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AIC International Crystallography School 2019

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SPACE-GROUP SYMMETRY

International Tables for Crystallography, Volume A

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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 $\triangleleft$ G

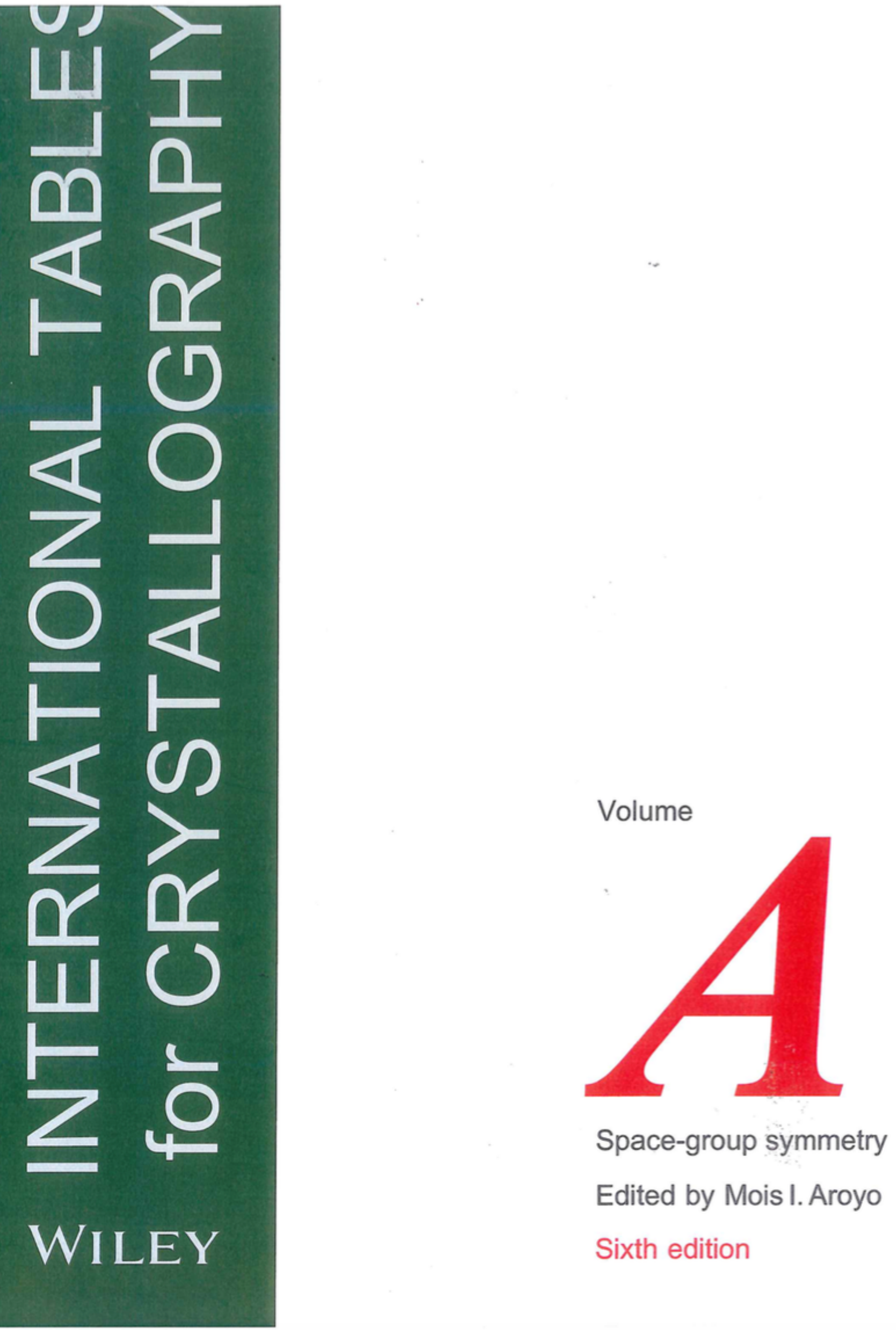
The infinite set of all translations that are symmetry operations of the crystal pattern

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

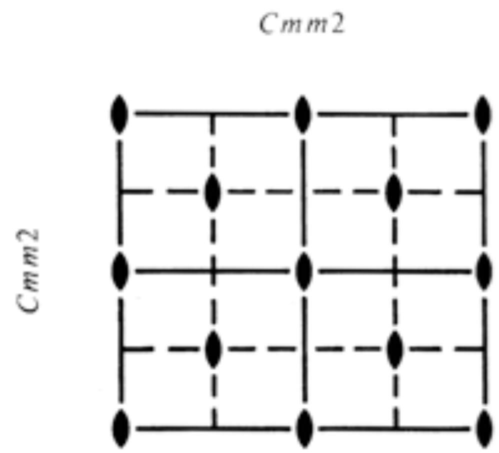
- headline with the relevant group symbols;
- diagrams of the symmetry elements and of the general position;
- specification of the origin and the asymmetric unit;
- list of symmetry operations;
- generators;
- general and special positions with multiplicities, site symmetries, coordinates and reflection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

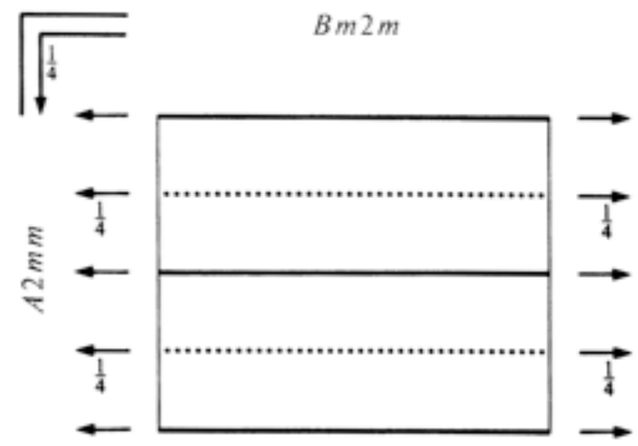
GENERAL LAYOUT: LEFT-HAND PAGE

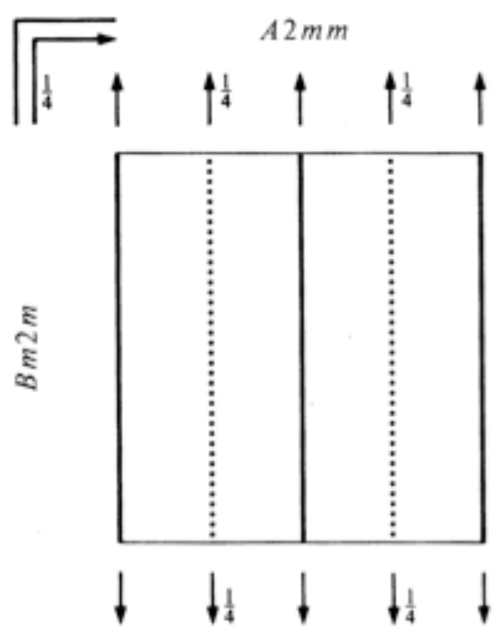
① $Cmm2$ C_{2v}^{11} $mm2$ Orthorhombic

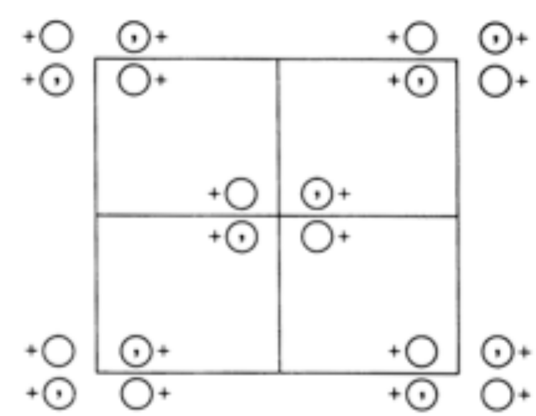
② No. 35 $Cmm2$ Patterson symmetry $Cmmm$

③









④ **Origin** on $mm2$

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	$m\,m\,2$	$0,\frac{1}{2},z$				no extra conditions
2	a	$m\,m\,2$	$0,0,z$				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 FOR SPACE GROUPS

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:

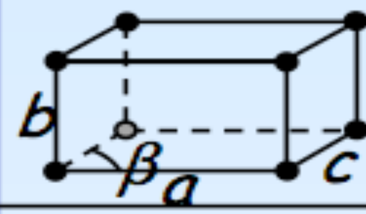
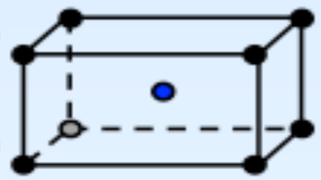
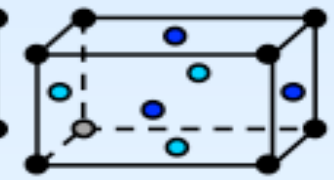
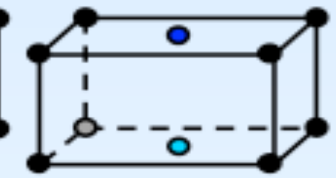
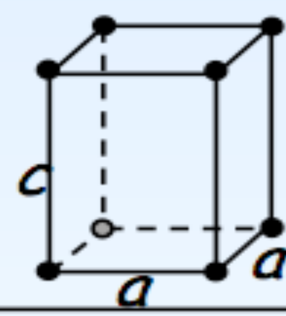
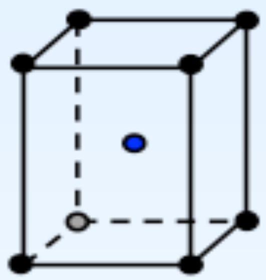
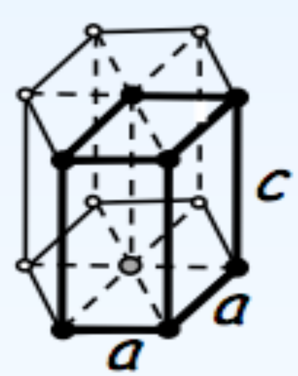
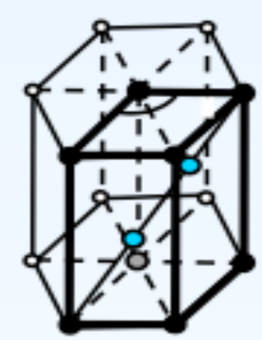
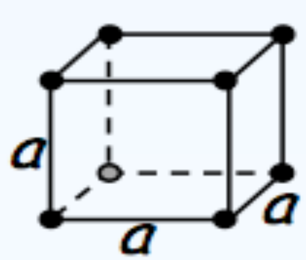
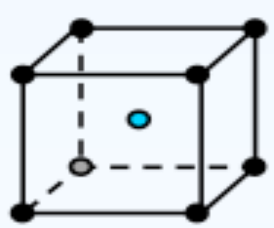
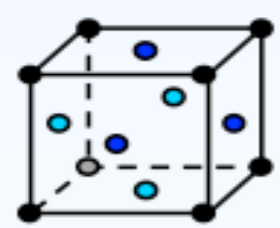
pure rotations > screw rotations;

pure rotations > rotoinversions

reflection m > a; b; c > n

'>' means 'has priority'

14 Bravais Lattices

crystal family	P	I	F	C	R
triclinic					
monoclinic					
orthorhombic					
tetragonal					
hexagonal					
cubic					

Lattice types: P, I, F, C, R

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.

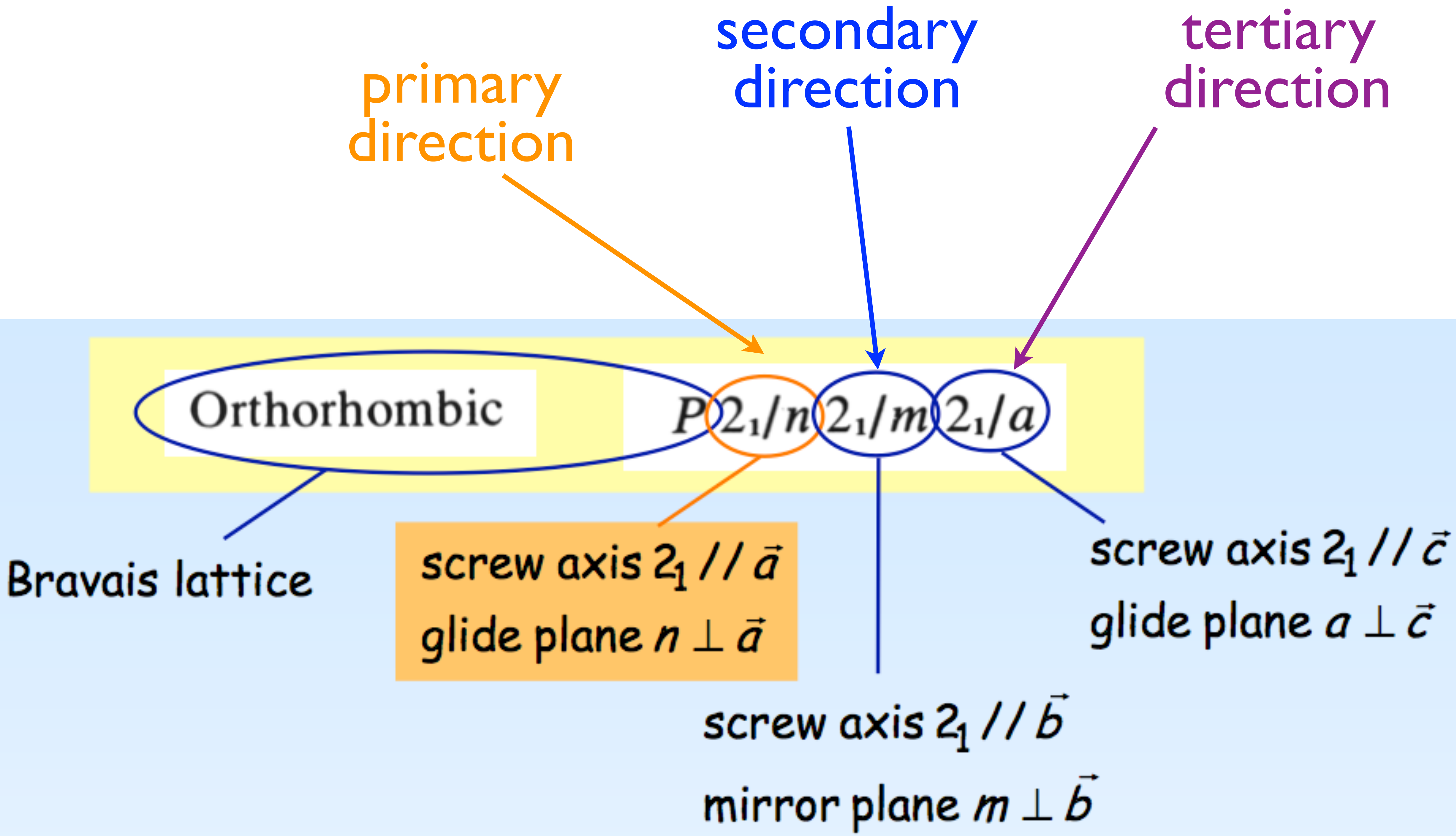
Hermann-Mauguin symbols for space groups

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]	{ [100] [010] }	{ $[1\bar{1}0]$ [110] }
Hexagonal	[001]	{ [100] [010] $[\bar{1}\bar{1}0]$ }	{ $[1\bar{1}0]$ [120] $[\bar{2}\bar{1}0]$ }
Rhombohedral (hexagonal axes)	[001]	{ [100] [010] $[\bar{1}\bar{1}0]$ }	
Rhombohedral (rhombohedral axes)	[111]	{ $[1\bar{1}0]$ $[01\bar{1}]$ $[\bar{1}01]$ }	
Cubic	{ [100] [010] [001] }	{ [111] $[1\bar{1}\bar{1}]$ $[\bar{1}1\bar{1}]$ $[\bar{1}\bar{1}1]$ }	{ $[1\bar{1}0]$ [110] $[01\bar{1}]$ [011] $[\bar{1}01]$ [101] }

Example:

Hermann-Mauguin symbols for space groups



PRESENTATION OF SPACE-GROUP SYMMETRY OPERATIONS

IN INTERNATIONAL TABLES FOR CRYSTALLOGRAPHY, VOL. A

Symmetry Operations

KIND of the symmetry operation

TYPE of the symmetry operation

SCREW/GLIDE component

ORIENTATION of the geometric element

LOCATION of the geometric element

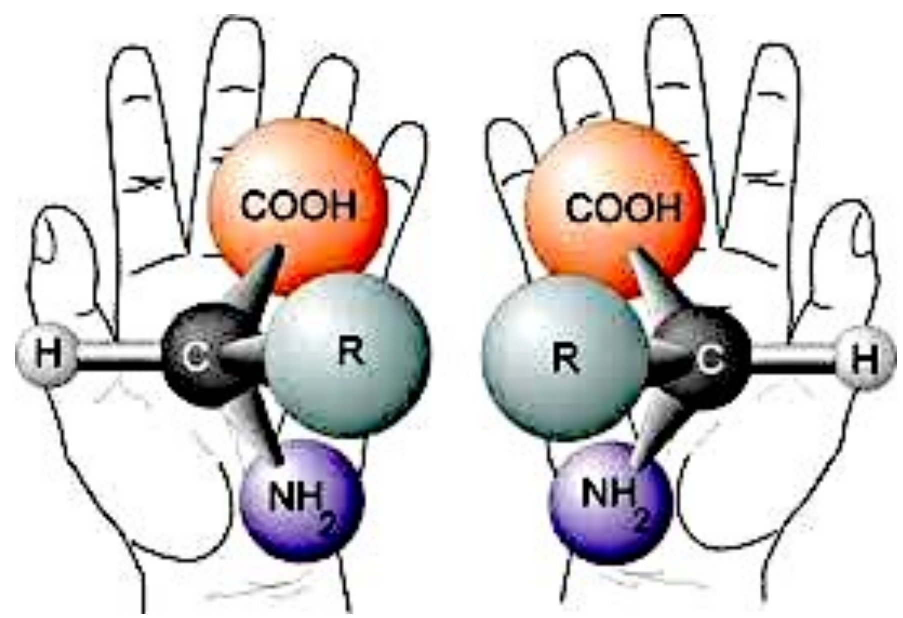
Kinds of Symmetry Operations

Symmetry operations of 1st kind (proper):

chirality (handedness)
preserving

Symmetry operations of 2nd kind (improper):

chirality (handedness)
non-preserving



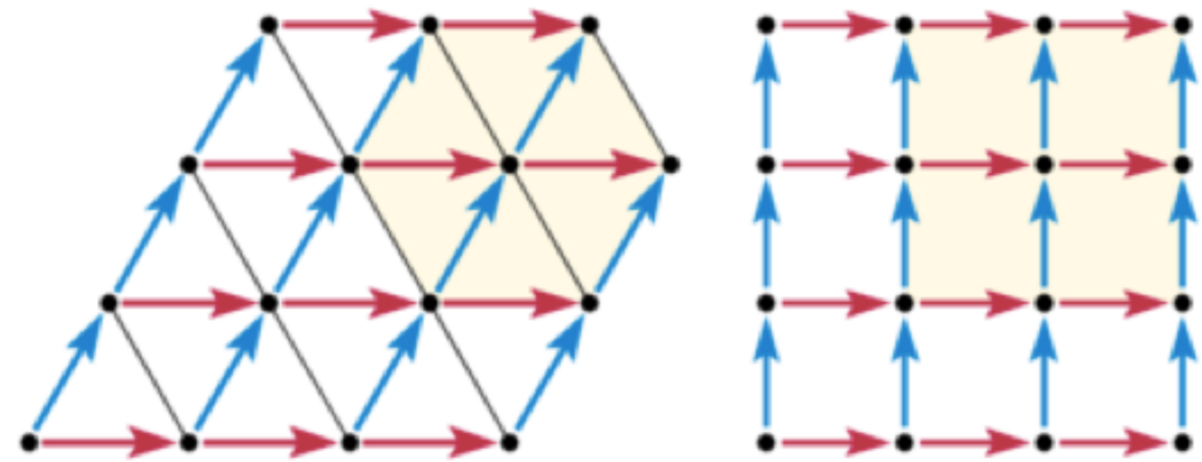
Chirality is the geometric property of a rigid object of being non-superposable on its mirror image. An object displaying chirality is called **chiral**; the opposite term is **achiral**.

Crystallographic symmetry operations

Crystallographic restriction theorem

The rotational symmetries of a crystal pattern are limited to 2-fold, 3-fold, 4-fold, and 6-fold.

Matrix proof:



Rotation with respect to orthonormal basis

$$R = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}$$

Rotation with respect to lattice basis

R: integer matrix

In a lattice basis, because the rotation must map lattice points to lattice points, each matrix entry — and hence the trace — must be an integer.

$$\mathrm{Tr}\, R = 2\cos\theta = \text{integer}$$

m	$m/2 = \cos\theta$	θ (°)	$n = 360°/\theta$
0	0	90	Fourfold
1	1/2	60	Sixfold
2	1	0 = 360	Identity (onefold)
−1	−1/2	120	Threefold
−2	−1	180	Twofold

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

Types of isometries do not preserve handedness

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

QUIZ

Referred to an 'orthorhombic' coordinated system ($a \neq b \neq c$; $\alpha=\beta=\gamma=90$) 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

HINTS

QUIZ

Characterization of the symmetry operations:

$$\det\left(\begin{array}{|c|c|c|}\hline -1 & & \\ \hline & 1 & \\ \hline & & -1 \\ \hline\end{array}\right) = ? \qquad \mathrm{tr}\left(\begin{array}{|c|c|c|}\hline -1 & & \\ \hline & 1 & \\ \hline & & -1 \\ \hline\end{array}\right) = ?$$

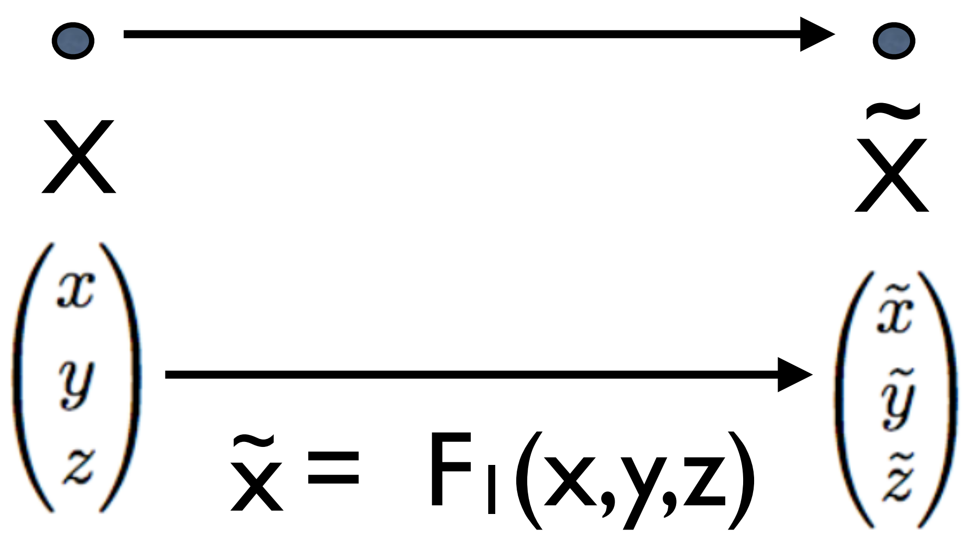
What are the fixed points of (W_1,w_1) and (W_2,w_2) ?

$$\left(\begin{array}{|c|c|c|}\hline -1 & & \\ \hline & 1 & \\ \hline & & -1 \\ \hline\end{array}\ \begin{array}{|c|}\hline 1/2 \\ \hline 0 \\ \hline 1/2 \\ \hline\end{array}\right)\begin{array}{|c|}\hline x_f \\ \hline y_f \\ \hline z_f \\ \hline\end{array} = \begin{array}{|c|}\hline x_f \\ \hline y_f \\ \hline z_f \\ \hline\end{array}$$

Description of isometries: 3D

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

isometry:



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

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

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

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

matrix-column pair

Seitz symbol

Short-hand notation for the description of isometries

isometry:

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

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

notation rules:

-left-hand side: omitted

-coefficients 0, +1, -1

-different rows in one line

examples:

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

→ { -x+1/2, y, -z+1/2
$\bar{x}$+1/2, y, $\bar{z}$+1/2

QUICK QUIZ

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

Space group *Cmm*2 (No. 35)

How are the symmetry operations represented in ITA ?

Diagram of symmetry elements

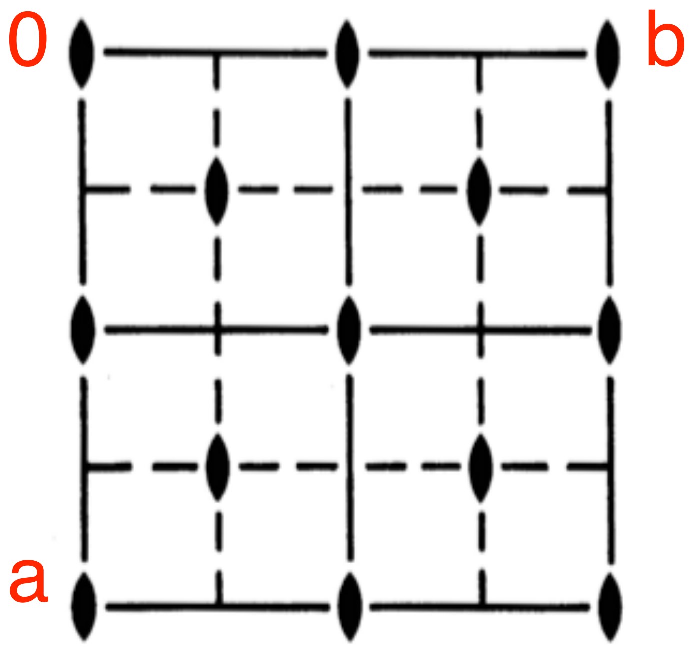
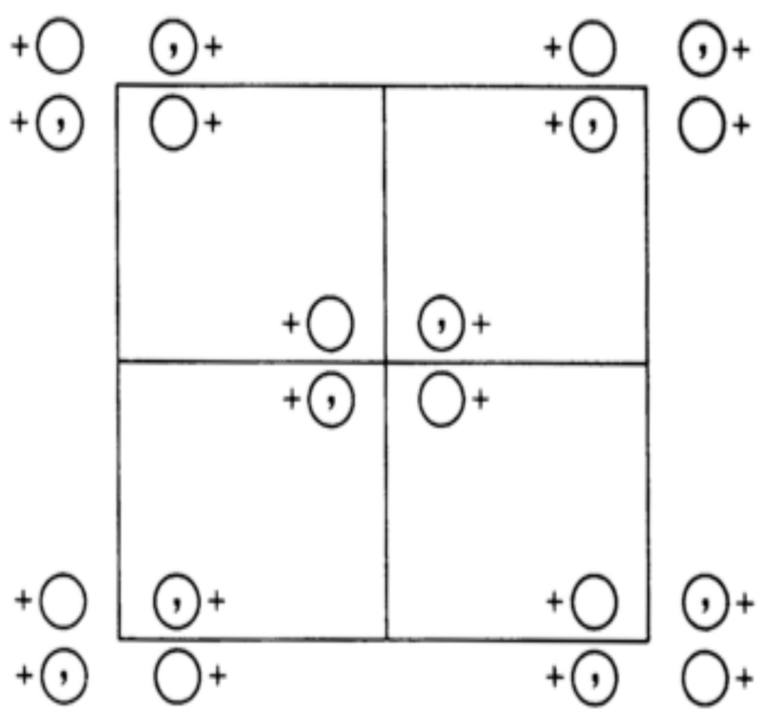


Diagram of general position points



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) $\bar{x},y,z$

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

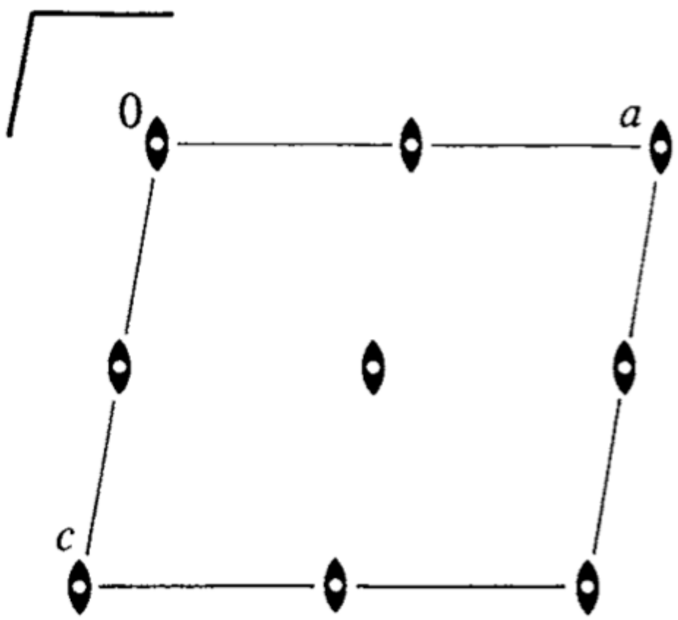
$(I,0)$	(W_2,w_2)	...	(W_m,w_m)	...	(W_i,w_i)
(I,t_1)	(W_2,w_2+t_1)	...	(W_m,w_m+t_1)	...	(W_i,w_i+t_1)
(I,t_2)	(W_2,w_2+t_2)	...	(W_m,w_m+t_2)	...	(W_i,w_i+t_2)
...	...	...	...	...	...
(I,t_j)	(W_2,w_2+t_j)	...	(W_m,w_m+t_j)	...	(W_i,w_i+t_j)
...	...	...	...	...	...

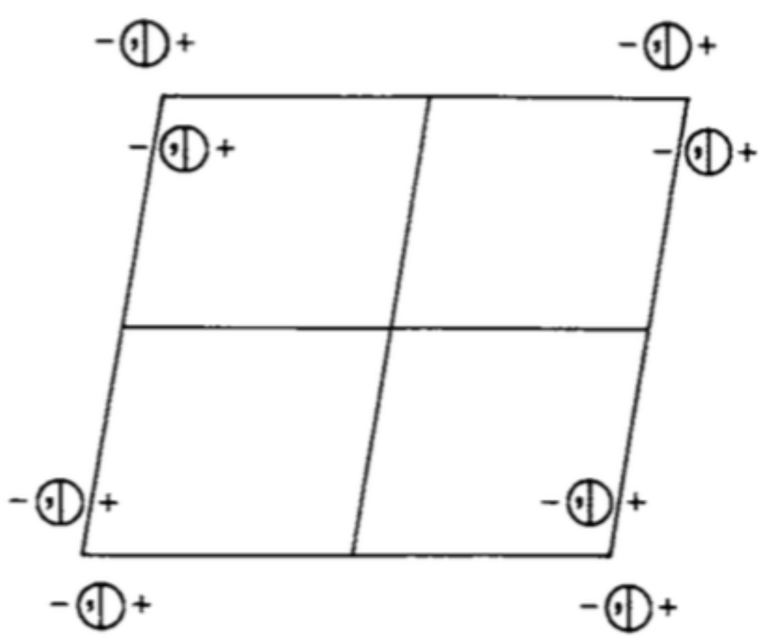
Factor group G/T_G

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)
...	...	...	...

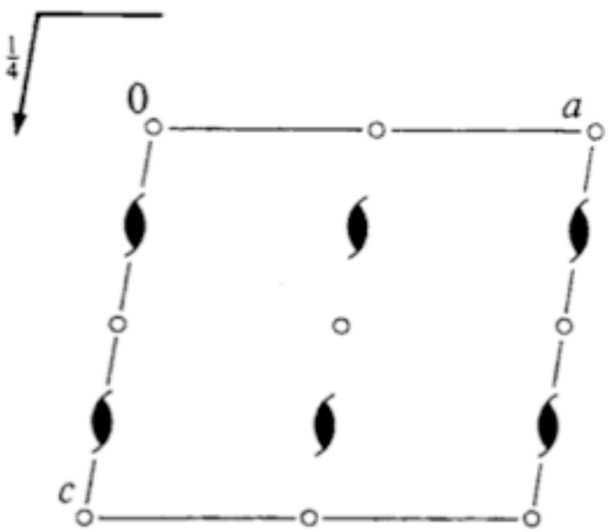
$$\left(\begin{array}{ccc|c} -1 & & & n_1 \\ & -1 & & n_2 \\ & & -1 & n_3 \end{array}\right) \xrightarrow{\bar{1} \text{ at}} \begin{pmatrix} n_1/2 \\ n_2/2 \\ n_3/2 \end{pmatrix}$$

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

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

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

inversion centers

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

2_1 screw axes

$(2,u\ \frac{1}{2}+v\ \frac{1}{2}+w)$ → $(2,0\ \frac{1}{2}+v\ \frac{1}{2})$

→ $(2,u\ \frac{1}{2}\ \frac{1}{2}+w)$

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

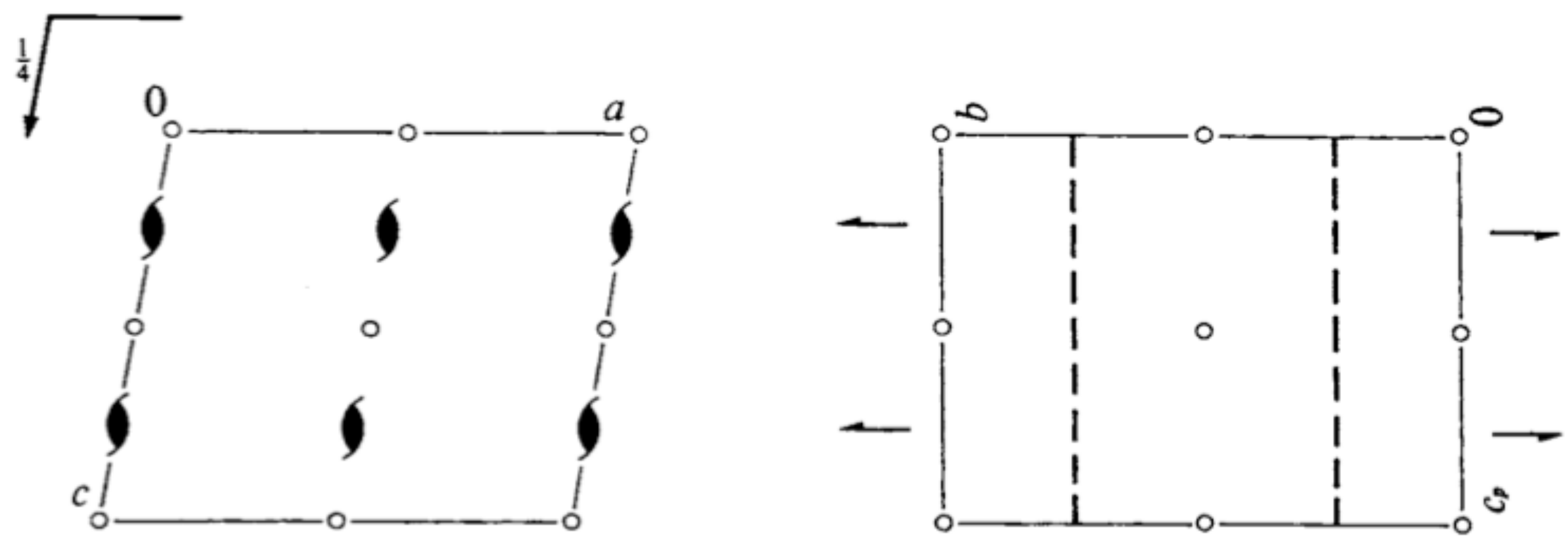
Space group $P2_1/c$ (No. 14)

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

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

Symmetry operations

Geometric interpretation

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

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

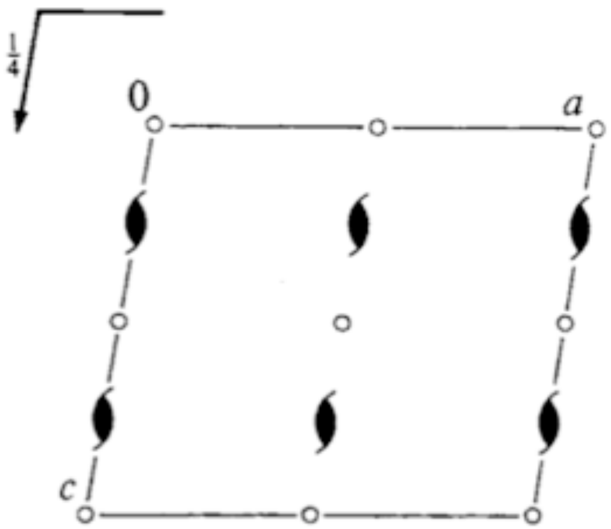
ITA description				Seitz symbol
No.	coord. triplet	type	orien-tation	
1)	x, y, z	1		1
2)	$\bar{y}, x-y, z$	3^+	$0,0,z$	3^+_{001}
3)	$\bar{x}+y, \bar{x}, z$	3^-	$0,0,z$	3^-_{001}
4)	$\bar{x}, \bar{y}, z$	2	$0,0,z$	2_{001}
5)	$y, \bar{x}+y, z$	6^-	$0,0,z$	6^-_{001}
6)	$x-y, x, z$	6^+	$0,0,z$	6^+_{001}
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

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



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

No. 14 $P12_1/c1$ 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 (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 $x,\frac{1}{4},z$

Seitz symbols

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

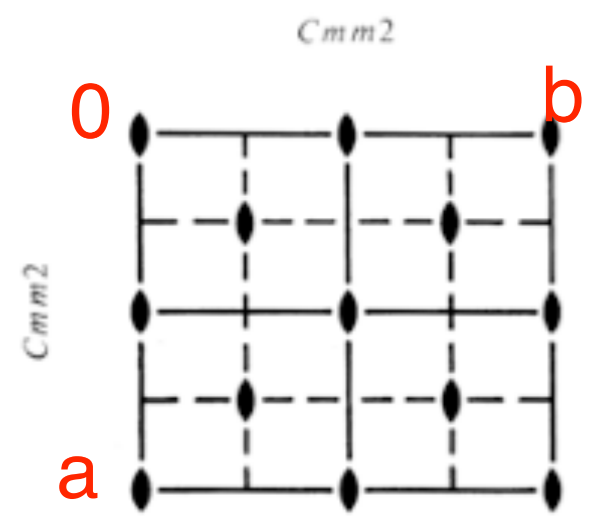
NOT in ITA

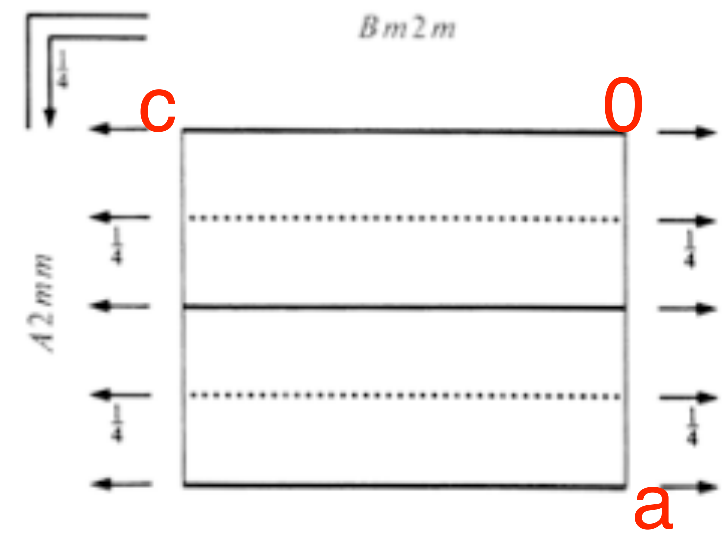
SPACE-GROUPS DIAGRAMS

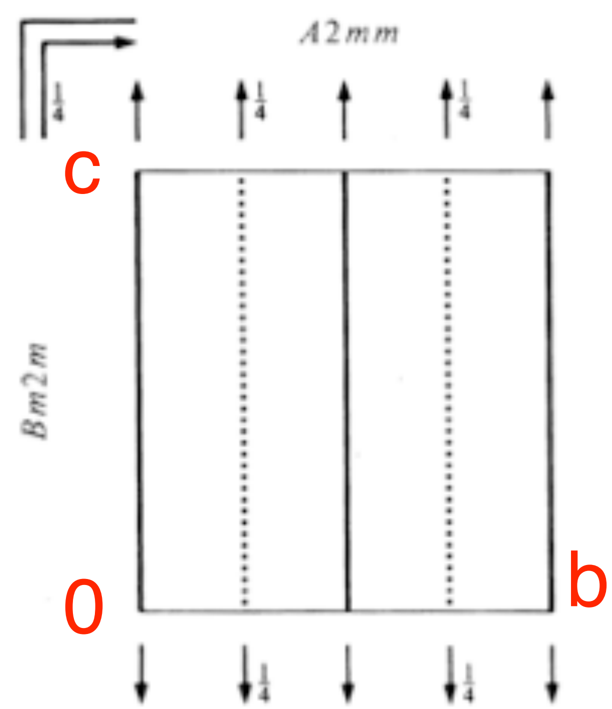
Diagrams of symmetry elements

three different settings

permutations of ***a,b,c***







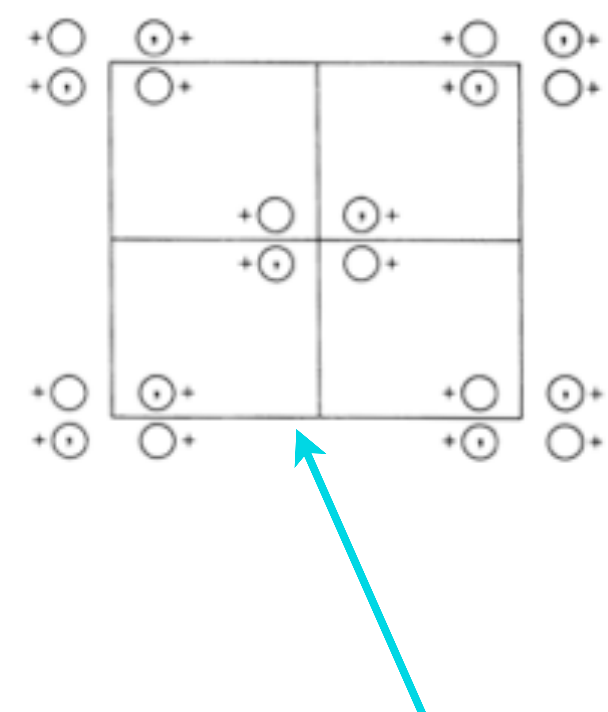
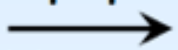


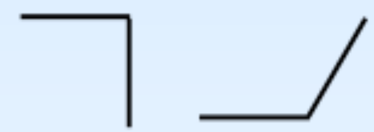
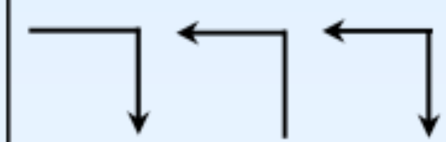
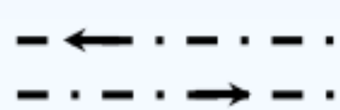
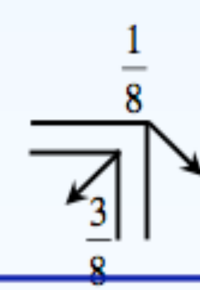
Diagram of general position points

The various rotation and screw axes and their symbol

printed symbol	symmetry axis	graphic symbol	nature of the screw translation
1	Identity	none	none
$\bar{1}$	Inversion	○	none
2	Rotation diad or twofold rotation axis	 (⊥ paper)  (// paper)	none
2_1	Screw diad or twofold screw axis	 (⊥ paper)  (// paper)	$c/2$ $a/2$ or $b/2$
3	Rotation triad	⊥ paper 	none
3_1	Screw triad		$c/3$
3_2	Screw triad		$2c/3$
$\bar{3}$	Inverse triad		none

printed symbol	symmetry axis	graphic symbol	nature of the screw translation
4	Rotation tetrad		none
4_1	Screw tetrads		$c/4$
4_2	Screw tetrads		$2c/4$
4_3	Screw tetrads		$3c/4$
$\bar{4}$	Inverse tetrad		none
6	Rotation hexad		none
6_1	Screw hexads		$c/6$
6_2	Screw hexads		$2c/6$
6_3	Screw hexads		$3c/6$
6_4	Screw hexads		$4c/6$
6_5	Screw hexads		$5c/6$
$\bar{6}$	Inverse hexad		none

The various symmetry planes and their symbol

printed symbol	symmetry plane	graphical symbol: normal to plane of projection	graphical symbol: parallel to plane of projection	nature of glide translation
m	reflection plane (mirror)	———		none
a, *b*	axial glide plane	- - - - - -		*a*/2 or *b*/2
c	axial glide plane	··················	none	*c*/2
n	diagonal glide plane (*net*)	- · - · - · - · -		(*a*+*b*)/2, (*b*+*c*)/2 or (*c*+*a*)/2; OR (*a*+*b*+*c*)/2 for *t* and *c* systems
d	"diamond" glide plane			(*a*±*b*)/4, (*b*±*c*)/4 or (*c*±*a*)/4; OR (*a*±*b*±*c*)/4 for *t* and *c* systems

EXAMPLE

Space group *Cmm*2 (No. 35)

Geometric interpretation

⑥ Symmetry operations

For (0,0,0)+ set

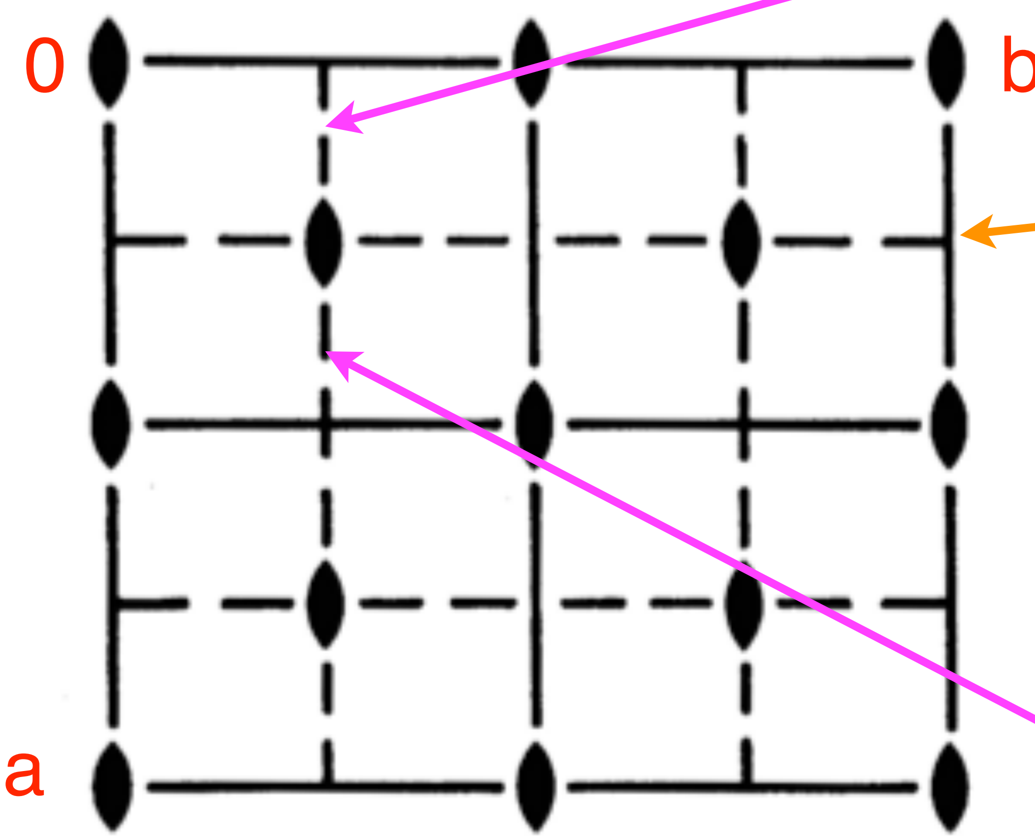
(1) 1 (2) 2 $0,0,z$ (3) m $x,0,z$ (4) m $0,y,z$

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

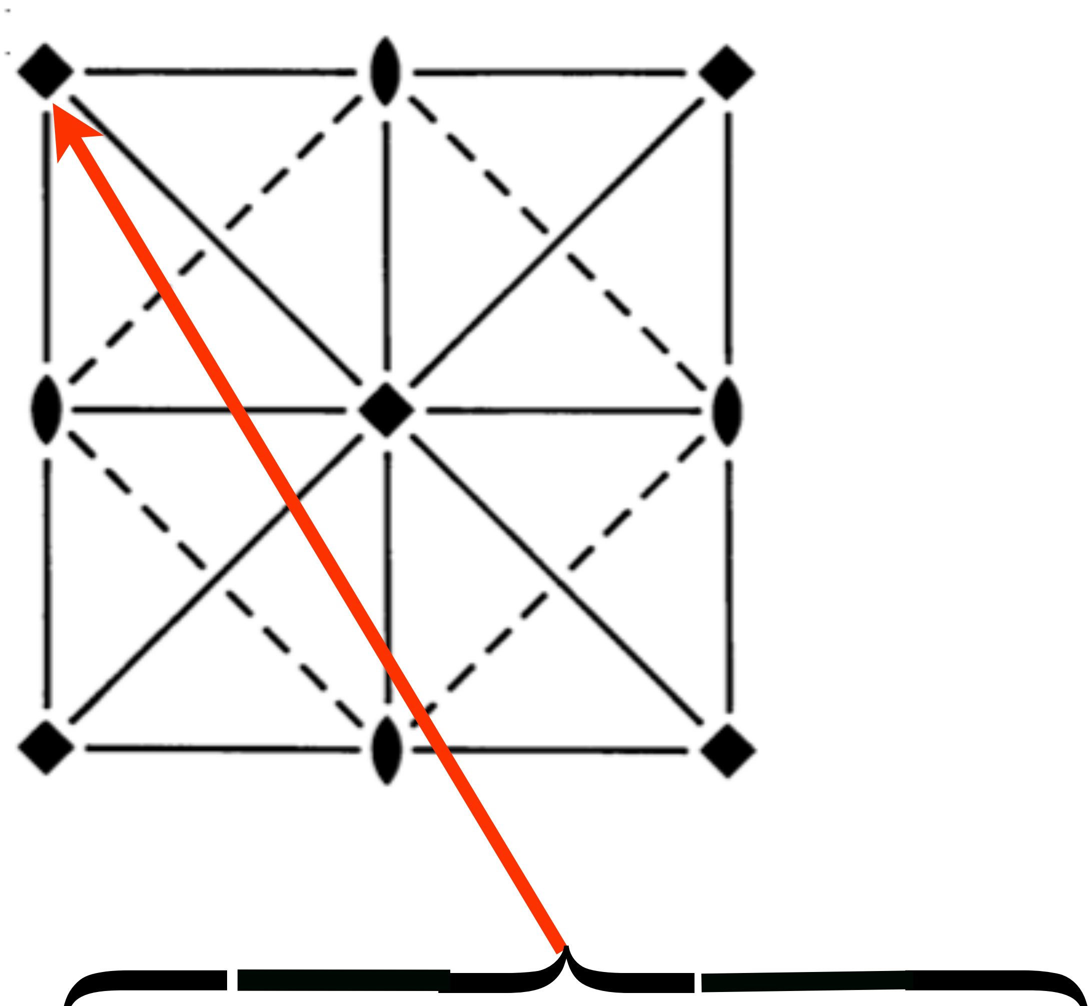
8 *f* 1 (1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $x,\bar{y},z$ (4) $\bar{x},y,z$

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

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

Example: P4mm

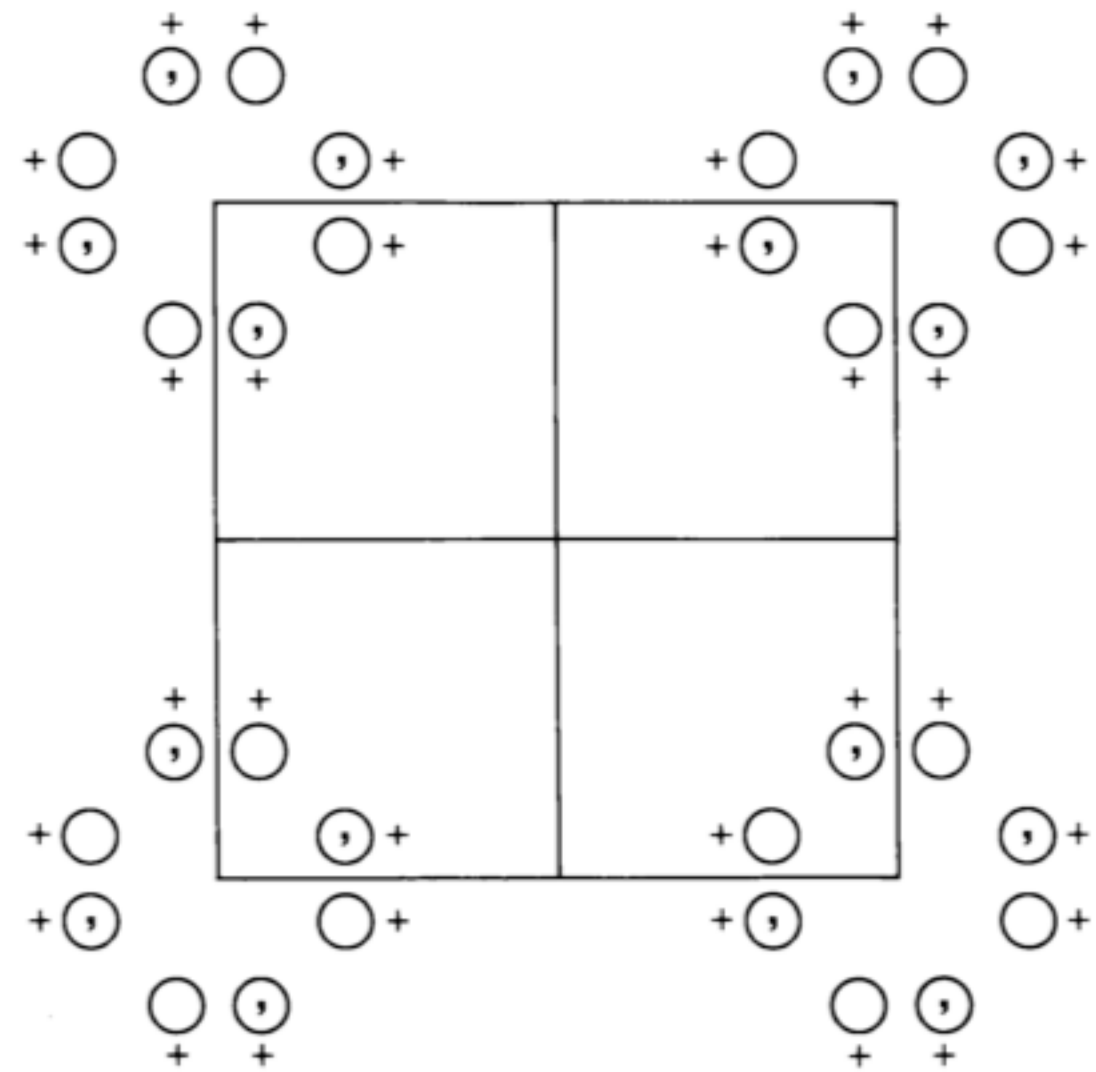
Diagram of symmetry elements



(1) 1 (2) $2 \quad 0,0,z$ (3) $4^{+} \quad 0,0,z$ (4) $4^{-} \quad 0,0,z$

(5) $m \quad x,0,z$ (6) $m \quad 0,y,z$ (7) $m \quad x,\bar{x},z$ (8) $m \quad x,x,z$

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

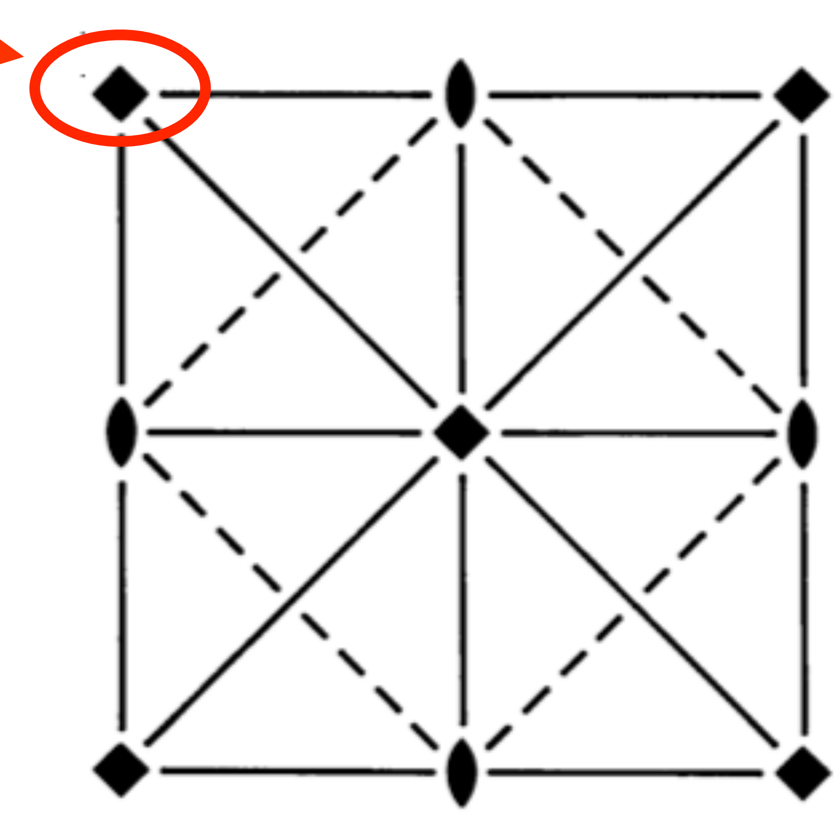
Diagram of symmetry elements

Symmetry operations that share (0,0,z) as geometric element } 1^{st}, 2^{nd}, 3^{rd} 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.

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**
...	**...**



Example: P2

Diagram of symmetry elements

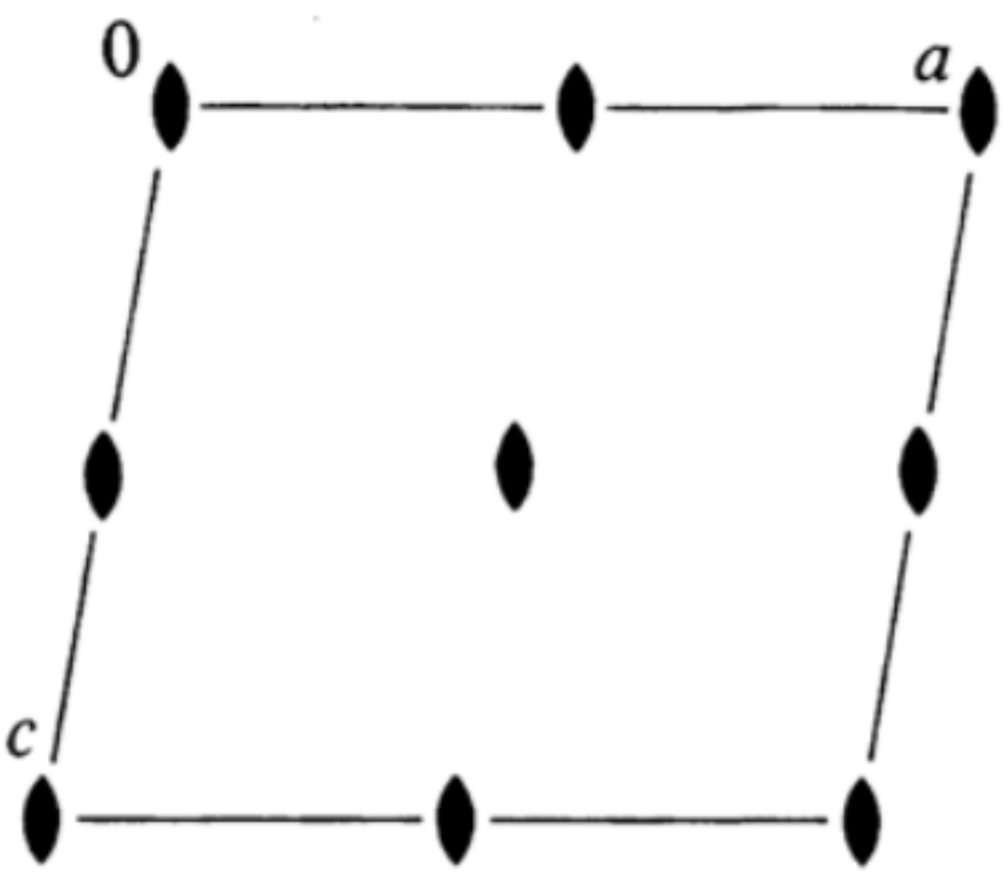
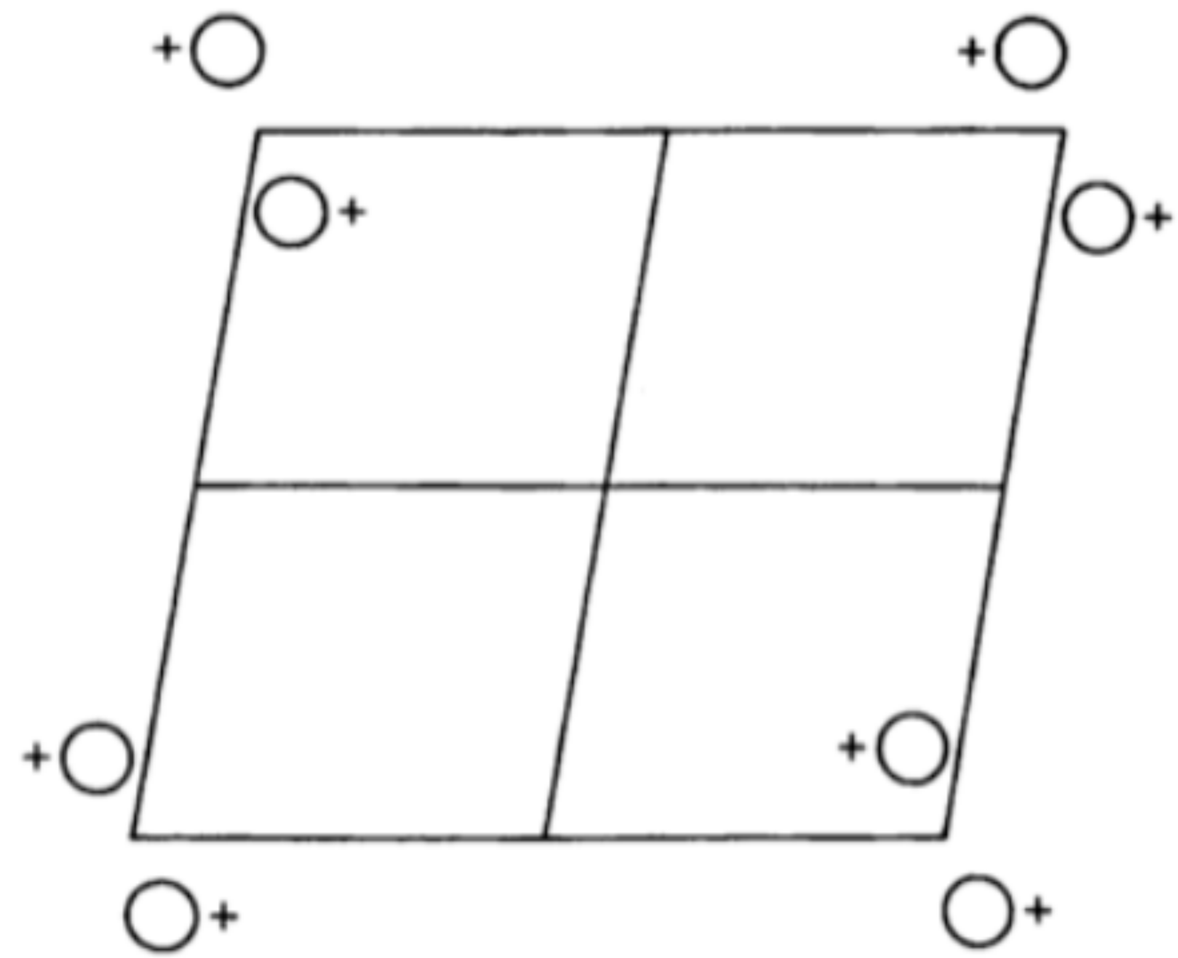


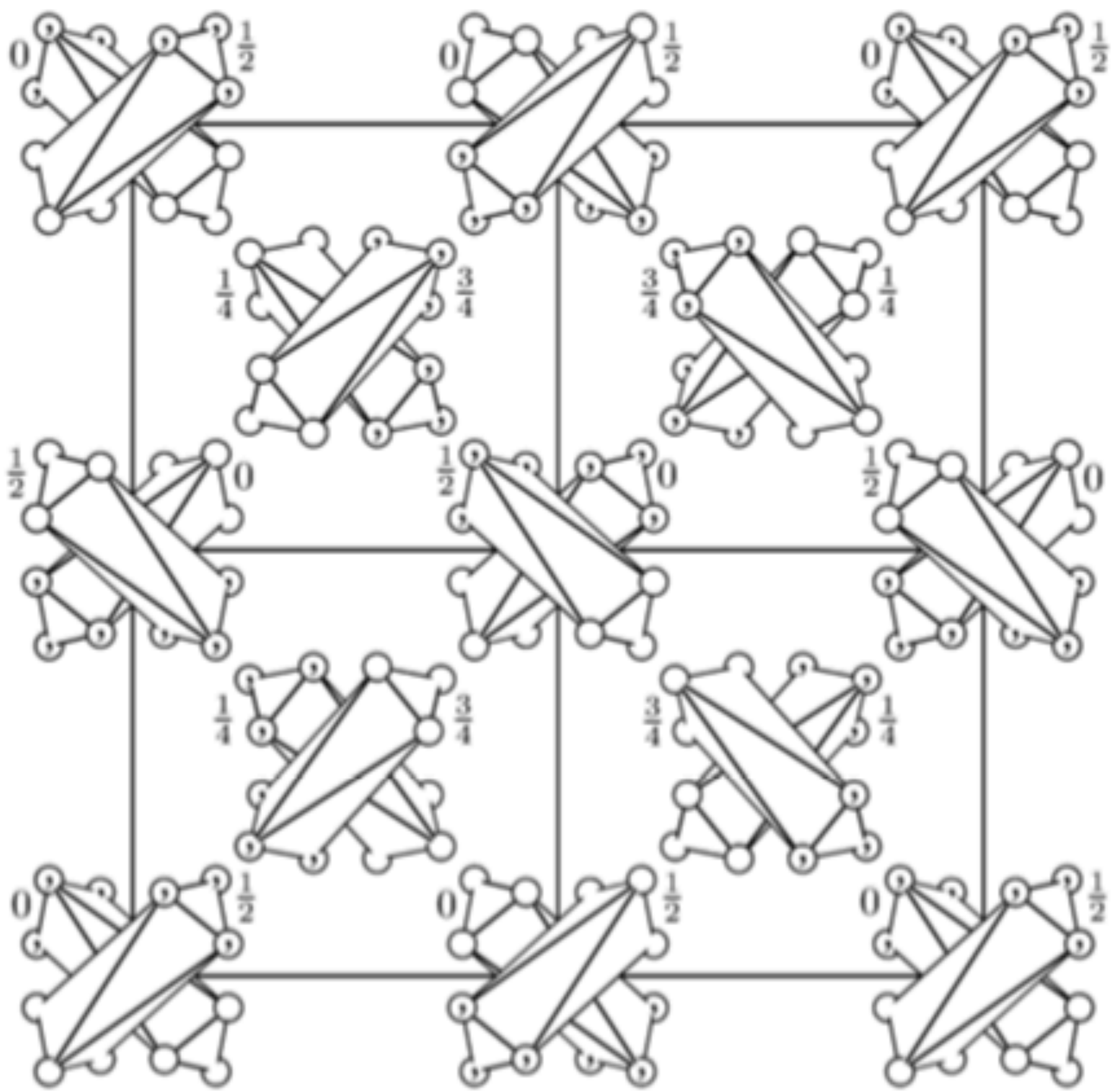
Diagram of general position points



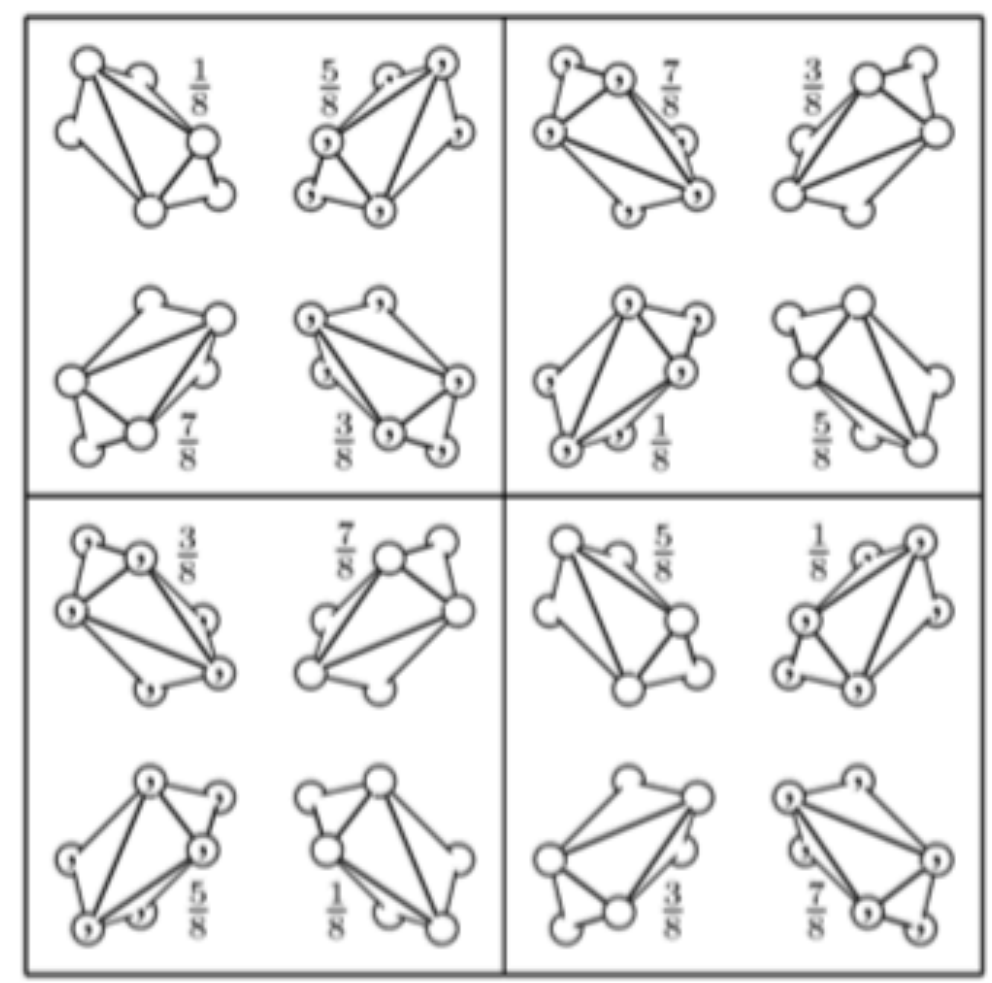
Symmetry element diagram (left) and *General position* diagram (right) of the space group $P2$, No. 3 (unique axis b, cell choice 1).

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

Diagrams of general position points



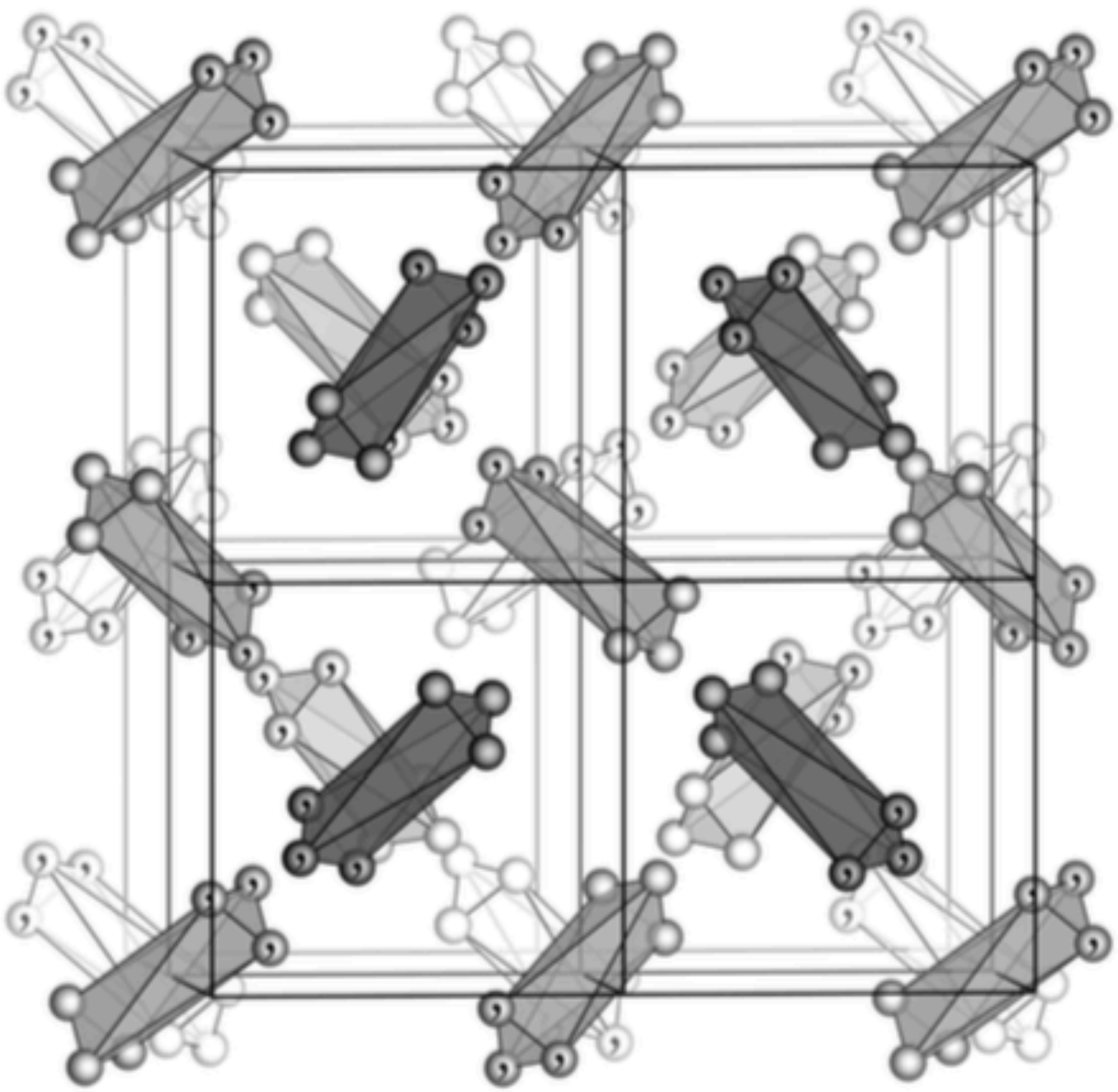
Polyhedron centre at 0, 0, 0



Polyhedron centre at $\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$

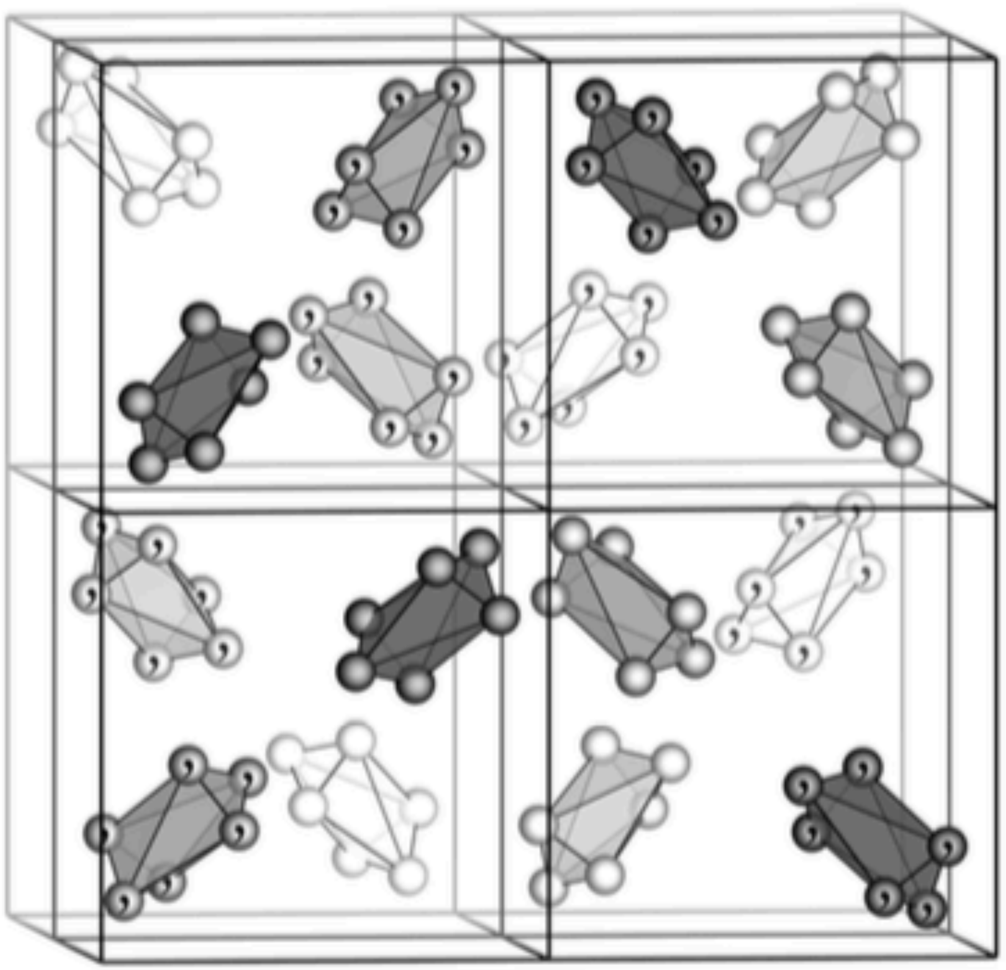
Example: Ia$\bar{3}$d (No. 230)

General-position diagrams in perspective projection



Polyhedron centre at 0, 0, 0

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



Polyhedron centre at $\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$

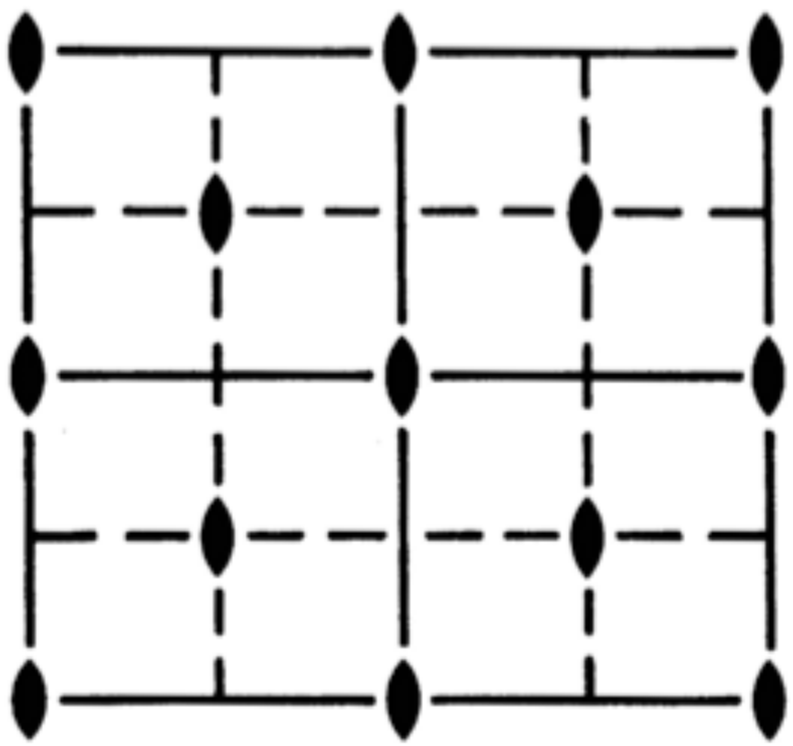
polyhedra (twisted trigonal antiprism) centres at (1/8,1/8,1/8) and its equivalent points, site symmetry .32.

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

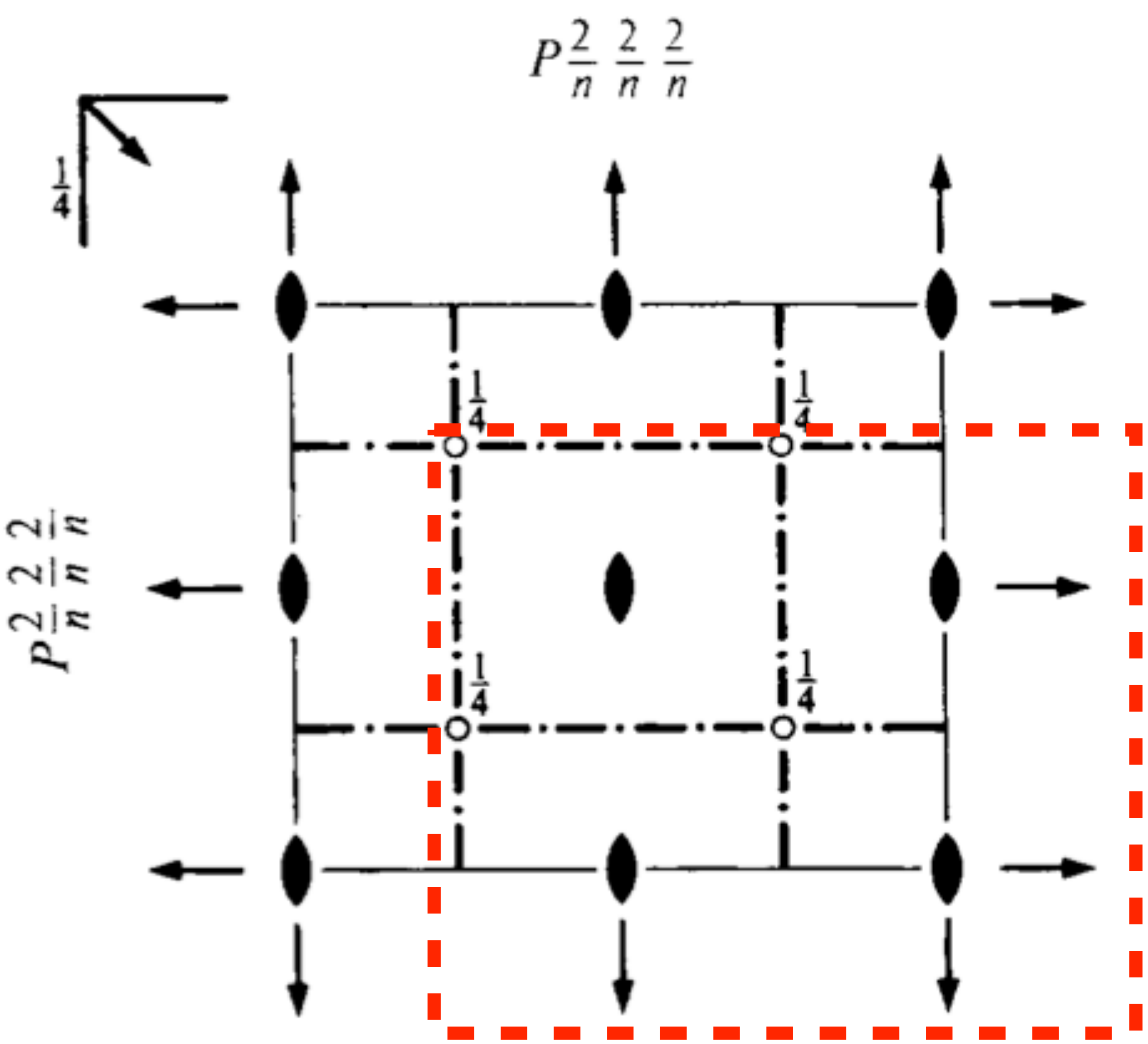
For each of the two origins the location relative to the other origin is also given.

Example: Different origins for *Pnnn*

Pnnn D_{2h}^2 *mmm* Orthorhombic

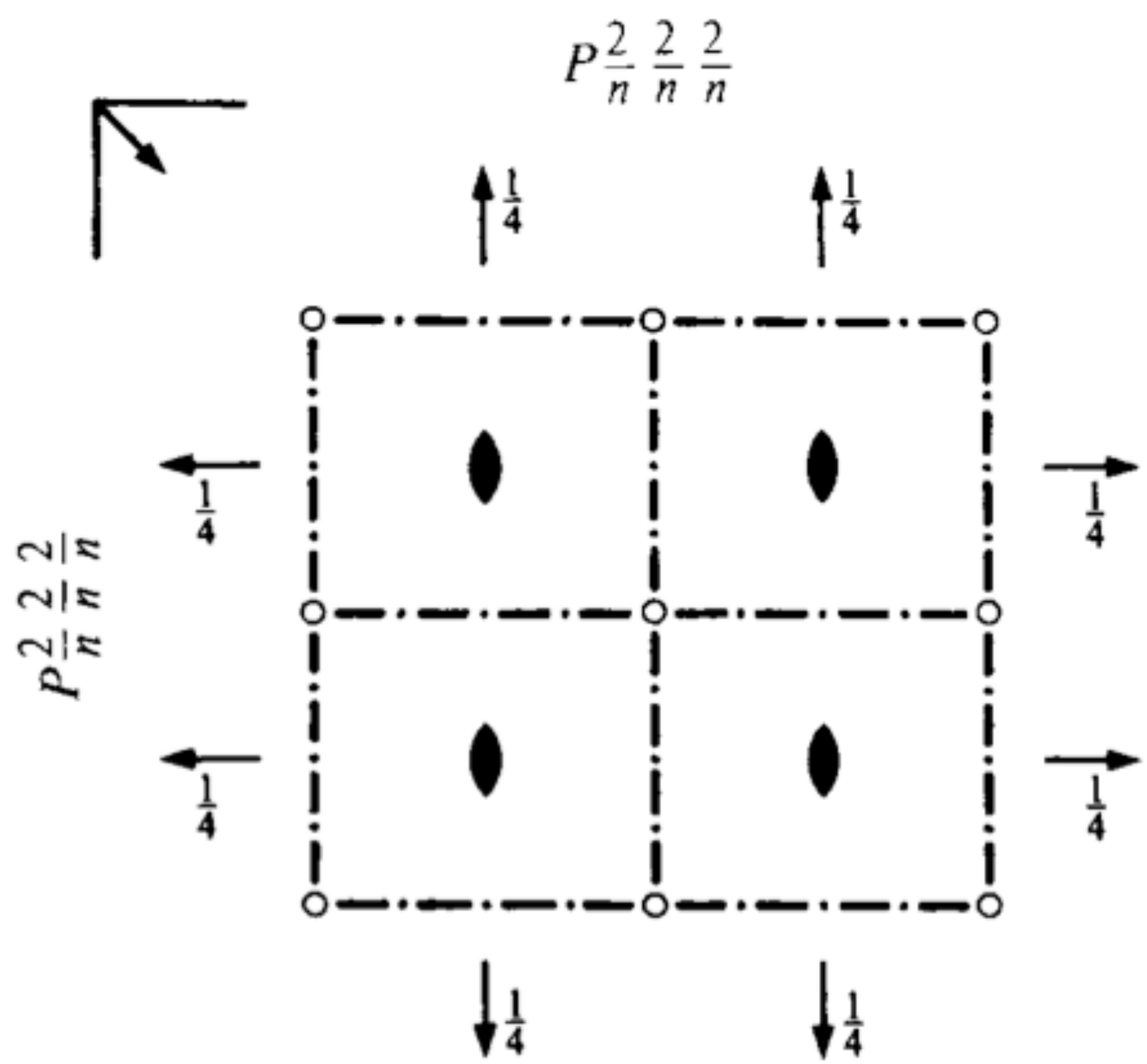
No. 48 $P\ 2/n\ 2/n\ 2/n$ Patterson symmetry *Pmmm*

ORIGIN CHOICE 1



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

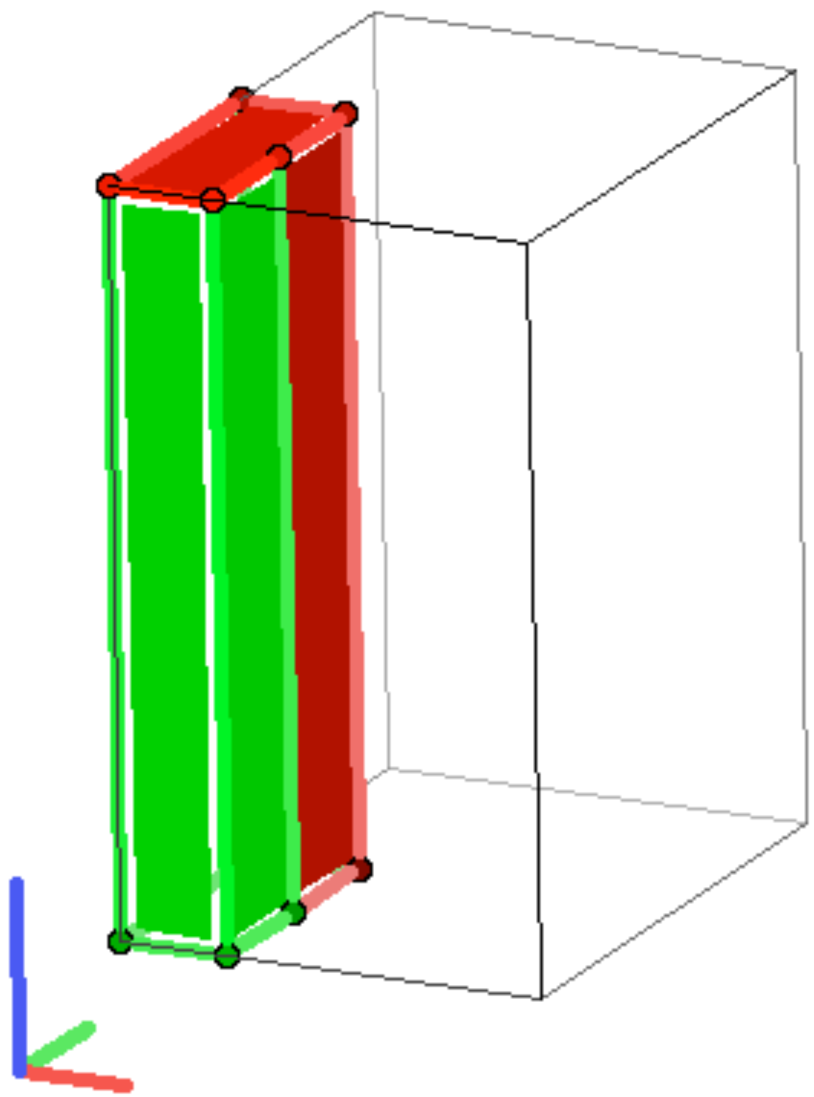
ORIGIN CHOICE 2



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

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

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



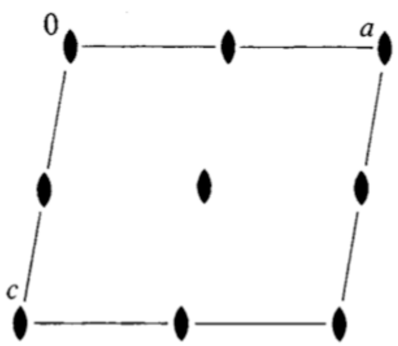
Surface area: green = inside the asymmetric unit, red = outside
Basis vectors: a = red, b = green, c = blue

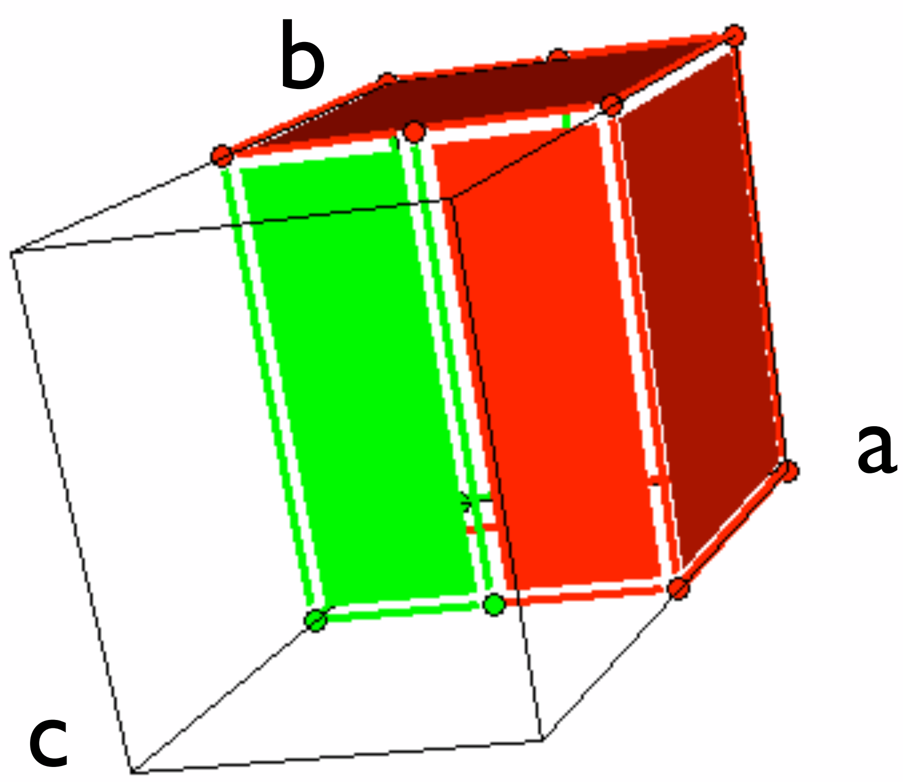
Number of vertices: 8	Number of facets: 6
0, 1/2, 0 0, 1/2, 1 1/4, 1/2, 1 1/4, 0, 1 0, 0, 0 1/4, 1/2, 0 0, 0, 1 1/4, 0, 0	x>=0 x<=1/4 [y<=1/4] y>=0 y<=1/2 z>=0 z<1 [Guide to notation]

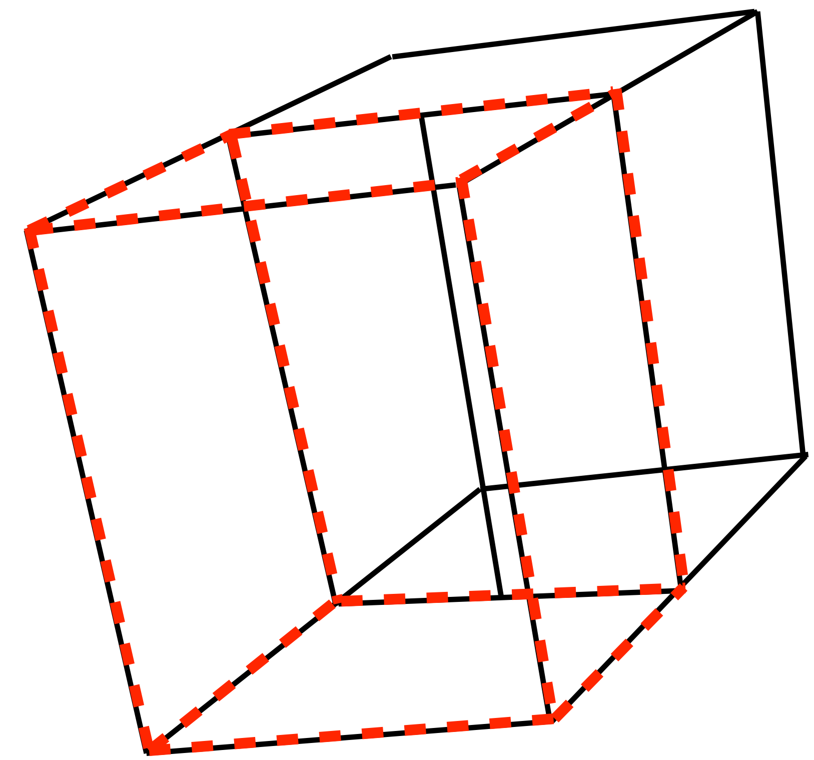
(output cctbx: Ralf Grosse-Kustelve)

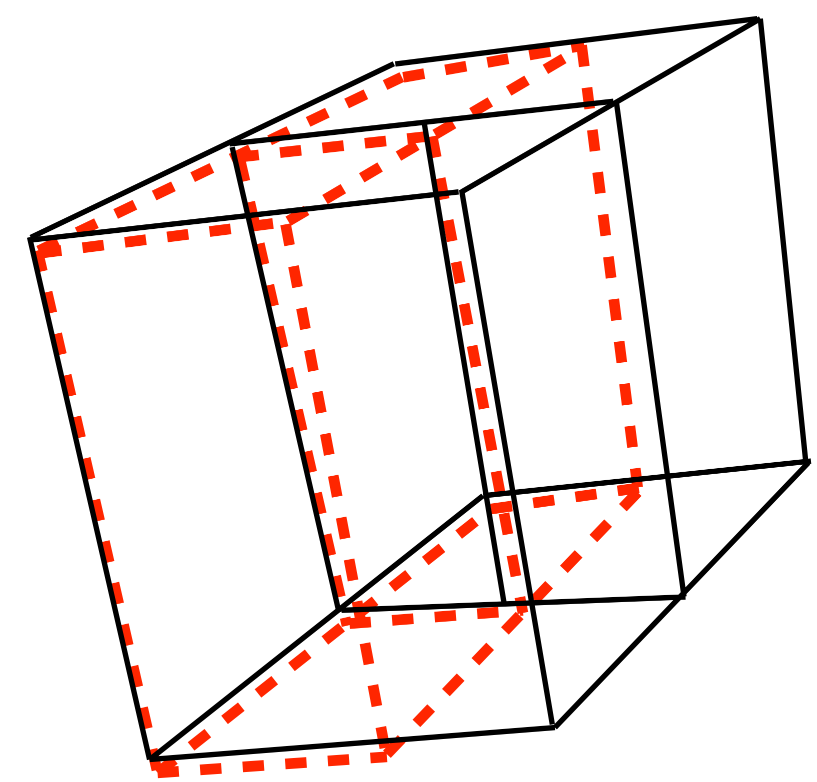
ITA: An asymmetric unit of a space group is a (simply connected) smallest closed part of space from which, by application of all symmetry operations of the space group, the whole of space is filled.

Example: Asymmetric units for the space group P121









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)

GENERAL
AND
SPECIAL WYCKOFF
POSITIONS
SITE-SYMMETRY

Group Actions

Group Actions

. A *group action* of a group $\mathcal{G}$ on a set $\Omega = \{\omega \mid \omega \in \Omega\}$ assigns to each pair (g, ω) an object $\omega' = g(\omega)$ of Ω such that the following hold:

(i) applying two group elements g and g' consecutively has the same effect as applying the product $g'g$, *i.e.* $g'(g(\omega)) = (g'g)(\omega)$

(ii) applying the identity element e of $\mathcal{G}$ has no effect on ω, *i.e.* $e(\omega) = \omega$ for all ω in Ω.

Orbit and Stabilizer

The set $\omega^{\mathcal{G}} := \{g(\omega) \mid g \in \mathcal{G}\}$ of all objects in the orbit of ω is called the *orbit of ω under $\mathcal{G}$*.

The set $S_{\mathcal{G}}(\omega) := \{g \in \mathcal{G} \mid g(\omega) = \omega\}$ of group elements that do not move the object ω is a subgroup of $\mathcal{G}$ called the *stabilizer* of ω in $\mathcal{G}$.

Equivalence classes

Via this equivalence relation, the action of $\mathcal{G}$ partitions the objects in Ω into equivalence classes

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

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

Multiplicity: $|P|$

Special position X_o

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

Multiplicity: $|P|/|S_o|$

Site-symmetry groups: oriented symbols

General position

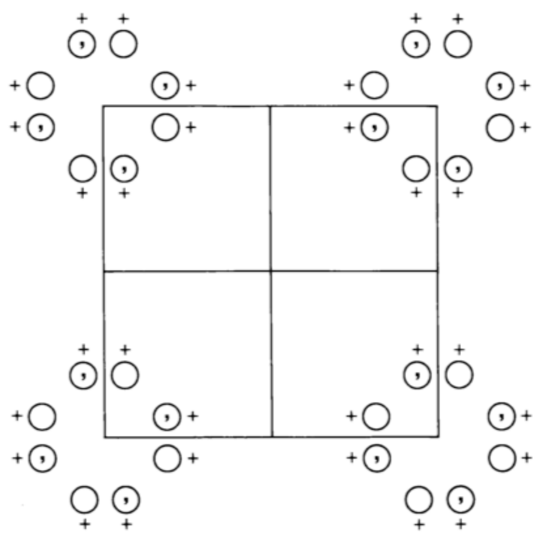
(i) coordinate triplets of an image point $\tilde{X}$ of the original point $X = \begin{pmatrix} x \\ y \\ z \end{pmatrix}$ under (W,w) of G

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

(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



As 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

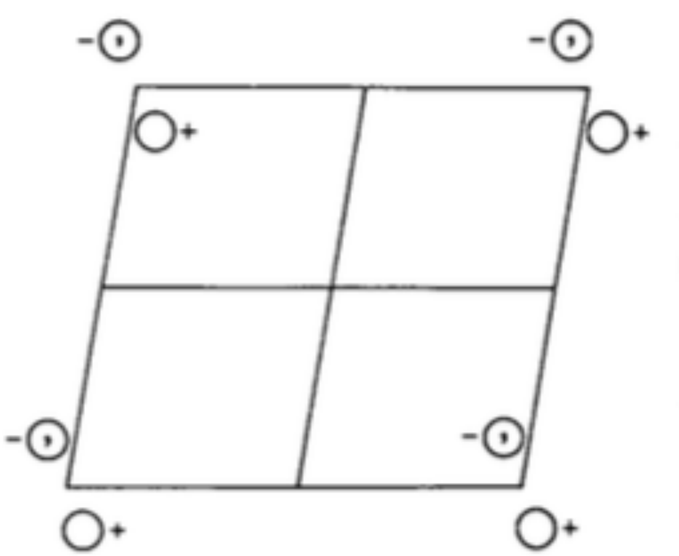
General position

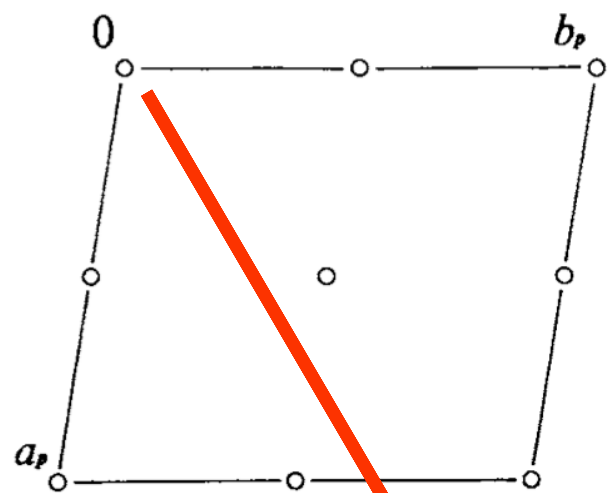
$(I,0)X$	$(W_2,w_2)X$	...	$(W_m,w_m)X$	...	$(W_i,w_i)X$	
$(I,t_1)X$	$(W_2,w_2+t_1)X$	...	$(W_m,w_m+t_1)X$	...	$(W_i,w_i+t_1)X$	
$(I,t_2)X$	$(W_2,w_2+t_2)X$	...	$(W_m,w_m+t_2)X$	...	$(W_i,w_i+t_2)X$	
...	...	...	...	...	...	
$(I,t_j)X$	$(W_2,w_2+t_j)X$	...	$(W_m,w_m+t_j)X$	...	$(W_i,w_i+t_j)X$	
...	...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

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

Example: Calculation of the Site-symmetry groups

Group P-1





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

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

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

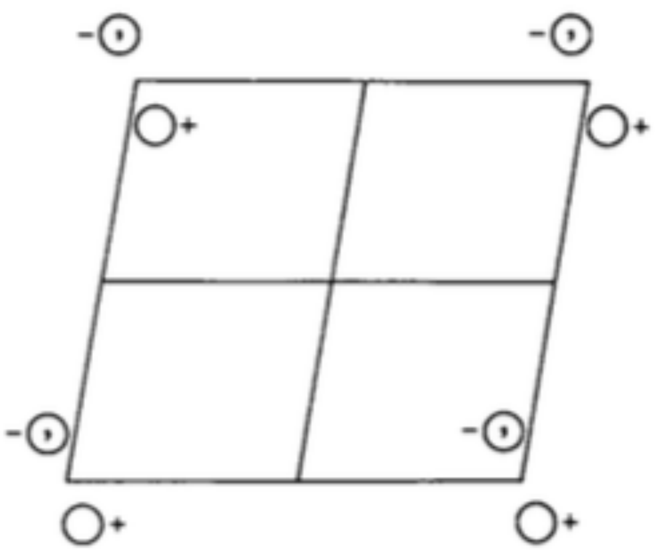
$$S_f \simeq \{1, -1\}$$ isomorphic

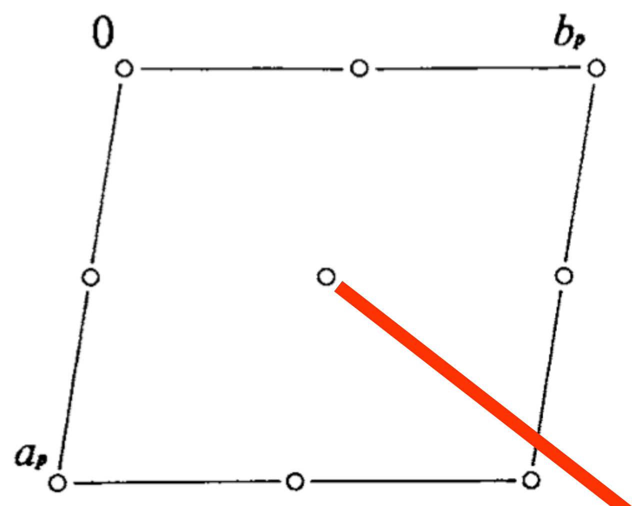
Positions

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*	$\bar{1}$	$0,0,0$	

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*	$\bar{1}$	$0,0,0$	

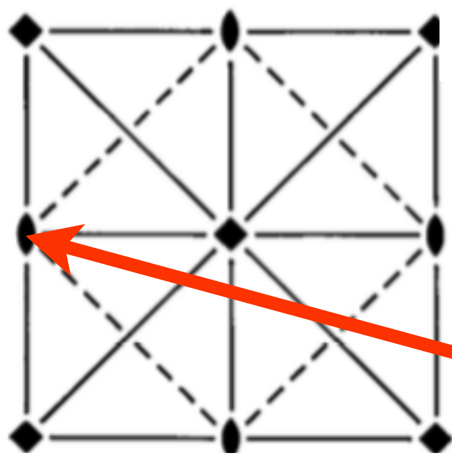
Determine the site symmetry group of the point $X_o = \begin{pmatrix} 1/2 \\ 0 \\ 1/2 \end{pmatrix}$

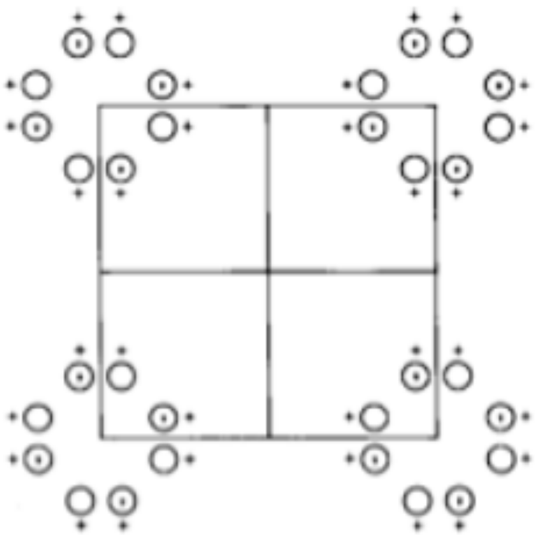
$$S=\{(W,w), (W,w)X_o = X_o\}$$

QUICK QUIZ

Space group P4mm

Site symmetry groups of special Wyckoff positions





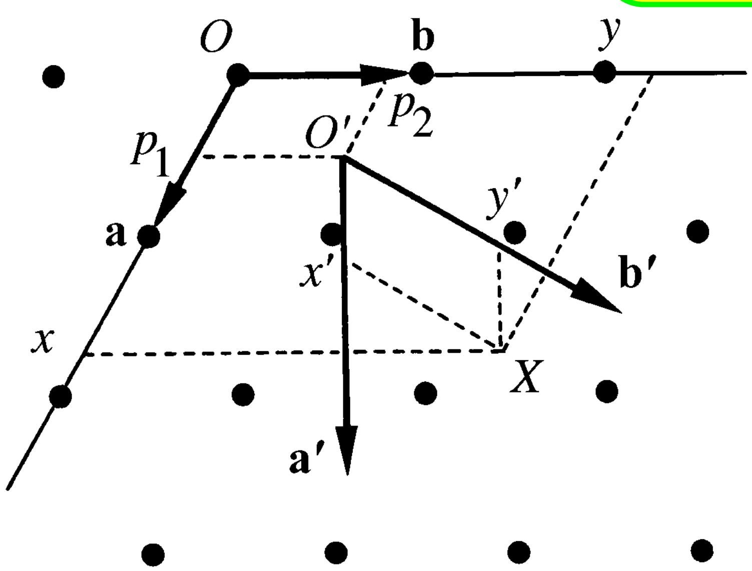
8	*g*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$
			(5) $x,\bar{y},z$	(6) $\bar{x},y,z$	(7) $\bar{y},\bar{x},z$	(8) y,x,z
4	*f*	$.m.$	$x,\frac{1}{2},z$	$\bar{x},\frac{1}{2},z$	$\frac{1}{2},x,z$	$\frac{1}{2},\bar{x},z$
4	*e*	$.m.$	$x,0,z$	$\bar{x},0,z$	$0,x,z$	$0,\bar{x},z$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

Symmetry 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

CO-ORDINATE TRANSFORMATIONS IN CRYSTALLOGRAPHY

Co-ordinate transformation



3-dimensional space

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

$\downarrow$ (P,p)

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

Transformation matrix-column pair (P,p)

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

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

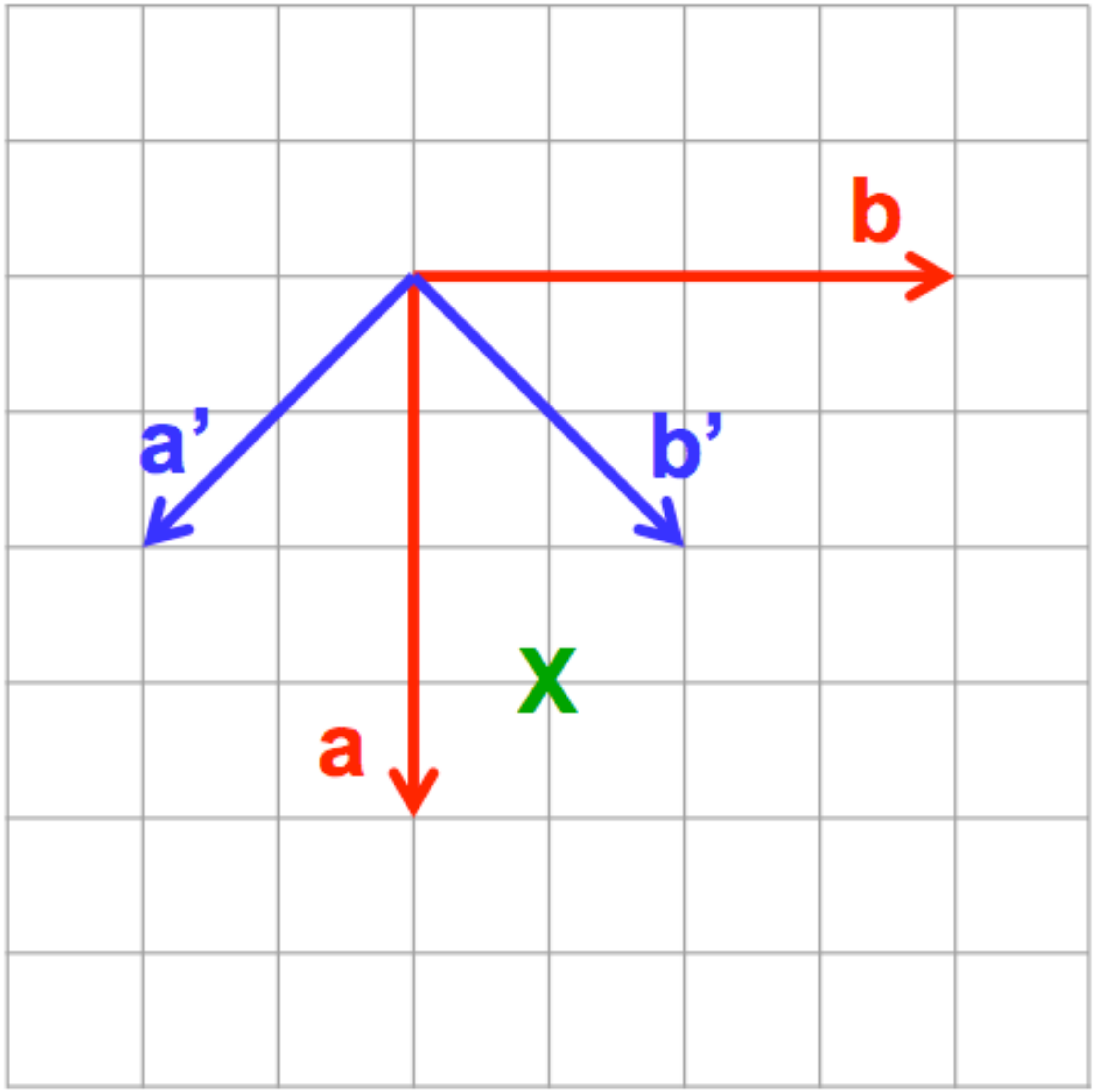
$$= (\mathbf{a}, \mathbf{b}, \mathbf{c}) \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix} = (P_{11}\mathbf{a} + P_{21}\mathbf{b} + P_{31}\mathbf{c}, \; P_{12}\mathbf{a} + P_{22}\mathbf{b} + P_{32}\mathbf{c}, \; P_{13}\mathbf{a} + P_{23}\mathbf{b}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

(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

QUICK QUIZ



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

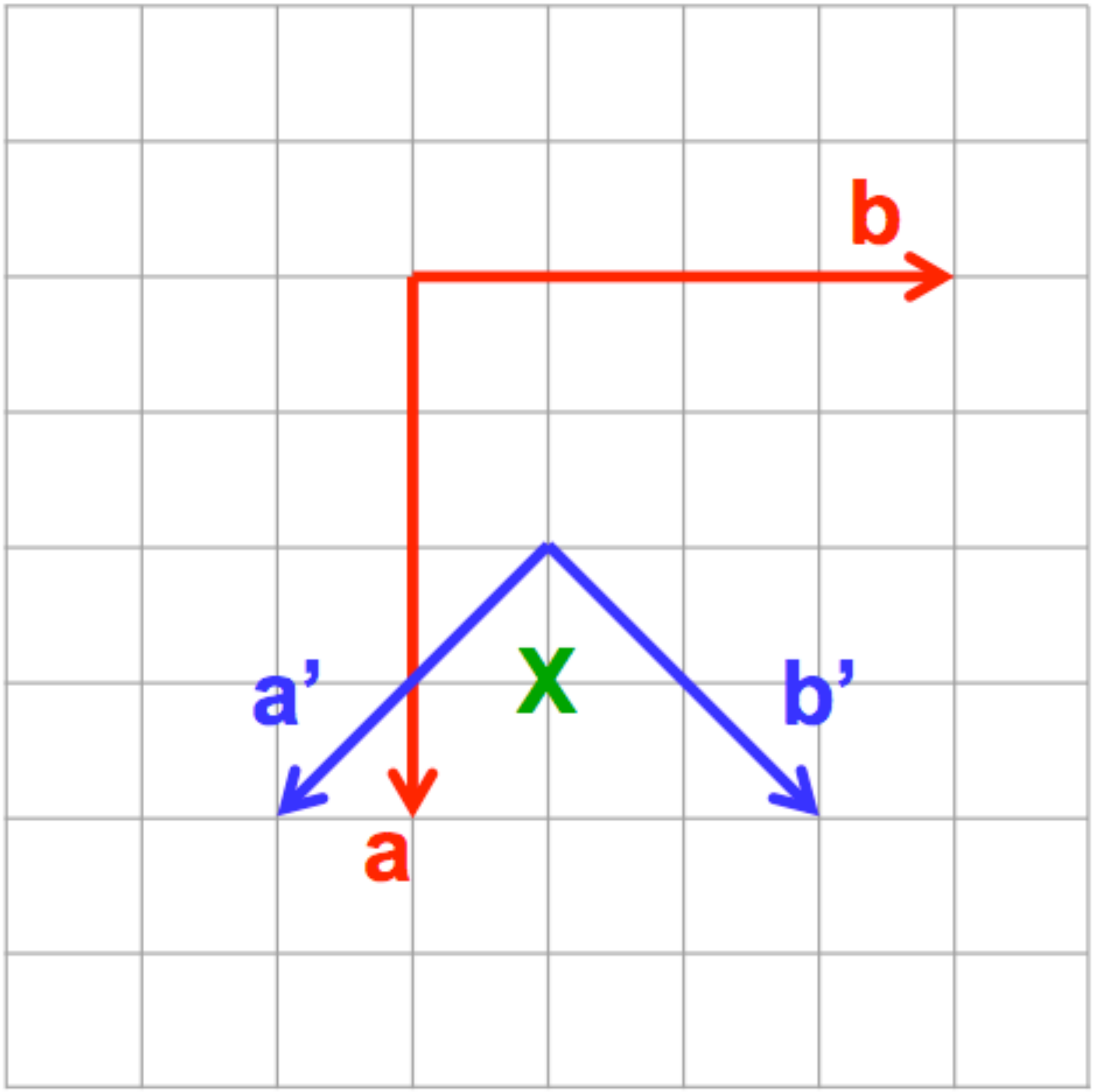
$$(a, b, c) = (a', b', c')\begin{pmatrix} ? \end{pmatrix}$$

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

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

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

QUICK QUIZ



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

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

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

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

Linear parts as before.

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

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

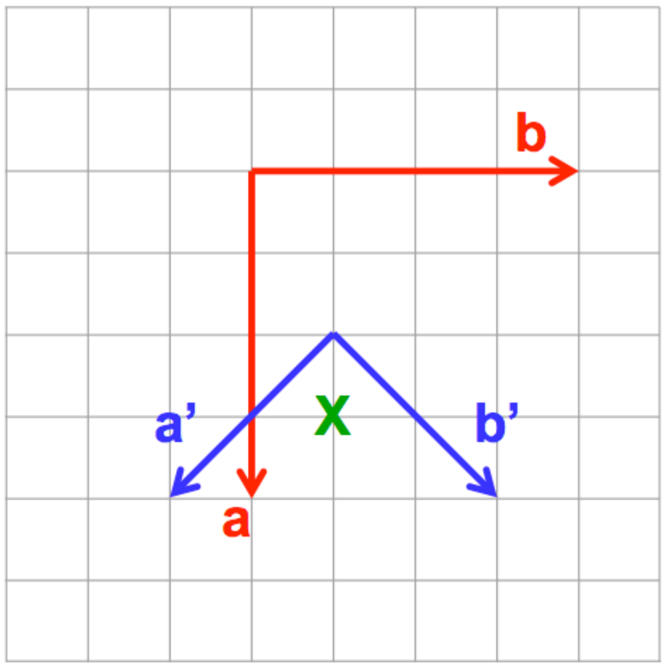
$$(P,p)^{-1}=\left(\begin{array}{ccc|c} 1 & -1 & 0 & -1/4 \\ 1 & 1 & 0 & -3/4 \\ 0 & 0 & 1 & 0 \end{array}\right)$$

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'

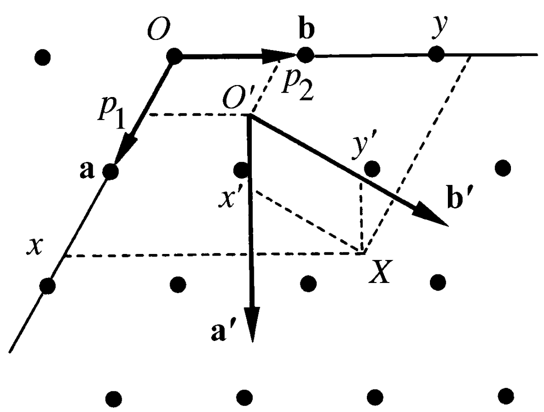
b=-a'+b'

c=c'

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

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:

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

Transformation of the coordinates of a point X(x,y,z):

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

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} P_{11} & P_{12} & P_{13} & p_1 \\ P_{21} & P_{22} & P_{23} & p_2 \\ P_{31} & P_{32} & P_{33} & p_3 \end{pmatrix}^{-1} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

special cases

-origin shift (***P***=***I***): $x' = x - p$

-change of basis (***p***=**o**) : $x' = P^{-1}x$

EXAMPLE

$$X' = (P,p)^{-1}X = \left(\begin{pmatrix} 1 & -1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} -1/4 \\ -3/4 \\ 0 \end{pmatrix} \right) \begin{pmatrix} 3/4 \\ 1/4 \\ 0 \end{pmatrix} = \begin{pmatrix} 1/4 \\ 1/4 \\ 0 \end{pmatrix}$$

QUICK QUIZ

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

0,70
0,31
0,95

Hint

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

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

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

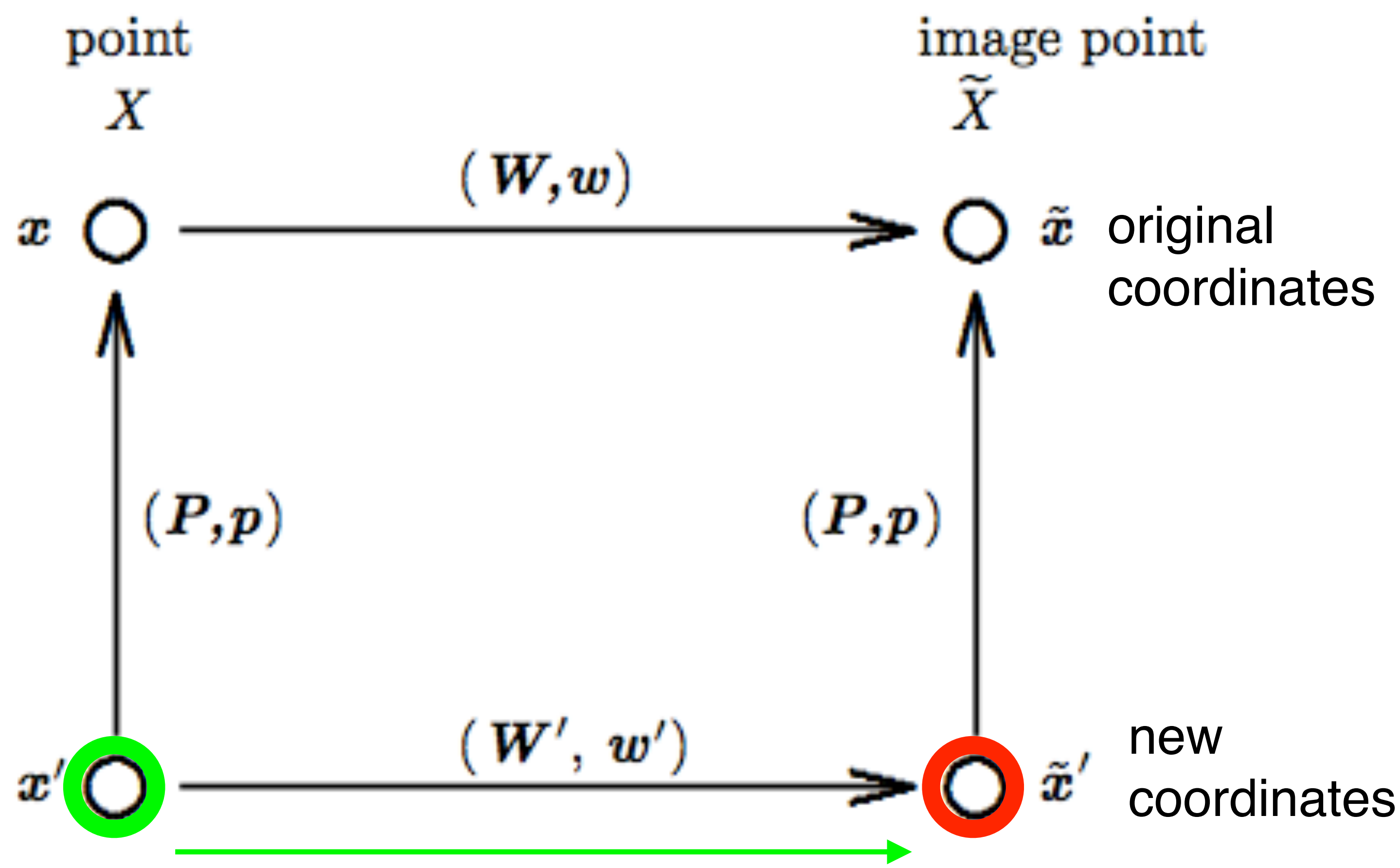
covariant to crystal basis: Miller indices

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

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

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

Transformation of symmetry operations (W,w)



i. $\tilde{\boldsymbol{x}}' = (\boldsymbol{W}', \boldsymbol{w}')\boldsymbol{x}'$;

ii. $\tilde{\boldsymbol{x}}' = (\boldsymbol{P}, \boldsymbol{p})^{-1}\tilde{\boldsymbol{x}} = (\boldsymbol{P}, \boldsymbol{p})^{-1}(\boldsymbol{W}, \boldsymbol{w})\boldsymbol{x} = (\boldsymbol{P}, \boldsymbol{p})^{-1}(\boldsymbol{W}, \boldsymbol{w})(\boldsymbol{P}, \boldsymbol{p})\boldsymbol{x}'$.

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

QUIZ

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

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**.

Hint

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

Problem: SYMMETRY DATA ITA SETTINGS

530 ITA settings of orthorhombic and monoclinic groups

Monoclinic descriptions

	Transf.	**abc**	**c$\bar{\mathbf{b}}$a**	**abc**	**ba$\bar{\mathbf{c}}$**	**abc**	**$\bar{\mathbf{a}}$cb**	Monoclinic axis b Monoclinic axis c Monoclinic axis a
HM	$C2/c$	$C12/c1$ $A12/n1$ $I12/a1$	$A12/a1$ $C12/n1$ $I12/c1$	$A112/a$ $B112/n$ $I112/b$	$B112/b$ $A112/n$ $I112/a$	$B2/b11$ $C2/n11$ $I2/c11$	$C2/c11$ $B2/n11$ $I2/b11$	Cell type 1 Cell type 2 Cell type 3

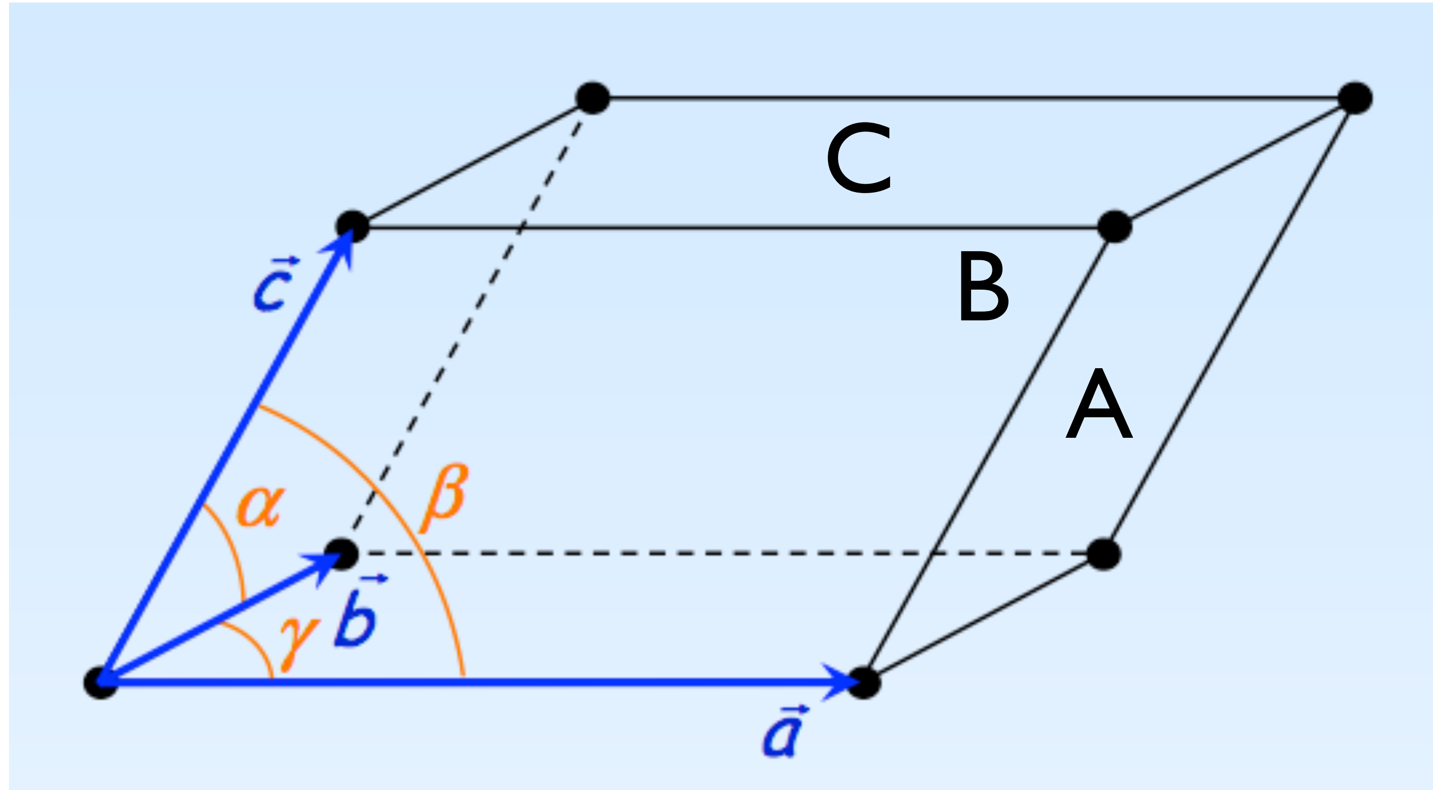
Orthorhombic descriptions

No.	HM	**abc**	**ba$\bar{\mathbf{c}}$**	**cab**	**$\bar{\mathbf{c}}$ba**	**bca**	**a$\bar{\mathbf{c}}$b**
33	$Pna2_1$	$Pna2_1$	$Pbn2_1$	$P2_1nb$	$P2_1cn$	$Pc2_1n$	$Pn2_1a$

METRIC TENSOR

3D-unit cell and lattice parameters

lattice basis:
{**a**, **b**, **c**}



unit cell:
the parallelepiped defined by the basis vectors

primitive P and **centred** unit cells:
A,B,C,F, I, R

number of lattice points per unit cell

Lattice parameters

lengths of the unit translations:	angles between them:
a	$\alpha = (\widehat{\vec{b}, \vec{c}})$
b	$\beta = (\widehat{\vec{c}, \vec{a}})$
c	$\gamma = (\widehat{\vec{a}, \vec{b}})$

Lattice parameters (3D)

An alternative way to define the metric properties of a lattice **L**

Given a lattice **L** of $\mathbf{V}^3$ with a lattice basis: $\{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3\}$

Definition (D 1.5.3) The quantities

$$a_1 = |\mathbf{a}_1| = +\sqrt{(\mathbf{a}_1\,,\,\mathbf{a}_1)}, \qquad a_2 = |\mathbf{a}_2| = +\sqrt{(\mathbf{a}_2\,,\,\mathbf{a}_2)},$$

$$a_3 = |\mathbf{a}_3| = +\sqrt{(\mathbf{a}_3\,,\,\mathbf{a}_3)},$$

$$\alpha_1 = \arccos\left(|\mathbf{a}_2|^{-1}|\mathbf{a}_3|^{-1}(\mathbf{a}_2\,,\,\mathbf{a}_3)\right), \qquad \alpha_2 = \arccos\left(|\mathbf{a}_3|^{-1}|\mathbf{a}_1|^{-1}(\mathbf{a}_3\,,\,\mathbf{a}_1)\right),$$

$$\text{and} \quad \alpha_3 = \arccos\left(|\mathbf{a}_1|^{-1}|\mathbf{a}_2|^{-1}(\mathbf{a}_1\,,\,\mathbf{a}_2)\right)$$

are called the *lattice parameters* of the lattice.

Remark: the lengths of basis vectors are measured in

nm (1*nm*=10^{-9} m) Å (1Å=10^{-10} m) *pm* (1*pm*=10^{-12} m)

Metric tensor *G* in terms of lattice parameters

$$G = \begin{pmatrix} \mathbf{a}\cdot\mathbf{a} & \mathbf{a}\cdot\mathbf{b} & \mathbf{a}\cdot\mathbf{c} \\ \mathbf{b}\cdot\mathbf{a} & \mathbf{b}\cdot\mathbf{b} & \mathbf{b}\cdot\mathbf{c} \\ \mathbf{c}\cdot\mathbf{a} & \mathbf{c}\cdot\mathbf{b} & \mathbf{c}\cdot\mathbf{c} \end{pmatrix} \quad G = \begin{pmatrix} a^2 & ab\cos\gamma & ac\cos\beta \\ ab\cos\gamma & b^2 & bc\cos\alpha \\ ac\cos\beta & bc\cos\alpha & c^2 \end{pmatrix}$$

Crystal families, crystal systems, lattice systems and Bravais lattices in 3D

Crystal family	Symbol*	Crystal system	Crystallographic point groups†	No. of space groups	Conventional coordinate system		Bravais lattices*
					Restrictions on cell parameters	Parameters to be determined	
Triclinic (anorthic)	*a*	Triclinic	$1, \bar{1}$	2	None	$a, b, c,$ α, β, γ	*aP*
Monoclinic	*m*	Monoclinic	$2, m, 2/m$	13	*b*-unique setting $\alpha = \gamma = 90°$	a, b, c β‡	*mP* *mS* (*mC*, *mA*, *mI*)
					c-unique setting $\alpha = \beta = 90°$	$a, b, c,$ γ‡	*mP* *mS* (*mA*, *mB*, *mI*)
Orthorhombic	*o*	Orthorhombic	$222, mm2, mmm$	59	$\alpha = \beta = \gamma = 90°$	a, b, c	*oP* *oS* (*oC*, *oA*, *oB*) *oI* *oF*
Tetragonal	*t*	Tetragonal	$4, \bar{4}, 4/m$ $422, 4mm, \bar{4}2m,$ $4/mmm$	68	$a = b$ $\alpha = \beta = \gamma = 90°$	a, c	*tP* *tI*
Hexagonal	*h*	Trigonal	$3, \bar{3}$ $32, 3m, \bar{3}m$	18	$a = b$ $\alpha = \beta = 90°,\ \gamma = 120°$	a, c	*hP*
				7	$a = b = c$ $\alpha = \beta = \gamma$ (rhombohedral axes, primitive cell) $a = b$ $\alpha = \beta = 90°, \gamma = 120°$ (hexagonal axes, triple obverse cell)	a, α	*hR*
		Hexagonal	$6, \bar{6}, 6/m$ $622, 6mm, \bar{6}2m,$ $6/mmm$	27	$a = b$ $\alpha = \beta = 90°, \gamma = 120°$	a, c	*hP*
Cubic	*c*	Cubic	$23, m\bar{3}$ $432, \bar{4}3m, m\bar{3}m$	36	$a = b = c$ $\alpha = \beta = \gamma = 90°$	a	*cP* *cI* *cF*

Crystallographic calculations: Volume of the unit cell

Volume of the unit cell:

The volume V of the unit cell of a crystal structure, *i.e.* the body containing all points with coordinates $0 \le x_1, x_2, x_3 < 1$, can be calculated by the formula

$$\det(\boldsymbol{G}) = V^2.$$

Scalar product of arbitrary vectors:

$$(\mathbf{r},\mathbf{t})=\mathbf{r}^T\boldsymbol{G}\mathbf{t}$$

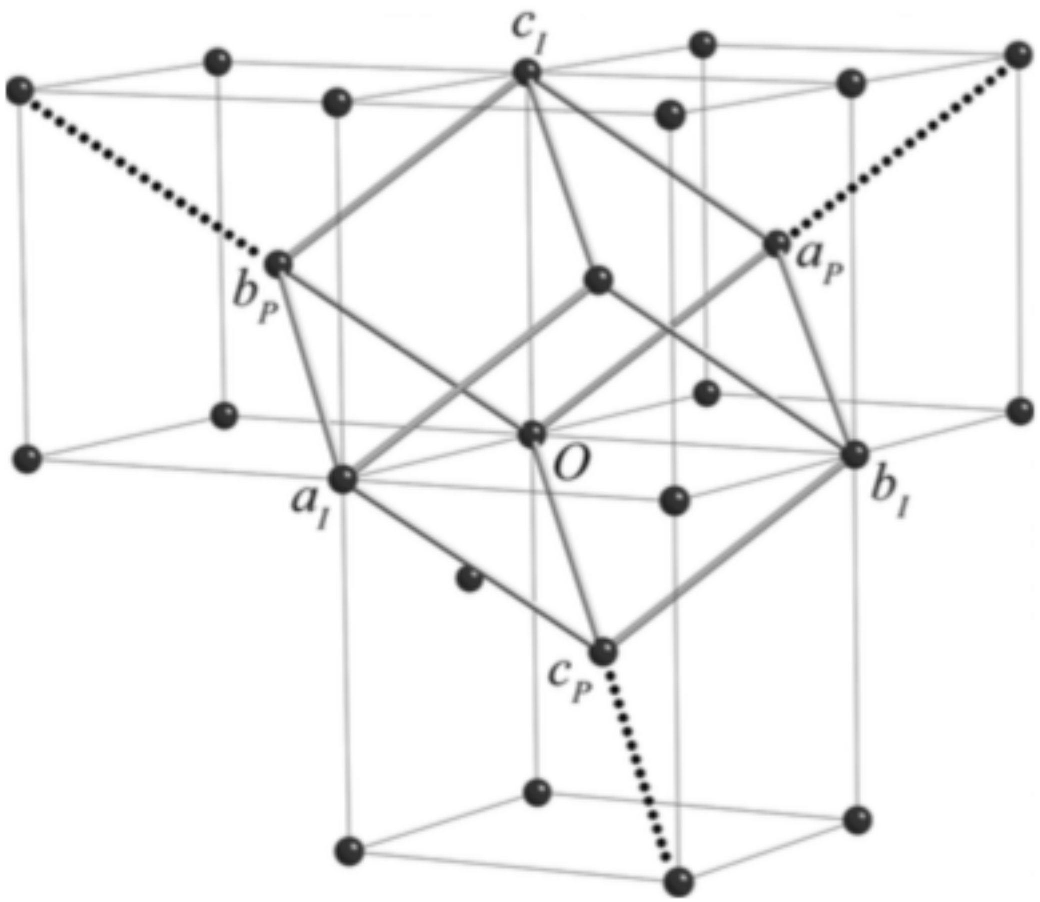
Transformation properties of *G* under basis transformation

$$\{\mathbf{a'}_1, \mathbf{a'}_2, \mathbf{a'}_3\}= \{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3\}\boldsymbol{P}$$

$$\boldsymbol{G'}=\boldsymbol{P}^T \boldsymbol{G}\ \boldsymbol{P}$$

QUIZ

Body-centred cubic cell



A body-centred cubic lattice (*cI*) has as its conventional basis the conventional basis $(\mathbf{a_P},\mathbf{b_P},\mathbf{c_P})$ of a primitive cubic lattice, but the lattice also contains the centring vector $1/2\mathbf{a_P}+1/2\mathbf{b_P}+1/2\mathbf{c_P}$ which points to the centre of the conventional cell.

Calculate the coefficients of the metric tensor for the body-centred cubic lattice:

(i) for the conventional basis $(\mathbf{a_P},\mathbf{b_P},\mathbf{c_P})$;

(ii) for the primitive basis:

$\mathbf{a_I}=1/2(-\mathbf{a_P}+\mathbf{b_P}+\mathbf{c_P})$, $\mathbf{b_I}=1/2(\mathbf{a_P}-\mathbf{b_P}+\mathbf{c_P})$, $\mathbf{c_I}=1/2(\mathbf{a_P}+\mathbf{b_P}-\mathbf{c_P})$

(iii) determine the lattice parameters of the primitive cell if a_P=4 Å

Hint

metric tensor transformation $\mathbf{G'}=\mathbf{P^t}\,\mathbf{G}\,\mathbf{P}$