International Union of Crystallography

Commission on Mathematical and Theoretical Crystallography

Universidad de los Andes

Facultad de Ciencias

International School on Fundamental Crystallography
Sixth MaThCryst school in Latin America
Workshop on the Applications of Group Theory in the Study of Phase Transitions

Bogotá, Colombia, 26 November - 1st December 2018

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SPACE GROUPS II

International Tables for Crystallography, Volume A: Space-group Symmetry

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SPACE GROUPS

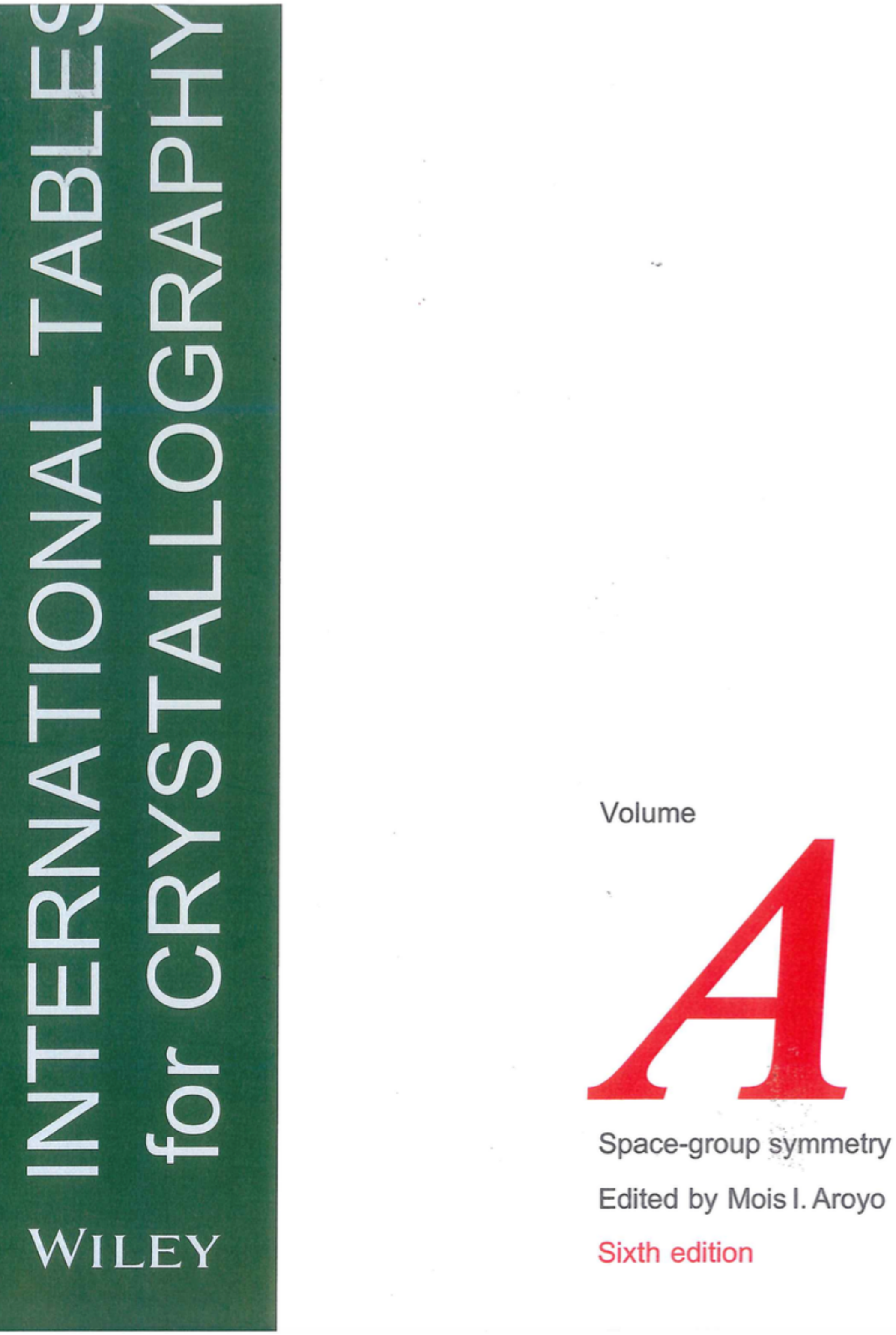
Crystal pattern: A model of the ideal crystal (crystal structure) in point space consisting of a strictly 3-dimensional periodic set of points

Space group G: The set of all symmetry operations (isometries) of a crystal pattern

Translation subgroup $H \triangleleft G$: 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: $P_G \cong G/H$

INTERNATIONAL TABLES FOR CRYSTALLOGRAPHY VOLUME A: SPACE-GROUP SYMMETRY



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

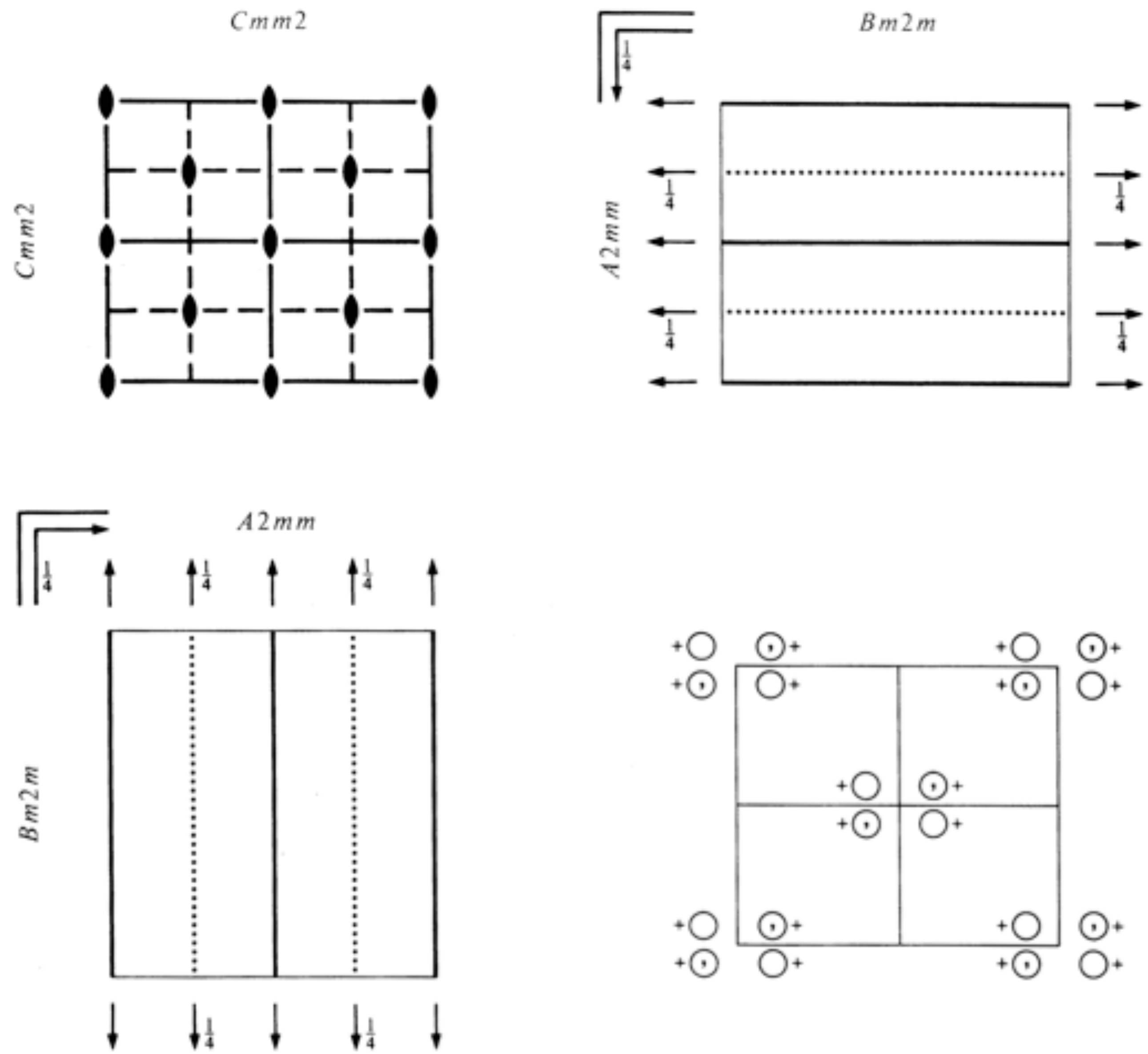
- headline with the relevant group symbols;
- diagrams of the symmetry elements and of the general position;
- specification of the origin and the asymmetric unit;
- list of symmetry operations;
- generators;
- general and special positions with multiplicities, site symmetries, coordinates and reflection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

(1) CONTINUED — No. 35 — $Cmm2$

(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 $0,y,0$

Primitive and centred lattice basis in 2D

$\{\mathbf{a}_1, \mathbf{a}_2\}$: two translation vectors, linearly independent, form a *lattice basis*

Primitive basis: If all lattice vectors are expressed as integer linear combinations of the basis vectors

Centred basis: If some lattice vectors are expressed as linear combinations of the basis vectors with *rational*, *non-integer* coefficients

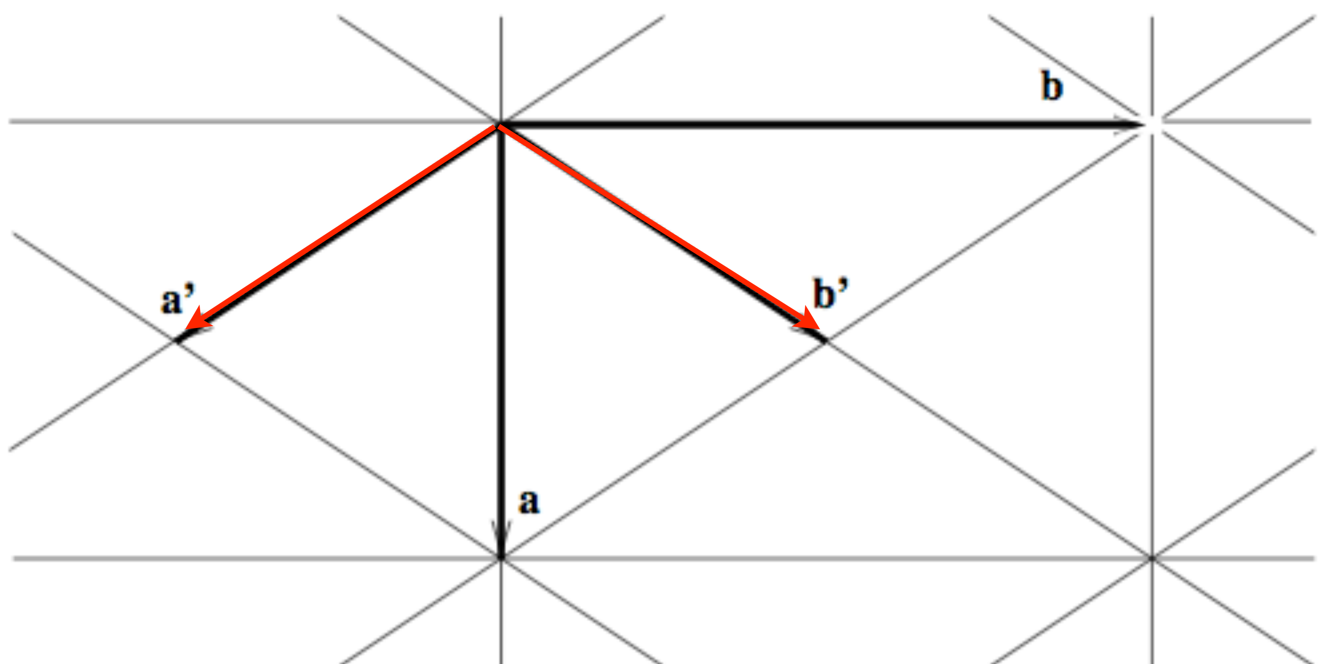


Fig. 1.5.2 c-centred lattice (net) in the plane with conventional **a**, **b** and primitive **a'**, **b'** bases.

Conventional centred basis (2D): *c*

Number of lattice points per primitive and centred cells

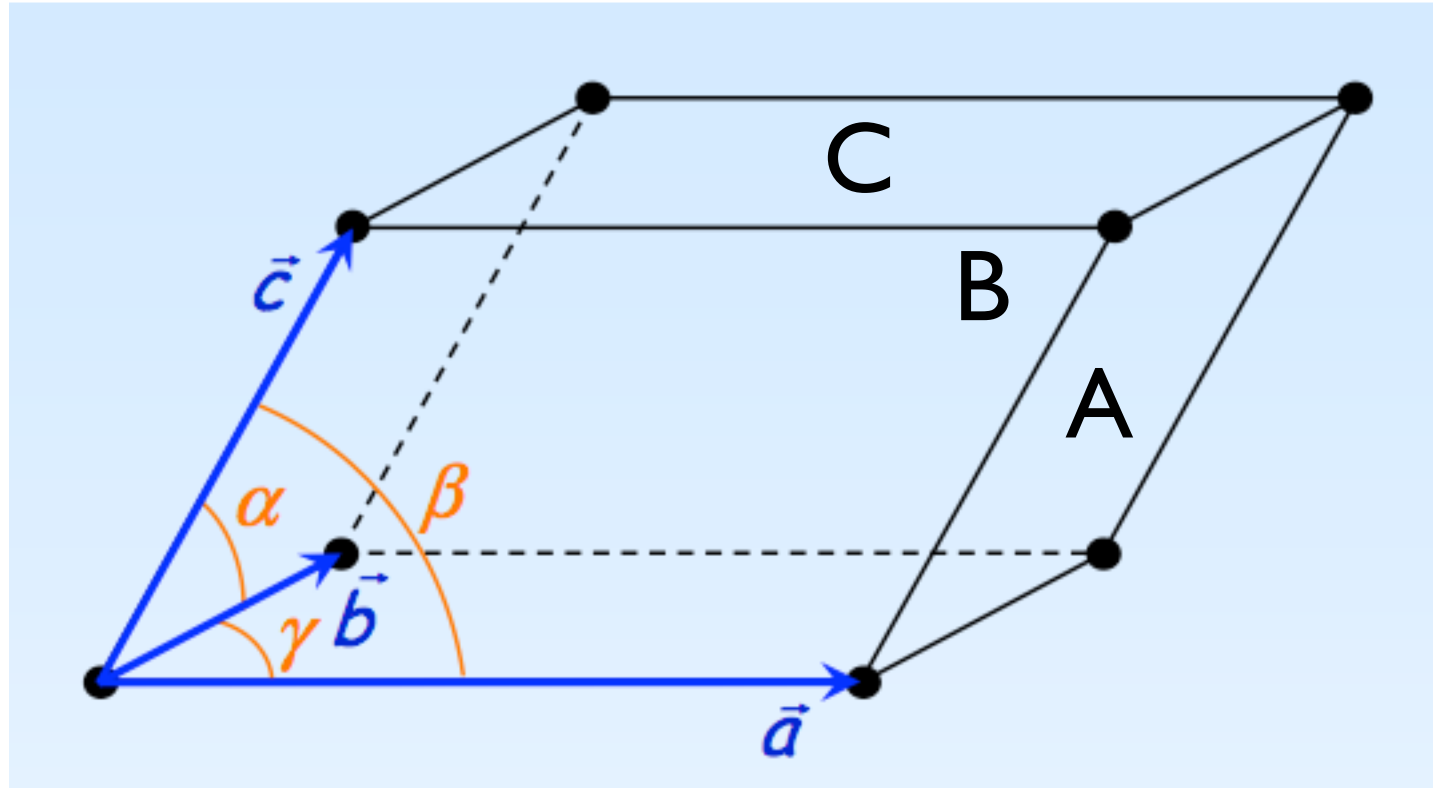
Crystal families, crystal systems, conventional coordinate system and Bravais lattices in 2D

Crystal family	Symbol*	Crystal system	Crystallographic point groups†	No. of space groups	Conventional coordinate system: Restrictions on cell parameters	Conventional coordinate system: Parameters to be determined	Bravais lattices*
One dimension							
–	–	–	1, m	2	None	a	p
Two dimensions							
Oblique (monoclinic)	m	Oblique	1, 2	2	None	a, b γ‡	mp
Rectangular (orthorhombic)	o	Rectangular	m, $2mm$	7	$\gamma = 90°$	a, b	op oc
Square (tetragonal)	t	Square	4, $4mm$	3	$a = b$ $\gamma = 90°$	a	tp
Hexagonal	h	Hexagonal	3, 6 $3m$, $6mm$	5	$a = b$ $\gamma = 120°$	a	hp

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

Lattice parameters

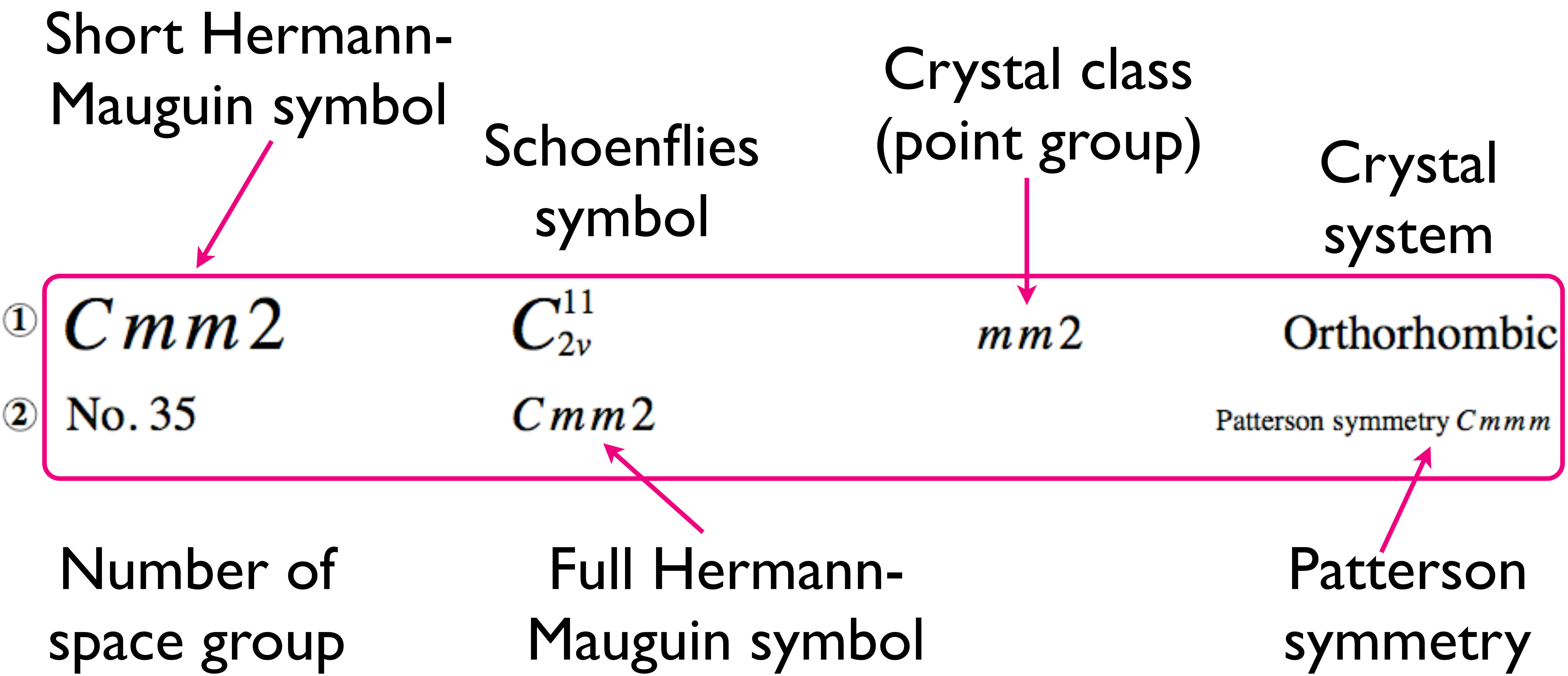
lengths of the unit translations:	angles between them:
a	$\alpha = (\widehat{\vec{b}, \vec{c}})$
b	$\beta = (\widehat{\vec{c}, \vec{a}})$
c	$\gamma = (\widehat{\vec{a}, \vec{b}})$

number of lattice points per unit cell

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

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:

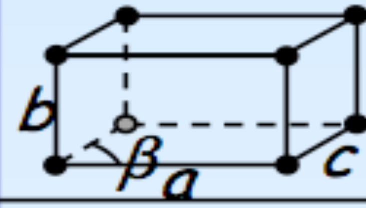
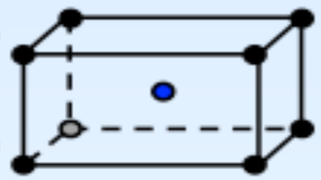
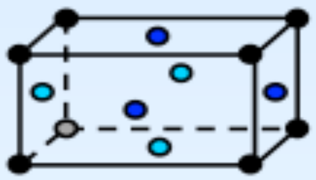
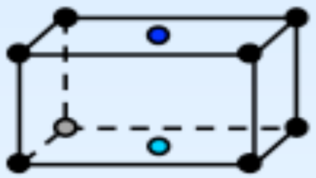
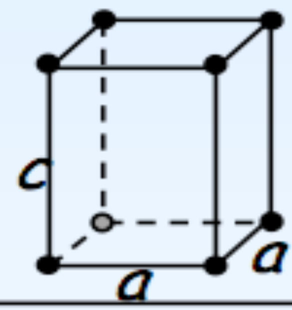
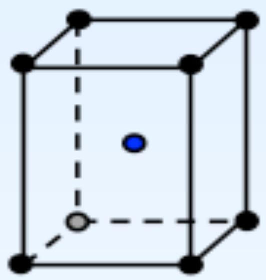
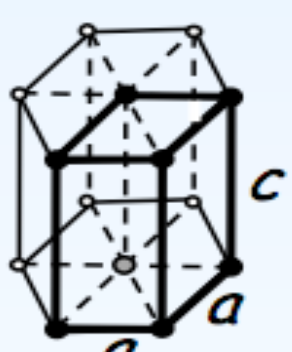
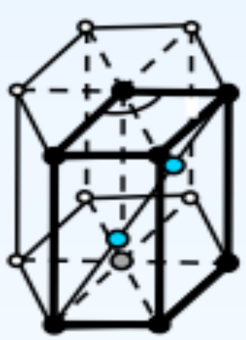
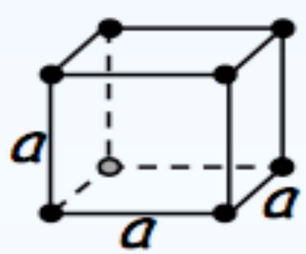
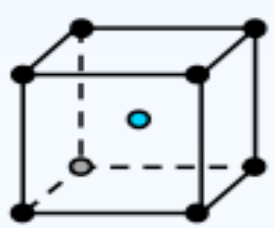
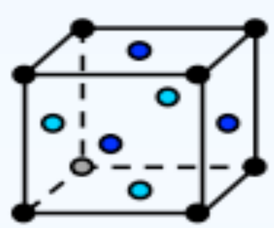
pure rotations > screw rotations;

pure rotations > rotoinversions

reflection m > a; b; c > n

'>' means 'has priority'

14 Bravais Lattices

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

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.

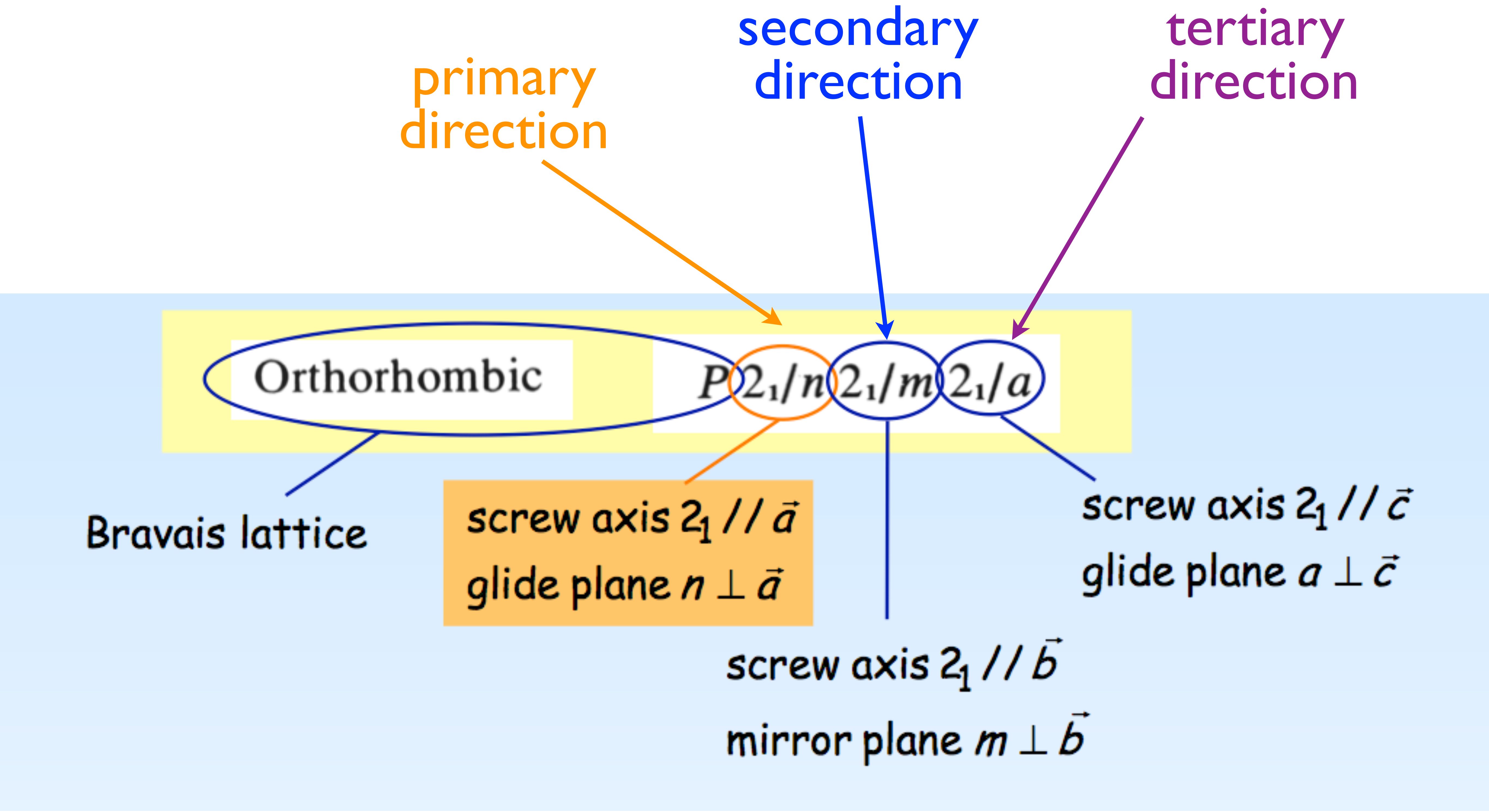
Hermann-Mauguin symbols for space groups

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



PRESENTATION OF SPACE-GROUP SYMMETRY OPERATIONS

IN INTERNATIONAL TABLES FOR CRYSTALLOGRAPHY, VOL. A

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

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

Space group *Cmm*2 (No. 35)

How are the symmetry operations represented in ITA ?

Diagram of symmetry elements

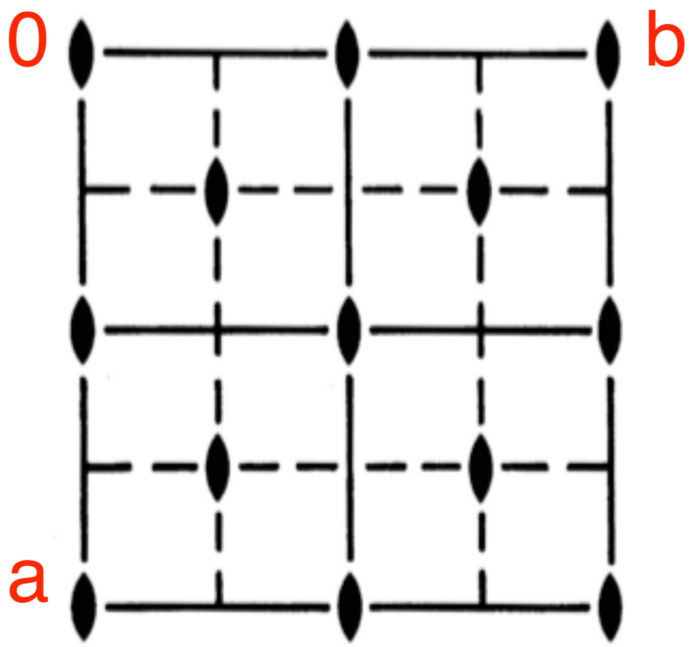
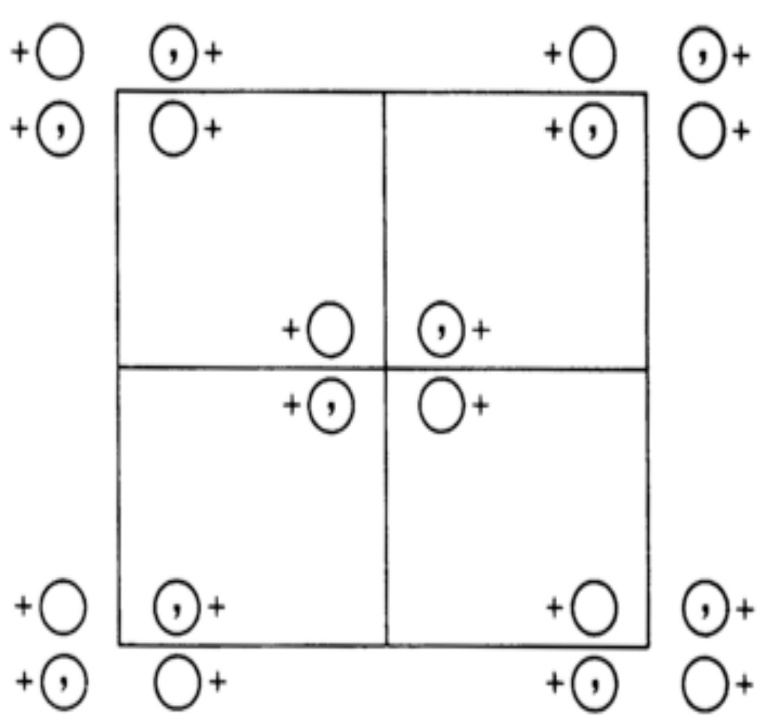


Diagram of general position points



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

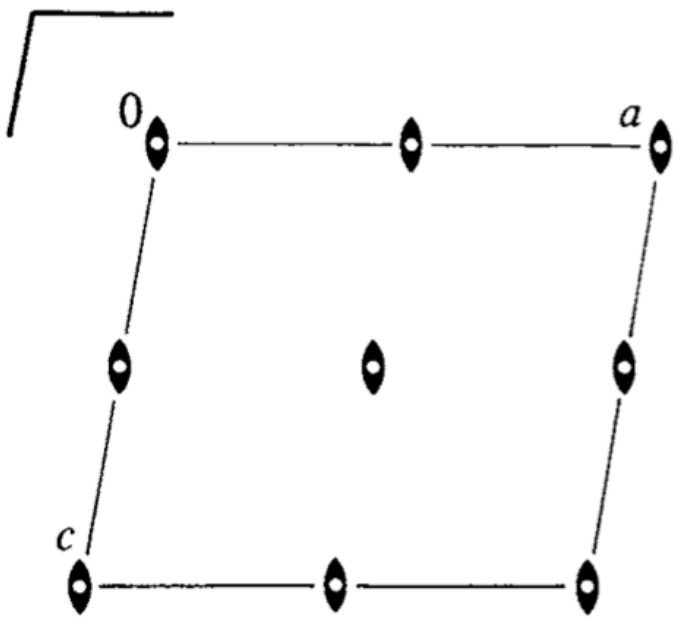
$(I,0)$	(W_2,w_2)	...	(W_m,w_m)	...	(W_i,w_i)
(I,t_1)	(W_2,w_2+t_1)	...	(W_m,w_m+t_1)	...	(W_i,w_i+t_1)
(I,t_2)	(W_2,w_2+t_2)	...	(W_m,w_m+t_2)	...	(W_i,w_i+t_2)
...	...	...	...	...	...
(I,t_j)	(W_2,w_2+t_j)	...	(W_m,w_m+t_j)	...	(W_i,w_i+t_j)
...	...	...	...	...	...

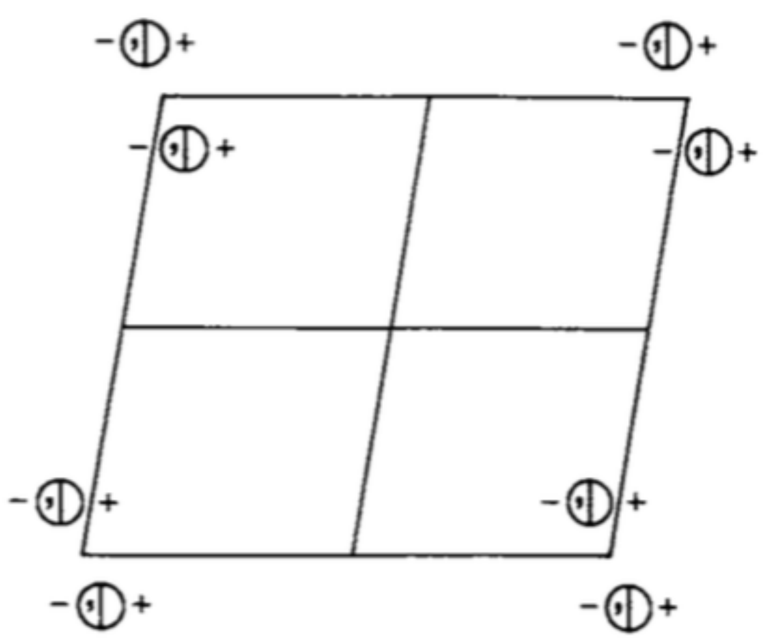
Factor group G/T_G

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

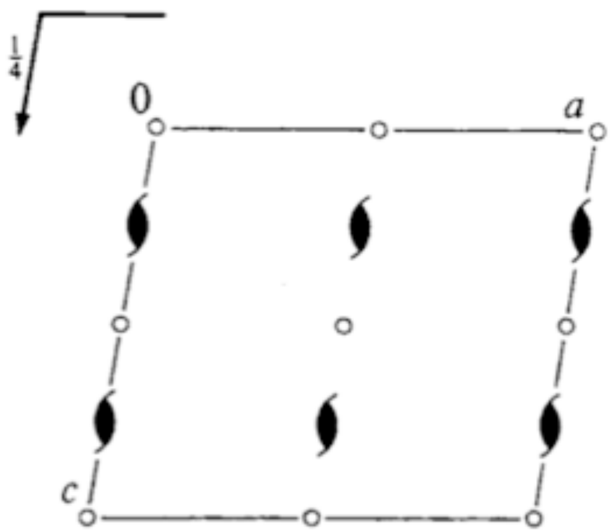
inversion centres ($\bar{1}$,t):

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

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

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

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

TYPE of the symmetry operation

SCREW/GLIDE component

ORIENTATION of the geometric element

LOCATION of the geometric element

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

Example: Cmm2

Diagram of symmetry elements

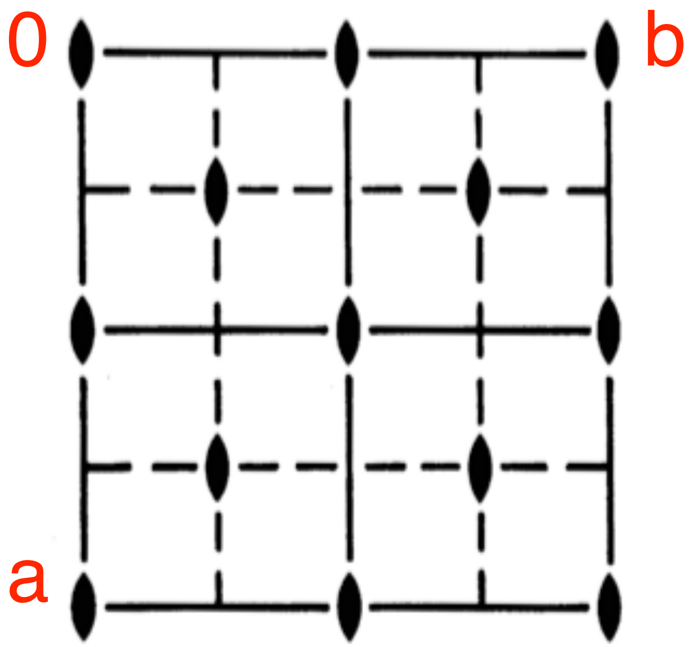
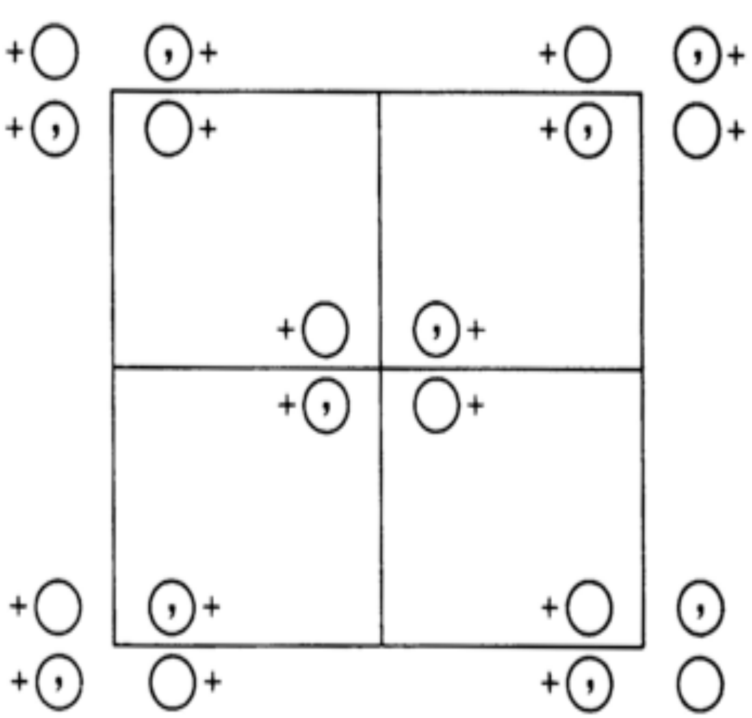


Diagram of
general position points



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

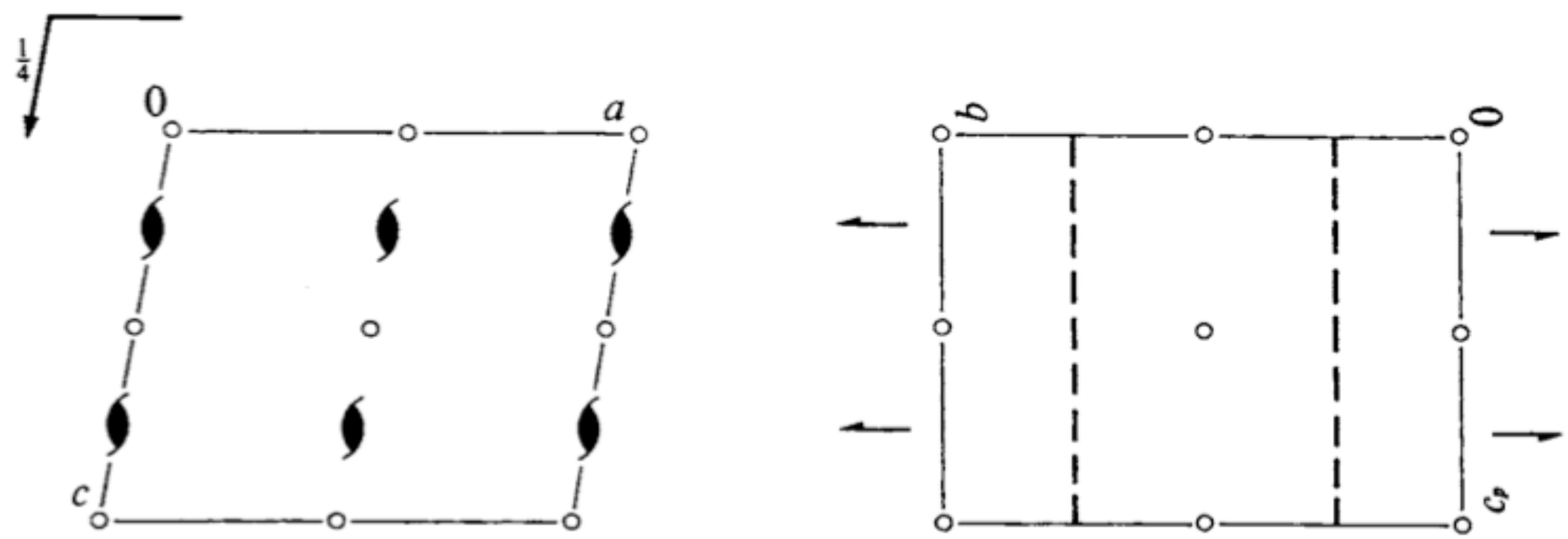
Space group $P2_1/c$ (No. 14)

$P2_1/c$ 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 $x,\frac{1}{4},z$

FCT/ZTF

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20-21 August 2018

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

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

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

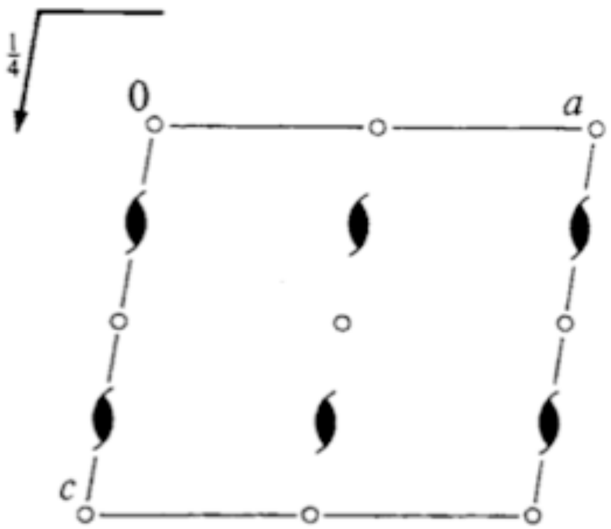
International Tables for Crystallography (2006). Vol. A, Space gro

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

$P2_1/c$ 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) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$

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

Seitz symbols

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

EXERCISES

Problem 2.16 (b)

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.

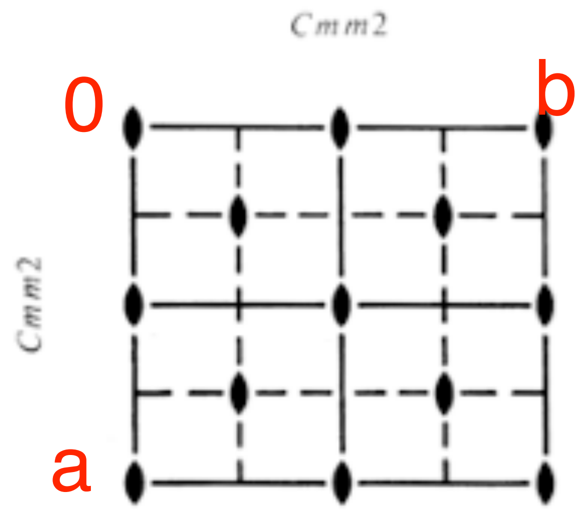
3. Compare your results with the results of the program SYMMETRY OPERATIONS

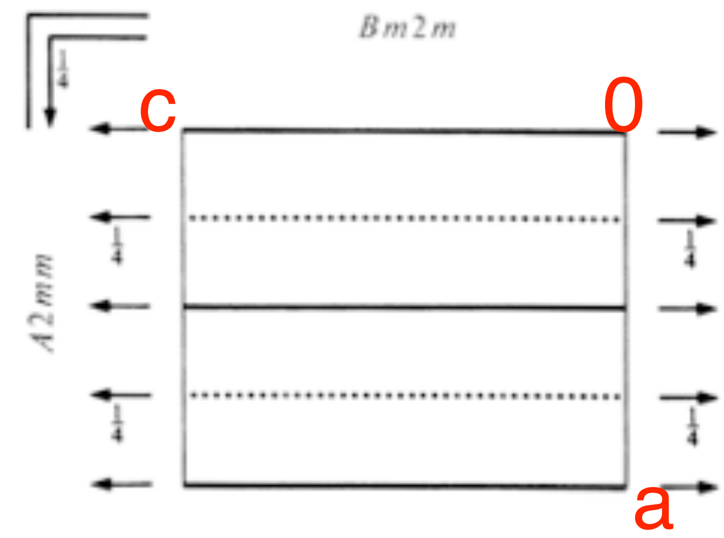
SPACE-GROUPS DIAGRAMS

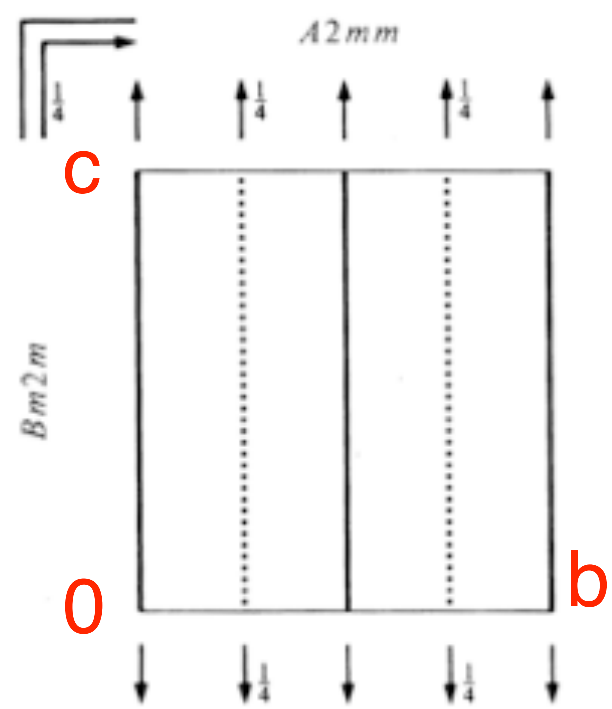
Diagrams of symmetry elements

three different settings

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







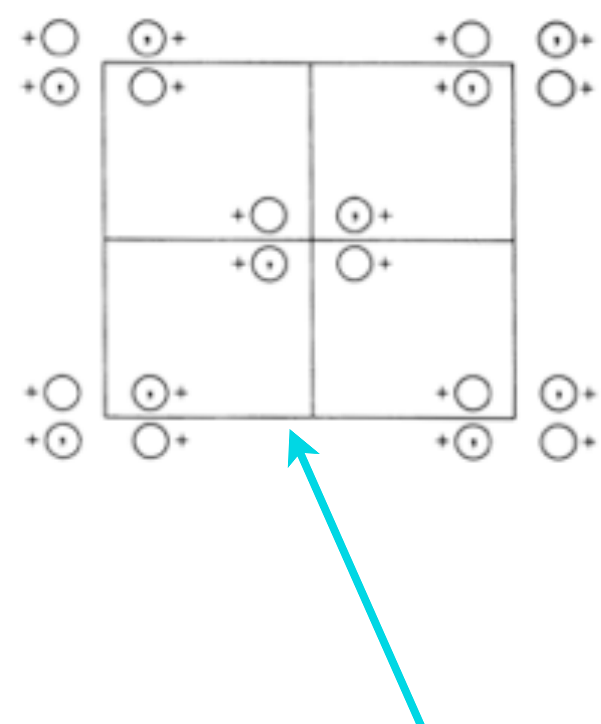


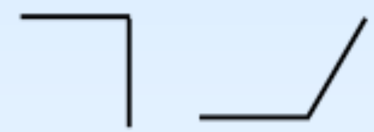
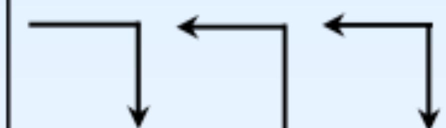
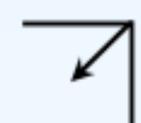
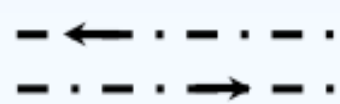
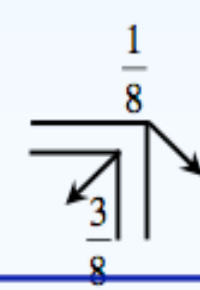
Diagram of general position points

The various rotation and screw axes and their symbol

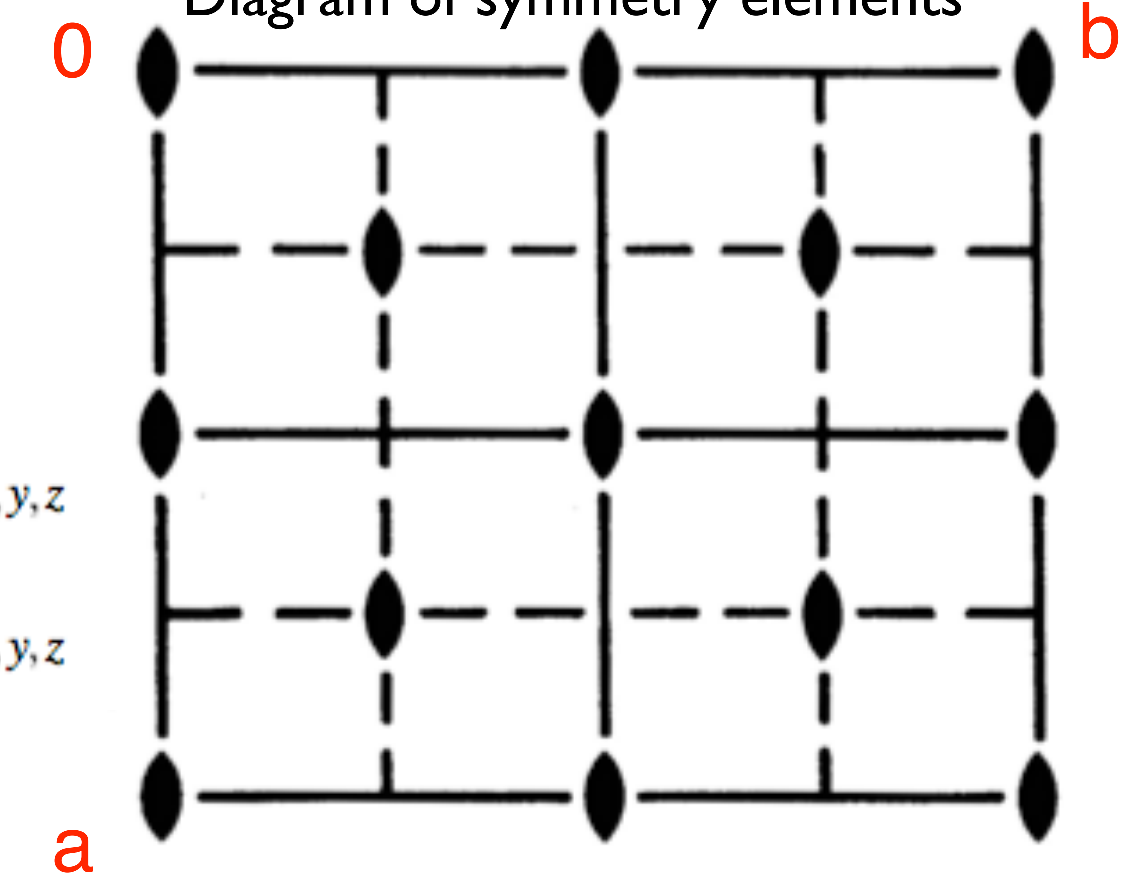
printed symbol	symmetry axis	graphic symbol	nature of the screw translation
1	Identity	none	none
$\bar{1}$	Inversion	○	none
2	Rotation diad or twofold rotation axis	 (⊥ paper)  (// paper)	none
2_1	Screw diad or twofold screw axis	 (⊥ paper) (// paper)	$c/2$ $a/2$ or $b/2$
3	Rotation triad	⊥ paper 	none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

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

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

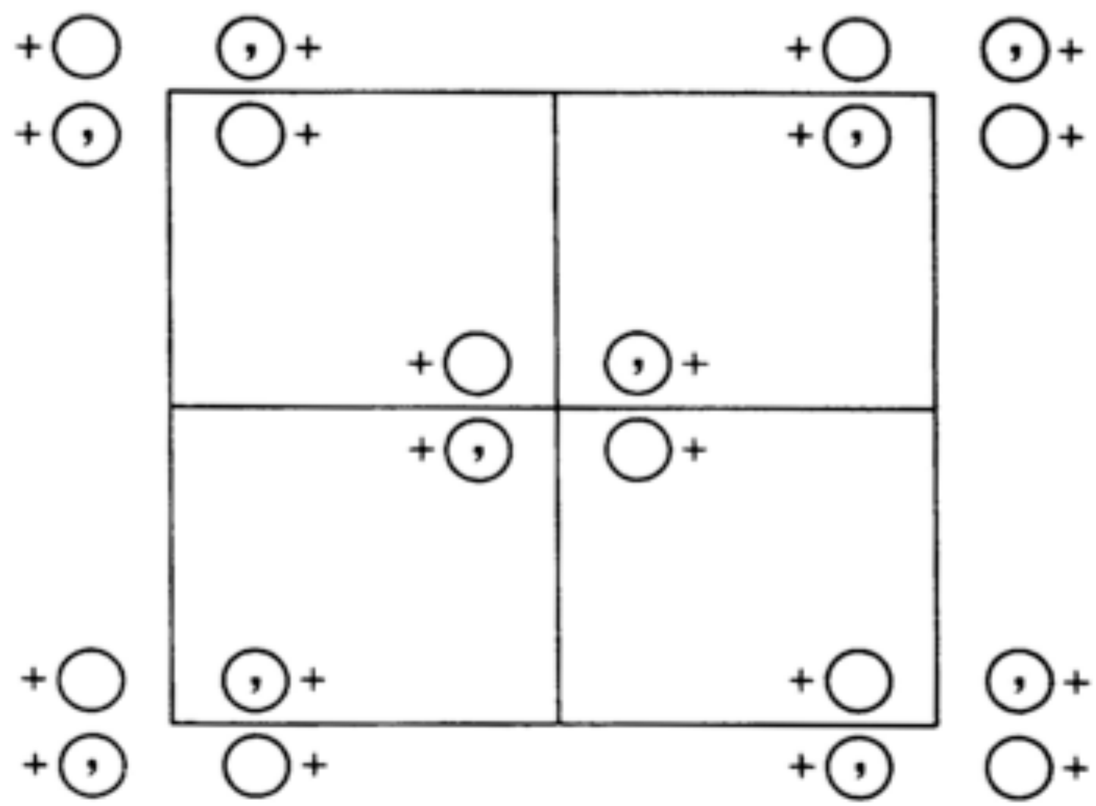
(1) t($\frac{1}{2}$,$\frac{1}{2}$,0) (2) 2 $\frac{1}{4}$,$\frac{1}{4}$,z (3) a x,$\frac{1}{4}$,z (4) b $\frac{1}{4}$,y,z

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

Space group *Cmm*2 (No. 35)

Geometric interpretation

⑥ Symmetry operations

For (0,0,0)+ set

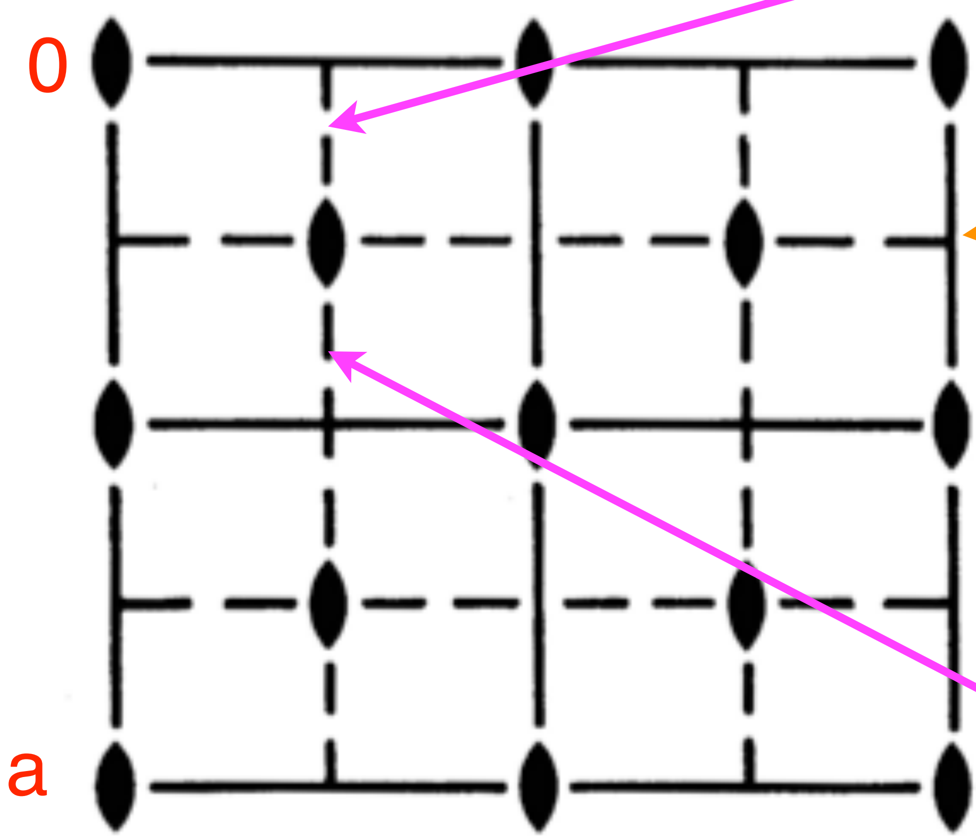
(1) 1 (2) 2 0,0,z (3) m x,0,z (4) m 0,y,z

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

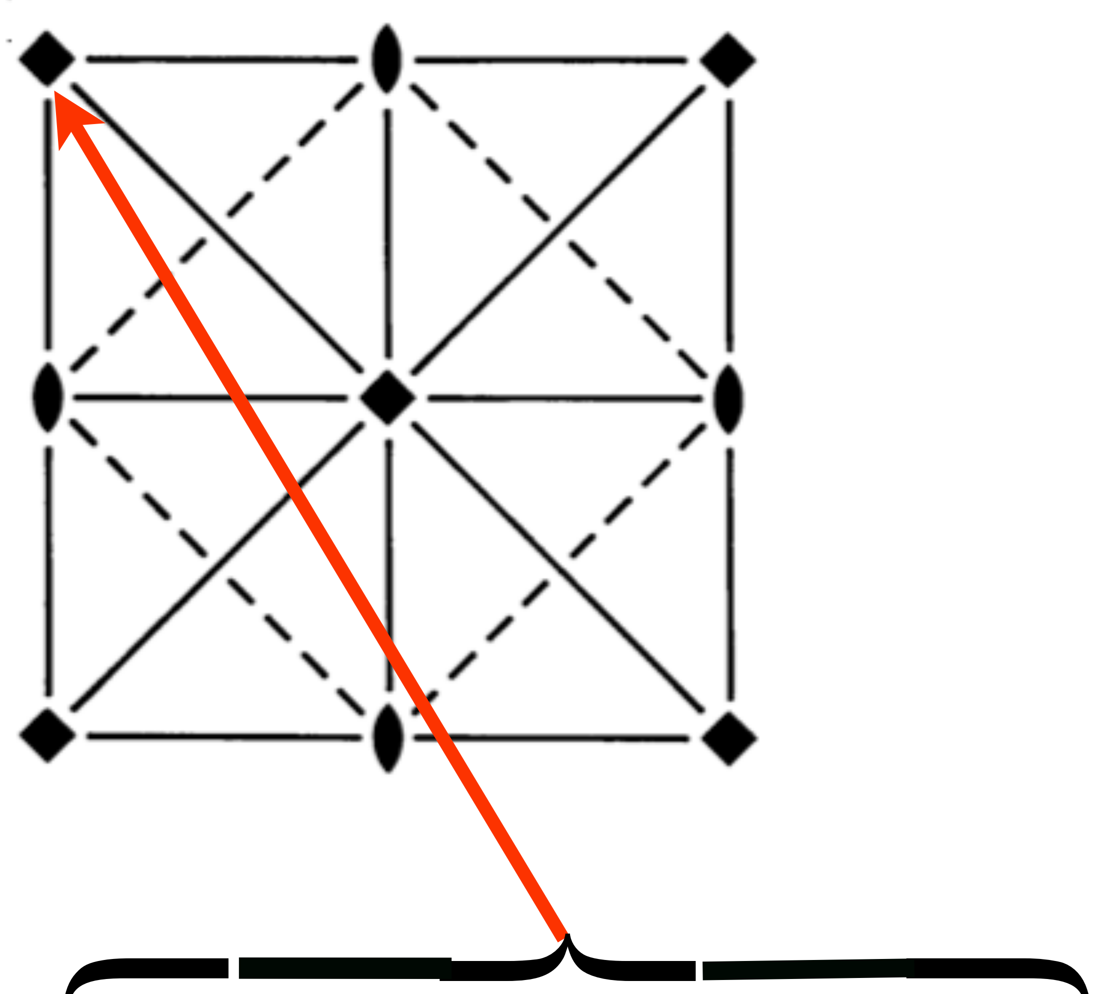
8 f 1 (1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $x,\bar{y},z$ (4) $\bar{x},y,z$

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

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

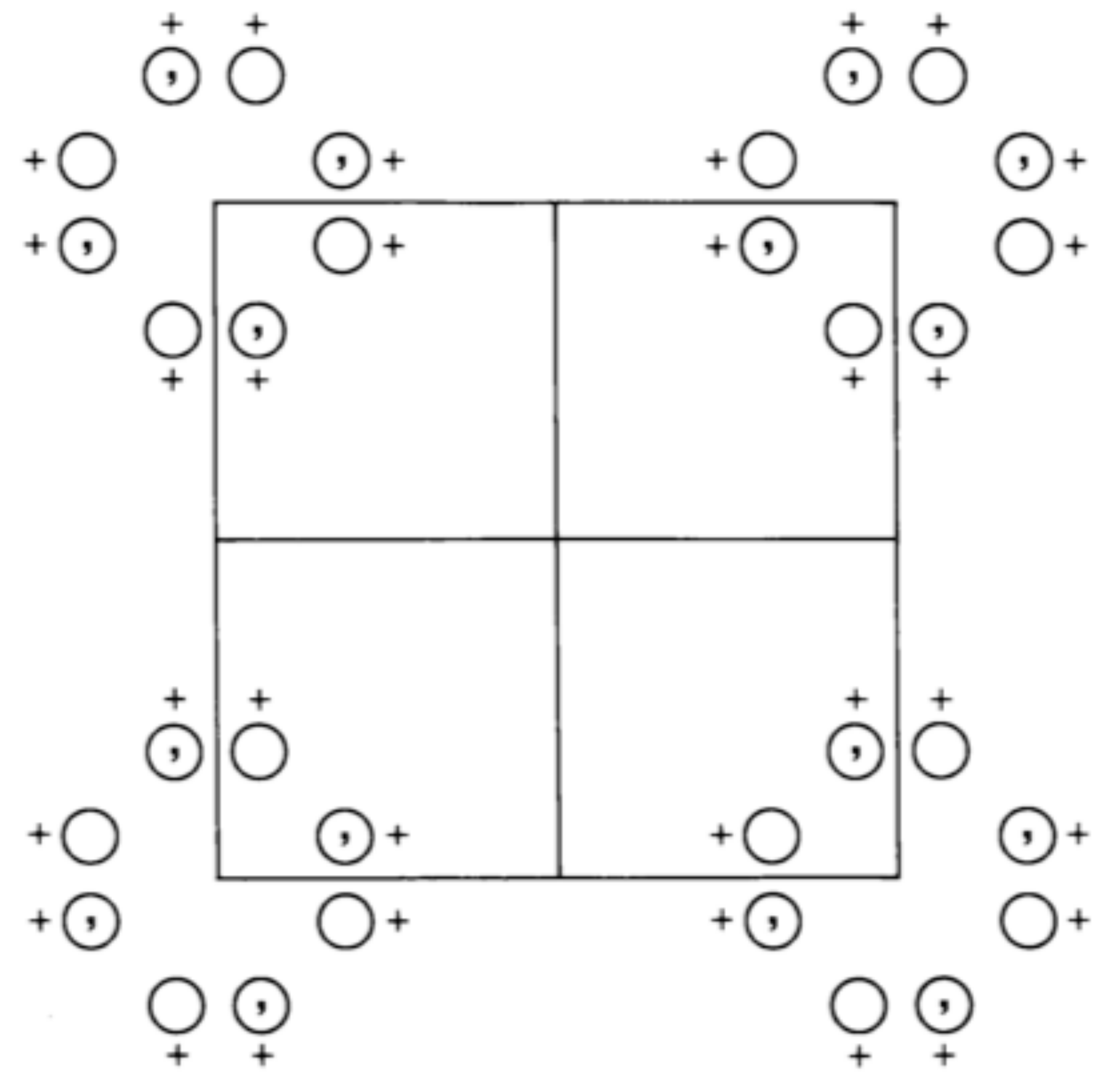
Example: P4mm

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

Diagram of symmetry elements

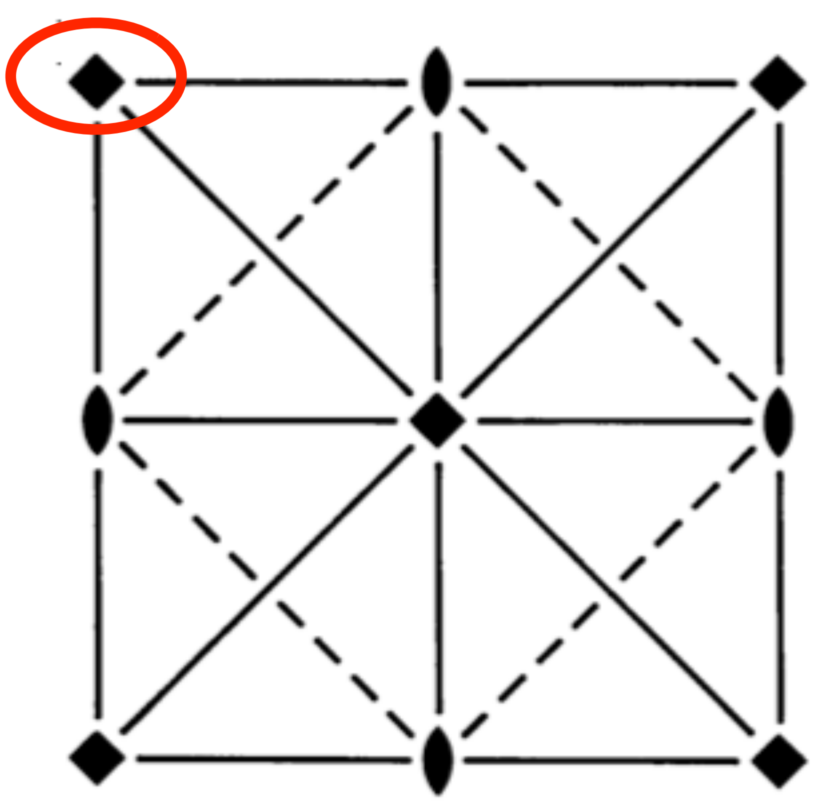
Element set of (00z) line

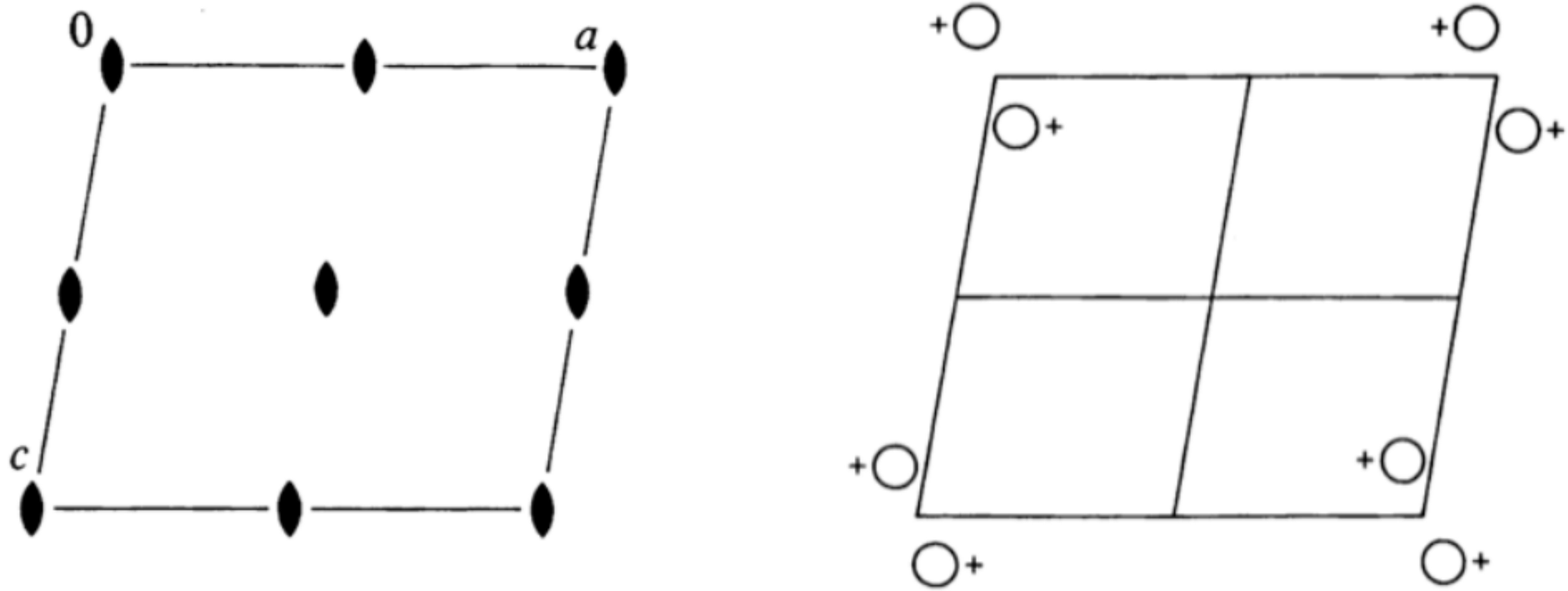
Symmetry operations that share (0,0,z) as geometric element } 1st, 2nd, 3rd powers + all coaxial equivalents

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





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

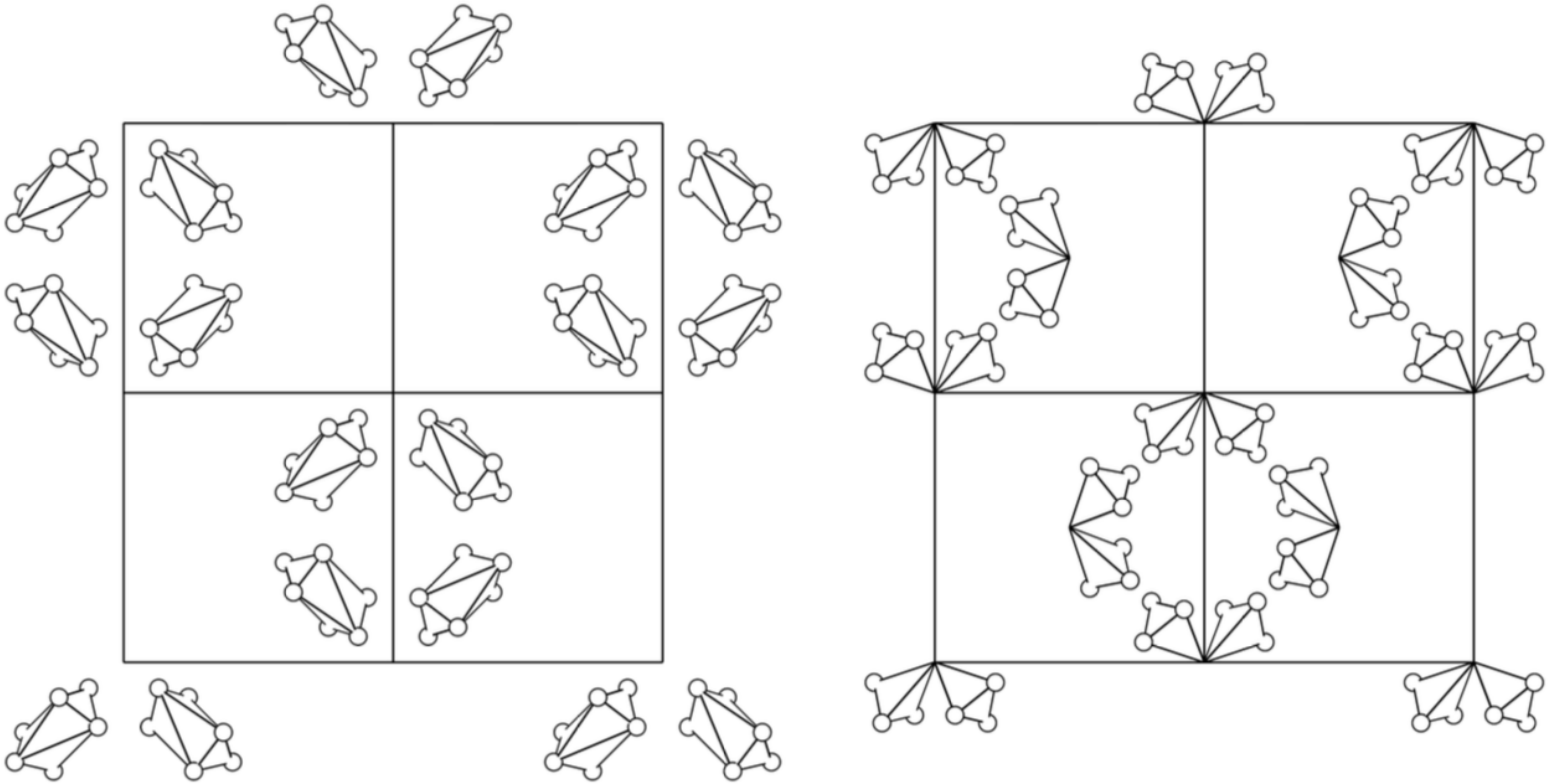
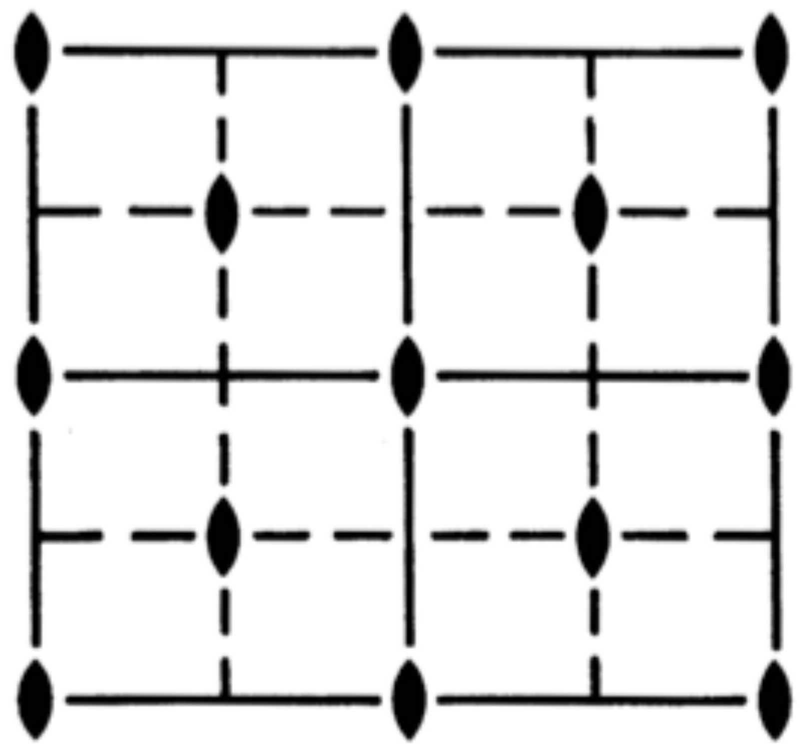


Figure 2.5 *General position* diagrams of the space group $I4_132$, No. 214. Left diagram: polyhedra (twisted trigonal antiprisms) centres at $(\frac{1}{8}, \frac{1}{8}, \frac{1}{8})$ and its equivalent points, site-symmetry group $.32$. Right diagram: polyhedra (sphenoids) attached to (0, 0, 0) and its equivalent points, site-symmetry group $.3..$

ORIGINS AND ASYMMETRIC UNITS

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

*Cmm*2	C_{2v}^{11}	*mm*2	Orthorhombic
No. 35	*Cmm*2		Patterson symmetry *Cmmm*



Origin on *mm*2

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

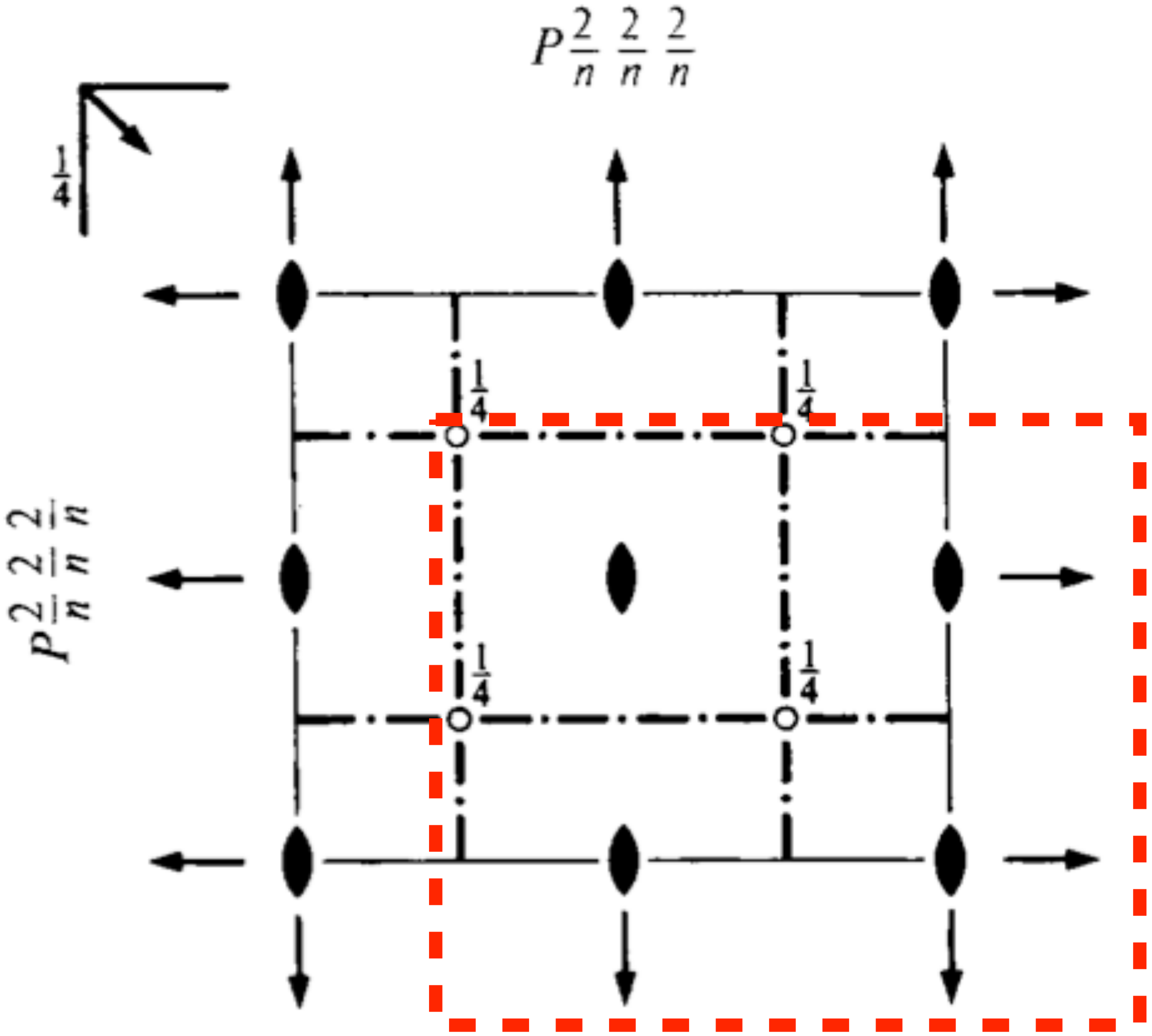
For each of the two origins the location relative to the other origin is also given.

Example: Different origins for *Pnnn*

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

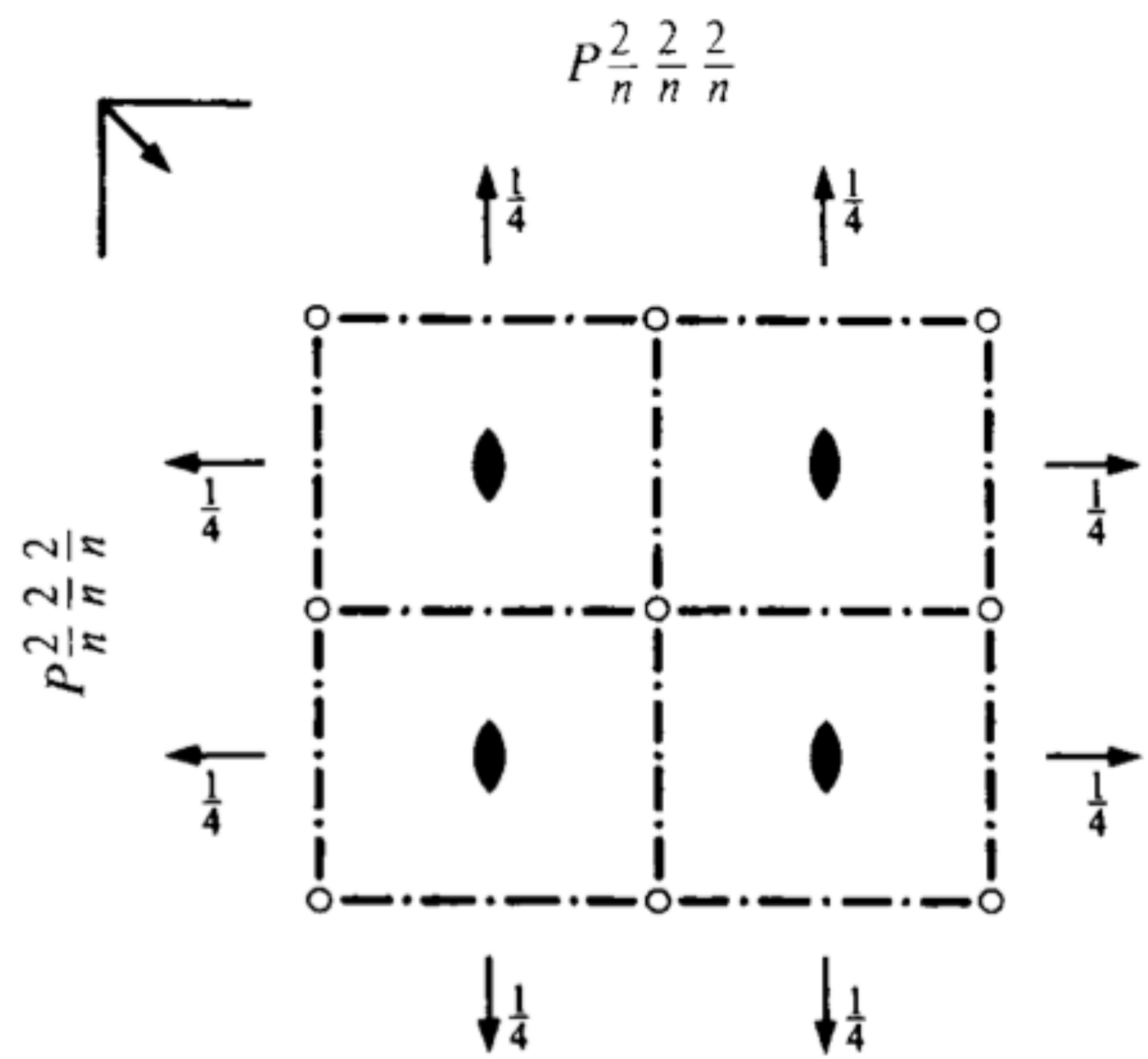
No. 48 $P\ 2/n\ 2/n\ 2/n$ Patterson symmetry *Pmmm*

ORIGIN CHOICE 1



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

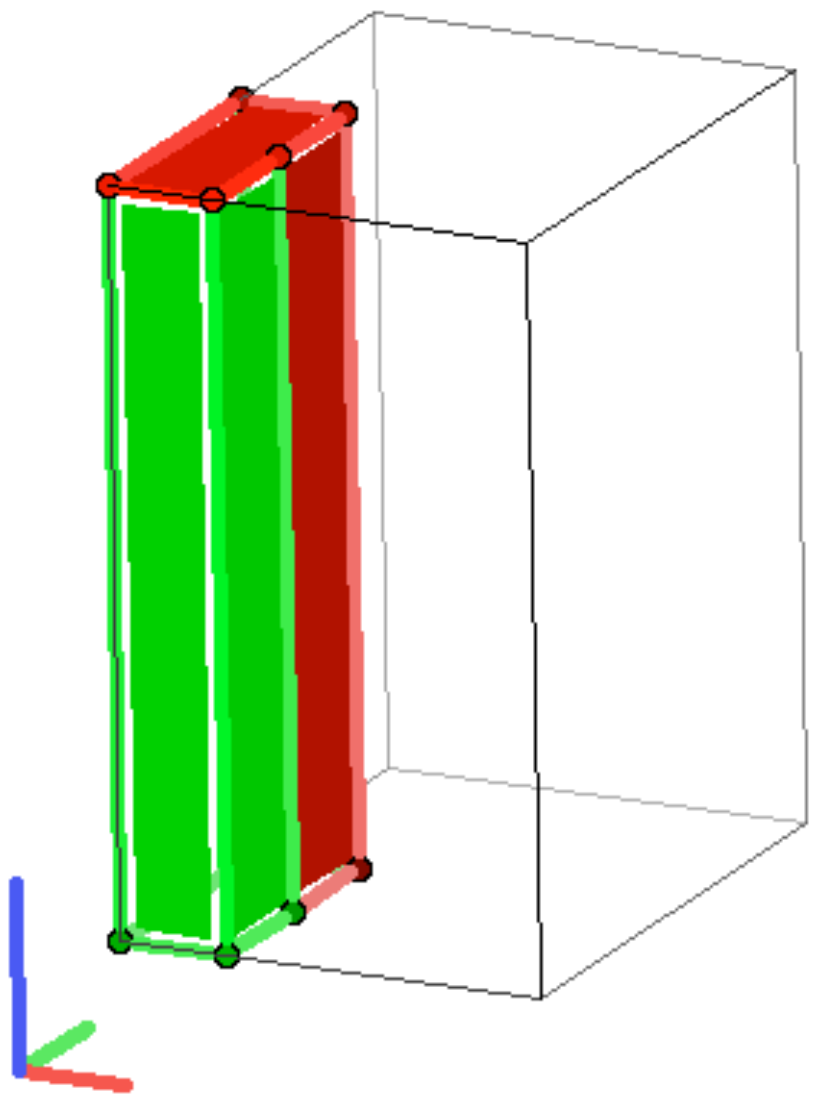
ORIGIN CHOICE 2



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



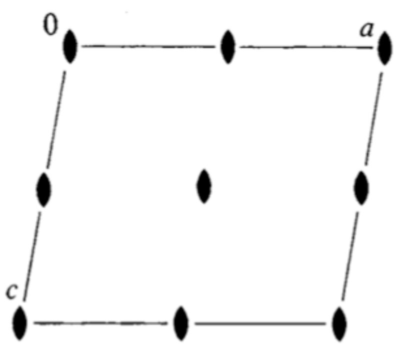
Surface area: green = inside the asymmetric unit, red = outside
Basis vectors: a = red, b = green, c = blue

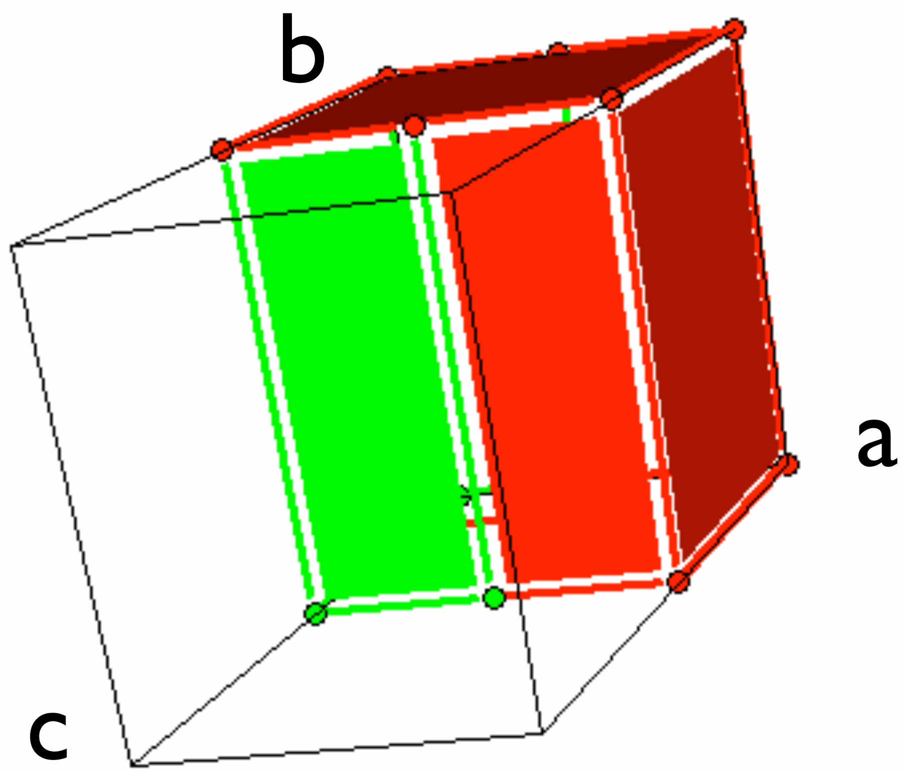
Number of vertices: 8	Number of facets: 6
0, 1/2, 0	x>=0
0, 1/2, 1	x<=1/4 [y<=1/4]
1/4, 1/2, 1	y>=0
1/4, 0, 1	y<=1/2
0, 0, 0	z>=0
1/4, 1/2, 0	z<1
0, 0, 1	
1/4, 0, 0	[Guide to notation]

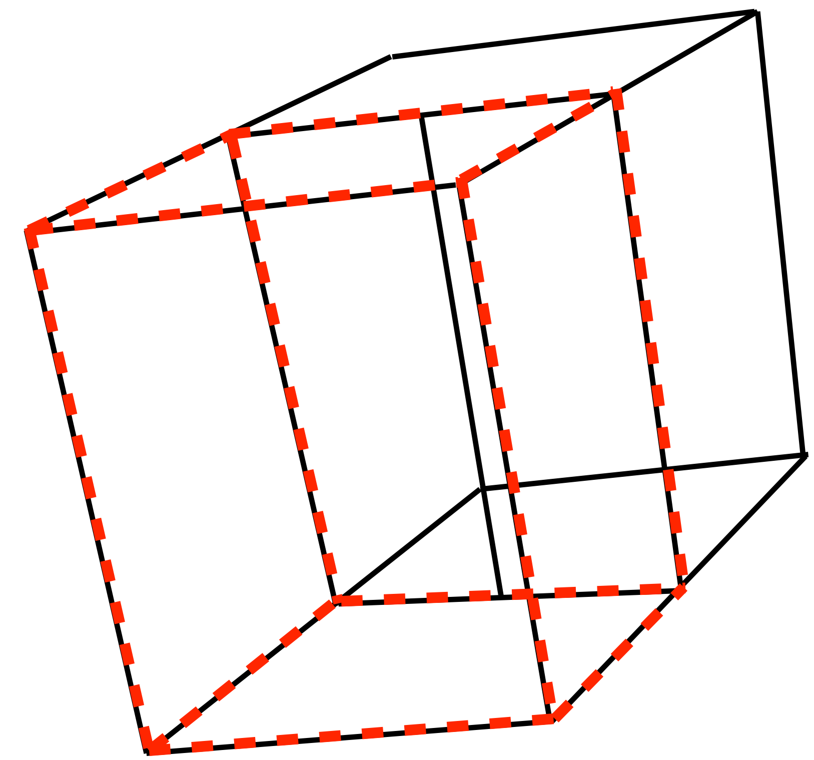
(output cctbx: Ralf Grosse-Kustelve)

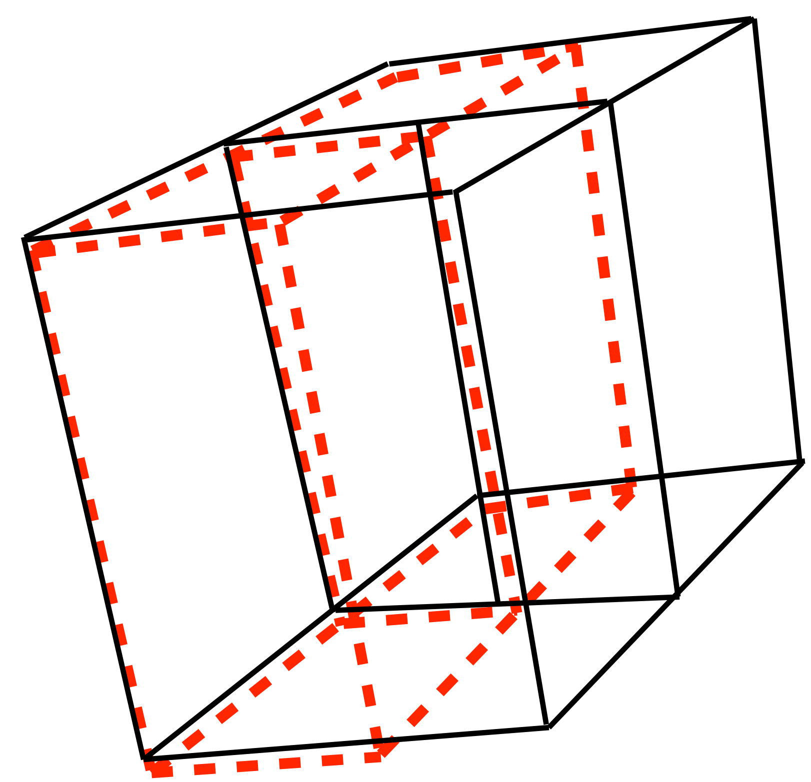
ITA: An asymmetric unit of a space group is a (simply connected) smallest closed part of space from which, by application of all symmetry operations of the space group, the whole of space is filled.

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

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

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

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

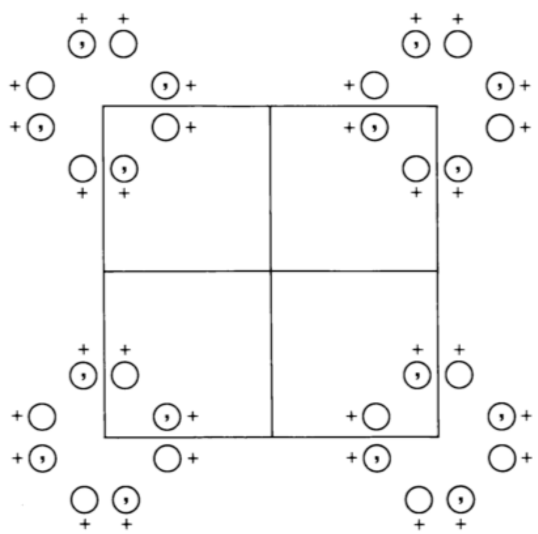
(i) coordinate triplets of an image point $\tilde{X}$ of the original point $X = \begin{pmatrix} x \\ y \\ z \end{pmatrix}$ under (W,w) of G

-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

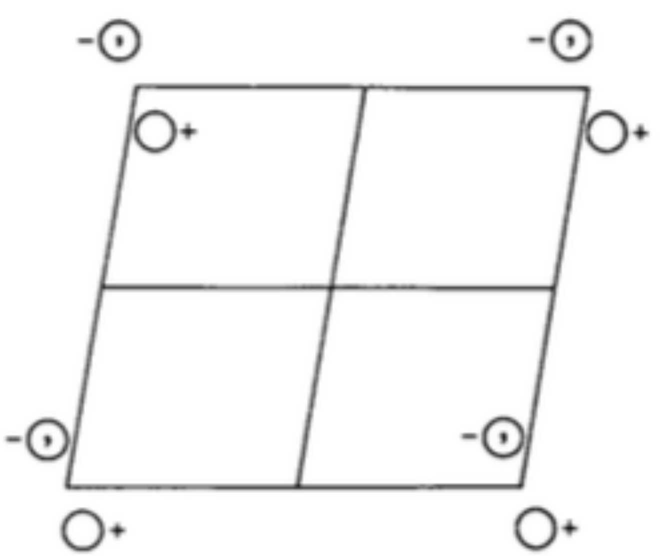
General position

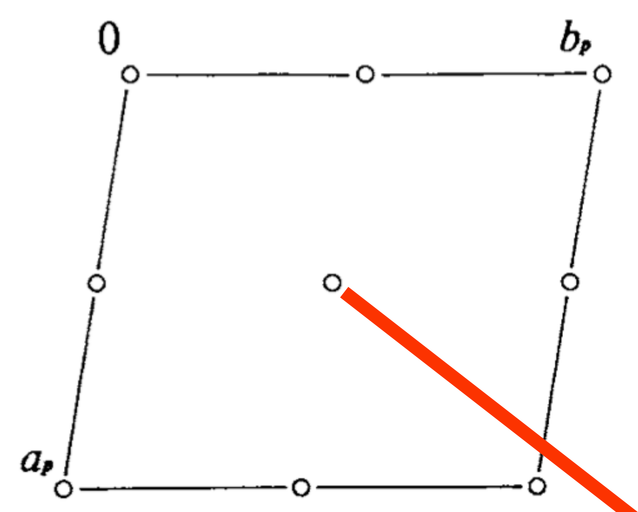
$(I,0)X$	$(W_2,w_2)X$	...	$(W_m,w_m)X$	...	$(W_i,w_i)X$
$(I,t_1)X$	$(W_2,w_2+t_1)X$	...	$(W_m,w_m+t_1)X$	...	$(W_i,w_i+t_1)X$
$(I,t_2)X$	$(W_2,w_2+t_2)X$	...	$(W_m,w_m+t_2)X$	...	$(W_i,w_i+t_2)X$
...	...	...	...	...	...
$(I,t_j)X$	$(W_2,w_2+t_j)X$	...	$(W_m,w_m+t_j)X$	...	$(W_i,w_i+t_j)X$
...	...	...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

-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





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

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

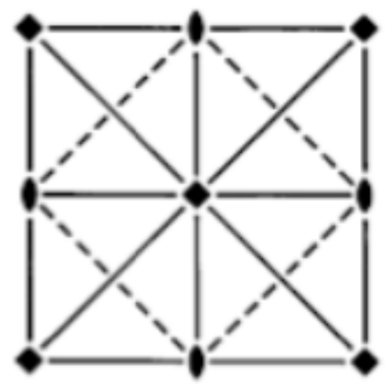
$$\left(\begin{pmatrix} -1 & & \\ & -1 & \\ & & -1 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}\right) \begin{pmatrix} 1/2 \\ 0 \\ 1/2 \end{pmatrix} = \begin{pmatrix} -1/2 \\ 0 \\ -1/2 \end{pmatrix}$$

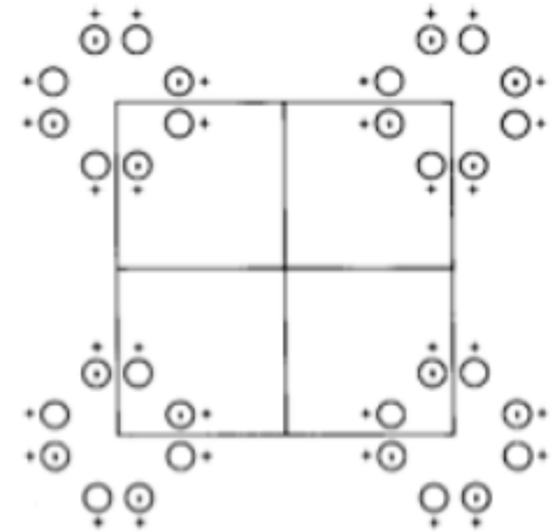
$S_f=\{(1,0),\ (-1,101)X_f = X_f\}$

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

Example

Space group P4mm





No. 99

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

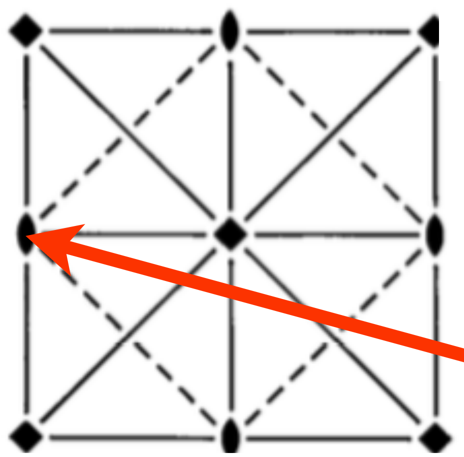
Positions

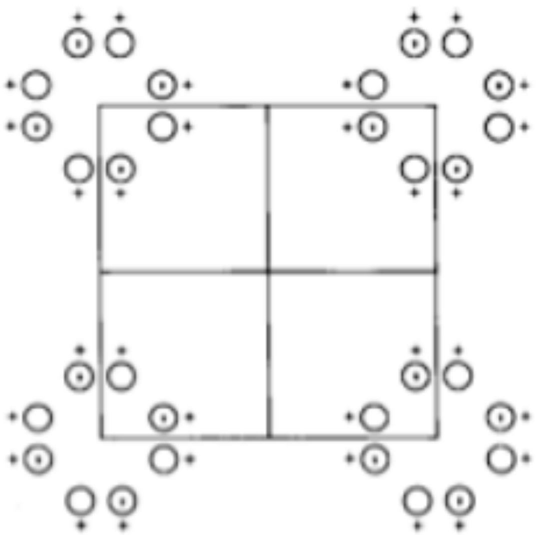
Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	*g*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$
			(5) $x,\bar{y},z$	(6) $\bar{x},y,z$	(7) $\bar{y},\bar{x},z$	(8) y,x,z
4	*f*	$.m.$	$x,\frac{1}{2},z$	$\bar{x},\frac{1}{2},z$	$\frac{1}{2},x,z$	$\frac{1}{2},\bar{x},z$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

EXAMPLE

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

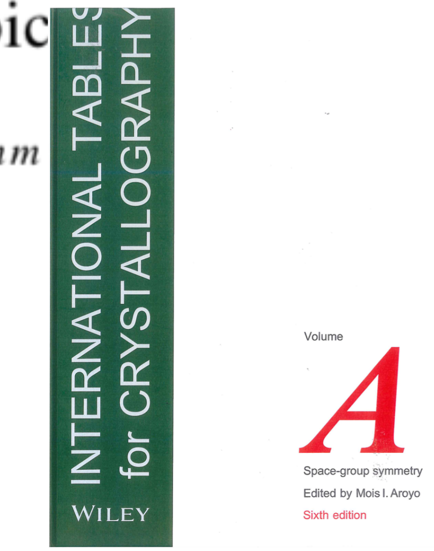
ces must be read by columns. **P** is the transformation f

(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)

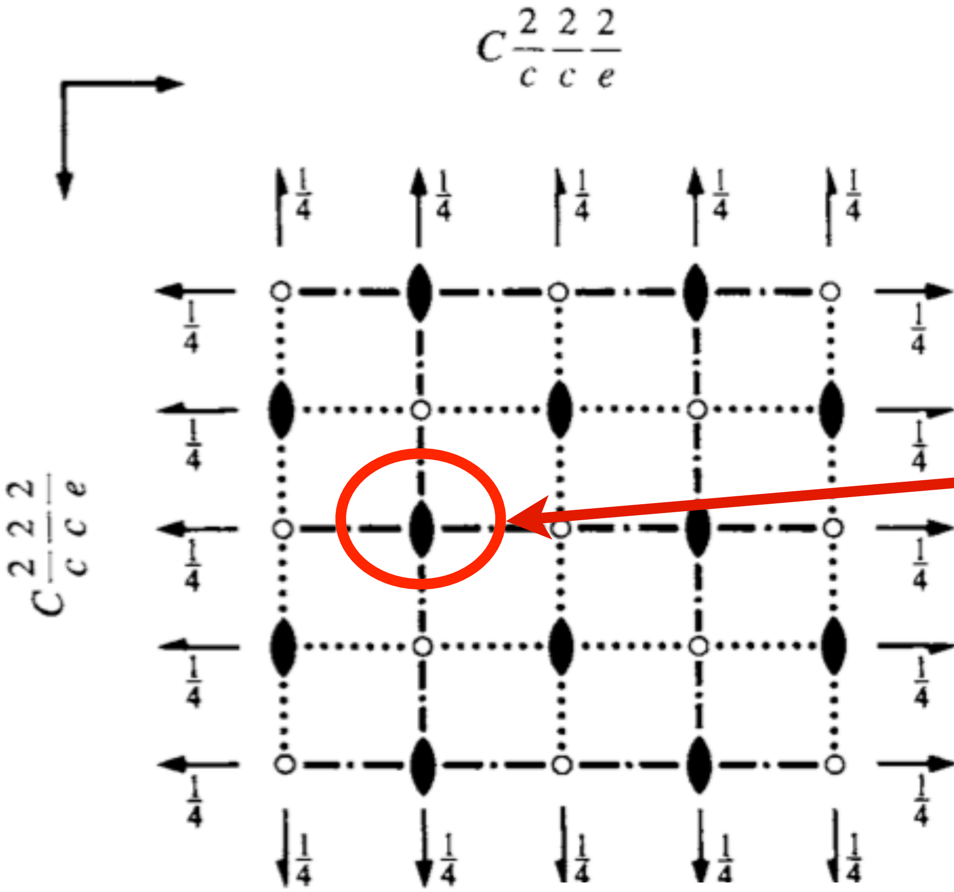
Space Group : 68 (*Ccce*) [origin choice 2
Point : (0,1/4,1/4)
Wyckoff Position : 4a

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

EXERCISES

Problem 2.17

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.

EXERCISES

Problem 2.18

Consider the Wyckoff-positions data of the space group *$I4_1/amd$ (No. 141), origin choice 2.*

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

Compare your results with the results of the program WYCKPOS.

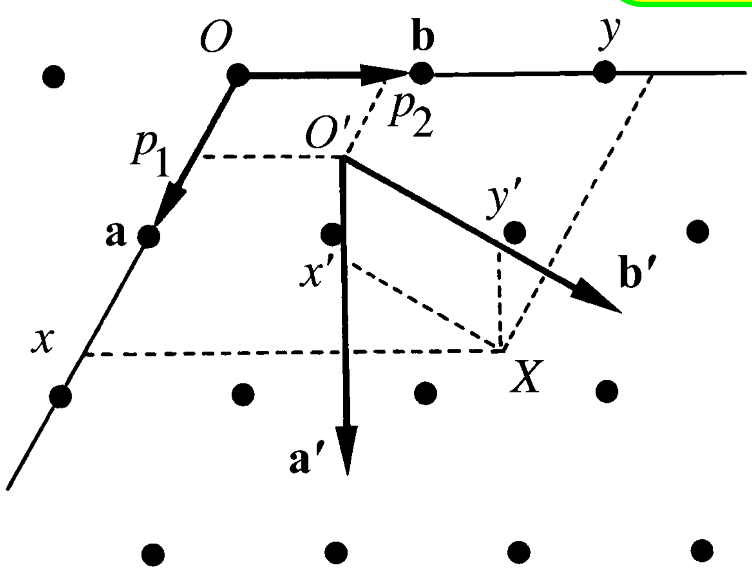
Characterize geometrically the isometries (3), (7), (12), (13) and (16) as listed under General Position. Compare the results with the corresponding geometric descriptions listed under Symmetry operations block in ITA. Comment on the differences between the corresponding symmetry operations listed under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

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

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

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:

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

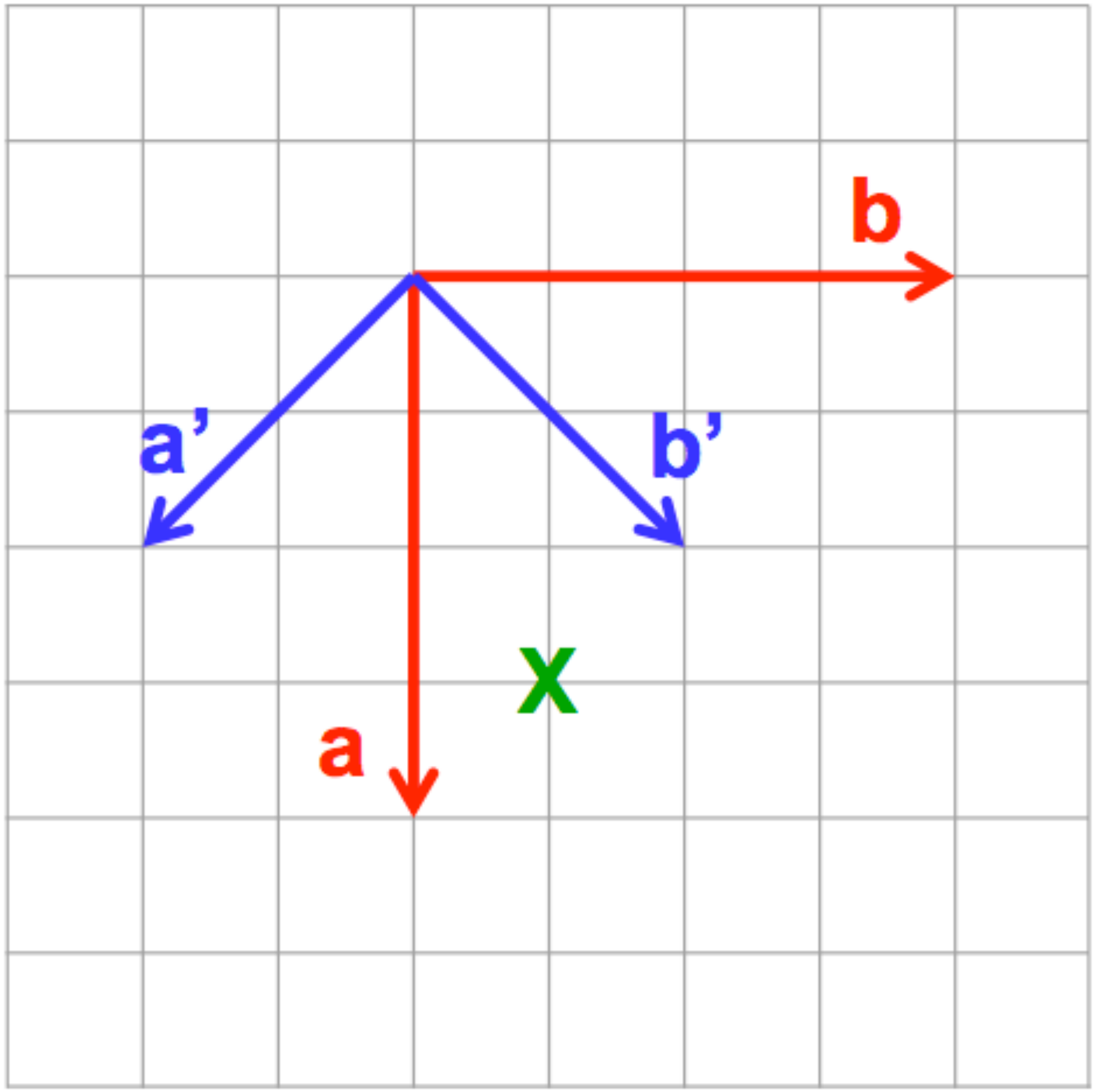
$$= (\mathbf{a}, \mathbf{b}, \mathbf{c}) \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix} = (P_{11}\mathbf{a} + P_{21}\mathbf{b} + P_{31}\mathbf{c}, \; P_{12}\mathbf{a} + P_{22}\mathbf{b} + P_{32}\mathbf{c}, \; P_{13}\mathbf{a} + P_{23}\mathbf{b}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

(ii) origin shift by a shift vector ***p***(p_1,p_2,p_3):

$$O' = O + p$$

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

EXAMPLE



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

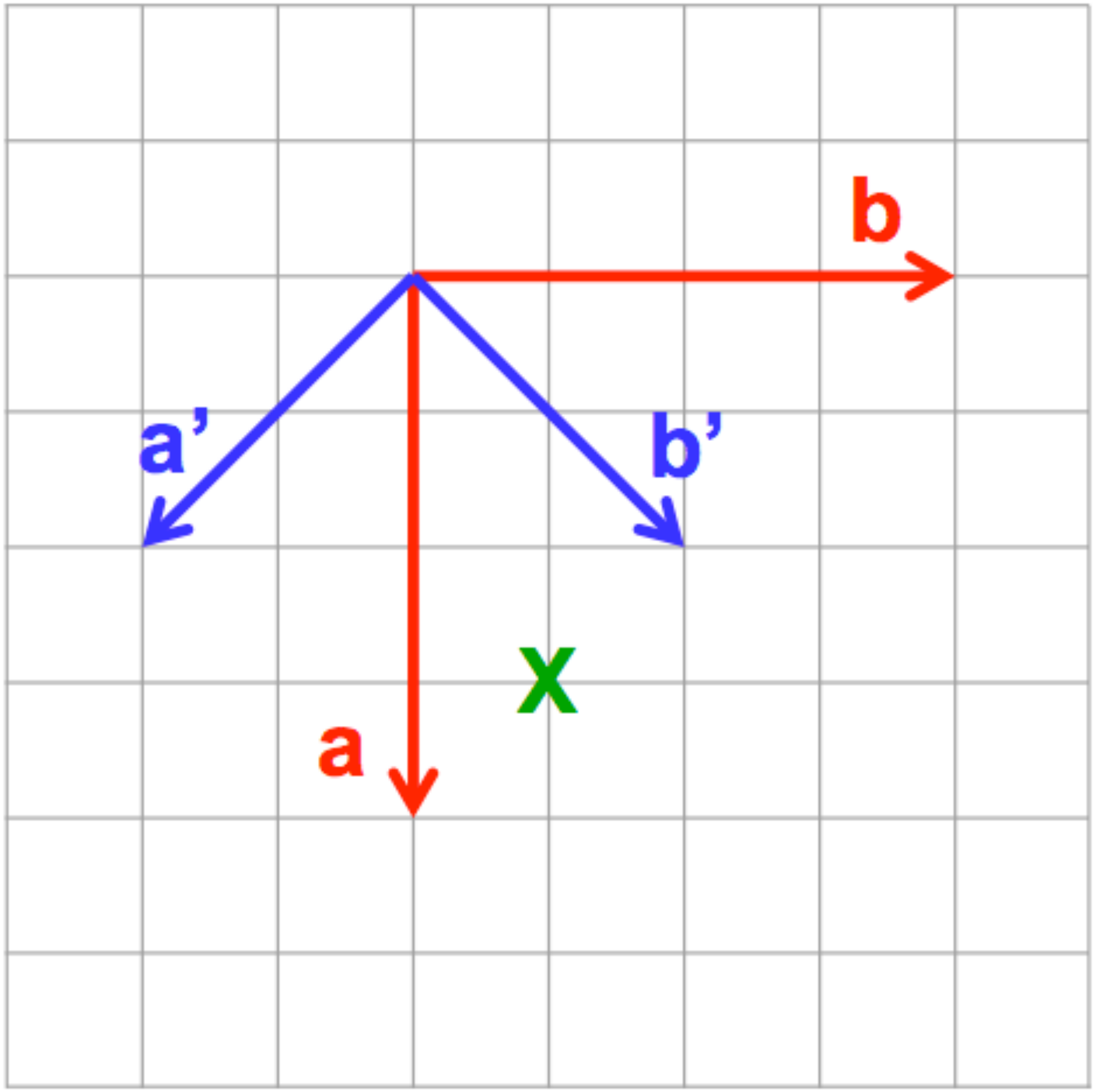
$$(a,b,c) = (a',b',c')\begin{pmatrix} ? \end{pmatrix}$$

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

$$X' = (?)$$

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

EXAMPLE



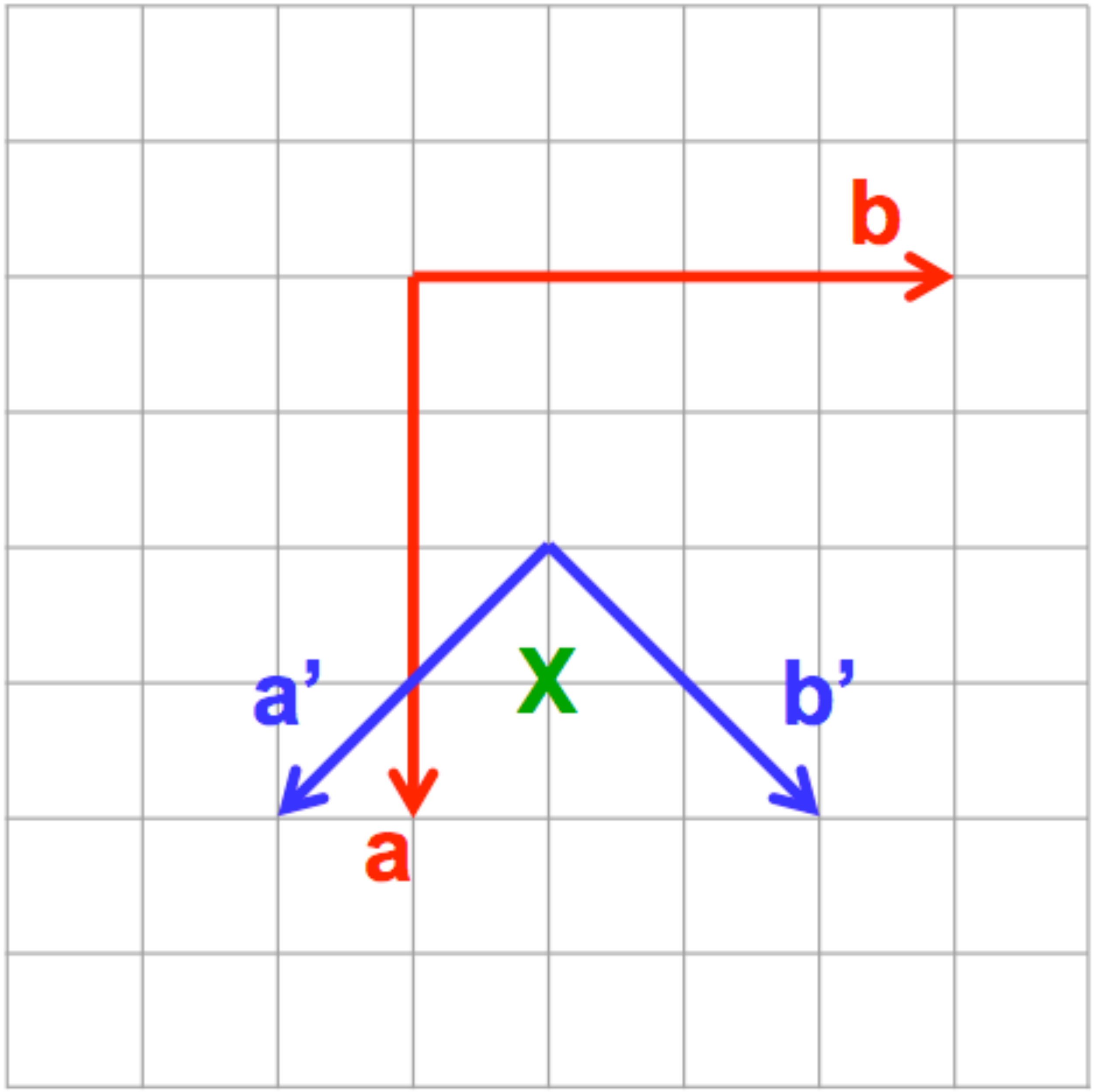
$$(\boldsymbol{a}',\boldsymbol{b}',\boldsymbol{c}') = (\boldsymbol{a},\boldsymbol{b},\boldsymbol{c})\begin{pmatrix} 1/2 & 1/2 & 0 \\ -1/2 & 1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$(\boldsymbol{a},\boldsymbol{b},\boldsymbol{c}) = (\boldsymbol{a}',\boldsymbol{b}',\boldsymbol{c}')\begin{pmatrix} 1 & -1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\boldsymbol{X} = (3/4, 1/4, 0)$$

$$\boldsymbol{X}' = (1/2, 1, 0)$$

EXAMPLE



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

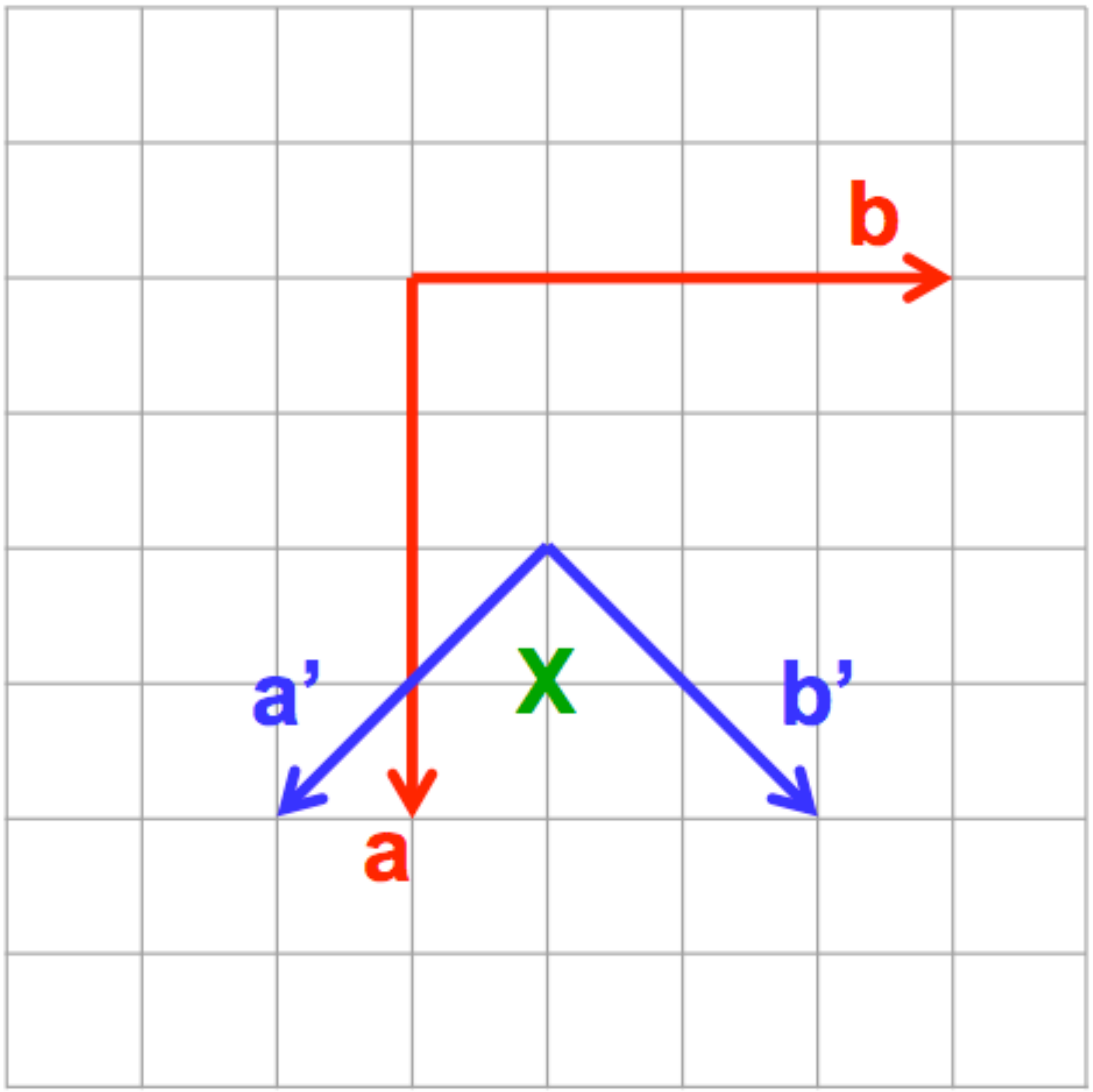
$$q = \begin{pmatrix} ? \end{pmatrix}$$

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

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

Linear parts as before.

EXAMPLE



$$p = \begin{pmatrix} 1/2 \\ 1/4 \\ 0 \end{pmatrix}$$

$$q = \begin{pmatrix} -1/4 \\ -3/4 \\ 0 \end{pmatrix}$$

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

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

Linear parts as before.

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

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

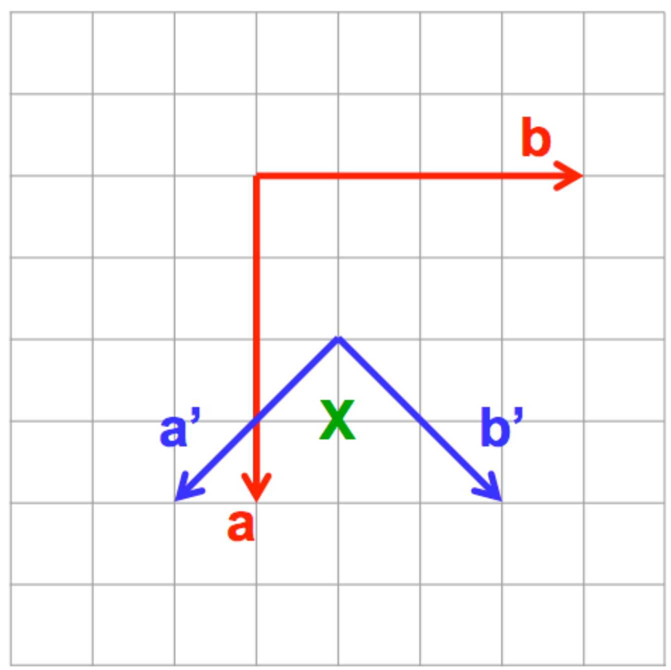
$$(P,p)^{-1}=\left(\begin{array}{ccc|c} 1 & -1 & 0 & -1/4 \\ 1 & 1 & 0 & -3/4 \\ 0 & 0 & 1 & 0 \end{array}\right)$$

a'=1/2a-1/2b

b'=1/2a+1/2b

c'=c

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



a=a'+b'

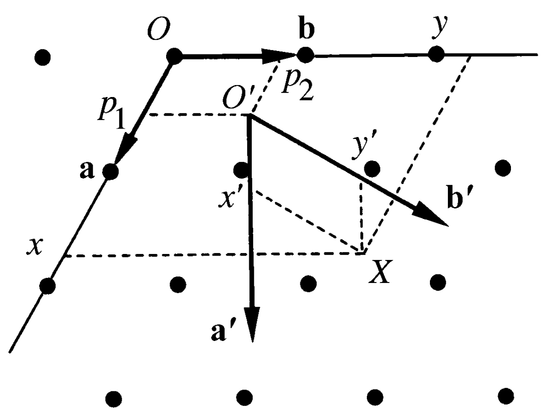
b=-a'+b'

c=c'

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

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:

1	-1		-1/4
1	1		-3/4
		1	0

→ { 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***): $\boldsymbol{x}' = \boldsymbol{x} - \boldsymbol{p}$

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

EXAMPLE

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

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

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

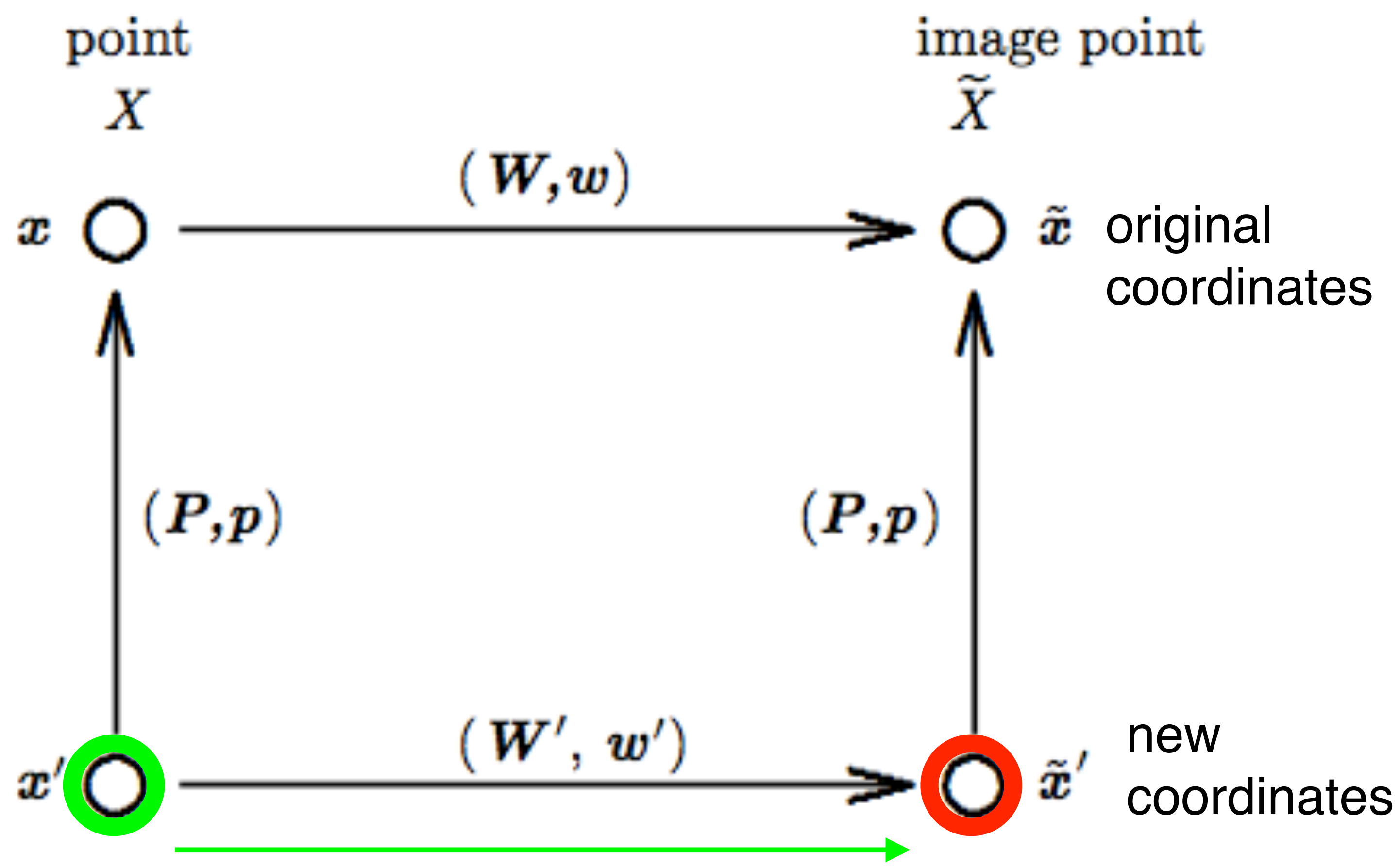
covariant to crystal basis: Miller indices

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

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

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

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***): $$\boldsymbol{x}' = \boldsymbol{x} - \boldsymbol{p}$$

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

Transformation of symmetry operations (*W*,*w*):

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

Transformation by (***P***,***p***) of the unit cell parameters:

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

EXERCISES

Problem 2.19

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: SYMMETRY DATA ITA SETTINGS

530 ITA settings of **orthorhombic** and **monoclinic** groups

Table 4.3.1 (*cont.*)

MONOCLINIC SYSTEM

No. of space group	Schoenflies symbol	Standard short Hermann–Mauguin symbol	Extended Hermann–Mauguin symbols for various settings and cell choices						
			a<u>b</u>c	c<u>b̄</u>a	ab<u>c</u>	ba<u>c̄</u>	<u>a</u>bc	<u>ā</u>cb	Unique axis *b* Unique axis *c* Unique axis *a*
3	C_2^1	$P2$	$P121$	$P121$	$P112$	$P112$	$P211$	$P211$	
4	C_2^2	$P2_1$	$P12_11$	$P12_11$	$P112_1$	$P112_1$	$P2_111$	$P2_111$	
5	C_2^3	$C2$	$C121$ 2_1	$A121$ 2_1	$A112$ 2_1	$B112$ 2_1	$B211$ 2_1	$C211$ 2_1	Cell choice 1
			$A121$ 2_1	$C121$ 2_1	$B112$ 2_1	$A112$ 2_1	$C211$ 2_1	$B211$ 2_1	Cell choice 2
			$I121$ 2_1	$I121$ 2_1	$I112$ 2_1	$I112$ 2_1	$I211$ 2_1	$I211$ 2_1	Cell choice 3
6	C_s^1	Pm	$P1m1$	$P1m1$	$P11m$	$P11m$	$Pm11$	$Pm11$	
7	C_s^2	Pc	$P1c1$	$P1a1$	$P11a$	$P11b$	$Pb11$	$Pc11$	Cell choice 1
			$P1n1$	$P1n1$	$P11n$	$P11n$	$Pn11$	$Pn11$	Cell choice 2
			$P1a1$	$P1c1$	$P11b$	$P11a$	$Pc11$	$Pb11$	Cell choice 3
8	C_s^3	Cm	$C1m1$ a	$A1m1$ c	$A11m$ b	$B11m$ a	$Bm11$ c	$Cm11$ b	Cell choice 1
			$A1m1$ c	$C1m1$ a	$B11m$ a	$A11m$ b	$Cm11$ b	$Bm11$ c	Cell choice 2
			$I1m1$ n	$I1m1$ n	$I11m$ n	$I11m$ n	$Im11$ n	$Im11$ n	Cell choice 3
9	C_s^4	Cc	$C1c1$ n	$A1a1$ n	$A11a$ n	$B11b$ n	$Bb11$ n	$Cc11$ n	Cell choice 1
			$A1n1$ a	$C1n1$ c	$B11n$ b	$A11n$ a	$Cn11$ c	$Bn11$ b	Cell choice 2
			$I1a1$ c	$I1c1$ a	$I11b$ a	$I11a$ b	$Ic11$ b	$Ib11$ c	Cell choice 3
10	C_{2h}^1	$P2/m$	$P1\frac{2}{m}1$	$P1\frac{2}{m}1$	$P11\frac{2}{m}$	$P11\frac{2}{m}$	$P\frac{2}{m}11$	$P\frac{2}{m}11$	
11	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	

Monoclinic descriptions

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

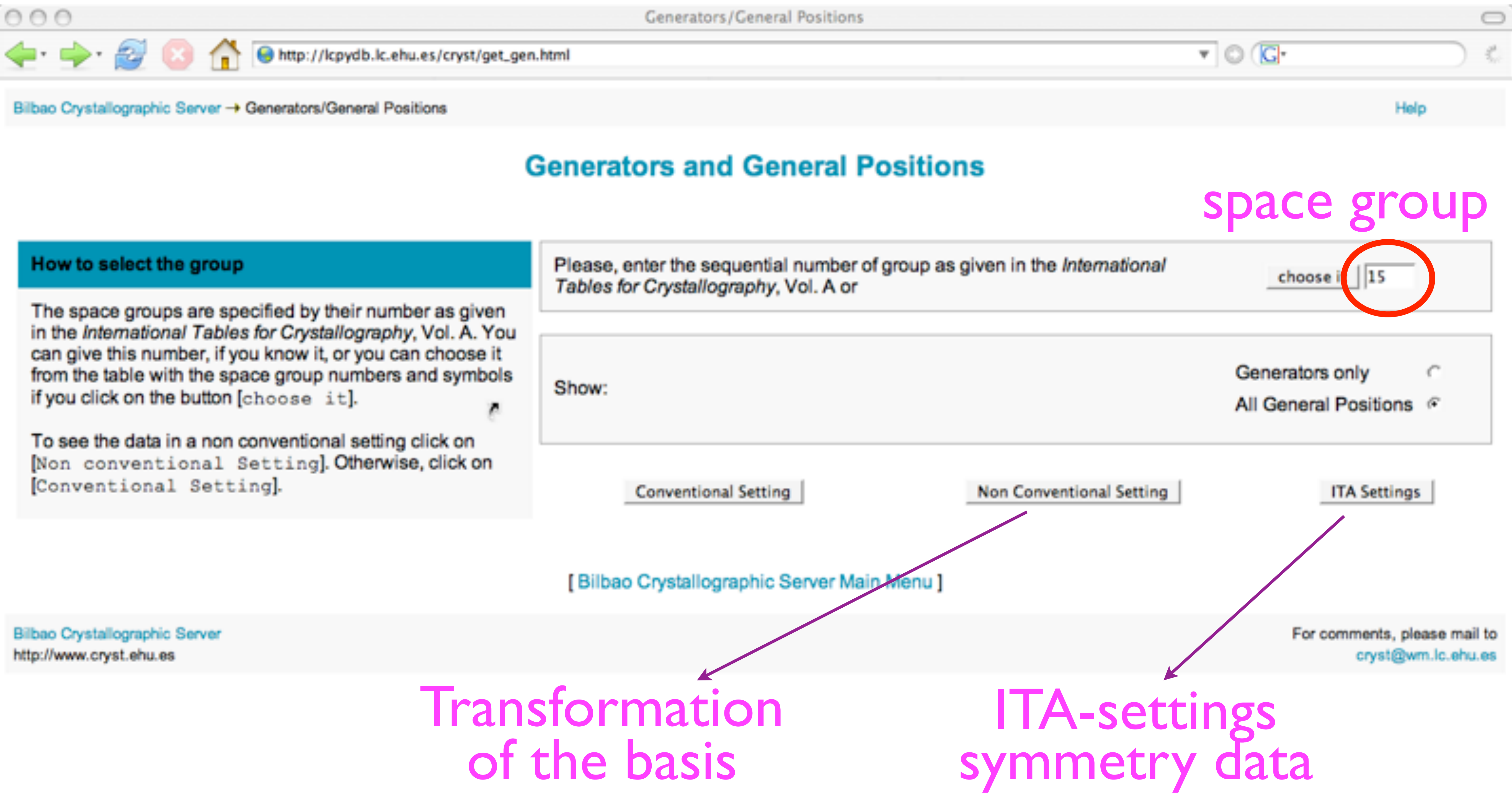
Orthorhombic descriptions

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

Bilbao Crystallographic Server

Problem: Coordinate transformations
Generators
General positions

GENPOS



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.

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

Example GENPOS:

default setting C12/c1

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

final setting A112/a

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

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

ITA number	Setting	P	P^{-1}
68	*C c c e* [origin 1]	**a,b,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 2.23

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 $\boldsymbol{P} = \boldsymbol{c},\boldsymbol{a},\boldsymbol{b}$.

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

EXERCISES

Problem 2.24

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

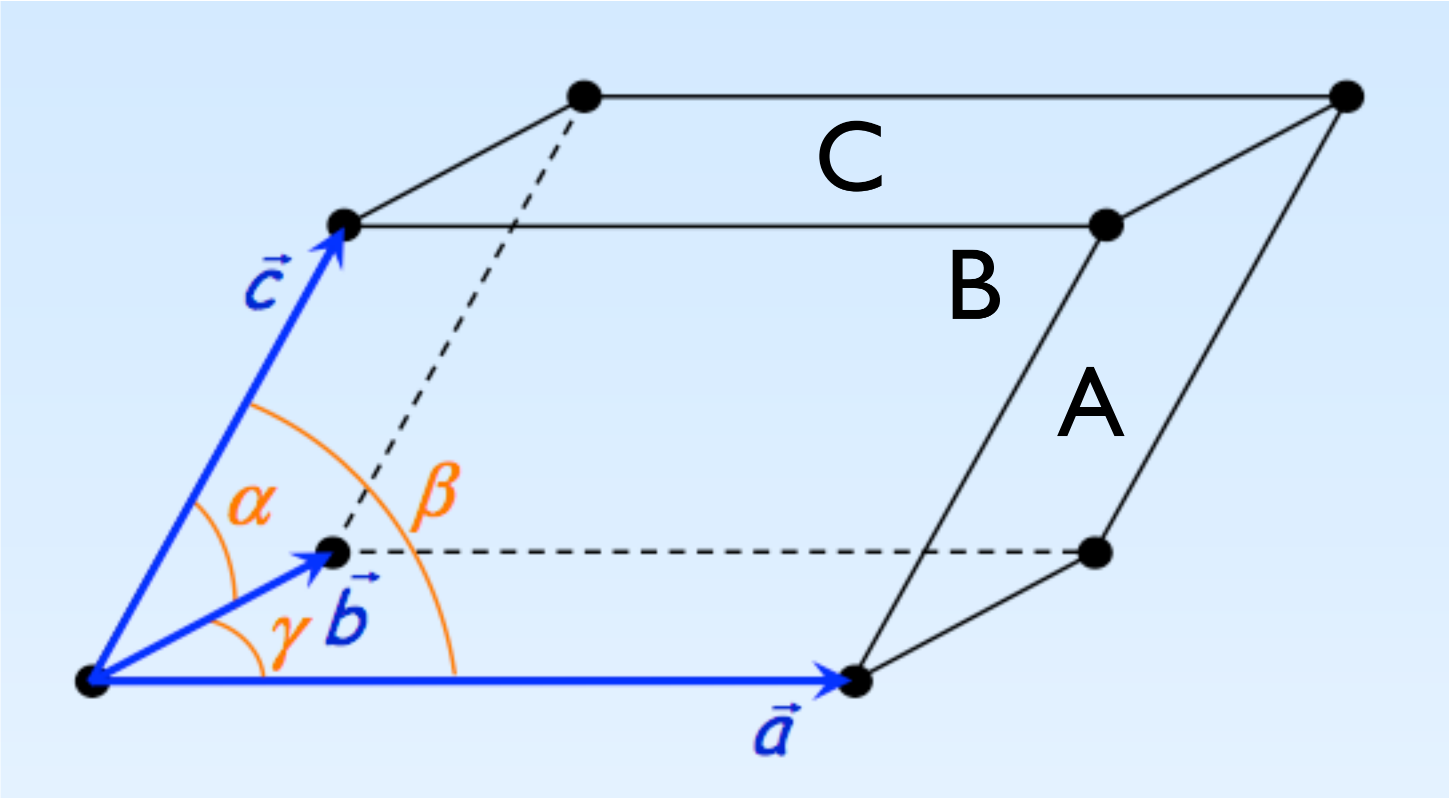
Consider the General position data of the space group *Im-3m* (No. 229). Using the option *Non-conventional setting* obtain the matrix-column pairs of the symmetry operations with respect to a primitive basis, applying the transformation $(\mathbf{a}',\mathbf{b}',\mathbf{c}') = 1/2(-\mathbf{a}+\mathbf{b}+\mathbf{c},\mathbf{a}-\mathbf{b}+\mathbf{c},\mathbf{a}+\ma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

METRIC TENSOR

3D-unit cell and lattice parameters

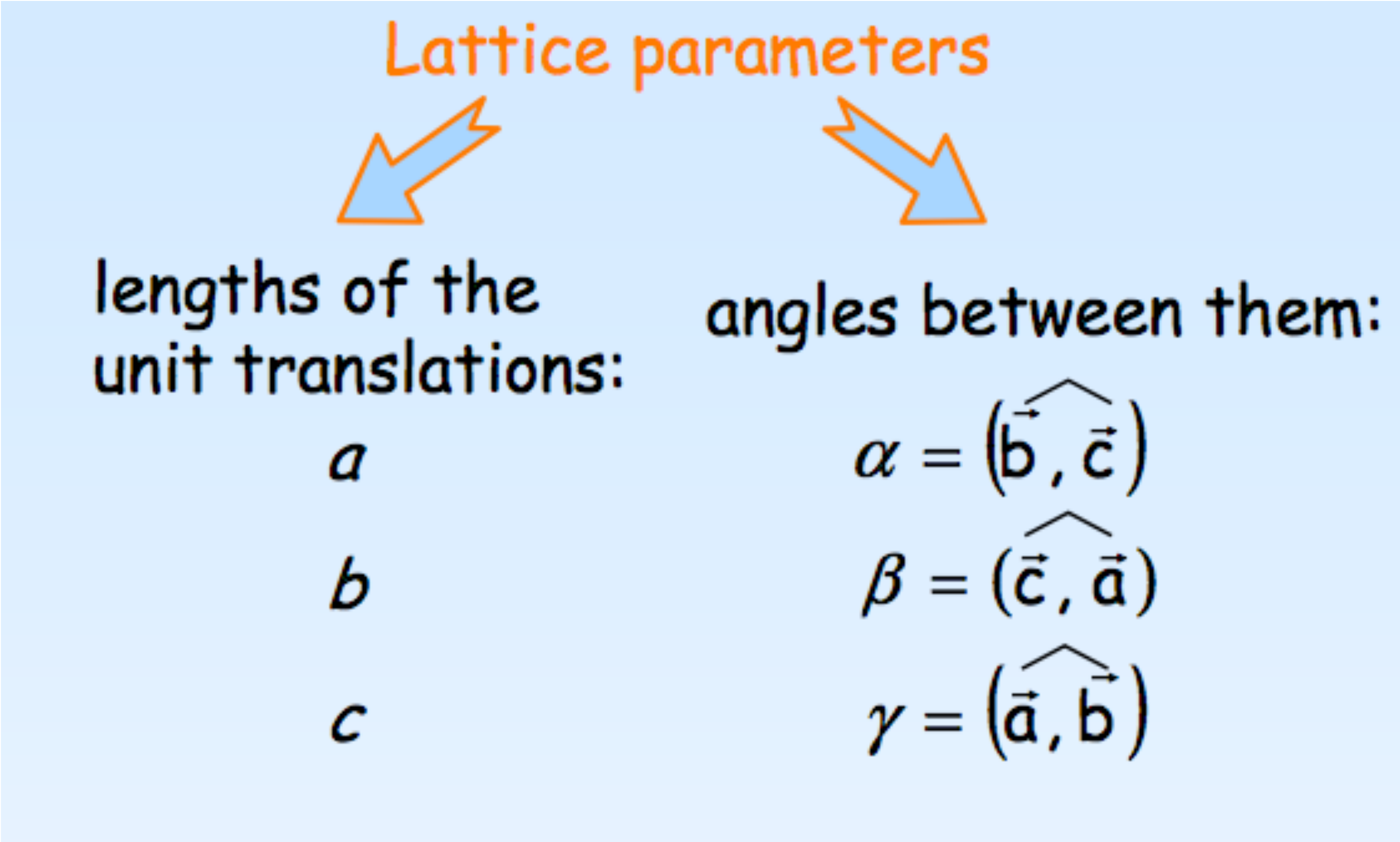
lattice basis:
{**a**, **b**, **c**}

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 (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

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

METRIC TENSOR (FUNDAMENTAL MATRIX)

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

The lattice **L** inherits the metric properties of the Euclidean space and they are conveniently expressed with respect to a lattice basis (right-handed coordinate system)

Metric tensor *G* of *L*

$$\boldsymbol{G} = \{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3\}^T . \{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3\} = \begin{pmatrix} \mathbf{a}_1 \\ \mathbf{a}_2 \\ \mathbf{a}_3 \end{pmatrix} . \{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3\} = \begin{pmatrix} G_{11} & G_{12} & G_{13} \\ G_{21} & G_{22} & G_{23} \\ G_{31} & G_{32} & G_{33} \end{pmatrix}$$

Metric tensor ***G* is symmetric:** $\boldsymbol{G}_{ik} = \boldsymbol{G}_{ki}$

$$\mathbf{G}_{ik} = (\mathbf{a}_i, \mathbf{a}_k) = a_i a_k \cos\alpha_j,$$

Scalar product of arbitrary vectors:

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

Transformation properties of *G* under basis transformation

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

$$\boldsymbol{G}' = \{\mathbf{a'}_1, \mathbf{a'}_2, \mathbf{a'}_3\}^T . \{\mathbf{a'}_1, \mathbf{a'}_2, \mathbf{a'}_3\} = \boldsymbol{P}^T \{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3\}^T . \{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3\} \boldsymbol{P}$$

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

Crystallographic calculations: 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 $0 \leq x_1, x_2, x_3 < 1$, can be calculated by the formula

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

In the general case one obtains

$$V^2 = \begin{vmatrix} G_{11} & G_{12} & G_{13} \\ G_{21} & G_{22} & G_{23} \\ G_{31} & G_{32} & G_{33} \end{vmatrix} =$$

$$= a^2\, b^2\, c^2\, (1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2\cos\alpha\cos\beta\cos\gamma).$$

Volume of the unit cell in terms of lattice parameters (Buerger, 1941)

Basis vectors with respect to Cartesian basis

$$\mathbf{a} = \mathbf{i}a_x + \mathbf{j}a_y + \mathbf{k}a_z,$$
$$\mathbf{b} = \mathbf{i}b_x + \mathbf{j}b_y + \mathbf{k}b_z,$$
$$\mathbf{c} = \mathbf{i}c_x + \mathbf{j}c_y + \mathbf{k}c_z,$$

$$\rightarrow \quad V = \mathbf{a} \cdot (\mathbf{b} \times \mathbf{c}) = \begin{vmatrix} a_x & a_y & a_z \\ b_x & b_y & b_z \\ c_x & c_y & c_z \end{vmatrix}$$

det (A)=det(A^T)

$$V^2 = \begin{vmatrix} a_x & a_y & a_z \\ b_x & b_y & b_z \\ c_x & c_y & c_z \end{vmatrix} \begin{vmatrix} a_x & b_x & c_x \\ a_y & b_y & c_y \\ a_z & b_z & c_z \end{vmatrix} = \begin{vmatrix} \mathbf{a}\cdot\mathbf{a} & \mathbf{a}\cdot\mathbf{b} & \mathbf{a}\cdot\mathbf{c} \\ \mathbf{b}\cdot\mathbf{a} & \mathbf{b}\cdot\mathbf{b} & \mathbf{b}\cdot\mathbf{c} \\ \mathbf{c}\cdot\mathbf{a} & \mathbf{c}\cdot\mathbf{b} & \mathbf{c}\cdot\mathbf{c} \end{vmatrix} = \det(\boldsymbol{G})$$

$$= \begin{vmatrix} a^2 & ab\cos\gamma & ac\cos\beta \\ ba\cos\gamma & b^2 & bc\cos\alpha \\ ca\cos\beta & cb\cos\alpha & c^2 \end{vmatrix}$$

$$V = abc(1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2\cos\alpha\cos\beta\cos\gamma)^{1/2}$$

EXERCISE (Problem 2.20)

Write down the metric tensors of the seven crystal systems in parametric form using the general expressions for their lattice parameters. For each of the cases, express the volume of the unit cell as a function of the lattice parameters.

For example:

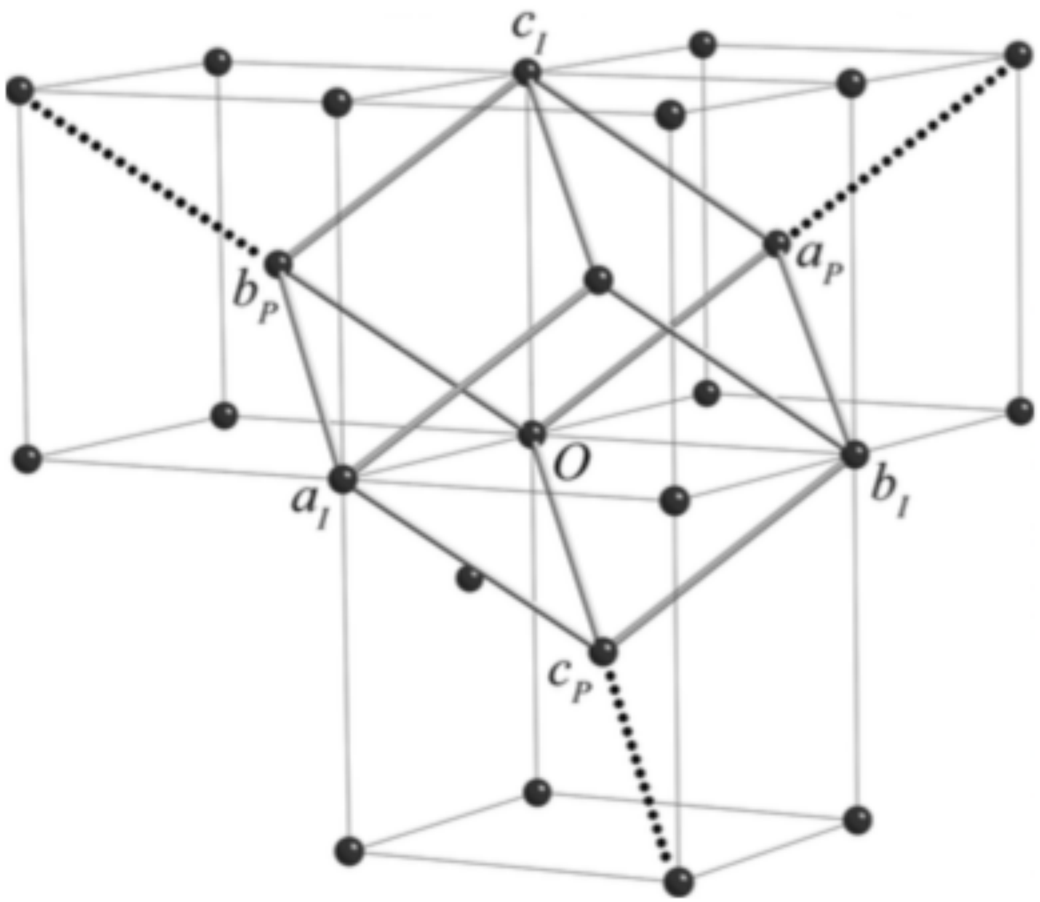
tetragonal crystal system: a=b, c, α=β=γ=90

$$\boldsymbol{G} = \begin{bmatrix} a^2 & 0 & 0 \\ 0 & a^2 & 0 \\ 0 & 0 & c^2 \end{bmatrix}$$

V=?

EXERCISES

Problem 2.21



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:

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

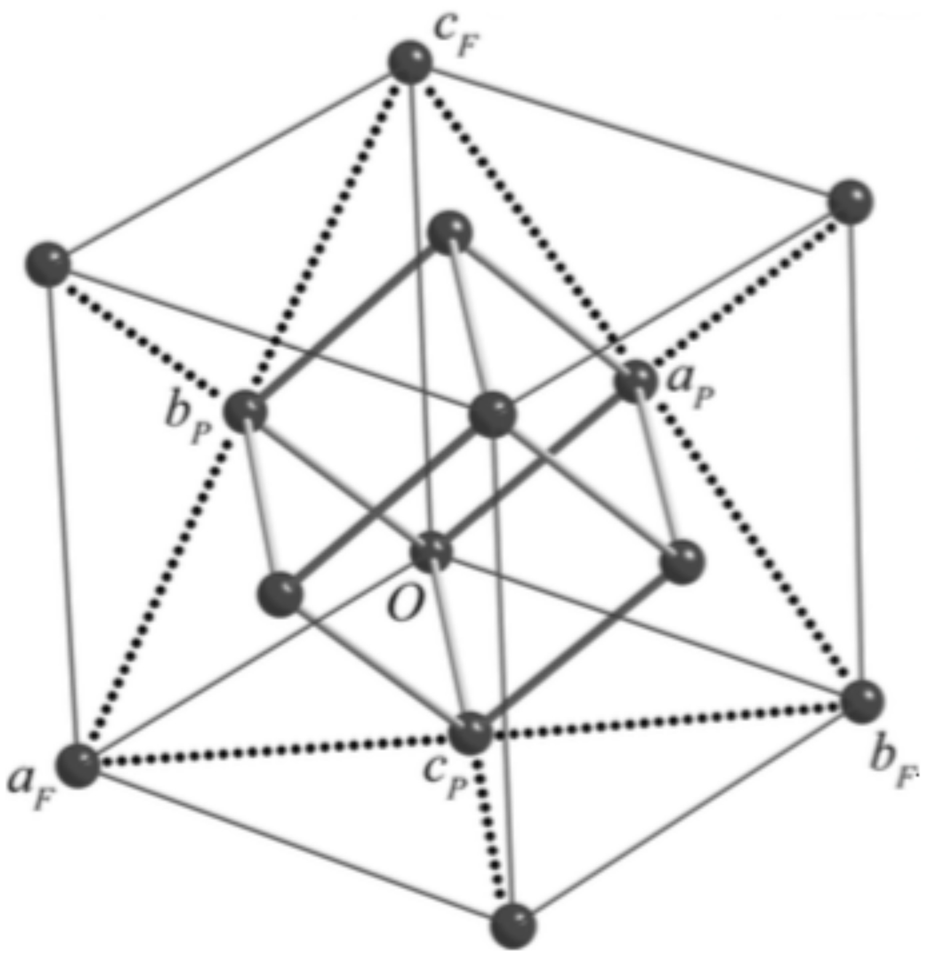
(iii) determine the lattice parameters of the primitive cell if a_P=4 Å

Hint

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

EXERCISES

Problem 2.22



A face-centred cubic lattice (*cF*) 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 vectors $1/2\mathbf{b_P}+1/2\mathbf{c_P}$, $1/2\mathbf{a_P}+1/2\mathbf{c_P}$, $1/2\mathbf{a_P}+1/2\mathbf{b_P}$, which point to the centres of the faces of the conventional cell.

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

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

(ii) for the primitive basis:

$$\mathbf{a_F}=1/2(\mathbf{b_P}+\mathbf{c_P}),\ \mathbf{b_F}=1/2(\mathbf{a_P}+\mathbf{c_P}),\ \mathbf{c_F}=1/2(\mathbf{a_P}+\mathbf{b_P})$$

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