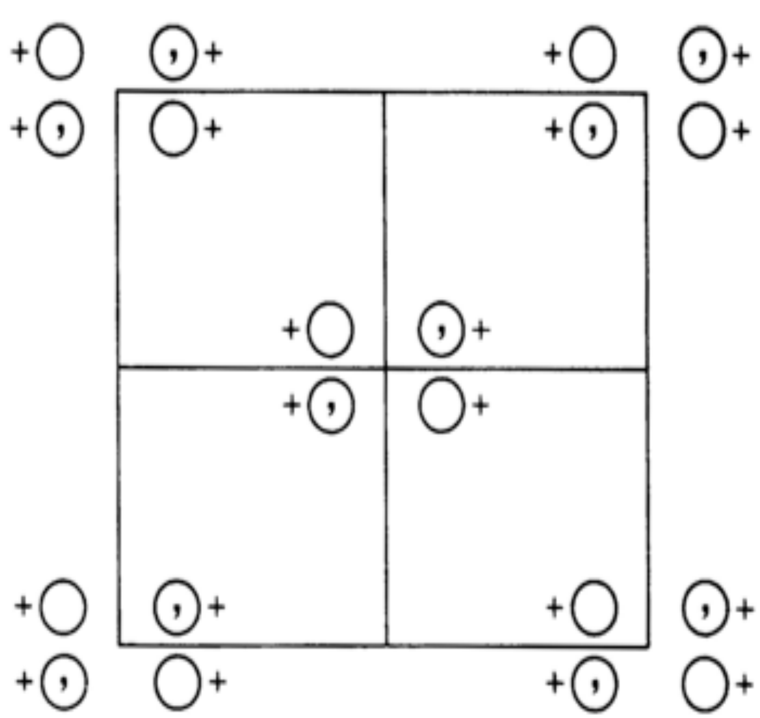
For (0,0,0)+ set

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

For $(\frac{1}{2},\frac{1}{2},0)$+ set

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

Diagram of general position points



General Position

Coordinates

$(0,0,0)+ \quad (\frac{1}{2},\frac{1}{2},0)+$

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

General position

(i) coordinate triplets of an image point $\tilde{X}$ of the original point X= $\begin{pmatrix} x \\ y \\ z \end{pmatrix}$ under (W,w) of G

-presentation of infinite image points $\tilde{X}$ under the action of (W,w) of G

(ii) short-hand notation of the matrix-column pairs (W,w) of the symmetry operations of G

-presentation of infinite symmetry operations of G

$(W,w) = (I,t_n)(W,w_0),\ 0 \leq w_{i0} < 1$

Space Groups: infinite order

Coset decomposition $G:T_G$

General position

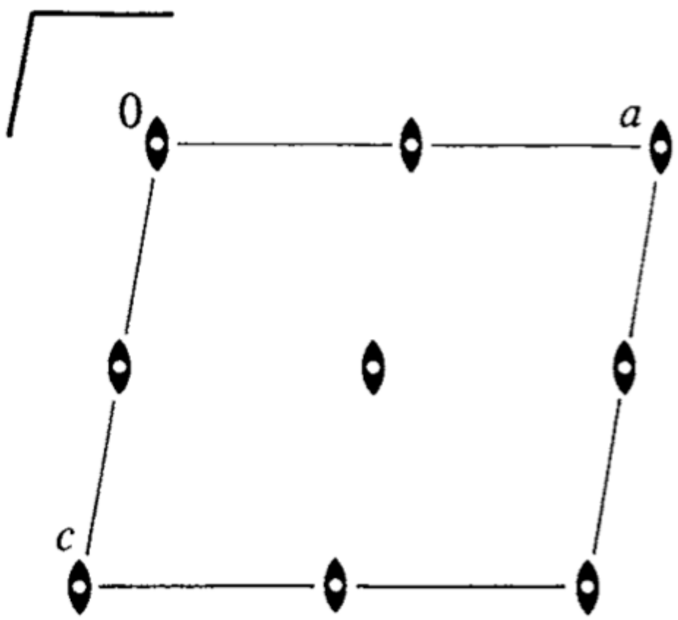
$(I,0)$	(W_2,w_2)	...	(W_m,w_m)	...	(W_i,w_i)
(I,t_1)	(W_2,w_2+t_1)	...	(W_m,w_m+t_1)	...	(W_i,w_i+t_1)
(I,t_2)	(W_2,w_2+t_2)	...	(W_m,w_m+t_2)	...	(W_i,w_i+t_2)
...	...	...	...	...	...
(I,t_j)	(W_2,w_2+t_j)	...	(W_m,w_m+t_j)	...	(W_i,w_i+t_j)
...	...	...	...	...	...

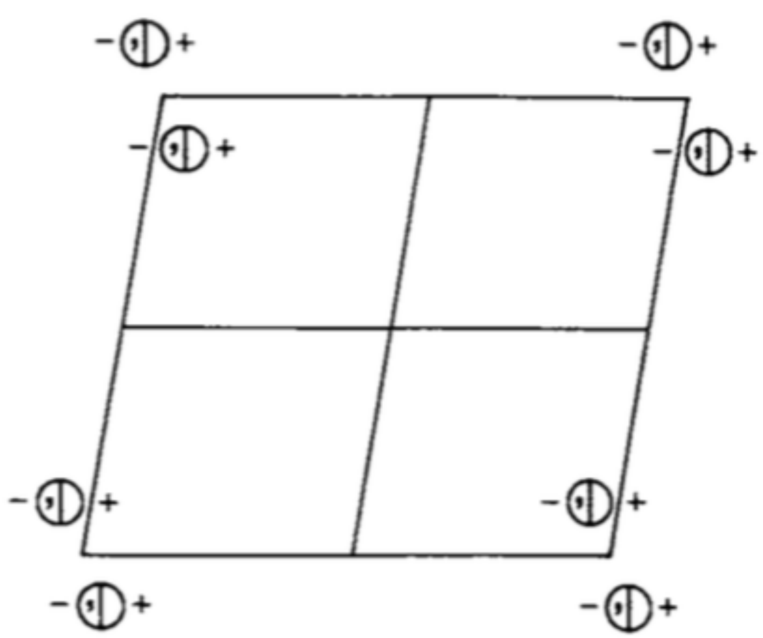
Factor group G/T_G

isomorphic to the point group P_G of G

Point group $P_G = \{I, W_2, W_3, \ldots, W_i\}$

Example: P12/m1





Coset decomposition G:T_G

Point group $P_G = \{1, 2, \bar{1}, m\}$

General position

T_G	$T_G\,2$	$T_G\,\bar{1}$	$T_G\,m$
(1,0)	(2,0)	($\bar{1}$,0)	(m,0)
(1,t_1)	(2,t_1)	($\bar{1}$, t_1)	(m, t_1)
(1,t_2)	(2,t_2)	($\bar{1}$, t_2)	(m,t_2)
...	...	...	...
(1,t_j)	(2,t_j)	($\bar{1}$, t_j)	(m, t_j)
...	...	...	...

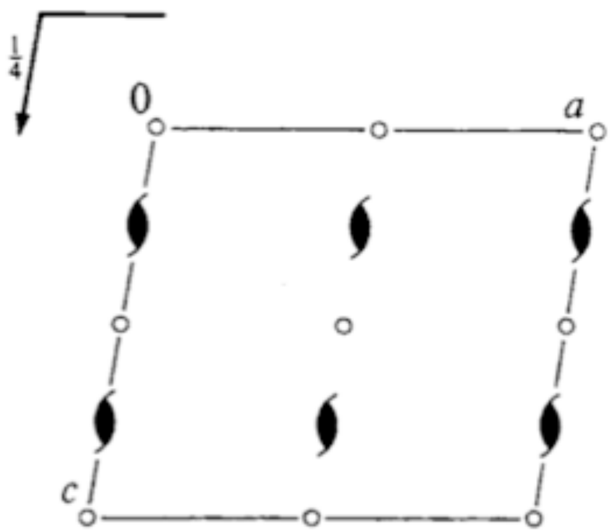
inversion centres ($\bar{1}$,t):

$$\begin{pmatrix} -1 & & \\ & -1 & \\ & & -1 \end{pmatrix} \begin{pmatrix} n_1 \\ n_2 \\ n_3 \end{pmatrix} \xrightarrow{\bar{1} \text{ at}} \begin{pmatrix} n_1/2 \\ n_2/2 \\ n_3/2 \end{pmatrix}$$

EXAMPLE

Coset decomposition $P12_1/c1:T$

Point group ?



General position

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

(1,0)	(2,0 ½ ½)	($\bar{1}$,0)	(m,0 ½ ½)
(1,t_1)	(2,0 ½ ½+t_1)	($\bar{1}$,t_1)	(m,0 ½ ½ +t_1)
(1,t_2)	(2,0 ½ ½ +t_2)	($\bar{1}$,t_2)	(m,0 ½ ½ +t_2)
…	… …	…	… …
(1,t_j)	(2,0 ½ ½ +t_j)	($\bar{1}$,t_j)	(m,0 ½ ½ +t_j)
…	… …	…	… …

inversion centers

($\bar{1}$,p q r): $\bar{1}$ at p/2,q/2,r/2

2_1screw axes

(2,u ½+v ½ +w) → (2,0 ½+v ½)

→ (2,u ½ ½ +w)

Symmetry Operations Block

GEOMETRIC INTERPRETATION OF THE MATRIX-COLUMN PRESENTATION OF THE SYMMETRY OPERATIONS

TYPE of the symmetry operation

SCREW/GLIDE component

ORIENTATION of the geometric element

LOCATION of the geometric element

Example: Cmm2

Diagram of symmetry elements

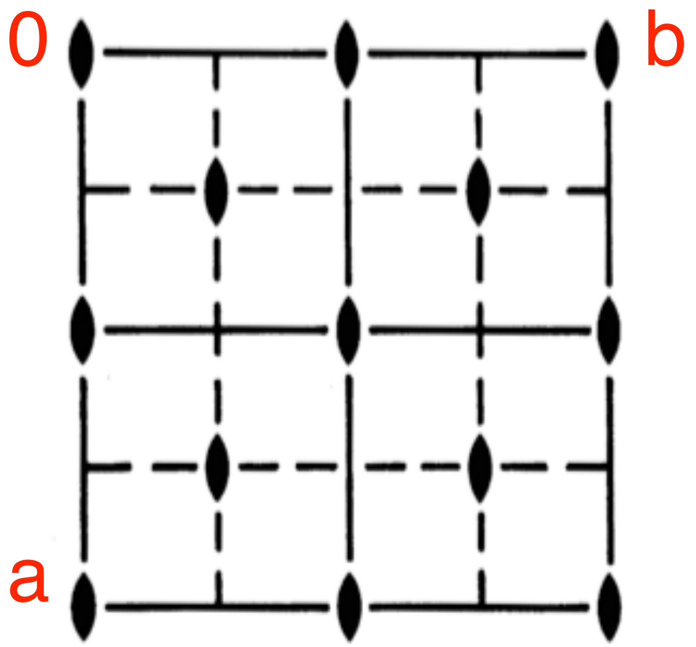
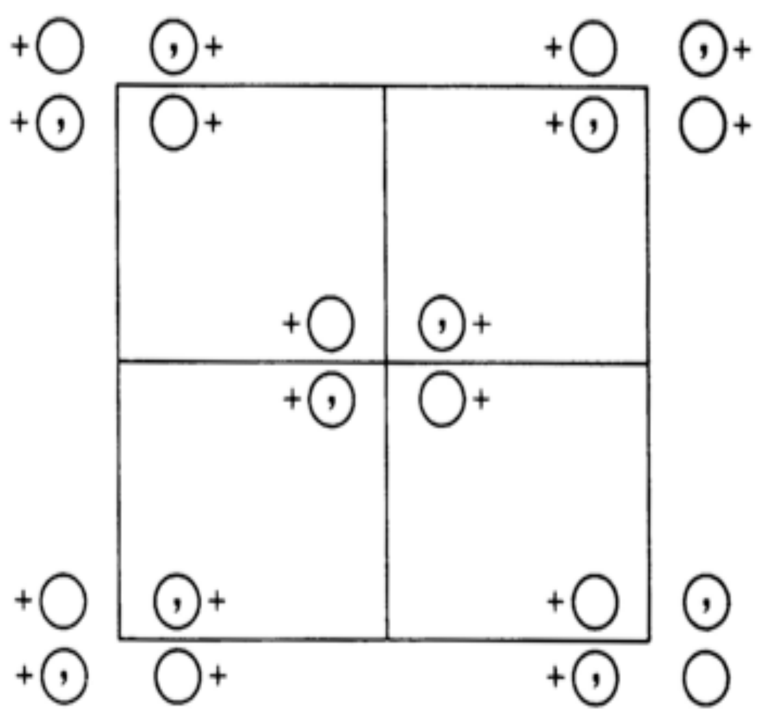


Diagram of general position points



Coordinates

$(0,0,0)+ \quad (\frac{1}{2},\frac{1}{2},0)+$

General position

8 *f* 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

For $(0,0,0)+$ set

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

For $(\frac{1}{2},\frac{1}{2},0)+$ set

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

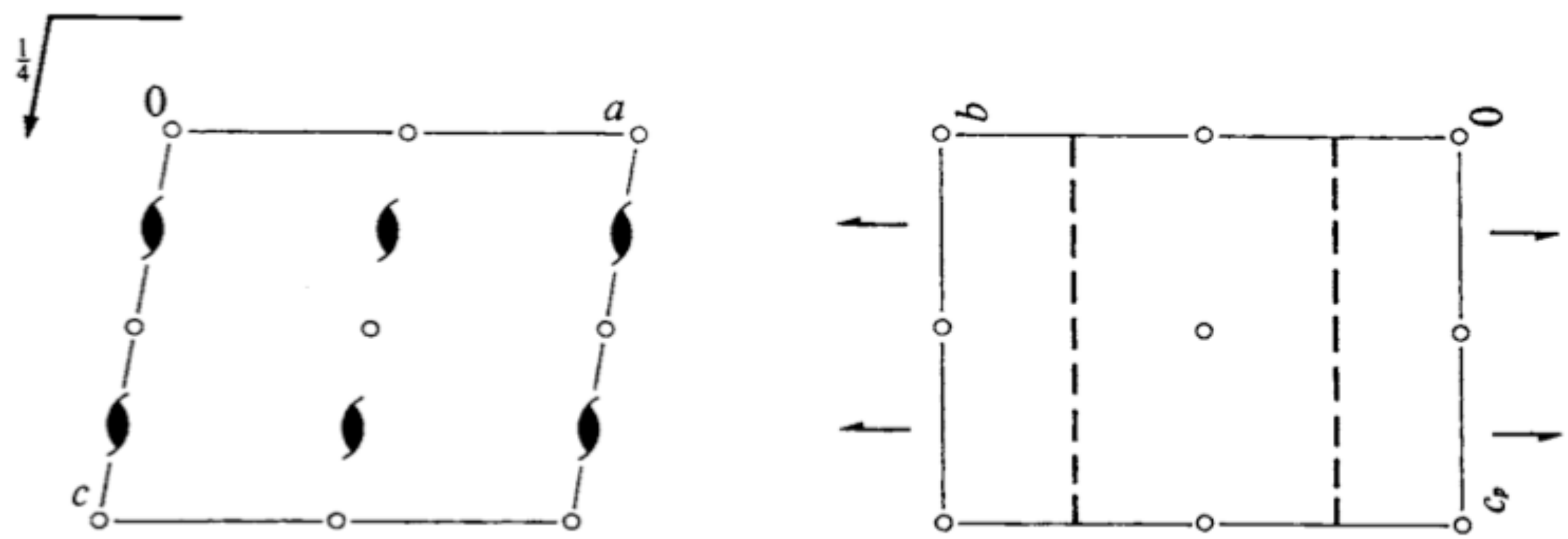
Space group $P2_1/c$ (No. 14)

$P2_1/c$ C_{2h}^5 $2/m$ I

No. 14 $P12_1/c1$ Patterson sy

UNIQUE AXIS b, CELL CHOICE 1

EXAMPLE



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

Geometric interpretation

Symmetry operations

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

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Space-group symmetry

Magnetic Symmetry and Applications

Group-Subgroup Relations of Space Groups

Representations and Applications

Solid State Theory Applications

Structure Utilities

Subperiodic Groups: Layer, Rod and Frieze Groups

Structure Databases

Raman and Hyper-Raman scattering

Point-group symmetry

Plane-group symmetry

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ews:

- **New Article in Nature**
  07/2017: Bradlyn *et al.* "Topological quantum chemistry" *Nature* (2017). **547**, 298-305.
- **New program: BANDREP**
  04/2017: Band representations and Elementary Band representations of Double Space Groups.
- **New section: Double point and space groups**
  - **New program: DGENPOS**
    04/2017: General positions of Double Space Groups
  - **New program: REPRESENTATIONS DPG**
    04/2017: Irreducible representations of

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  - New program: REPRESENTATIONS DPG
    04/2017: Irreducible representations of

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

Structure Utilities

Subperiodic Groups: Layer, Rod and Frieze Groups

Structure Databases

Raman and Hyper-Raman scattering

Point-group symmetry

Plane-group symmetry

Bilbao Crystallographic Server

Problem: Matrix-column presentation
Geometrical interpretation

GENPOS

Generators and General Positions

space group

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**].

To see the data in a non conventional setting click on [**Non conventional Setting**] or [**ITA Settings**] for checking the non

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

choose it 14

Show:

Generators only

All General Positions

Standard/Default Setting

Non Conventional Setting

ITA Settings

Example: Space group $P2_1/c$ (14)

BCS: GENPOS

Space-group symmetry operations

short-hand notation

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

Geometric interpretation

Seitz symbols

General Positions of the Group 14 ($P2_1/c$) [unique axis b]

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+1/2,-z+1/2	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1/2 \\ 0 & 0 & -1 & 1/2 \end{pmatrix}$	2 (0,1/2,0) 0,y,1/4	{ 2_{010} | 0 1/2 1/2 }
3	-x,-y,-z	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{pmatrix}$	-1 0,0,0	{ -1 | 0 }
4	x,-y+1/2,z+1/2	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 1/2 \\ 0 & 0 & 1 & 1/2 \end{pmatrix}$	c x,1/4,z	{ m_{010} | 0 1/2 1/2 }

ITA data

General positions

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

Symmetry operations

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

SEITZ SYMBOLS FOR SYMMETRY OPERATIONS

Seitz symbols { R | t }

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

rotation (or linear) 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* blocks

EXAMPLE

Seitz symbols for symmetry operations of hexagonal and trigonal crystal systems

ITA description				Seitz symbol
No.	coord. triplet	type	orien-tation	
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}

ITA description				Seitz symbol
No.	coord. triplet	type	orien-tation	
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 A 70, 300 (2014)

EXAMPLE

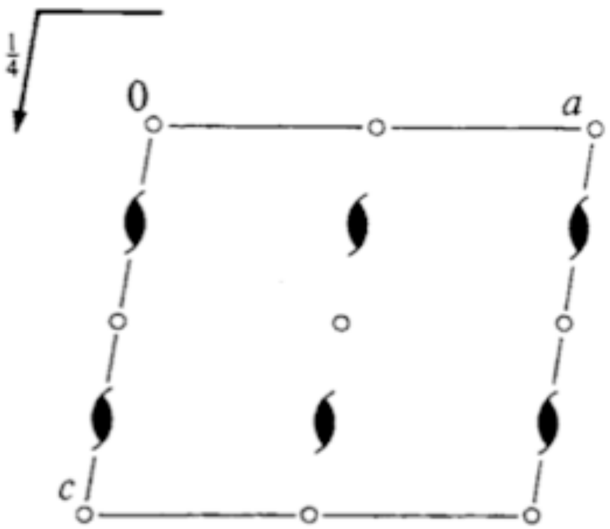
International Tables for Crystallography (2006). Vol. A, Space gro

Space group $P2_1/c$ (No. 14)

$P2_1/c$ $\qquad$ C_{2h}^5 $\qquad$ $2/m$ $\qquad$ Monoclinic

No. 14 $\qquad$ $P\,1\,2_1/c\,1$ $\qquad$ Patterson sy

UNIQUE AXIS *b*, CELL CHOICE 1



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

Symmetry operations

Geometric interpretation

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

Seitz symbols

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

NOT in ITA

Bilbao Crystallographic Server

Problem: Geometric Interpretation of (W,w) — 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.

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:

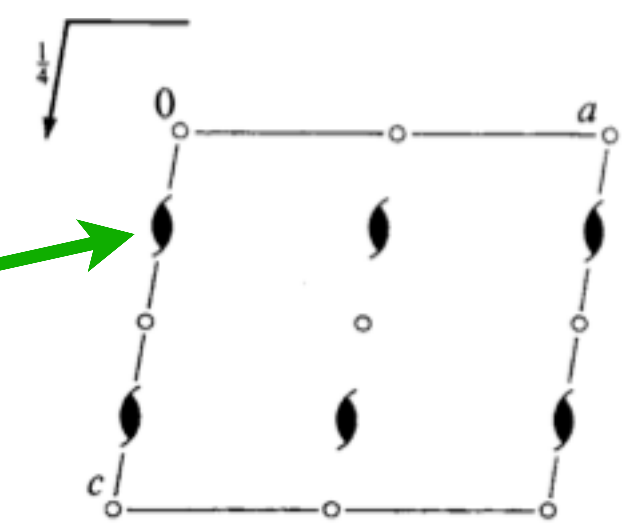
We obtain the geometric interpretation of the symmetry operation.

Introduce the crystal system	monoclinic
Or enter the sequential number of group as given in the *International Tables for Crystallography*, Vol. A	choose it
Matrix column representation of symmetry operation	-x,y+1/2,-z+1/2

In matrix form	Rotational part			Translation
	1	0	0	0
	0	1	0	0
	0	0	1	0

Standard/Default Setting — Non Conventional Setting — ITA Settings

-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 (0,1/2,0) 0,y,1/4



EXERCISES

Problem 1.6.2.3 (cont.)

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

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).

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

Problem 1.6.2.4

Determine the orientation and location of the three mutually perpendicular 2-fold rotation axes in the space groups $P222$, $P222_1$, $P2_12_12$ and $P2_12_12_1$.

EXERCISES

Problem 1.6.2.2

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

2. 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.

3. Compare your results with the results of the program SYMMETRY OPERATIONS

GENERAL
AND
SPECIAL WYCKOFF
POSITIONS
SITE-SYMMETRY

General and special Wyckoff positions

Orbit of a point X_o under G: $G(X_o)=\{(W,w)X_o,(W,w)\in G\}$

Multiplicity

Site-symmetry group $S_o=\{(W,w)\}$ of a point X_o

$$(W,w)X_o = X_o$$

$$\left(\begin{array}{ccc|c} a & b & c & w_1 \\ d & e & f & w_2 \\ g & h & i & w_3 \end{array}\right)\begin{pmatrix} x_0 \\ y_0 \\ z_0 \end{pmatrix} = \begin{pmatrix} x_0 \\ y_0 \\ z_0 \end{pmatrix}$$

Multiplicity: $|P|/|S_o|$

General position X_o

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

Multiplicity: $|P|$

Special position X_o

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

Multiplicity: $|P|/|S_o|$

Oriented symbols of site-symmetry groups

General position

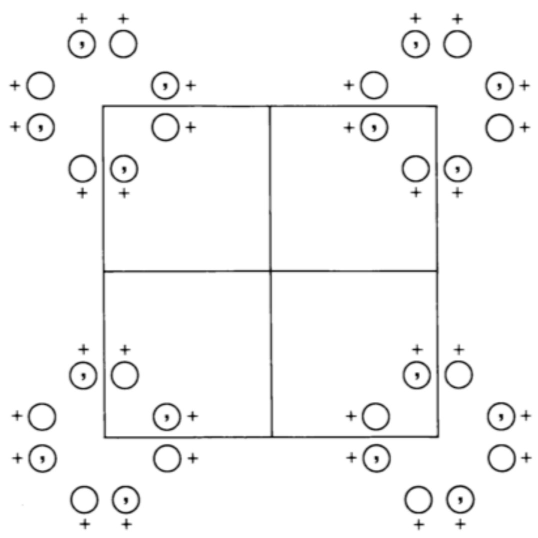
(i) **coordinate triplets** of an image point $\tilde{X}$ of the original point X= $\begin{bmatrix} x \\ y \\ z \end{bmatrix}$ under (W,w) of G

-presentation of infinite image points $\tilde{X}$ under the action of (W,w) of G: $0 \leq x_i < 1$

(ii) short-hand notation of the matrix-column pairs (W,w) of the **symmetry operations** of G

-presentation of infinite symmetry operations of G
$(W,w) = (I,t_n)(W,w_0)$, $0 \leq w_{i0} < 1$

General Position of Space groups



- the coordinate triplets of an image point $\tilde{X}$ of the original point $X = \begin{pmatrix} x \\ y \\ z \end{pmatrix}$ under (W,w) of G

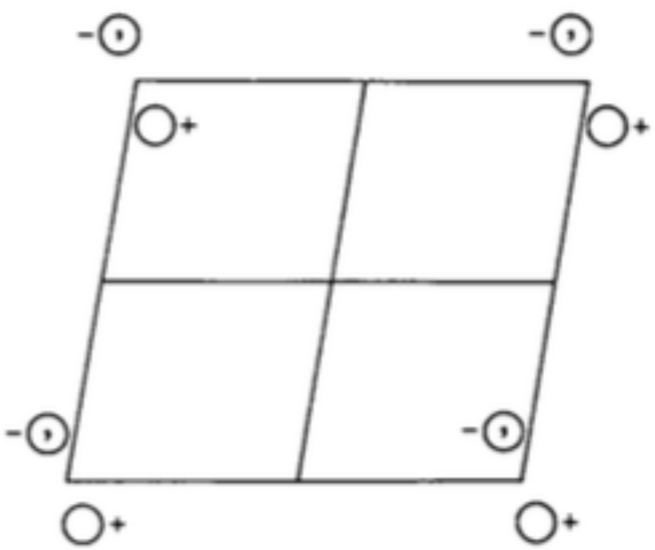
- presentation of infinite image points $\tilde{X}$ of X under the action of (W,w) of G: $0 \leq x_i < 1$

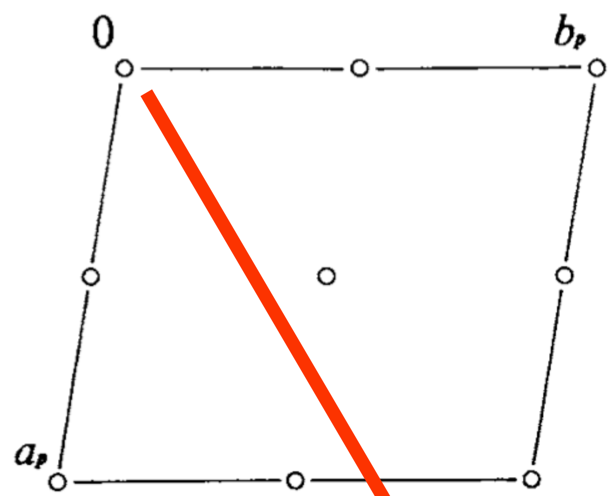
General position

$(I,0)X$	$(W_2,w_2)X$	...	$(W_m,w_m)X$	...	$(W_i,w_i)X$		
$(I,t_1)X$	$(W_2,w_2+t_1)X$	...	$(W_m,w_m+t_1)X$	...	$(W_i,w_i+t_1)X$		
$(I,t_2)X$	$(W_2,w_2+t_2)X$	...	$(W_m,w_m+t_2)X$	...	$(W_i,w_i+t_2)X$		
...	...	...	...	...	...		
$(I,t_j)X$	$(W_2,w_2+t_j)X$	...	$(W_m,w_m+t_j)X$	...	$(W_i,w_i+t_j)X$		
...	...	...	...	...	...		

Example: Calculation of the Site-symmetry groups

Group P-1





Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinate	
2	i	1	(1) x,y,z	(2) $\bar{x},\bar{y},\bar{z}$
1	h	$\bar{1}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	
1	g	$\bar{1}$	$0,\frac{1}{2},\frac{1}{2}$	
1	f	$\bar{1}$	$\frac{1}{2},0,\frac{1}{2}$	
1	e	$\bar{1}$	$\frac{1}{2},\frac{1}{2},0$	
1	d	$\bar{1}$	$\frac{1}{2},0,0$	
1	c	$\bar{1}$	$0,\frac{1}{2},0$	
1	b	$\bar{1}$	$0,0,\frac{1}{2}$	
1	a	$\bar{1}$	$0,0,0$	

$S=\{(W,w),\ (W,w)X_o = X_o\}$

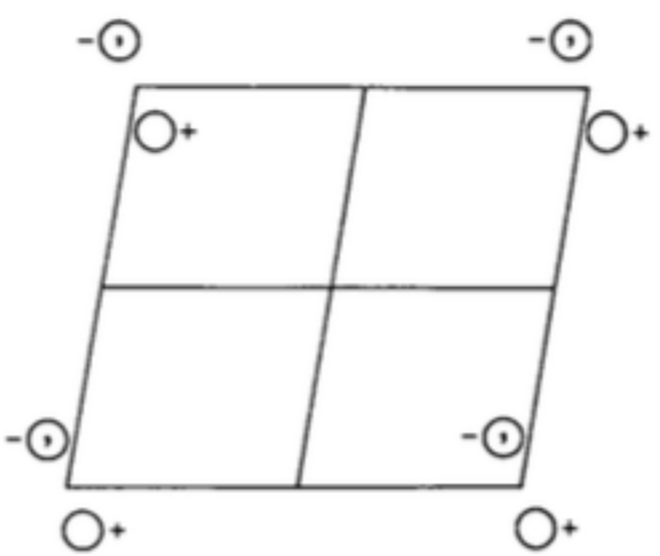
$$\left(\begin{array}{ccc|c} -1 & & & 0 \\ & -1 & & 0 \\ & & -1 & 0 \end{array}\right)\begin{pmatrix}0\\0\\0\end{pmatrix} = \begin{pmatrix}0\\0\\0\end{pmatrix}$$

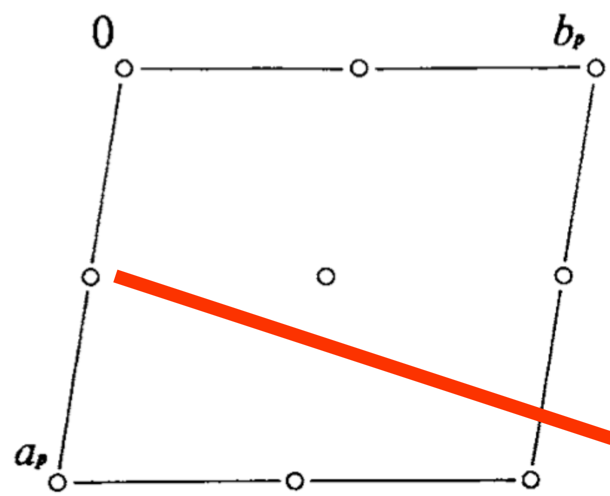
$S_f=\{(1,0),\ (-1,000)X_f = X_f\}$

$S_f \simeq \{1, -1\}$ isomorphic

QUIZ: Calculation of the Site-symmetry groups

Group P-1





Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates	
2	*i*	1	(1) x,y,z	(2) $\bar{x},\bar{y},\bar{z}$
1	*h*	$\bar{1}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	
1	*g*	$\bar{1}$	$0,\frac{1}{2},\frac{1}{2}$	
1	*f*	$\bar{1}$	$\frac{1}{2},0,\frac{1}{2}$	
1	*e*	$\bar{1}$	$\frac{1}{2},\frac{1}{2},0$	
1	*d*	$\bar{1}$	$\frac{1}{2},0,0$	
1	*c*	$\bar{1}$	$0,\frac{1}{2},0$	
1	*b*	$\bar{1}$	$0,0,\frac{1}{2}$	
1	*a*	$\bar{1}$	$0,0,0$	

Determine the site symmetry group of the point

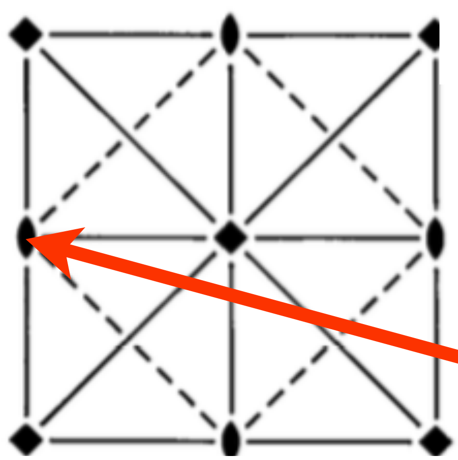
$$X_o = \begin{pmatrix} 1/2 \\ 0 \\ 1/2 \end{pmatrix}$$

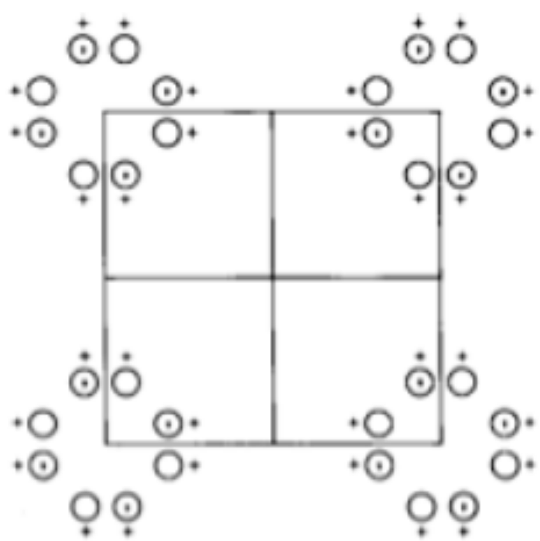
Hint: $S=\{(W,w), (W,w)X_o = X_o\}$

Problem 1.6.2.5

Space group P4mm

General and special Wyckoff positions of P4mm





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	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	$0,0,z$			

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

Bilbao Crystallographic Server

Problem: Wyckoff positions
Site-symmetry groups
Coordinate transformations

WYCKPOS

Wyckoff Positions

space group

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**.

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.

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 basis

Transformation of the basis

ITA settings

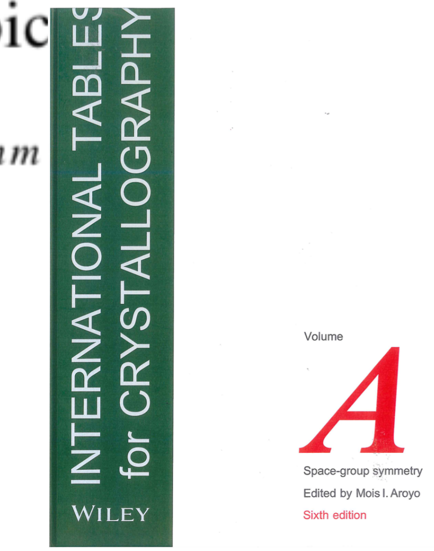
ITA-Settings for the Space Group 68

ces must be read by columns. **P** is the transformation f

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

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

$Ccce$	D_{2h}^{22}	mmm	Orthorhombic
No. 68	$C\ 2/c\ 2/c\ 2/e$		Patterson symmetry $Cmmm$



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.	$0,y,\frac{1}{4}$	$\frac{1}{2},\bar{y},\frac{1}{4}$	$0,\bar{y},\frac{3}{4}$	
8	e	2..	$x,\frac{1}{4},\frac{1}{4}$	$\bar{x}+\frac{1}{2},\frac{3}{4},\frac{1}{4}$	$\bar{x},\frac{3}{4},\frac{3}{4}$	
8	d	$\bar{1}$	$0,0,0$	$\frac{1}{2},0,0$	$0,0,\frac{1}{2}$	
8	c	$\bar{1}$	$\frac{1}{4},\frac{3}{4},0$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{3}{4},\frac{1}{2}$	
4	b	222	$0,\frac{1}{4},\frac{3}{4}$	$0,\frac{3}{4},\frac{1}{4}$		
4	a	222	$0,\frac{1}{4},\frac{1}{4}$	$0,\frac{3}{4},\frac{3}{4}$		

Wyckoff Positions of Group 68 (*Ccce*) [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)

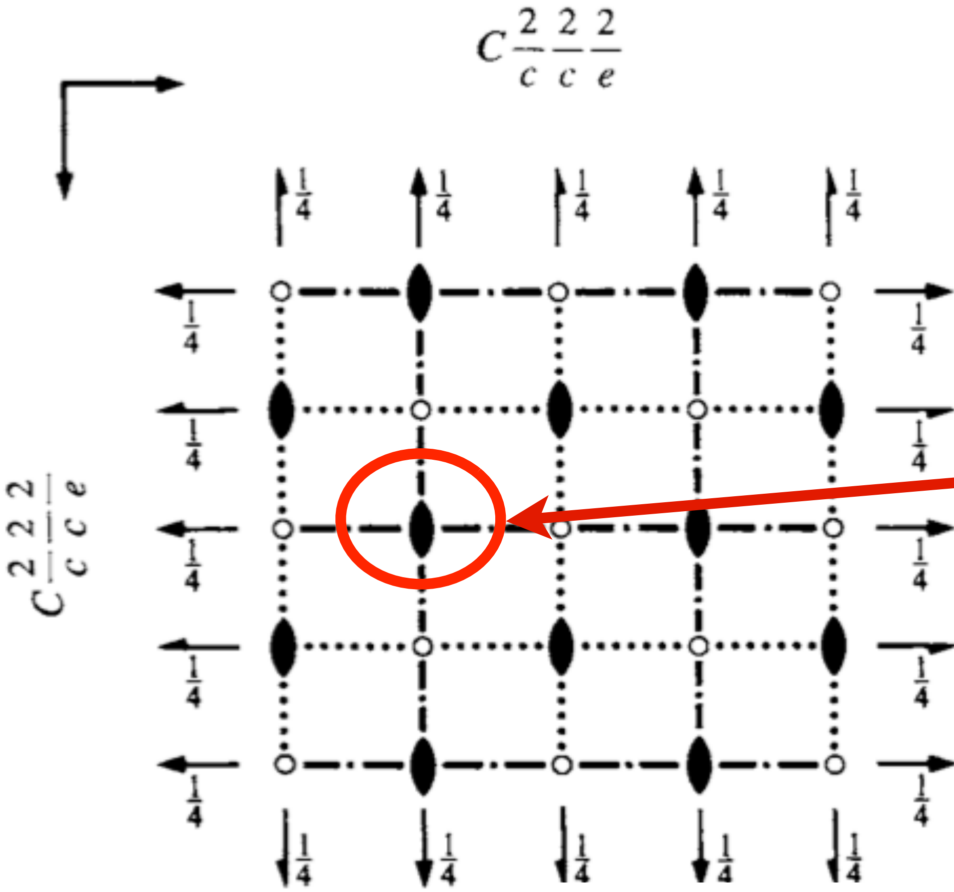
Space Group : 68 (*Ccce*) [origin choice 2
Point : (0,1/4,1/4)
Wyckoff Position : 4a

Site Symmetry Group 222

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

Bilbao Crystallographic Server

Example WYCKPOS: Wyckoff Positions Ccce (68)



2 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 : 68 (*Ccce*) [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

Problem 1.6.2.5 (cont.)

Consider the special Wyckoff positions of the the space group *P4mm*.

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

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

Compare your results with the results of the program WYCKPOS.

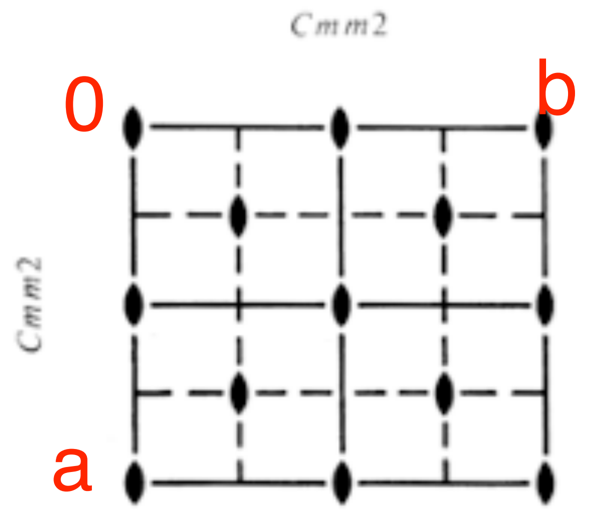
SPACE-GROUPS DIAGRAMS

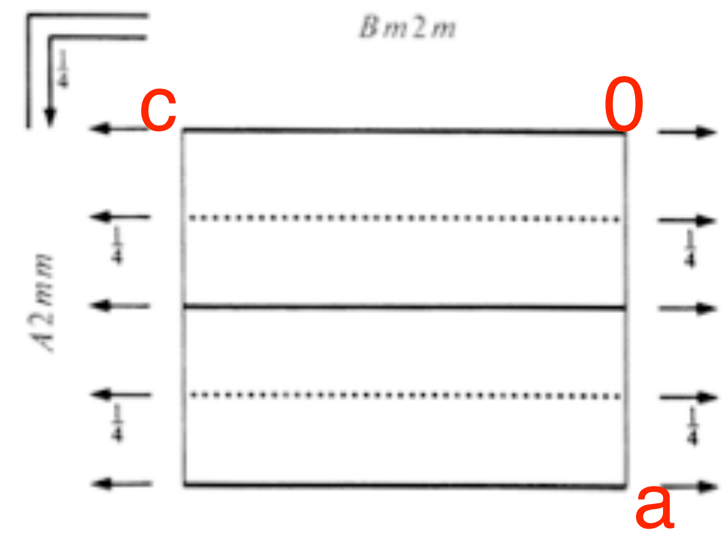
*Cmm*2 (No. 35)

Space-group diagrams

Symmetry-element diagrams

three different projections





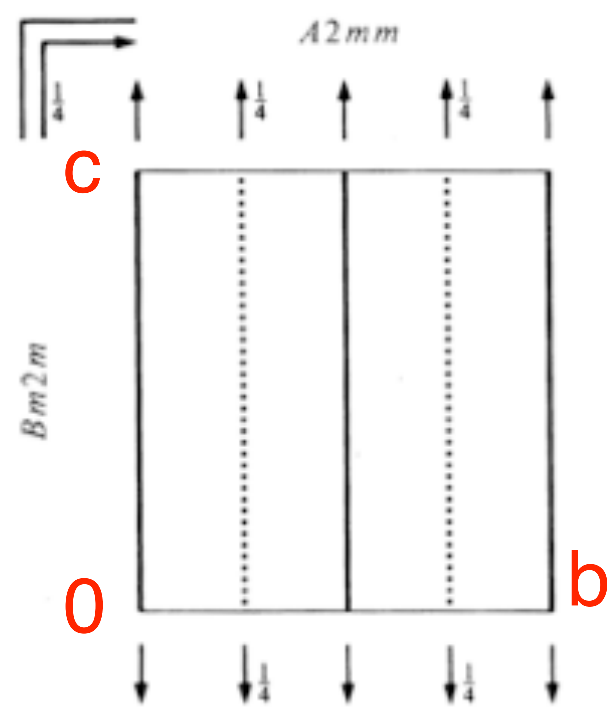
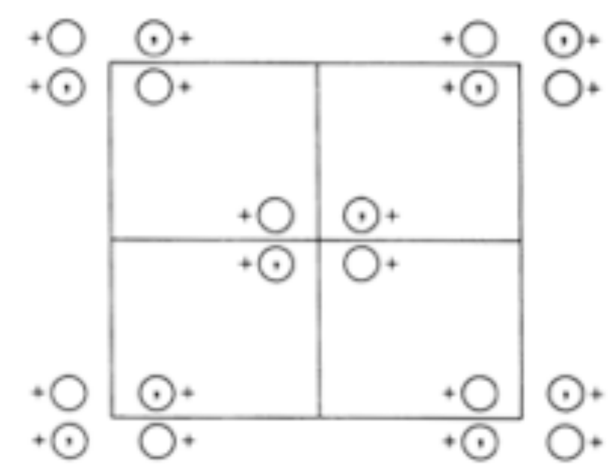


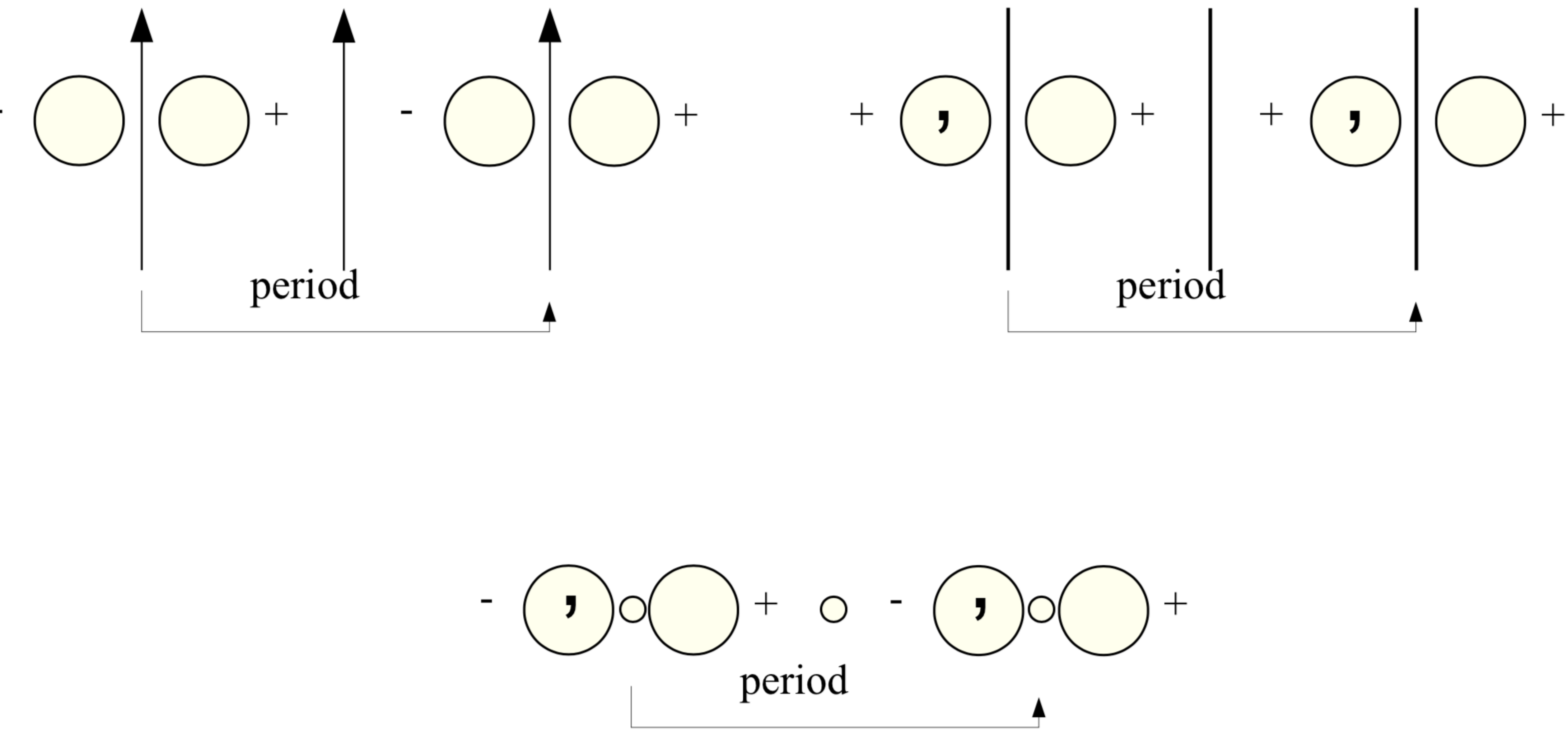
Diagram of general position points



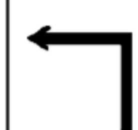
three different settings permutations of ***a,b,c***

No. of space group	Schoen-flies symbol	Standard full Hermann–Mauguin symbol **abc**	Extended Hermann–Mauguin symbols for the six settings of the same unit cell					
			abc (standard)	**ba$\bar{c}$**	**cab**	**$\bar{c}$ba**	**bca**	**a$\bar{c}$b**
35	C_{2v}^{11}	*Cmm*2	*Cmm*2 *ba*2	*Cmm*2 *ba*2	*A*2*mm* 2*cb*	*A*2*mm* 2*cb*	*Bm*2*m* *c*2*a*	*Bm*2*m* *c*2*a*

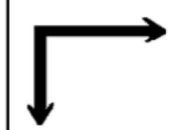
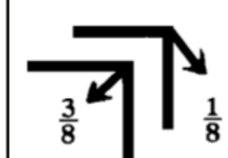
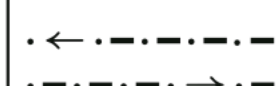
Symmetry elements corresponding to operations of order 2 occur every half a period



Mirror and glide planes

Symmetry element	Glide component $|\vec{g}|$	Symbol	Graphical symbol: ⊥ Plane of projection	Graphical symbol: ∥ Plane of projection[a]
Mirror plane Plane of symmetry	–	m		
Glide plane with axial glide component	$\frac{\vec{a}}{2}$	a		
	$\frac{\vec{b}}{2}$	b		
	$\frac{\vec{c}}{2}$	c		

Mirror and glide planes

Symmetry element	Glide component $\lvert\vec{g}\rvert$	Symbol	Graphical symbol	
			⊥ Plane of projection	∥ Plane of projection[a]
Double glide plane with two glide vectors	$\frac{\vec{a}}{2}, \frac{\vec{b}}{2}$	e		
Glide plane with diagonal glide component	$\frac{\vec{a}+\vec{b}}{2}$	n		
	$\frac{\vec{a}+\vec{c}}{2}$			
	$\frac{\vec{b}+\vec{c}}{2}$			
	$\frac{\vec{a}+\vec{b}+\vec{c}}{2}$[b]			
"Diamond" glide plane	$\frac{\vec{a}+\vec{b}}{4}$	d		
	$\frac{\vec{a}+\vec{c}}{4}$			
	$\frac{\vec{b}+\vec{c}}{4}$			
	$\frac{\vec{a}+\vec{b}+\vec{c}}{4}$[b]			

Rotation and screw-rotation axes

Symmetry element	**Screw component** $\|\vec{s}\|$	**Symbol**	**Graphical symbol**
Onefold rotation axis ≡ identity	–	1	
Inversion center Center of symmetry	–	$\bar{1}$	o[a]
Twofold rotation axis	–	2	 ⊥ Plane of Projection  || Plane of projection[a]
Twofold screw axis	$\frac{1}{2}\|\vec{\tau}\|$	2_1	 ⊥ Plane of Projection  || Plane of projection[a]

Rotation and screw-rotation axes

Symmetry element	Screw component $\lvert\vec{s}\rvert$	Symbol	Graphical symbol
Threefold rotation axis	–	3	
Threefold rotoinversion axis	–	$\bar{3}$	
Threefold screw axes	$\frac{1}{3}\lvert\vec{\tau}\rvert$	3_1	
	$\frac{2}{3}\lvert\vec{\tau}\rvert$	3_2	
Fourfold rotation axis	–	4	
Fourfold rotoinversion axis	–	$\bar{4}$	
Fourfold screw axes	$\frac{1}{4}\lvert\vec{\tau}\rvert$	4_1	
	$\frac{2}{4}\lvert\vec{\tau}\rvert$	4_2	
	$\frac{3}{4}\lvert\vec{\tau}\rvert$	4_3	
Sixfold rotation axis	–	6	
Sixfold rotoinversion axis	–	$\bar{6}$	
Sixfold screw axes	$\frac{1}{6}c_0$	6_1	
	$\frac{2}{6}c_0$	6_2	
	$\frac{3}{6}c_0$	6_3	
	$\frac{4}{6}c_0$	6_4	
	$\frac{5}{6}c_0$	6_5	

EXAMPLE

Space group *Cmm*2 (No. 35)

Geometric interpretation

⑥ Symmetry operations

For (0,0,0)+ set

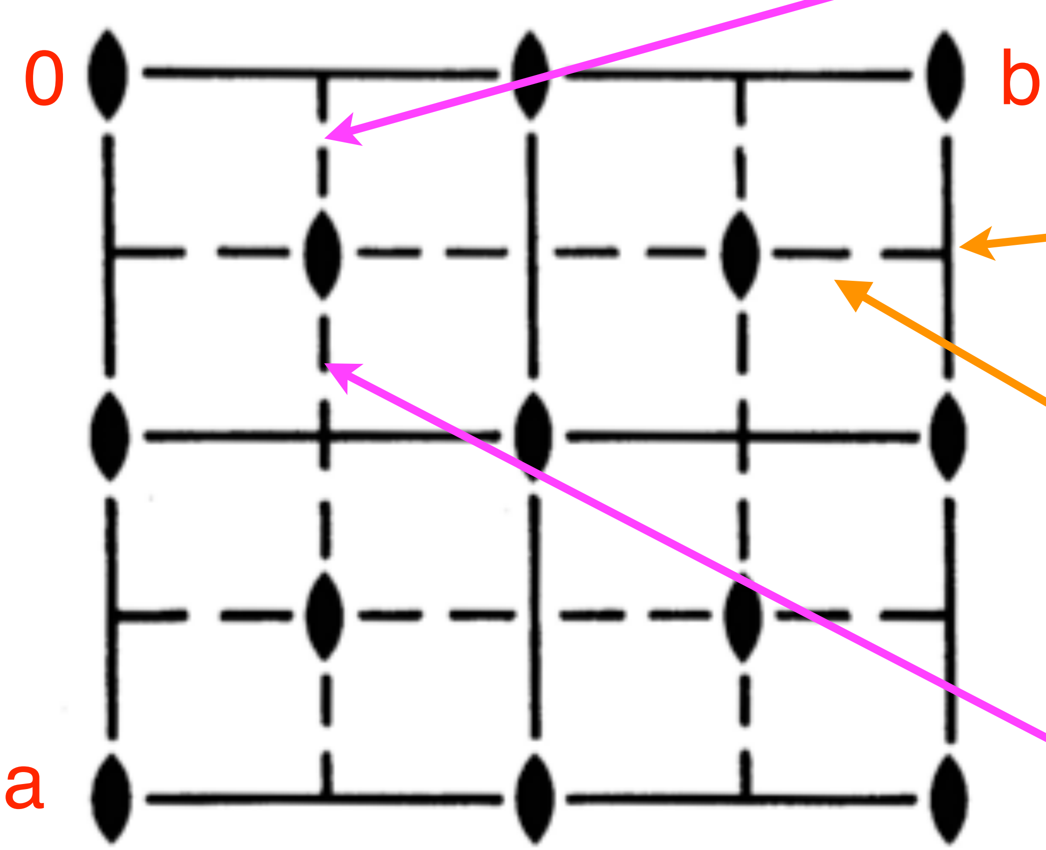
(1) 1 (2) 2 0,0,*z* (3) *m* *x*,0,*z* (4) *m* 0,*y*,*z*

For ($\frac{1}{2}$,$\frac{1}{2}$,0)+ set

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

glide plane, **t**=1/2**a** at y=1/4, ⊥**b**

glide plane, **t**=1/2**b** at x=1/4, ⊥**a**



General Position

Matrix-column presentation of symmetry operations

Coordinates

(0,0,0)+ ($\frac{1}{2}$,$\frac{1}{2}$,0)+

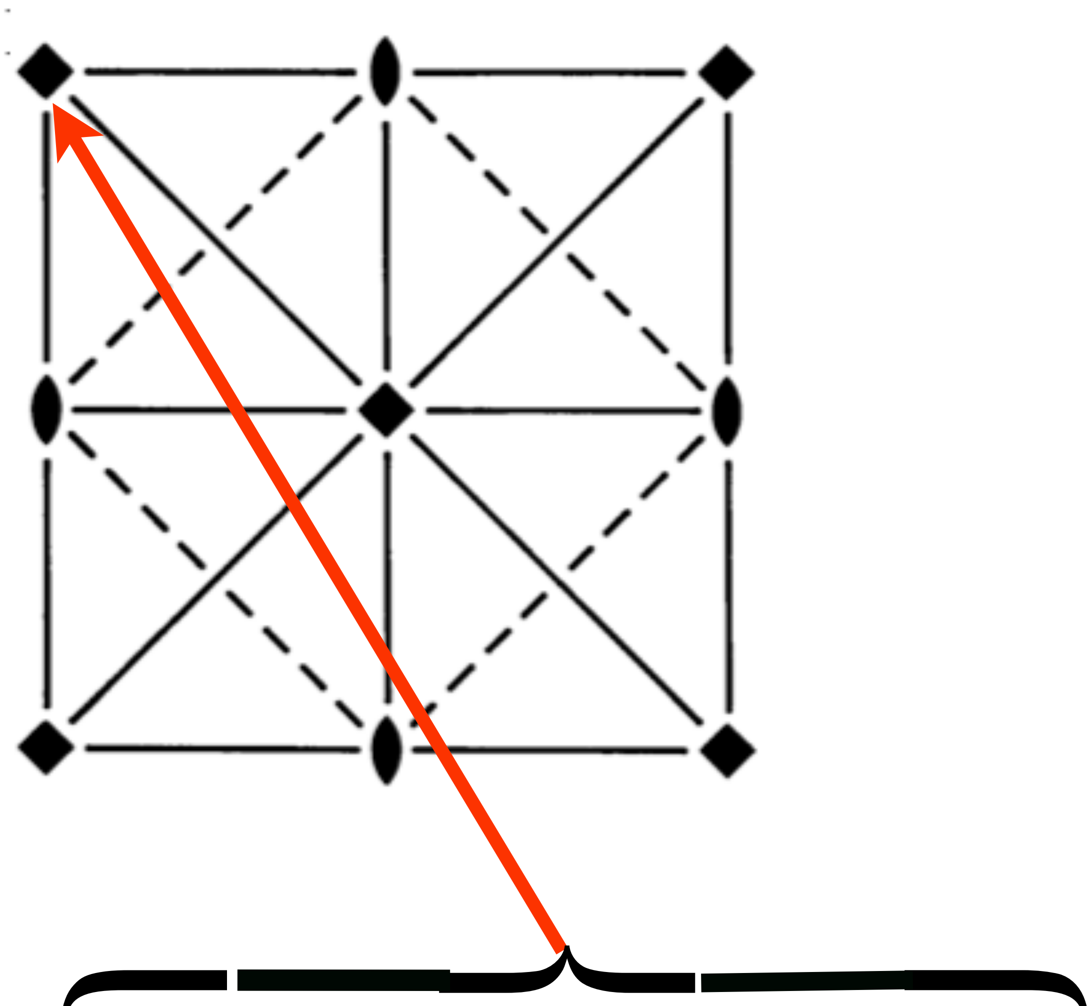
8 *f* 1 (1) *x*,*y*,*z* (2) $\bar{x}$,$\bar{y}$,*z* (3) *x*,$\bar{y}$,*z* (4) $\bar{x}$,*y*,*z*

x+1/2,-y+1/2,z

-x+1/2,y+1/2,z

Example: P4mm

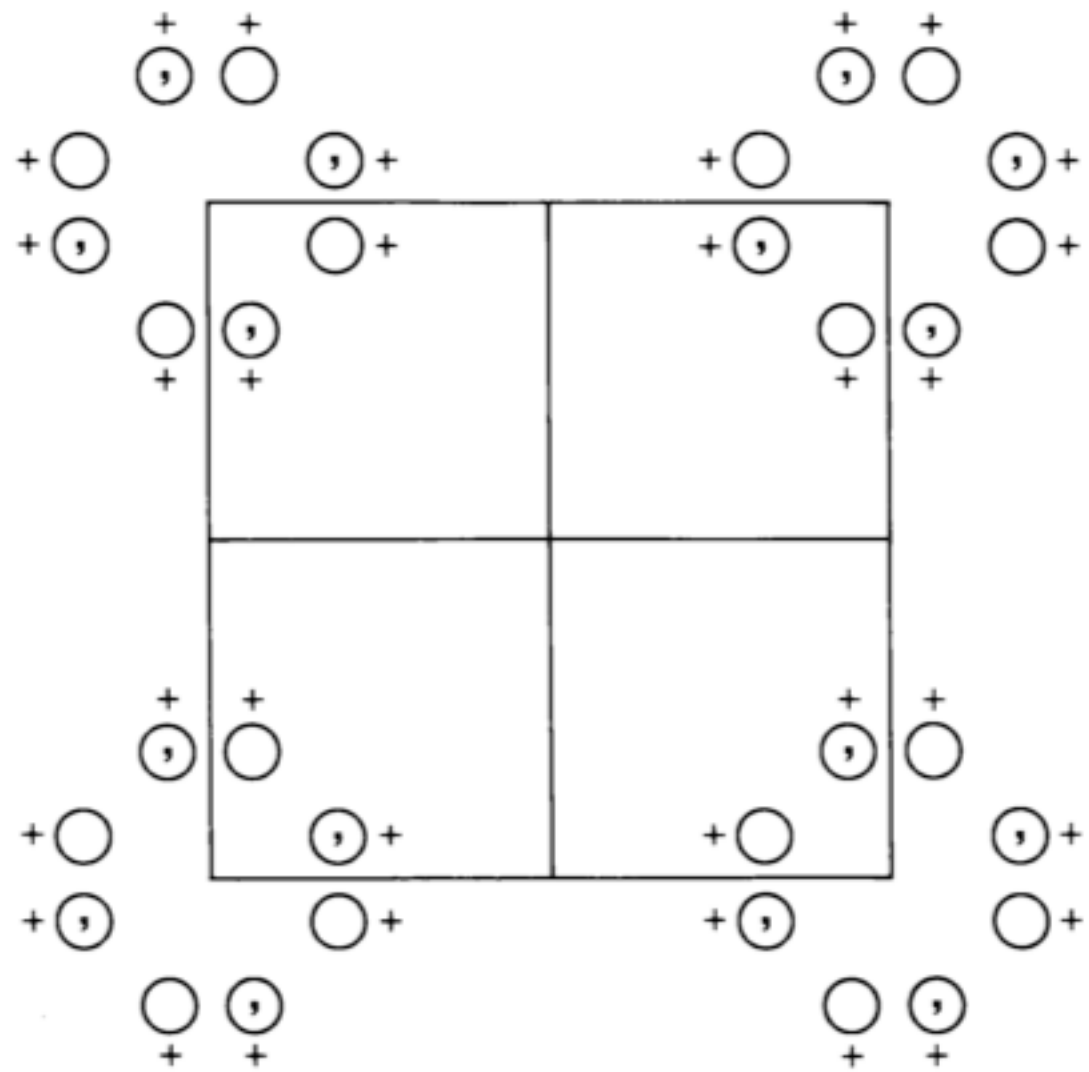
Diagram of symmetry elements



(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

Diagram of general position points



(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

Symmetry elements

Symmetry elements = Geometric element + Element set

Geometric element: Fixed points

Element set: Symmetry operations that share the same geometric element

Examples

Rotation axis

line

1st, ..., (n-1)th powers + all coaxial equivalents

All rotations and screw rotations with the same axis, the same angle and sense of rotation and the same screw vector (zero for rotation) up to a lattice translation vector.

Glide plane

plane

defining operation+ all coplanar equivalents

All glide reflections with the same reflection plane, with glide of d.o. (taken to be zero for reflections) by a lattice translation vector.

Symmetry operations and symmetry elements

Geometric elements and Element sets

Name of symmetry element	Geometric element	Defining operation (d.o)	Operations in element set
Mirror plane	Plane A	Reflection in A	D.o. and its coplanar equivalents*
Glide plane	Plane A	Glide reflection in A; 2ν (not ν) a lattice translation	D.o. and its coplanar equivalents*
Rotation axis	Line b	Rotation around b, angle $2\pi/n$ $n = 2, 3, 4$ or 6	1st, ..., $(n-1)$th powers of d.o. and their coaxial equivalents†
Screw axis	Line b	Screw rotation around b, angle $2\pi/n$, $u = j/n$ times shortest lattice translation along b, right-hand screw, $n = 2, 3, 4$ or 6, $j = 1, \ldots, (n-1)$	1st, ..., $(n-1)$th powers of d.o. and their coaxial equivalents†
Rotoinversion axis	Line b and point P on b	Rotoinversion: rotation around b, angle $2\pi/n$, and inversion through P, $n = 3, 4$ or 6	D.o. and its inverse
Center	Point P	Inversion through P	D.o. only

P. M. de Wolff *et al.* Acta Cryst (1992) A**48** 727

Example: P4mm

Element set of (00z) line

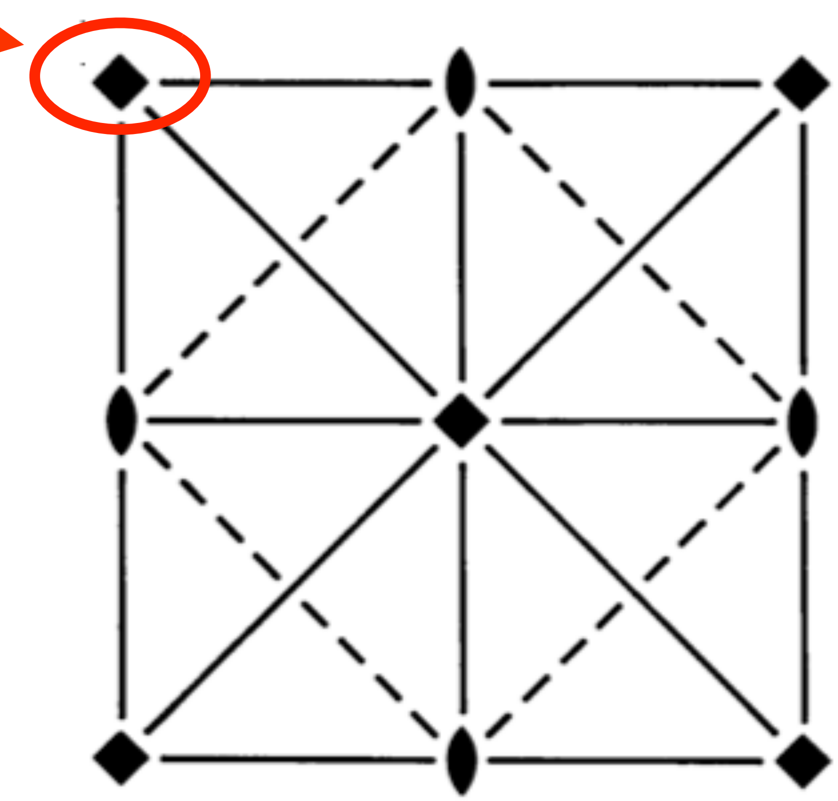
Symmetry operations that share (0,0,z) as geometric element } 1st, 2nd, 3rd powers + all coaxial equivalents

Diagram of symmetry elements

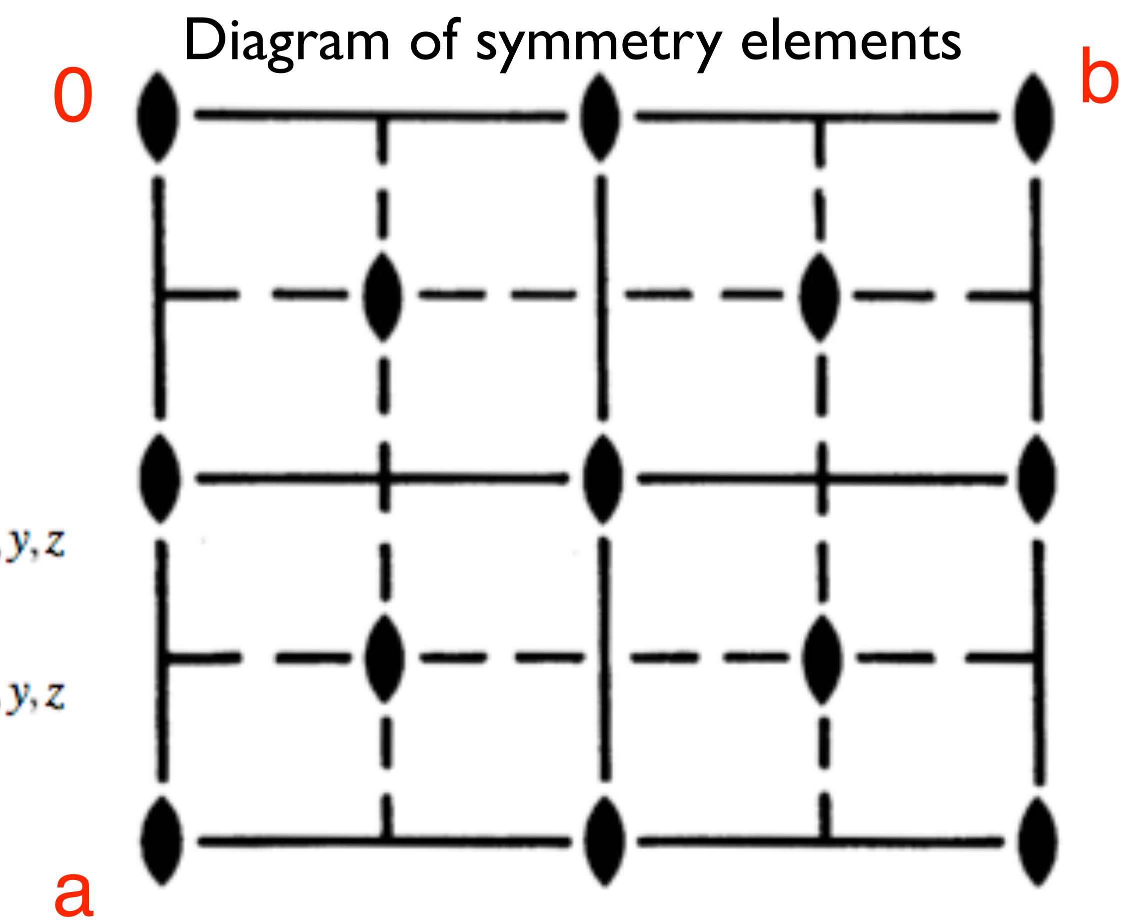
All rotations and screw rotations with the same axis, the same angle and sense of rotation and the same screw vector (zero for rotation) up to a lattice translation vector.

Element set of (0,0,z) line

2	**-x,-y,z**
4+	**-y,x,z**
4-	**y,-x,z**
2(0,0,1)	**-x,-y,z+1**
...	**...**



Space group *Cmm*2 (No. 35)



Symmetry operations

For (0,0,0)+ set

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

For ($\frac{1}{2}$,$\frac{1}{2}$,0)+ set

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

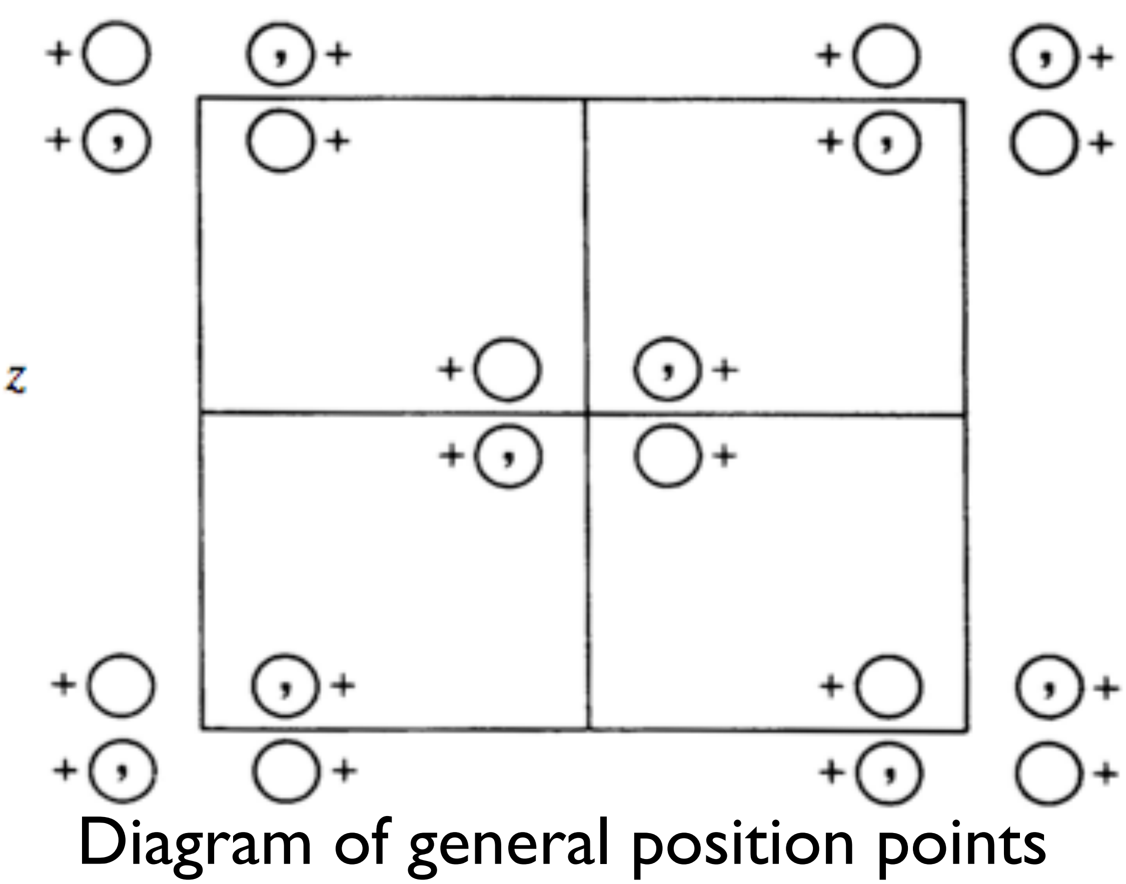
General Position

Coordinates

(0,0,0)+ ($\frac{1}{2}$,$\frac{1}{2}$,0)+

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

How many general position points per unit cell are there?

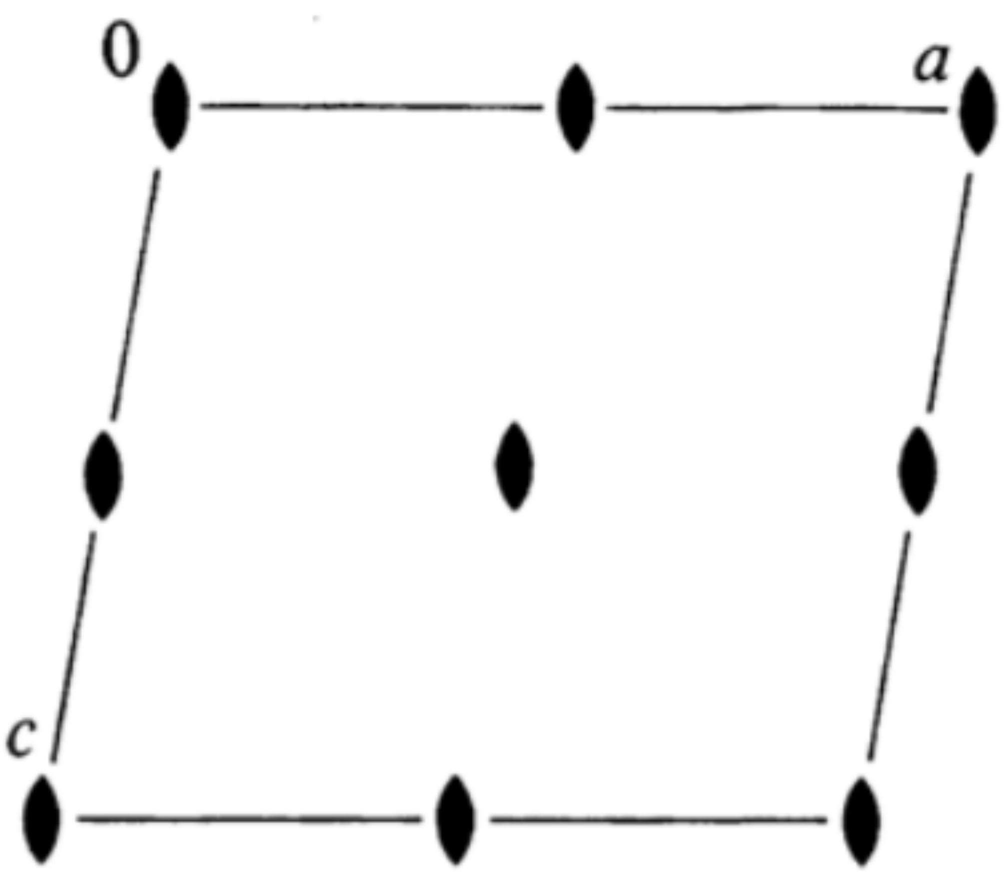


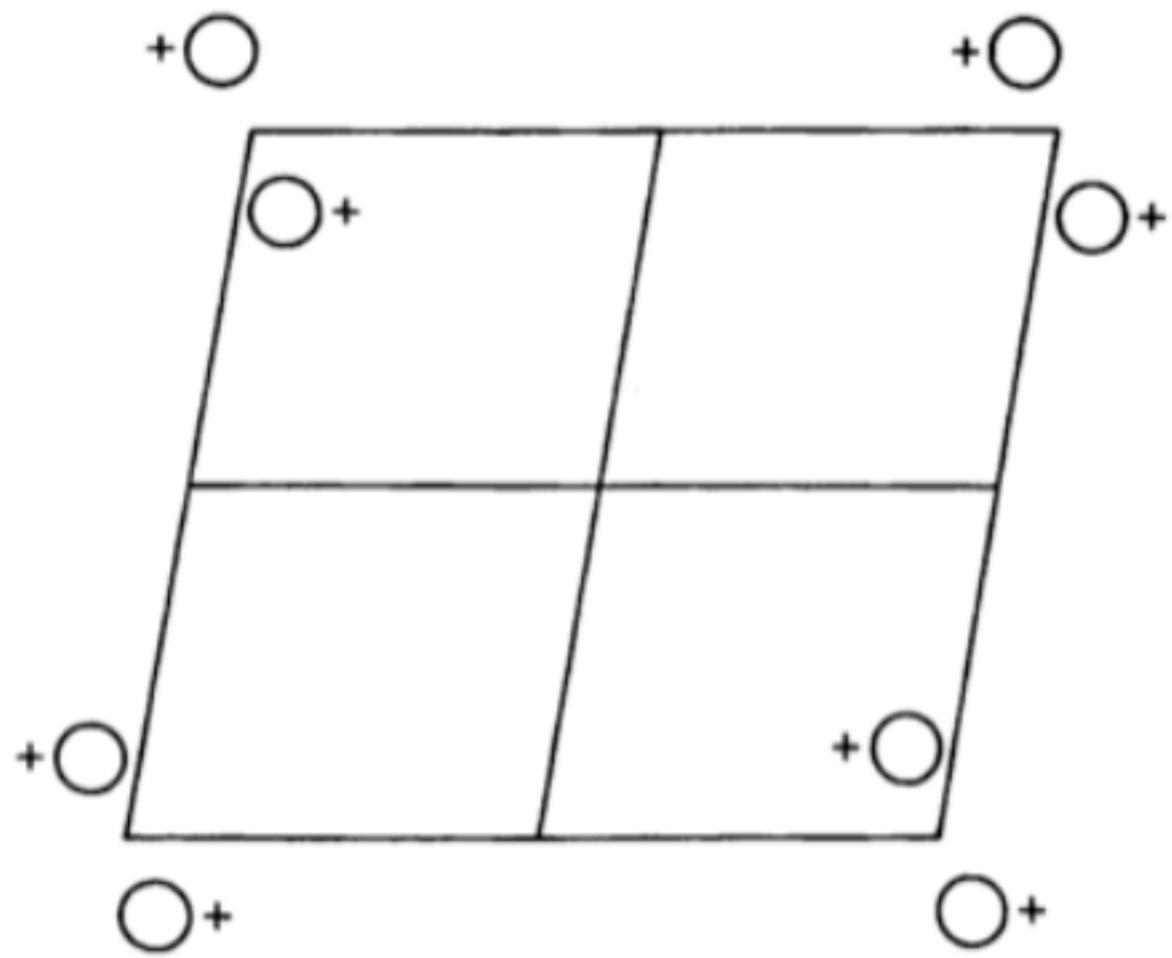
Example: P121

Diagram of general position points

Diagram of symmetry elements

Diagram of general position points

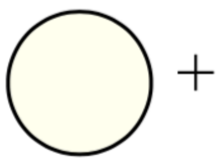




Symmetry element diagram (left) and *General position* diagram (right) of the space group $P2$, No. 3 (unique axis b, cell choice 1).

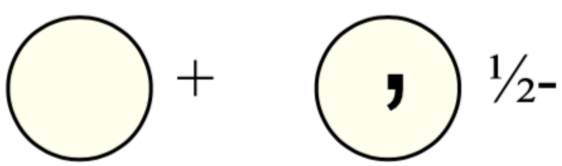
Diagram of general position points

Direction of projection *c* → vertical coordinate *z*.

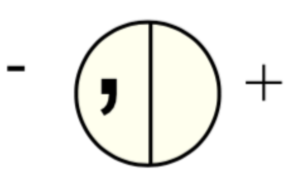


An atom with coordinate $z > 0$ ("+").

Two atoms mapped by an operation of the first kind (handedness preserving operation) with coordinates z (> 0) and ½+z respectively.



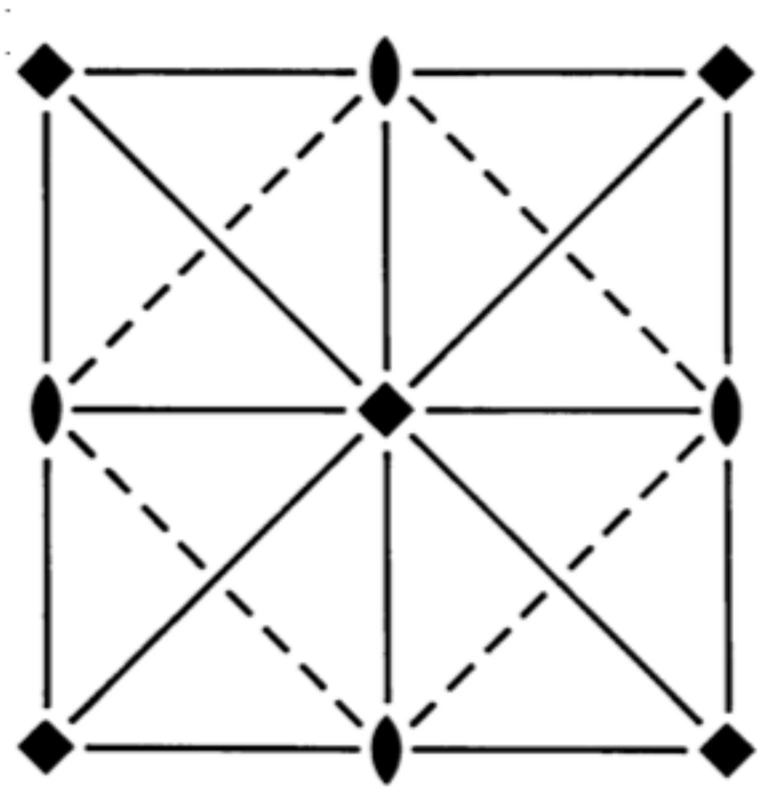
Two atoms mapped by an operation of the second kind (handedness reversing operation: note the "comma") with coordinates z (> 0) and ½-z respectively.



Two atoms mapped by an operation of the second kind (handedness reversing operation: note the "comma") with coordinates x,y,z and $x,y,\bar{z}$ respectively, overlapped in projection. The vertical segment represents a "cut" of the atom above (left) which allows to see half of the atom below (right).

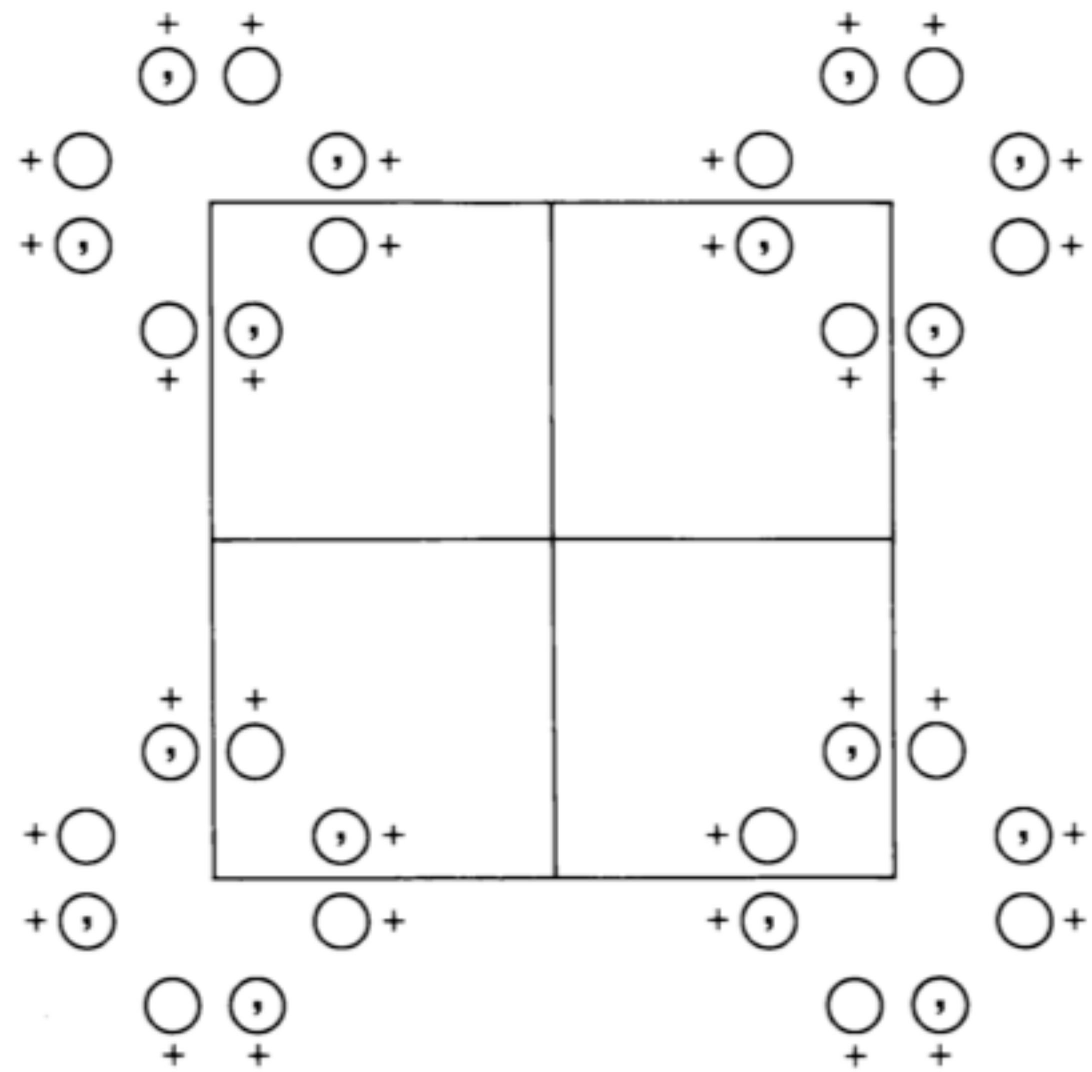
Example: P4mm

Diagram of symmetry elements



(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

Diagram of general position points



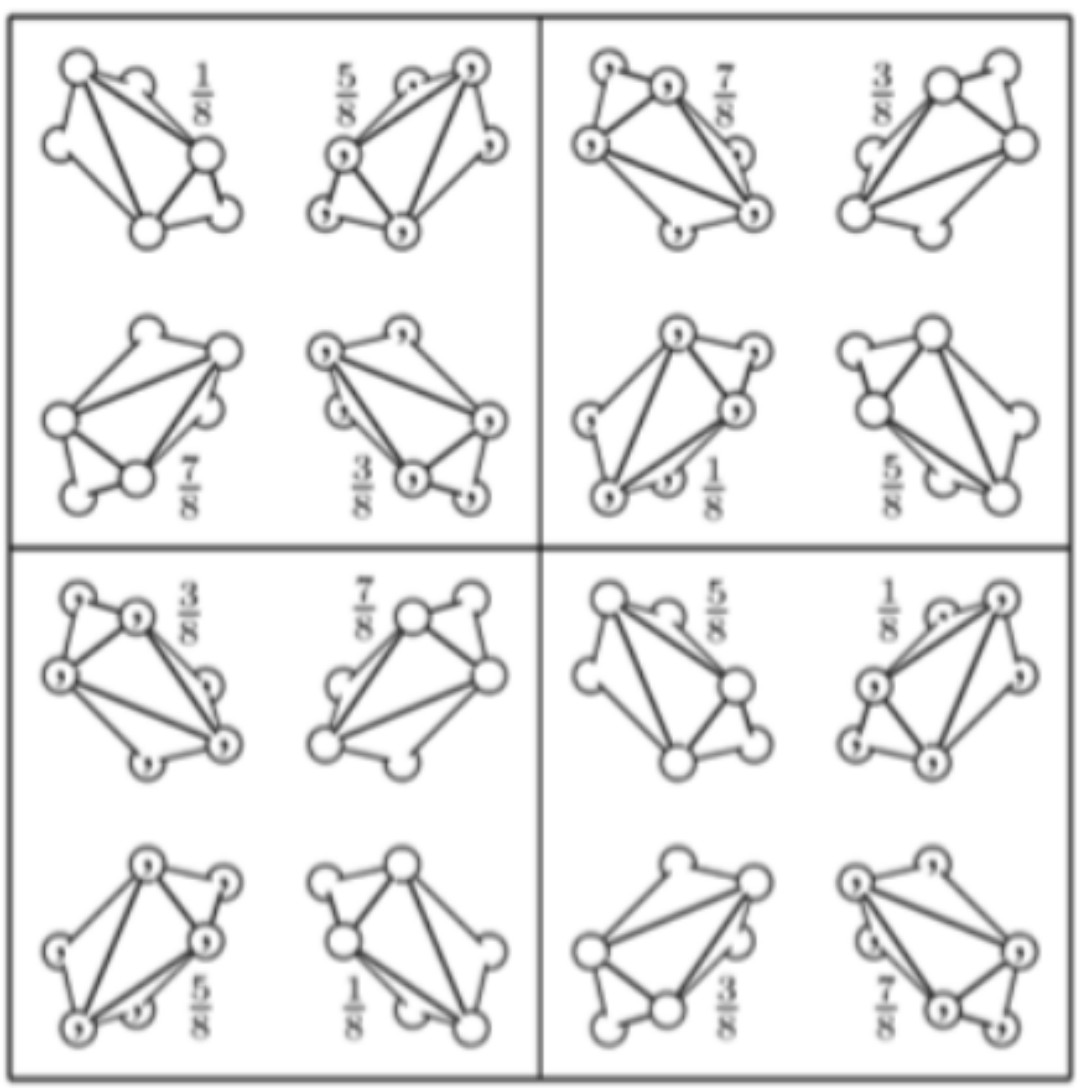
(1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $\bar{y},x,z$ (4) $y,\bar{x},z$
(5) $x,\bar{y},z$ (6) $\bar{x},y,z$ (7) $\bar{y},\bar{x},z$ (8) y,x,z

Example: $Ia\bar{3}d$ (No. 230)

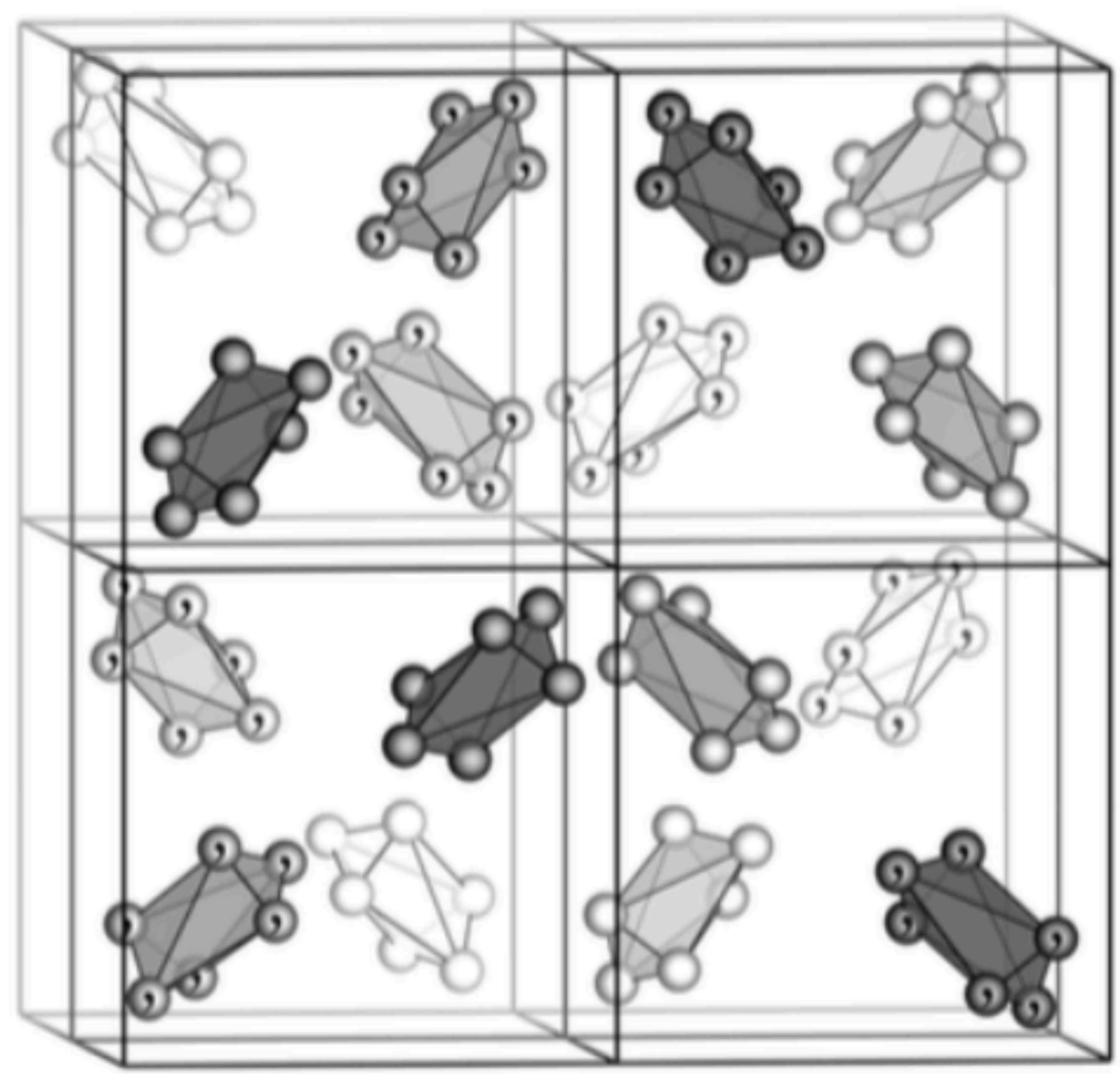
Diagrams of general position points

For the graphical presentation of the **general-position points of cubic groups,** the general-position points are grouped around points of higher site symmetry and represented in the form of **polyhedra**.

orthogonal projection



perspective projection

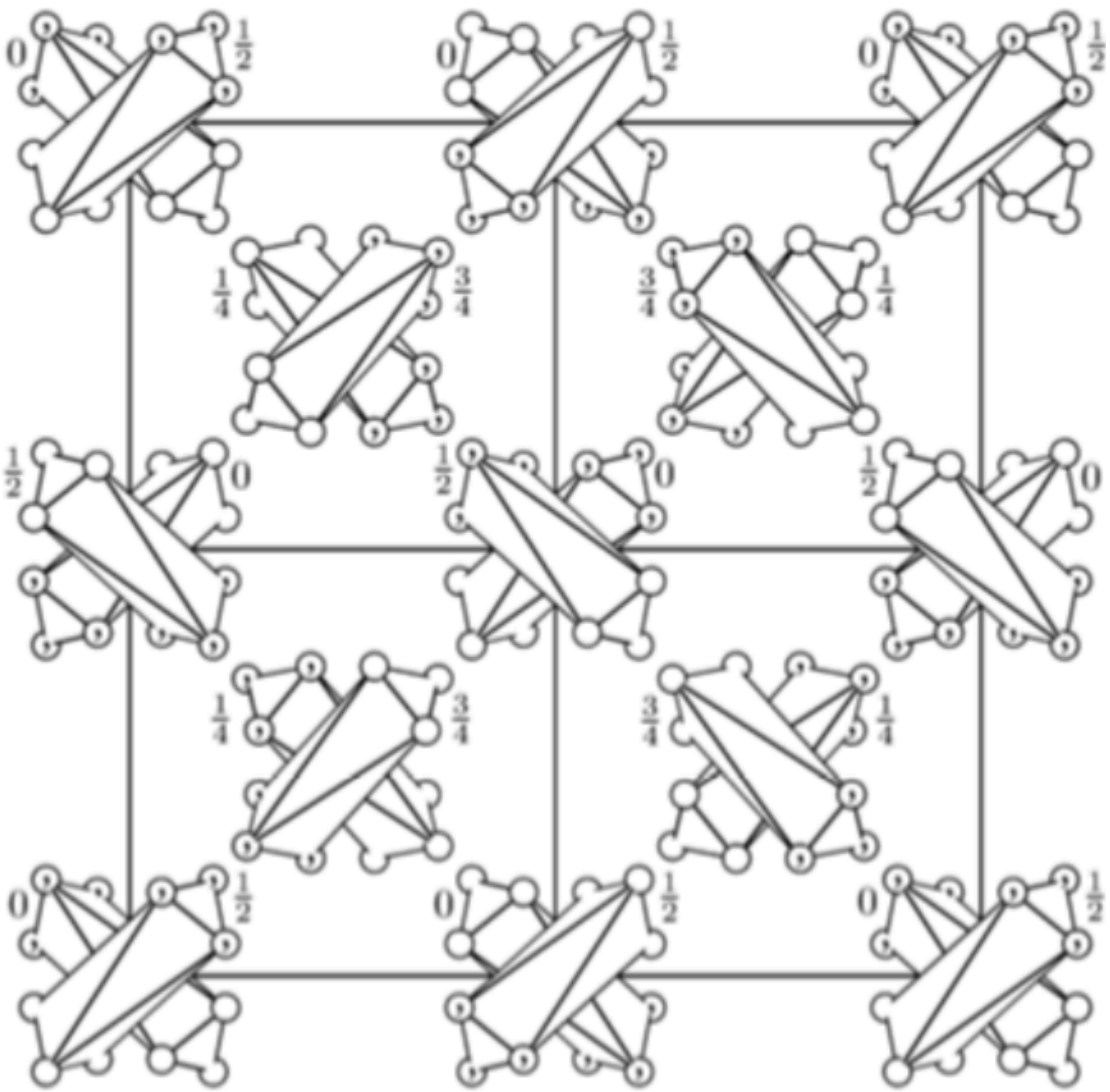


polyhedra (twisted trigonal antiprism) centres at (1/8,1/8,1/8) and its equivalent points, site symmetry .32.

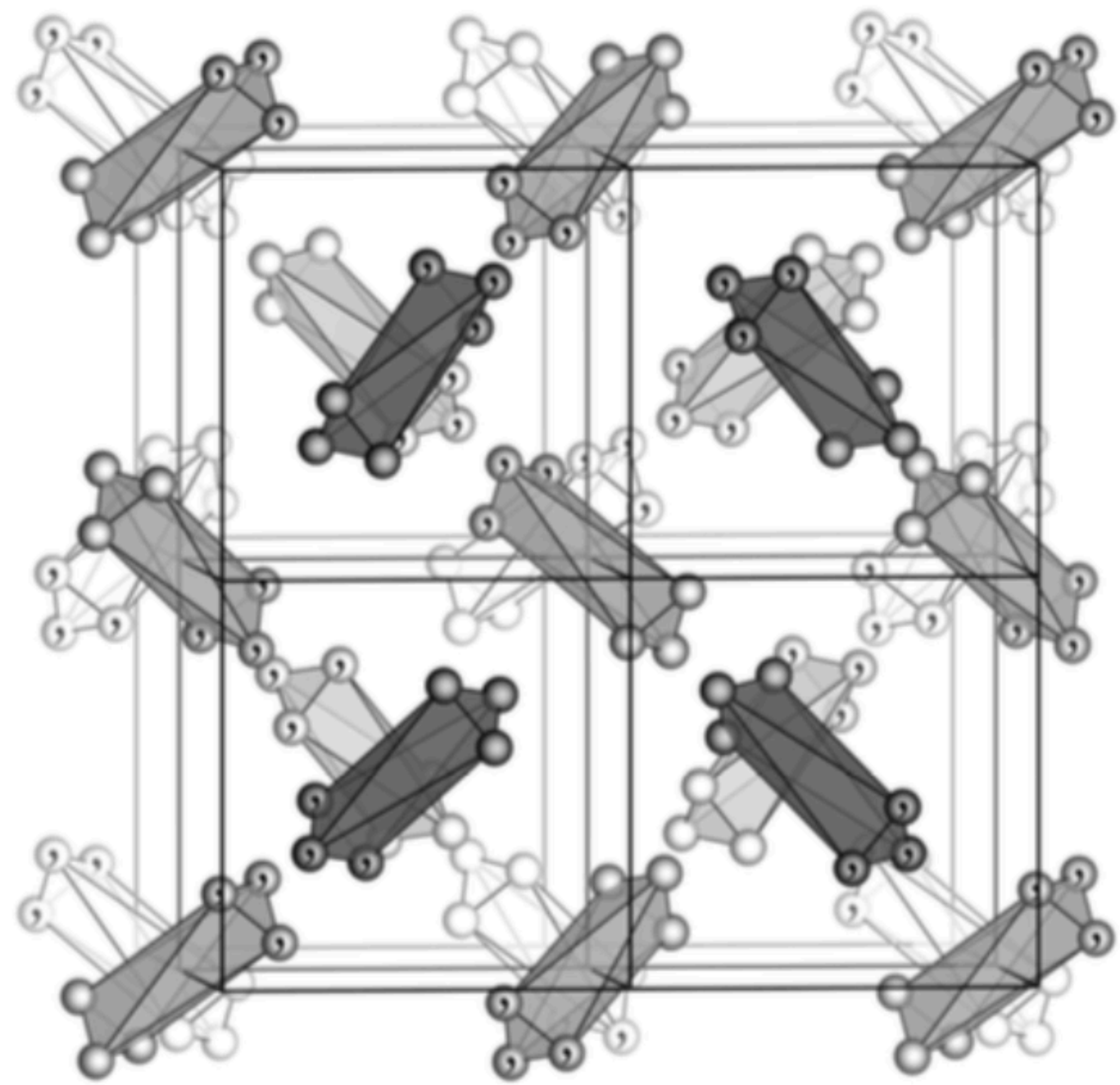
Example: Ia$\bar{3}$d (No. 230)

Diagrams of general position points

orthogonal projection



perspective projection

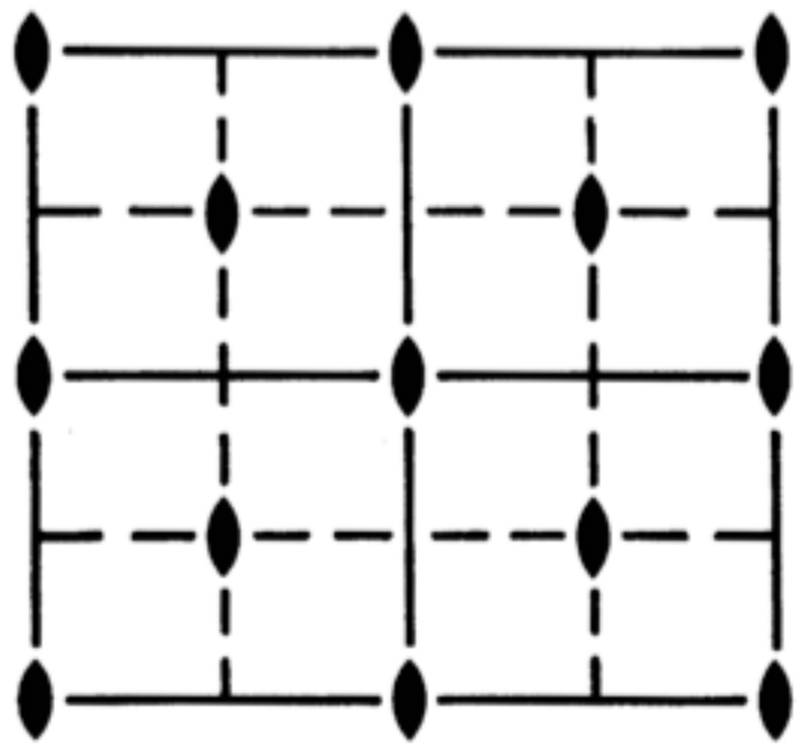


polyhedra (twisted trigonal antiprism) centres at (0,0,0) and its equivalent points, site symmetry .-3.

ORIGINS AND ASYMMETRIC UNITS

Space group *Cmm*2 (No. 35): left-hand page ITA

$Cmm2$	C_{2v}^{11}	$mm2$	Orthorhombic
No. 35	$Cmm2$		Patterson symmetry $Cmmm$



Origin on $mm2$

Origin statement

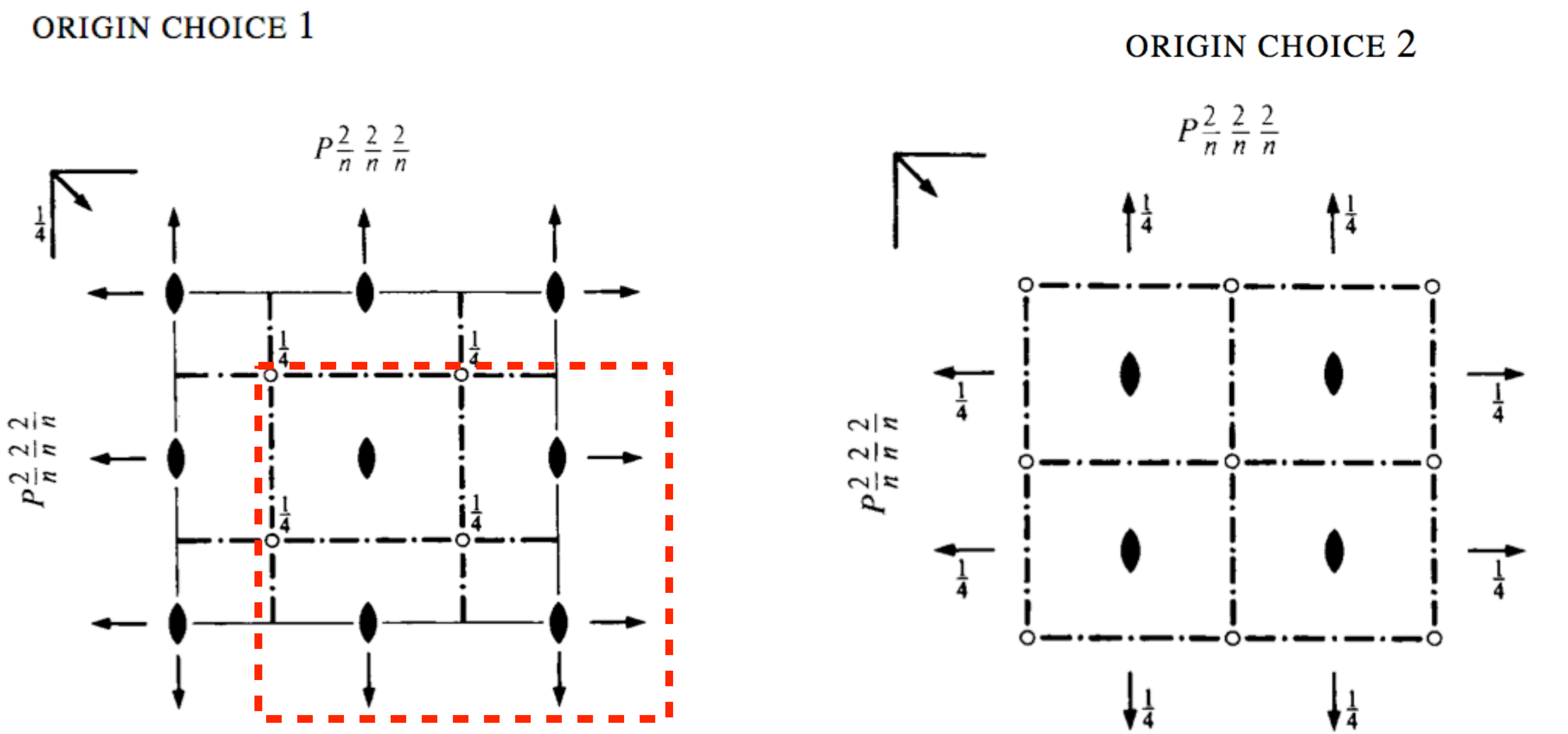
The site symmetry of the origin is stated, if different from the identity.
A further symbol indicates all symmetry elements (including glide planes and screw axes) that pass through the origin, if any.

Space groups with two origins

For each of the two origins the location relative to the other origin is also given.

Example: Different origins for *Pnnn*

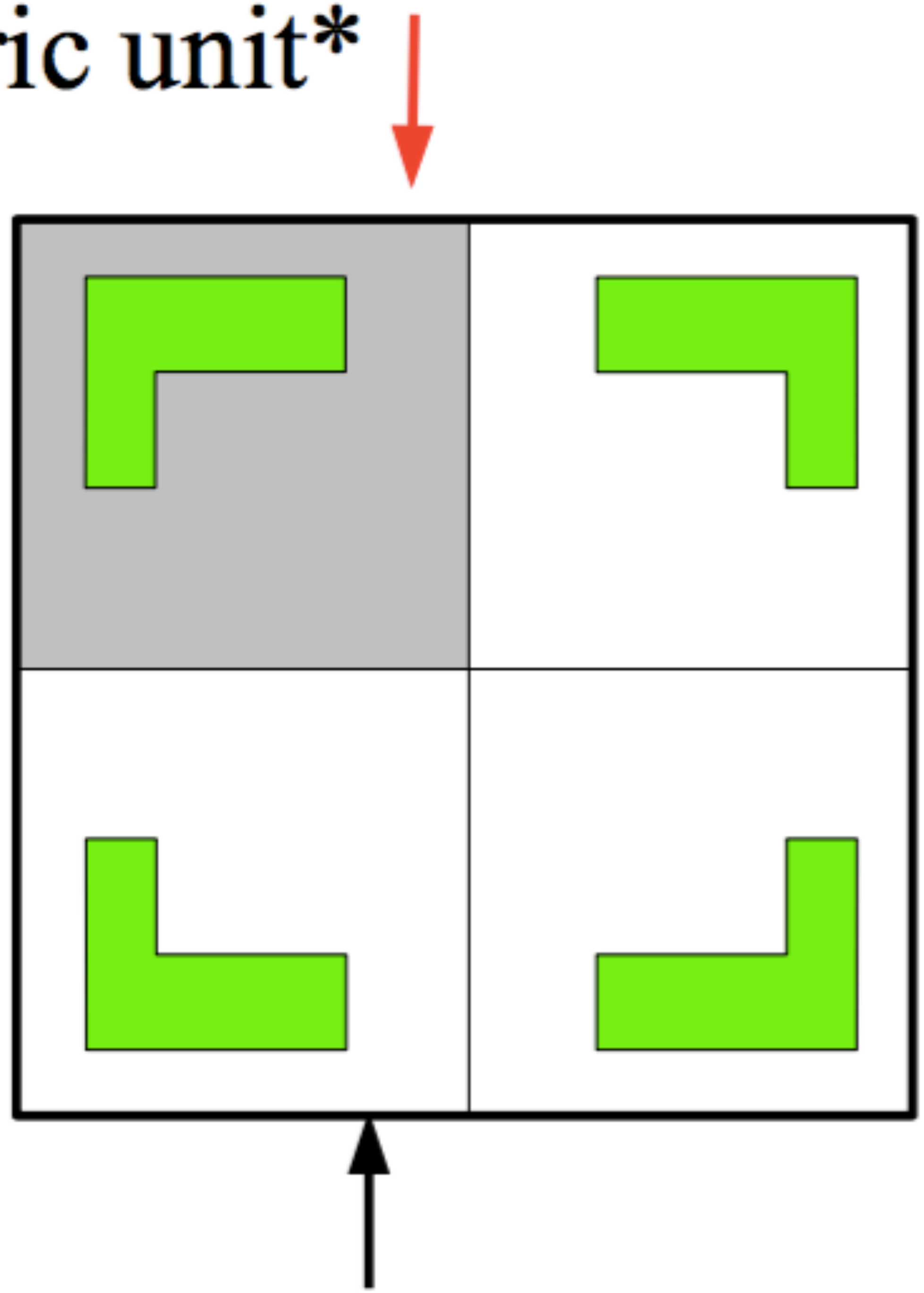
$Pnnn$	D_{2h}^{2}	mmm	Orthorhombic
No. 48	$P\ 2/n\ 2/n\ 2/n$		Patterson symmetry $Pmmm$



Origin at 222, at $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ from $\bar{1}$

Origin at $\bar{1}$ at nnn, at $-\frac{1}{4},-\frac{1}{4},-\frac{1}{4}$ from 222

Asymmetric unit*



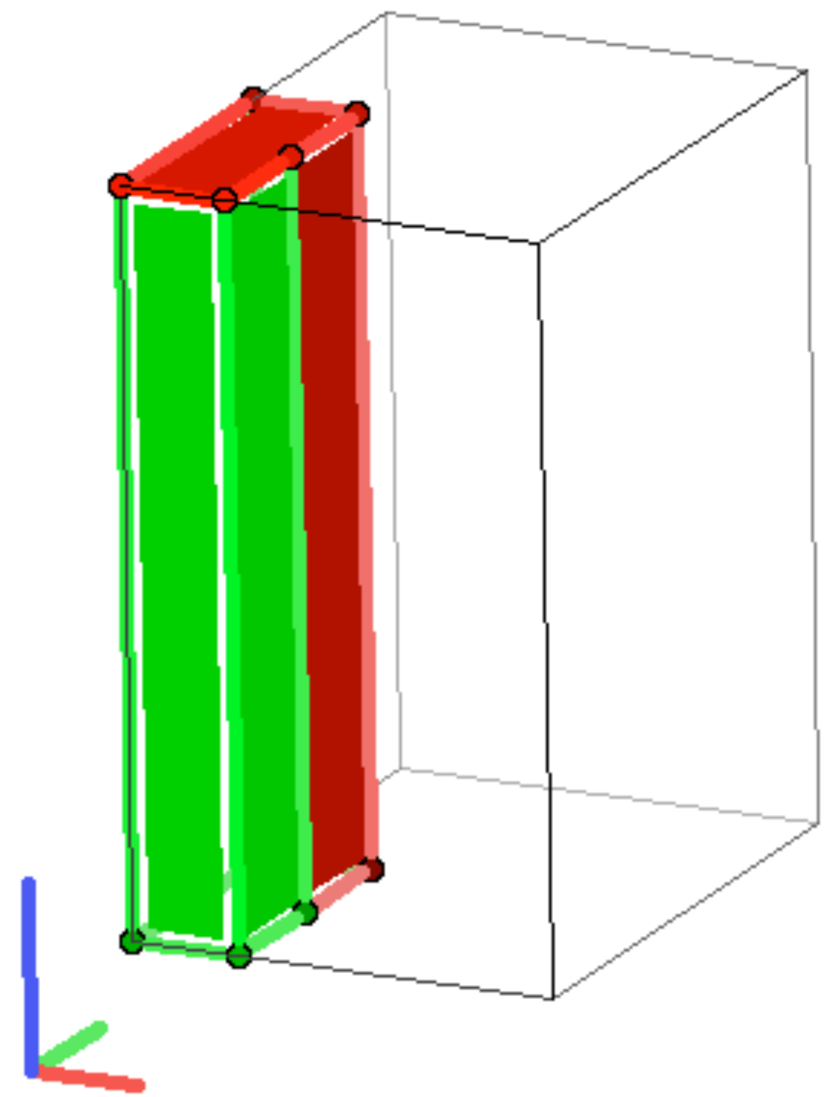
*In mathematics, it is called "fundamental region"

ITA:

An asymmetric unit of a space group is a (simply connected) smallest closed part of space from which, by application of all symmetry operations of the space group, the whole of space is filled.

Example: Asymmetric unit *Cmm*2 (No. 35)

ITA: **Asymmetric unit** $0 \leq x \leq \frac{1}{4}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq 1$



Surface area: green = inside the asymmetric unit, red = outside
Basis vectors: a = red, b = green, c = blue

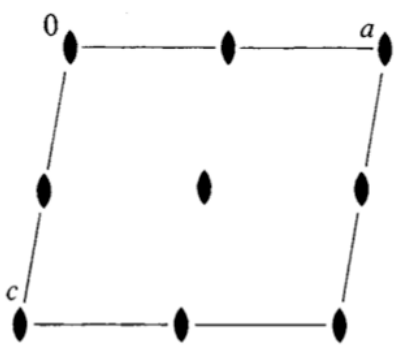
Number of vertices: 8	Number of facets: 6
0, 1/2, 0 0, 1/2, 1 1/4, 1/2, 1 1/4, 0, 1 0, 0, 0 1/4, 1/2, 0 0, 0, 1 1/4, 0, 0	x>=0 x<=1/4 [y<=1/4] y>=0 y<=1/2 z>=0 z<1 [Guide to notation]

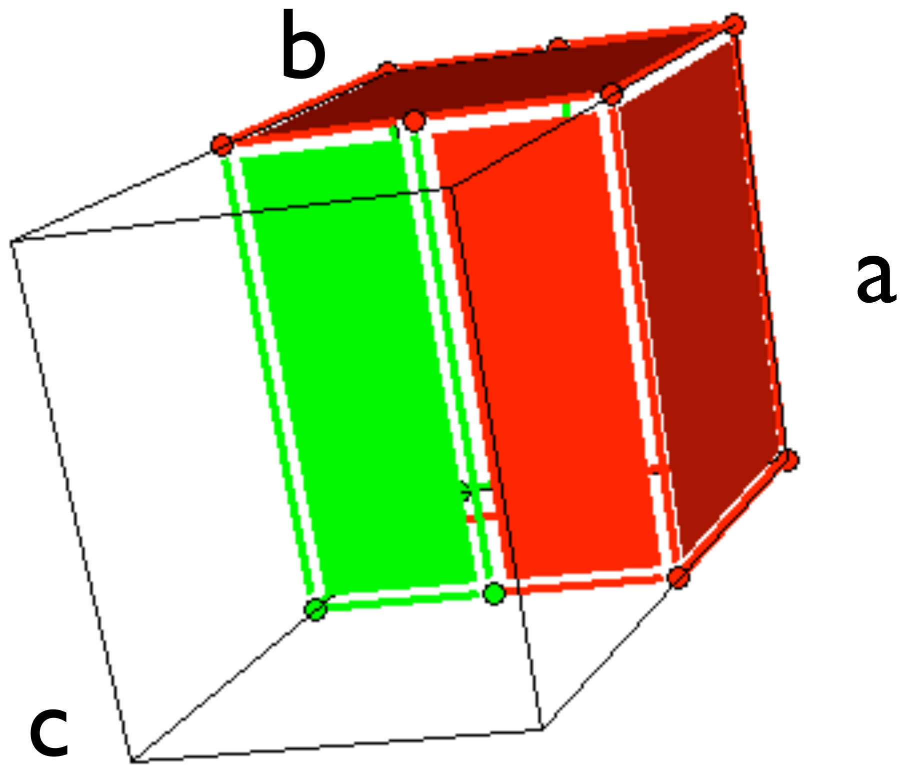
(output cctbx: Ralf Grosse-Kustelve)

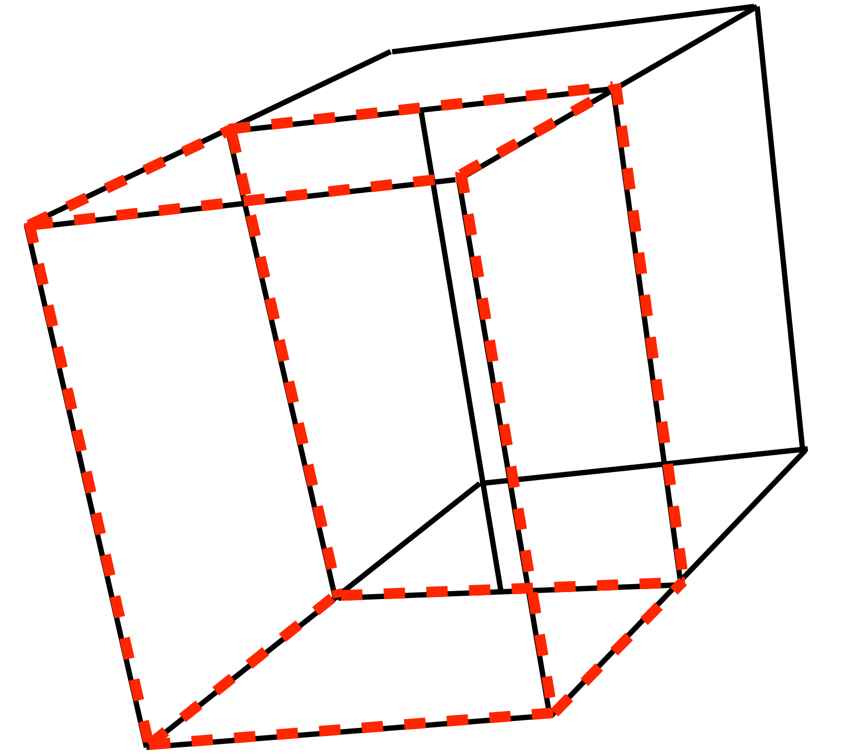
NOT in ITA: To avoid the overlap between the **boundaries of the asymmetric units** covering the unit cell (and the whole space), obtained by the application of the space-group symmetry operations, part of the boundaries have to be excluded from the asymmetric unit.

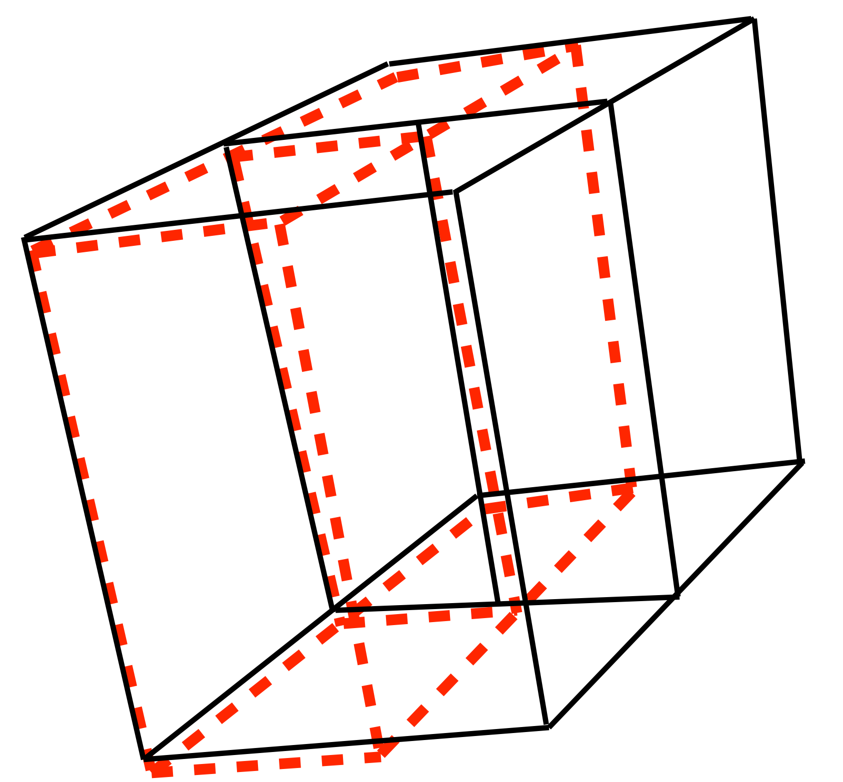
Example: Asymmetric units for the space group P121

non-uniqueness







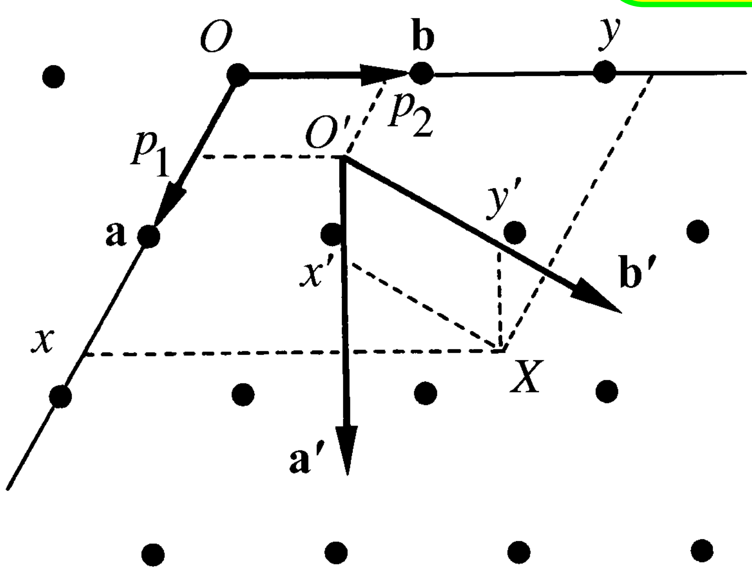


Number of vertices: 8	Number of facets: 6
0, 1, 1/2	x>=0
1, 1, 0	x<1
1, 0, 0	y>=0
0, 0, 1/2	y<1
1, 0, 1/2	z>=0 [x<=1/2]
0, 0, 0	z<=1/2 [x<=1/2]
0, 1, 0	
1, 1, 1/2	[Guide to notation]

(output cctbx: Ralf Grosse-Kustelve)

CO-ORDINATE TRANSFORMATIONS IN CRYSTALLOGRAPHY

Co-ordinate transformation



3-dimensional space

$(\mathbf{a}, \mathbf{b}, \mathbf{c})$, origin O: point $X(x, y, z)$

$\downarrow$ **(*P*,*p*)**

$(\mathbf{a}', \mathbf{b}', \mathbf{c}')$, origin O': point $X(x', y', z')$

Transformation matrix-column pair (*P*,*p*)

(i) linear part: change of orientation or length:

$$(\mathbf{a}', \mathbf{b}', \mathbf{c}') = (\mathbf{a}, \mathbf{b}, \mathbf{c})\boldsymbol{P}$$

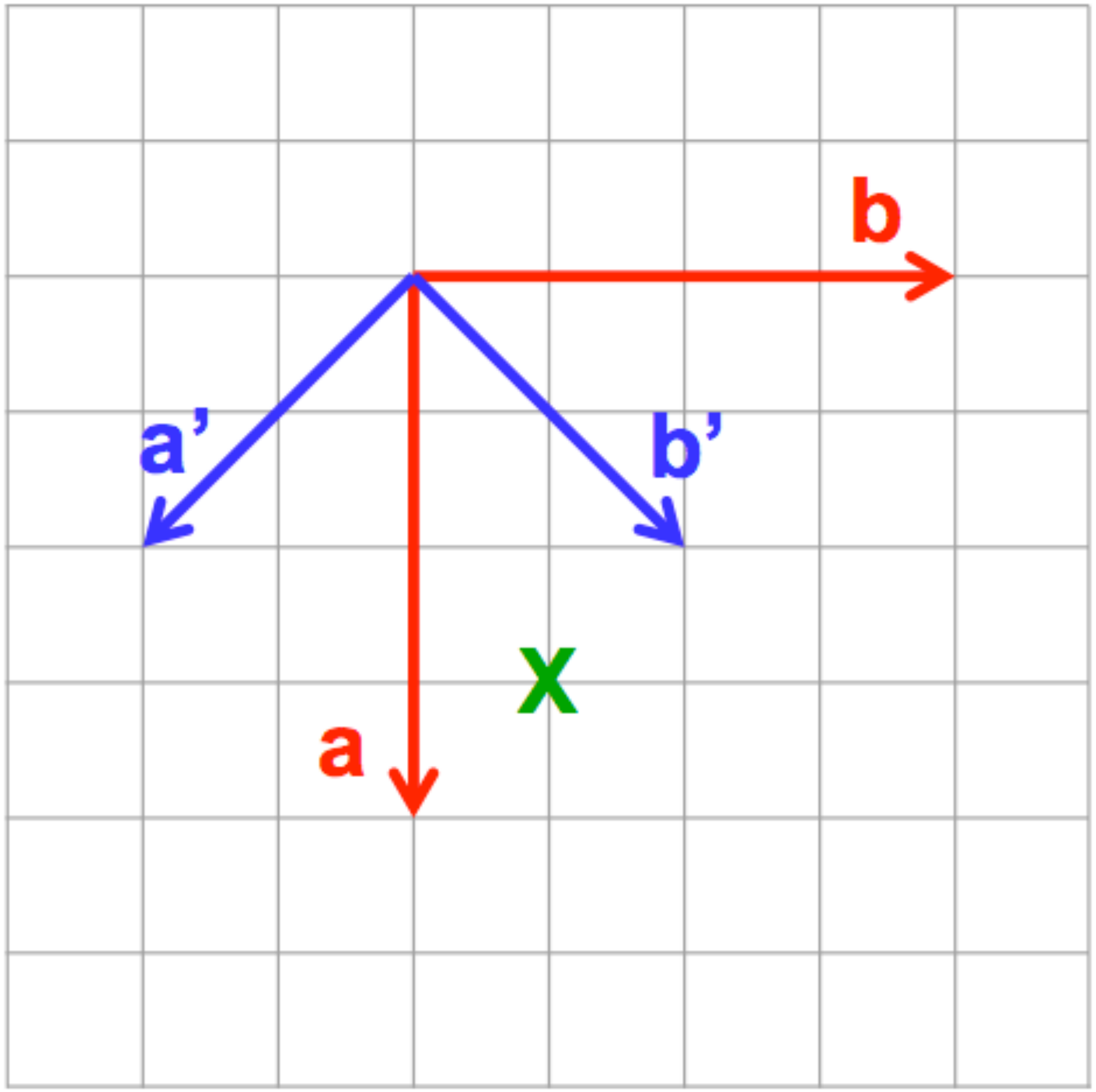
$$= (\mathbf{a}, \mathbf{b}, \mathbf{c}) \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix} = (P_{11}\mathbf{a} + P_{21}\mathbf{b} + P_{31}\mathbf{c}, \; P_{12}\mathbf{a} + P_{22}\mathbf{b} + P_{32}\mathbf{c}, \; P_{13}\mathbf{a} + P_{23}\mathbf{b} + P_{33}\mathbf{c}).$$

(ii) origin shift by a shift vector $\boldsymbol{p}(p_1,p_2,p_3)$:

$$\boldsymbol{O}' = \boldsymbol{O} + \boldsymbol{p}$$

the origin *O'* has coordinates (p_1,p_2,p_3) in the old coordinate system

EXAMPLE



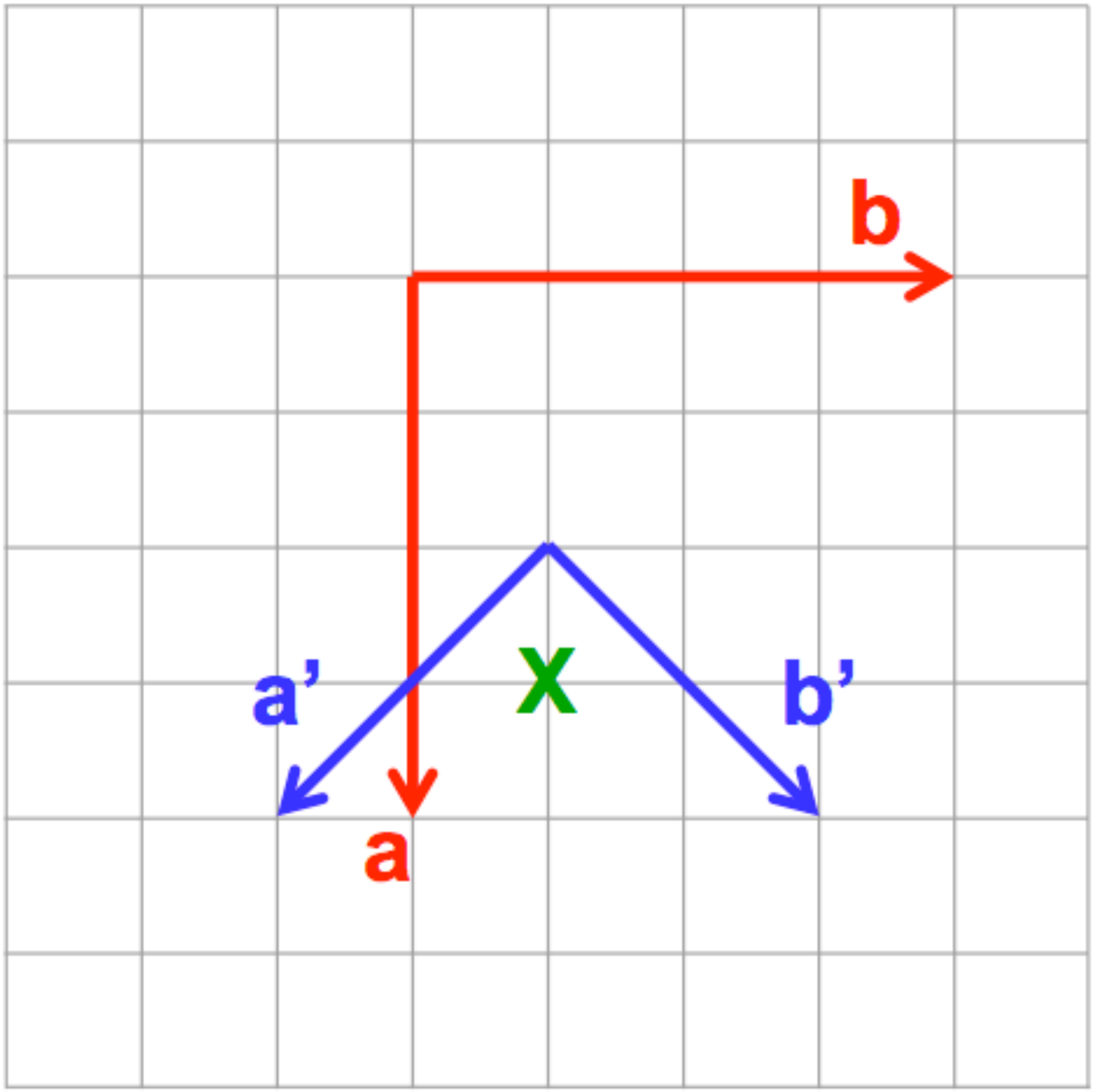
$$(a',b',c') = (a,b,c)\begin{pmatrix} ? \end{pmatrix}$$

$$(a,b,c) = (a',b',c')\begin{pmatrix} ? \end{pmatrix}$$

$$X = (3/4, 1/4, 0)$$

$$X' = (\; ? \;)$$

Write "new in terms of old" as column vectors.



$$p = \begin{pmatrix} ? \end{pmatrix}$$

$$q = \begin{pmatrix} ? \end{pmatrix}$$

$$X = (3/4, 1/4, 0)$$

$$X' = (\; ? \;)$$

Linear parts as before.

Transformation matrix-column pair (*P*,*p*)

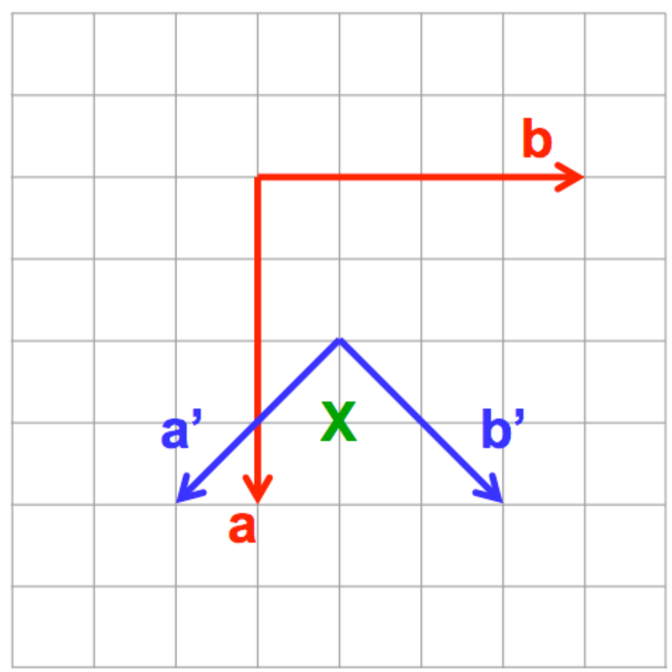
$$(P,p)=\left(\begin{array}{ccc|c} 1/2 & 1/2 & 0 & 1/2 \\ -1/2 & 1/2 & 0 & 1/4 \\ 0 & 0 & 1 & 0 \end{array}\right) \qquad (P,p)^{-1}=\left(\begin{array}{ccc|c} 1 & -1 & 0 & -1/4 \\ 1 & 1 & 0 & -3/4 \\ 0 & 0 & 1 & 0 \end{array}\right)$$

a’=1/2a-1/2b

b’=1/2a+1/2b

c’=c

$$\mathbf{O'}=\mathbf{O}+\begin{pmatrix}1/2\\1/4\\0\end{pmatrix}$$



a=a’+b’

b=-a’+b’

c=c’

$$\mathbf{O}=\mathbf{O'}+\begin{pmatrix}-1/4\\-3/4\\0\end{pmatrix}$$

Co-ordinate transformations in crystallography

Transformation of space-group operations (W,w) by $(\boldsymbol{P},\boldsymbol{p})$:

$$(W',w')=(P,p)^{-1}(W,w)(P,p)$$

Structure-description transformation by $(\boldsymbol{P},\boldsymbol{p})$

unit cell parameters:

metric tensor $\boldsymbol{G}$: $\boldsymbol{G}'=\boldsymbol{P}^t\,\boldsymbol{G}\,\boldsymbol{P}$

atomic coordinates X(x,y,z):

$$(X')=(P,p)^{-1}(X)$$

$$=(P^{-1},\,-P^{-1}p)(X)$$

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \left(\begin{array}{ccc|c} P_{11} & P_{12} & P_{13} & p_1 \\ P_{21} & P_{22} & P_{23} & p_2 \\ P_{31} & P_{32} & P_{33} & p_3 \end{array}\right)^{-1} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

Covariant and contravariant crystallographic quantities

direct or crystal basis

$$(\mathbf{a}',\mathbf{b}',\mathbf{c}')=(\mathbf{a},\mathbf{b},\mathbf{c})P=(\mathbf{a},\mathbf{b},\mathbf{c})\begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix}$$

reciprocal or dual basis

$$\begin{pmatrix} \mathbf{a}^{*\prime} \\ \mathbf{b}^{*\prime} \\ \mathbf{c}^{*\prime} \end{pmatrix} = P^{-1}\begin{pmatrix} \mathbf{a}^{*} \\ \mathbf{b}^{*} \\ \mathbf{c}^{*} \end{pmatrix} = \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix}^{-1}\begin{pmatrix} \mathbf{a}^{*} \\ \mathbf{b}^{*} \\ \mathbf{c}^{*} \end{pmatrix}$$

covariant to crystal basis: Miller indices

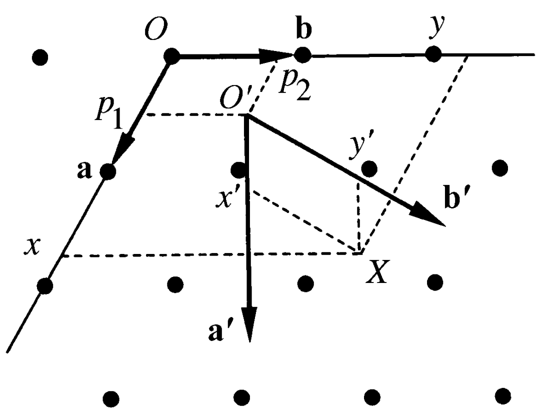
$$(h',k',l')=(h,k,l)P$$

contravariant to crystal basis: indices of a direction [u]

$$\begin{pmatrix} \mathbf{u}' \\ \mathbf{v}' \\ \mathbf{w}' \end{pmatrix} = \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix}^{-1}\begin{pmatrix} u \\ v \\ w \end{pmatrix}$$

Short-hand notation for the description of transformation matrices

Transformation matrix:



(**a**,**b**,**c**), origin O

$$(P,p)=\left(\begin{array}{ccc|c} P_{11} & P_{12} & P_{13} & p1 \\ P_{21} & P_{22} & P_{23} & p2 \\ P_{31} & P_{32} & P_{33} & p3 \end{array}\right)$$

(**a'**,**b'**,**c'**), origin O'

notation rules:

-written by columns

-coefficients 0, +1, -1

-different columns in one line

-origin shift

example:

$$\left(\begin{array}{ccc|c} 1 & -1 & & -1/4 \\ 1 & 1 & & -3/4 \\ & & 1 & 0 \end{array}\right) \longrightarrow \{\ a+b,\ -a+b,\ c;-1/4,-3/4,0$$

EXERCISES

Problem 1.6.2.6

The following matrix-column pairs (W,w) are referred with respect to a basis (**a**,**b**,**c**):

(1) x,y,z (2) -x,y+1/2,-z+1/2

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

(i) Determine the corresponding matrix-column pairs (W',w') with respect to the basis (**a'**,**b'**,**c'**)= (**a**,**b**,**c**)**P**, with **P**=**c**,**a**,**b**.

(ii) Determine the coordinates X' of a point X= with respect to the new basis (**a'**,**b'**,**c'**).

0,70
0,31
0,95

Hints

$(W',w')=(P,p)^{-1}(W,w)(P,p)$

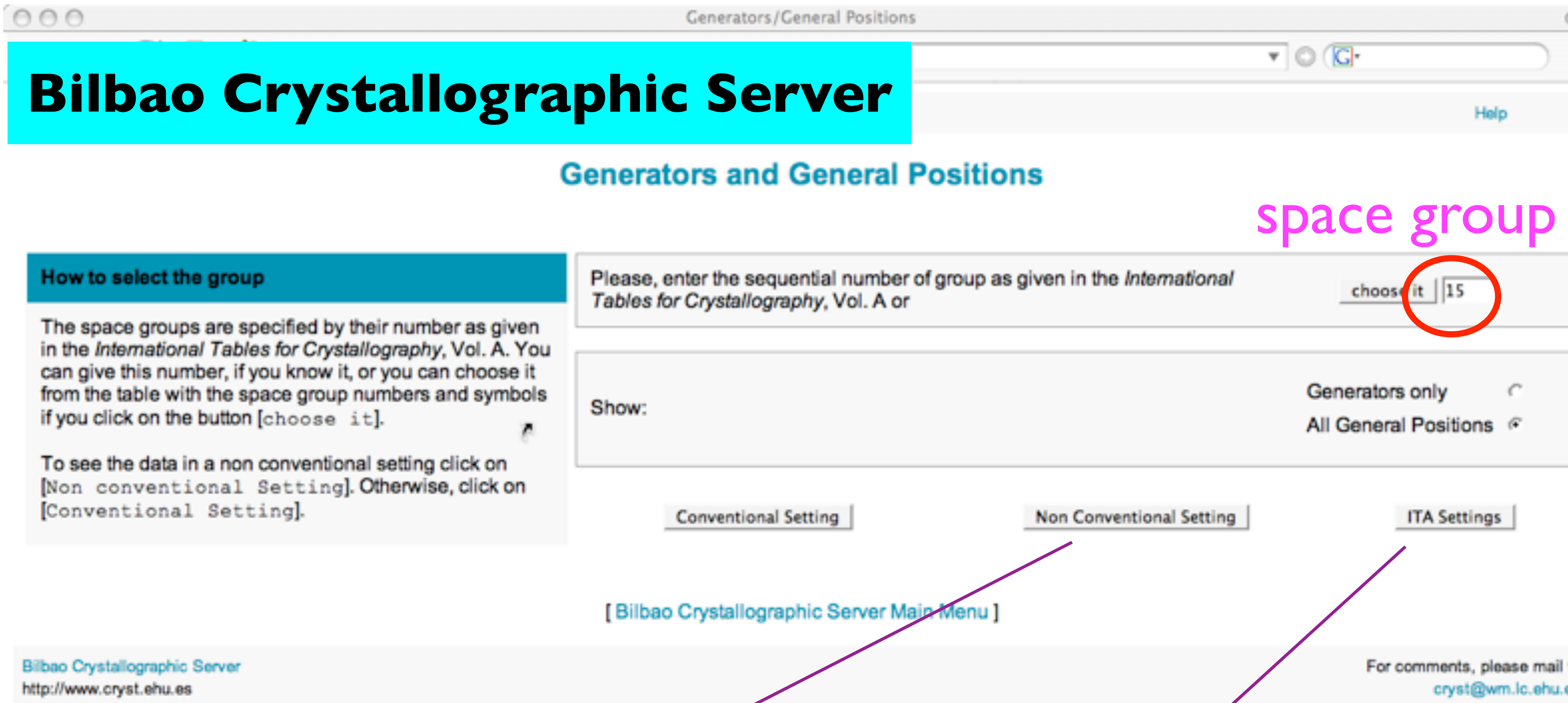
$(X')=(P,p)^{-1}(X)$

Problem: Co-ordinate transformations in crystallography

Generators
General positions

GENPOS

Bilbao Crystallographic Server



space group

Transformation of the basis

ITA-settings symmetry data

Example **GENPOS**:

default setting C12/c1

$(W,w)_{A112/a} = (P,p)^{-1}(W,w)_{C12/c1}(P,p)$

final setting A112/a

ITA-Settings for the Space Group 15

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}
15	*C* 1 2/*c* 1	a,b,c	a,b,c
15	*A* 1 2/*n* 1	-a-c,b,a	c,b,-a-c
15	*I* 1 2/*a* 1	c,b,-a-c	-a-c,b,a
15	*A* 1 2/*a* 1	c,-b,a	c,-b,a
15	*C* 1 2/*n* 1	a,-b,-a-c	a,-b,a-c
15	*I* 1 2/*c* 1	-a-c,-b,c	-a-c,-b,c
15	*A* 1 1 2/*a*	c,a,b	b,c,a
15	*B* 1 1 2/*n*	a,-a-c,b	a,c,-a-b
15	*I* 1 1 2/*b*	-a-c,c,b	-a-b,c,b
15	*B* 1 1 2/*b*	a,c,-b	a,-c,b
15	*A* 1 1 2/*n*	-a-c,a,-b	b,-c,-a-b
15	*I* 1 1 2/*a*	c,-a-c,-b	-a-b,-c,a
15	*B* 2/*b* 1 1	b,c,a	c,a,b
15	*C* 2/*n* 1 1	b,a,-a-c	b,a,-b-c
15	*I* 2/*c* 1 1	b,-a-c,c	-b-c,a,c
15	*C* 2/*c* 1 1	-b,a,c	b,-a,c
15	*B* 2/*n* 1 1	-b,-a-c,a	c,-a,-b-c
15	*I* 2/*b* 1 1	-b,c,-a-c	-b-c,-a,b

Example **GENPOS**: ITA settings of C2/c(15)

The general positions of the group 15 (*A* 1 1 2/*a*)

N	Standard/Default Setting *C2/c*			ITA-Setting *A* 1 1 2/*a*		
	(x,y,z) form	matrix form	symmetry operation	(x,y,z) form	matrix form	symmetry operation
1	x, y, z	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	1	x, y, z	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	1
2	-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+1/2, -y, z	$\begin{pmatrix} -1 & 0 & 0 & 1/2 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	2 1/4,0,z
3	-x, -y, -z	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{pmatrix}$	-1 0,0,0	-x, -y, -z	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{pmatrix}$	-1 0,0,0
4	x, -y, z+1/2	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 1/2 \end{pmatrix}$	c x,0,z	x+1/2, y, -z	$\begin{pmatrix} 1 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{pmatrix}$	a x,y,0
5	x+1/2, y+1/2, z	$\begin{pmatrix} 1 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 1/2 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	t (1/2,1/2,0)	x, y+1/2, z+1/2	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1/2 \\ 0 & 0 & 1 & 1/2 \end{pmatrix}$	t (0,1/2,1/2)
6	-x+1/2, y+1/2, -z+1/2	$\begin{pmatrix} -1 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 1/2 \\ 0 & 0 & -1 & 1/2 \end{pmatrix}$	2 (0,1/2,0) 1/4,y,1/4	-x+1/2, -y+1/2, z+1/2	$\begin{pmatrix} -1 & 0 & 0 & 1/2 \\ 0 & -1 & 0 & 1/2 \\ 0 & 0 & 1 & 1/2 \end{pmatrix}$	2 (0,0,1/2) 1/4,1/4,z
7	-x+1/2, -y+1/2, -z	$\begin{pmatrix} -1 & 0 & 0 & 1/2 \\ 0 & -1 & 0 & 1/2 \\ 0 & 0 & -1 & 0 \end{pmatrix}$	-1 1/4,1/4,0	-x, -y+1/2, -z+1/2	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 1/2 \\ 0 & 0 & -1 & 1/2 \end{pmatrix}$	-1 0,1/4,1/4
8	x+1/2, -y+1/2, z+1/2	$\begin{pmatrix} 1 & 0 & 0 & 1/2 \\ 0 & -1 & 0 & 1/2 \\ 0 & 0 & 1 & 1/2 \end{pmatrix}$	n (1/2,0,1/2) x,1/4,z	x+1/2, y+1/2, -z+1/2	$\begin{pmatrix} 1 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 1/2 \\ 0 & 0 & -1 & 1/2 \end{pmatrix}$	n (1/2,1/2,0) x,y,1/4

default setting **A112/*a* setting**

Bilbao Crystallographic Server

Problem: Coordinate transformations Wyckoff positions — WYCKPOS

Wyckoff Positions

space group

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**.

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.

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

Transformation of the basis

ITA settings

ITA-Settings for the Space Group 68

ces must be read by columns. **P** is the transformation f

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

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

EXERCISES

Problem 1.6.2.7

Consider the space group $P2_1/c$ (No. 14). Show that 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 $(\mathbf{a}',\mathbf{b}',\mathbf{c}')_{\mathbf{c}} = (\mathbf{a},\mathbf{b},\mathbf{c})_{\mathbf{b}}\boldsymbol{P}$, with $\boldsymbol{P}$= c,a,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*.

EXERCISES

Problem 1.2.6.8

Apart from the translation generators, the space group Im-3m (No. 229) can be generated by the following five generators (-x, -y, z), (-x, y, -z), (z,x,y), (y,x,-z) and (-x, -y, -z), where the matrix-column presentations of the generators are given with respect to the conventional I-centred basis.

1. Define a transformation matrix from the conventional to a primitive basis
2. What are the matrix-column pairs of the generators with respect to the primitive basis?
3. Consider the lattice points inside and at the border of the conventional unit cell: what are the coordinates of these points with respect to the chosen primitive basis?