University of Science and Technology, Beijung
Optical Material and Device Lab

2022 SPRING FESTIVAL BEIJING CRYSTALLOGRAPHY SCHOOL

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SPACE GROUPS

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

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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:
$T \triangleleft G$

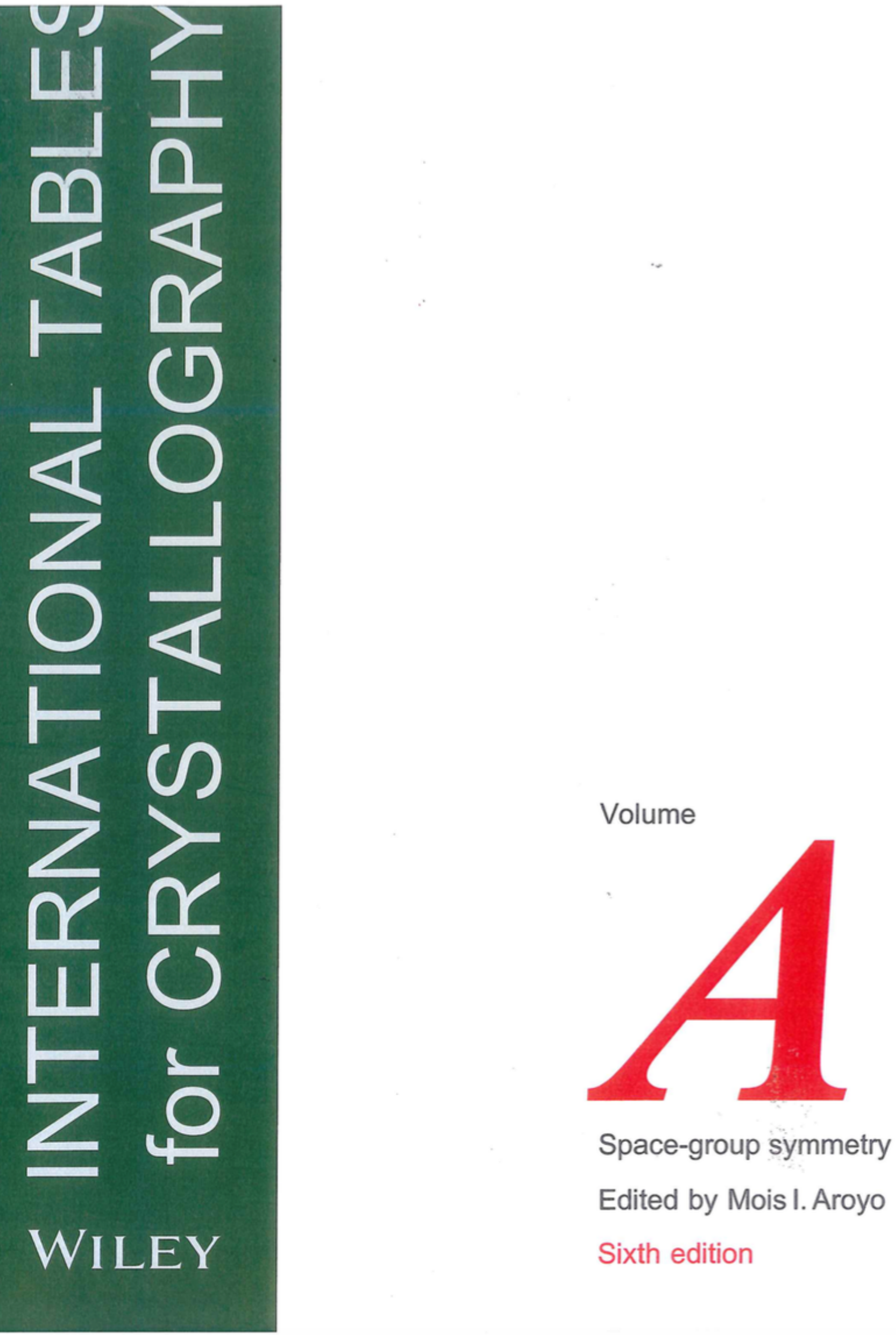
The infinite set of all translations that are symmetry operations of the crystal pattern

Point group of the space groups P_G:

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

$$(\boldsymbol{W},\boldsymbol{w}) \longrightarrow \boldsymbol{W} \qquad P_G=\{\boldsymbol{W} \mid (\boldsymbol{W},\boldsymbol{w}) \in G\}$$

INTERNATIONAL TABLES FOR CRYSTALLOGRAPHY
VOLUME A: SPACE-GROUP SYMMETRY



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

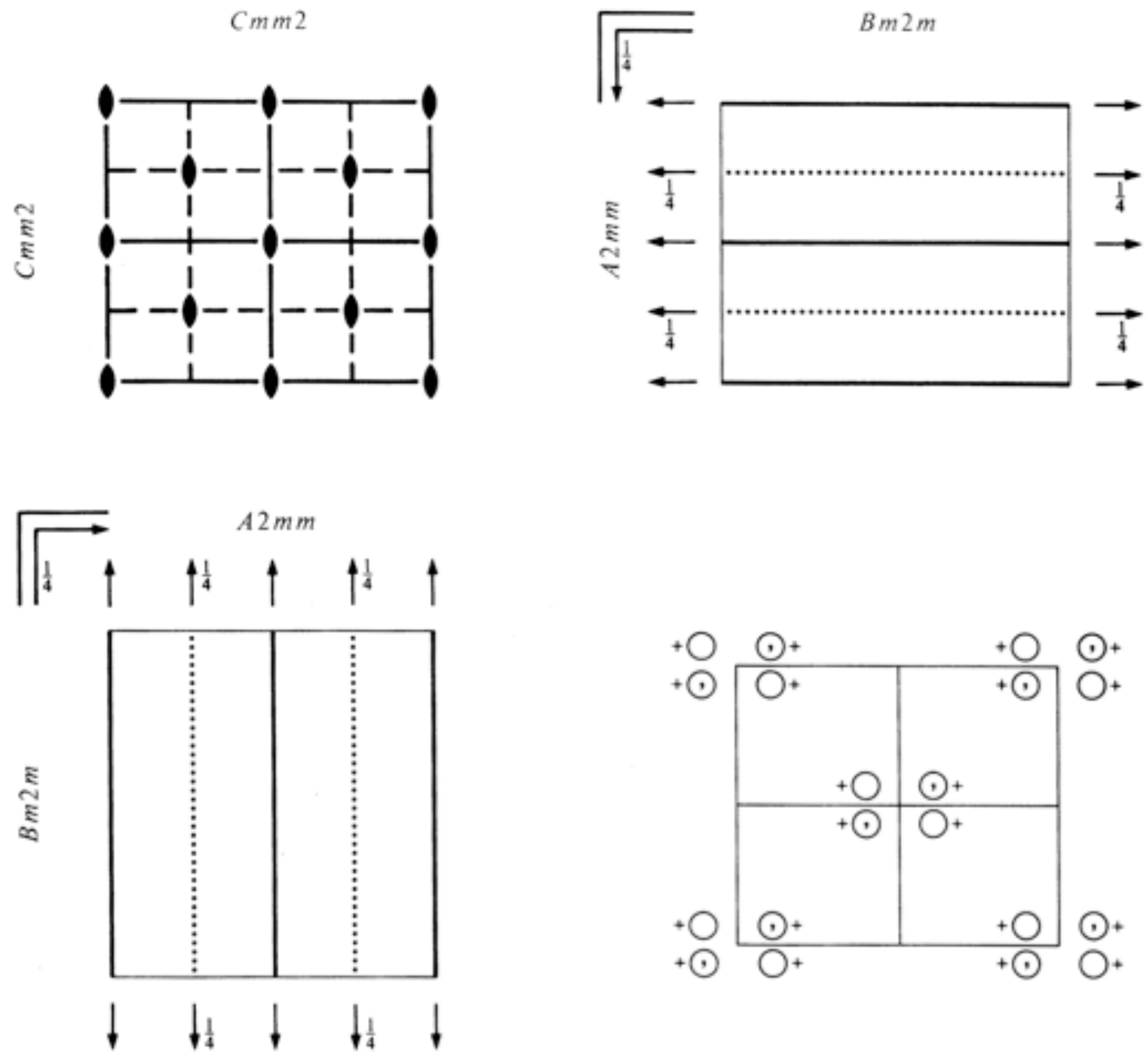
- headline with the relevant group symbols;
- diagrams of the symmetry elements and of the general position;
- specification of the origin and the asymmetric unit;
- list of symmetry operations;
- generators;
- general and special positions with multiplicities, site symmetries, coordinates and reflection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

(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	$m\,m\,2$	$0,\frac{1}{2},z$				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	$C\,m\,m\,2$		Patterson symmetry $C\,m\,m\,m$

Number of space group

Full Hermann-Mauguin symbol

Patterson symmetry

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	$1, \boxed{\bar{1}}$	2	None	$a, b, c,$ α, β, γ	aP
Monoclinic	m	Monoclinic	$2, m, \boxed{2/m}$	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	$222, mm2, \boxed{mmm}$	59	$\alpha = \beta = \gamma = 90°$	a, b, c	oP oS (oC, oA, oB) oI oF
Tetragonal	t	Tetragonal	$4, \bar{4}, \boxed{4/m}$ $422, 4mm, \bar{4}2m,$ $\boxed{4/mmm}$	68	$a = b$ $\alpha = \beta = \gamma = 90°$	a, c	tP tI
Hexagonal	h	Trigonal	$3, \boxed{\bar{3}}$ $32, 3m, \boxed{\bar{3}m}$	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	$6, \bar{6}, \boxed{6/m}$ $622, 6mm, \bar{6}2m,$ $\boxed{6/mmm}$	27	$a = b$ $\alpha = \beta = 90°, \gamma = 120°$	a, c	hP
Cubic	c	Cubic	$23, \boxed{m\bar{3}}$ $432, \bar{4}3m, \boxed{m\bar{3}m}$	36	$a = b = c$ $\alpha = \beta = \gamma = 90°$	a	cP cI cF

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:

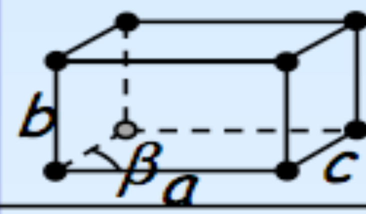
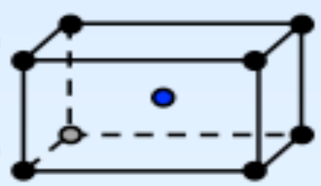
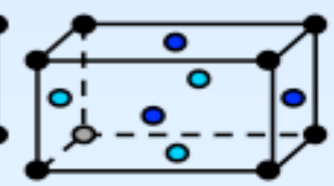
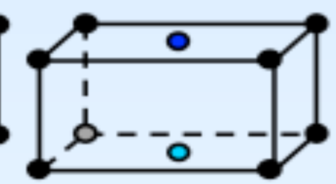
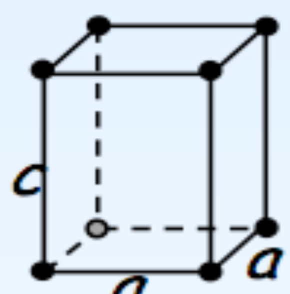
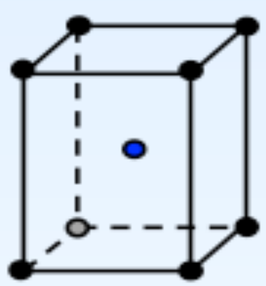
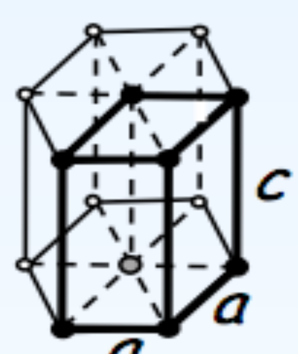
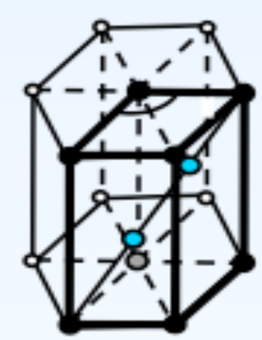
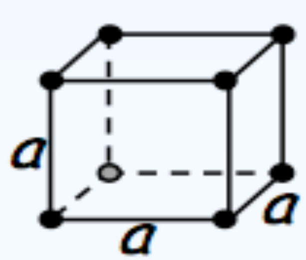
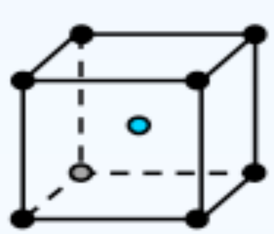
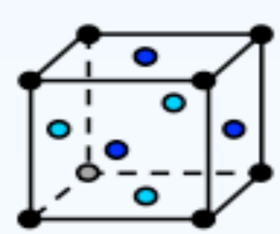
pure rotations > screw rotations;

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

primary direction

secondary direction

tertiary direction

Orthorhombic $P 2_1/n\, 2_1/m\, 2_1/a$

Bravais lattice

screw axis $2_1 // \vec{a}$
glide plane $n \perp \vec{a}$

screw axis $2_1 // \vec{b}$
mirror plane $m \perp \vec{b}$

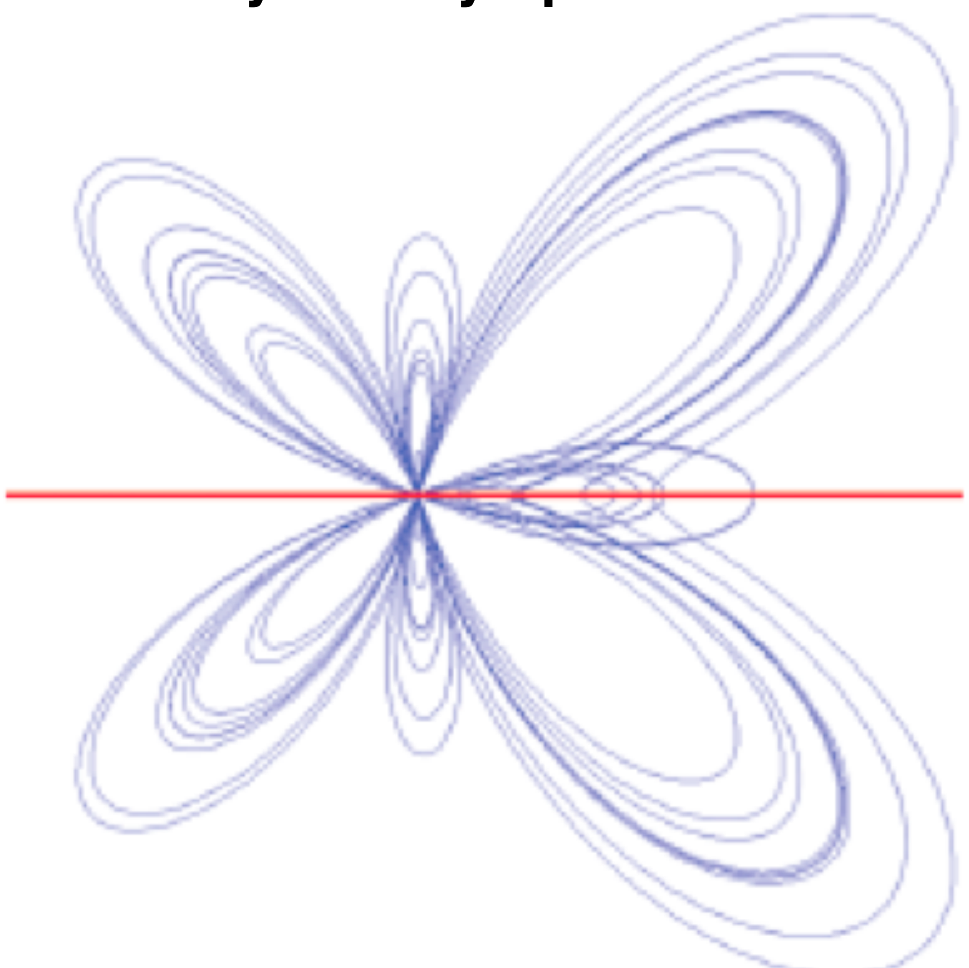
screw axis $2_1 // \vec{c}$
glide plane $a \perp \vec{c}$

PRESENTATION OF SPACE-GROUP SYMMETRY OPERATIONS

IN INTERNATIONAL TABLES FOR CRYSTALLOGRAPHY, VOL. A

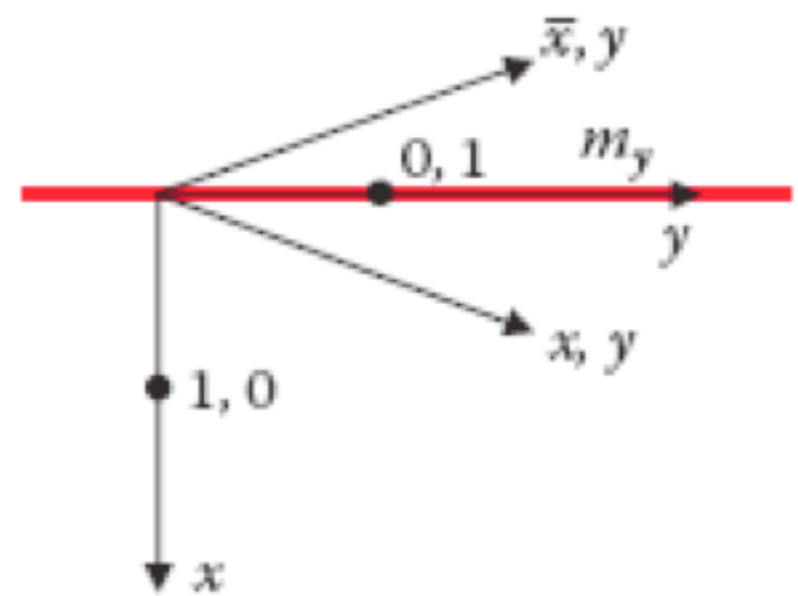
Example: Matrix presentation of symmetry operation

Mirror symmetry operation



drawing: M.M. Julian
Foundations of Crystallography
©Taylor & Francis, 2008

Mirror line m_y at 0,y



Matrix representation

$$m_y \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} -x \\ y \end{bmatrix} = \begin{bmatrix} -1 & \\ & 1 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix}$$

$$\det \begin{bmatrix} -1 & \\ & 1 \end{bmatrix} = \,? \qquad \mathrm{tr} \begin{bmatrix} -1 & \\ & 1 \end{bmatrix} = \,?$$

Fixed points

$$m_y \begin{bmatrix} x_f \\ y_f \end{bmatrix} = \begin{bmatrix} x_f \\ y_f \end{bmatrix}$$

Description of isometries: 3D

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

isometry:

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

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} \xrightarrow[\tilde{x} = F_1(x,y,z)]{} \begin{pmatrix} \tilde{x} \\ \tilde{y} \\ \tilde{z} \end{pmatrix}$$

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

Matrix notation for system of linear equations

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

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

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

QUICK QUIZ

Example

Referred to an 'orthorhombic' coordinate 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

Short-hand notation for the description of isometries

isometry:

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

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

notation rules:

-left-hand side: omitted

-coefficients 0, +1, -1

-different rows in one line

examples:

$$\left(\begin{array}{ccc|c} -1 & & & 1/2 \\ & 1 & & 0 \\ & & -1 & 1/2 \end{array}\right) \longrightarrow \left\{\begin{array}{l} -x+1/2,\ y,\ -z+1/2 \\ \bar{x}+1/2,\ y,\ \bar{z}+1/2 \end{array}\right.$$

(*x,y,z* notation)

EXAMPLE

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

Combination of isometries

$$\begin{tikzcd}
x \arrow[r, "{(U,u)}"] \arrow[dr, "{(W,w)}"'] & \tilde{x} \arrow[d, "{(V,v)}"] \\
& \tilde{\tilde{x}}
\end{tikzcd}$$

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

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

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

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

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

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

Example

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

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

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

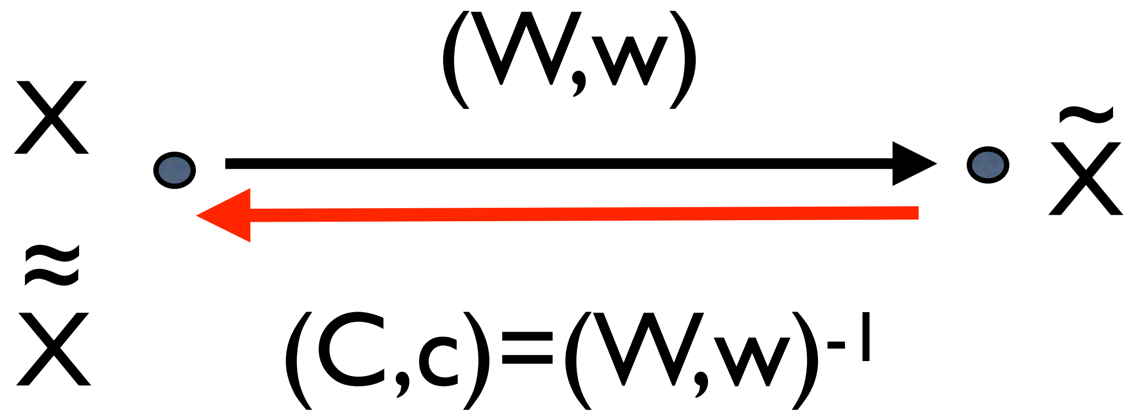
$$(W,w)=(W_1,w_1)(W_2,w_2)$$

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

combination of isometries:

$$\boxed{(\boldsymbol{V},\ \boldsymbol{v})(\boldsymbol{U},\ \boldsymbol{u}) = (\boldsymbol{VU},\ \boldsymbol{V}\boldsymbol{u}+\boldsymbol{v}).}$$

Inverse isometries



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

$\boldsymbol{o}$ = zero translation column

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

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

$CW=\boldsymbol{I}$ $\quad$ $Cw+c=\boldsymbol{o}$

$\boxed{C=W^{-1}}$ $\quad$ $\boxed{c=-Cw=-W^{-1}w}$

Example

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

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

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

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

inverse of isometries:

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

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

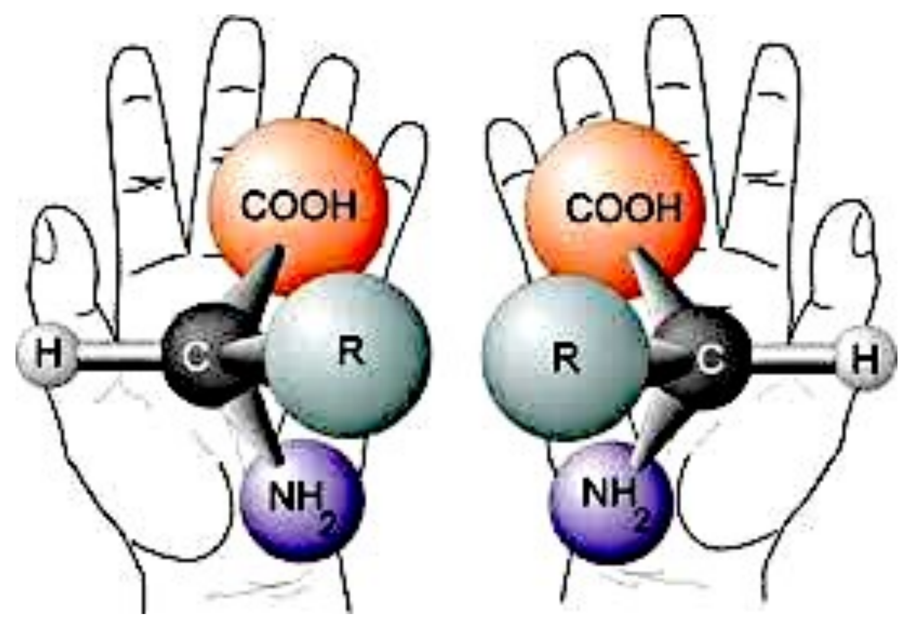
Kinds of Symmetry Operations

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

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 $\tilde{\mathbf{x}} = \mathbf{x} + \mathbf{t}$

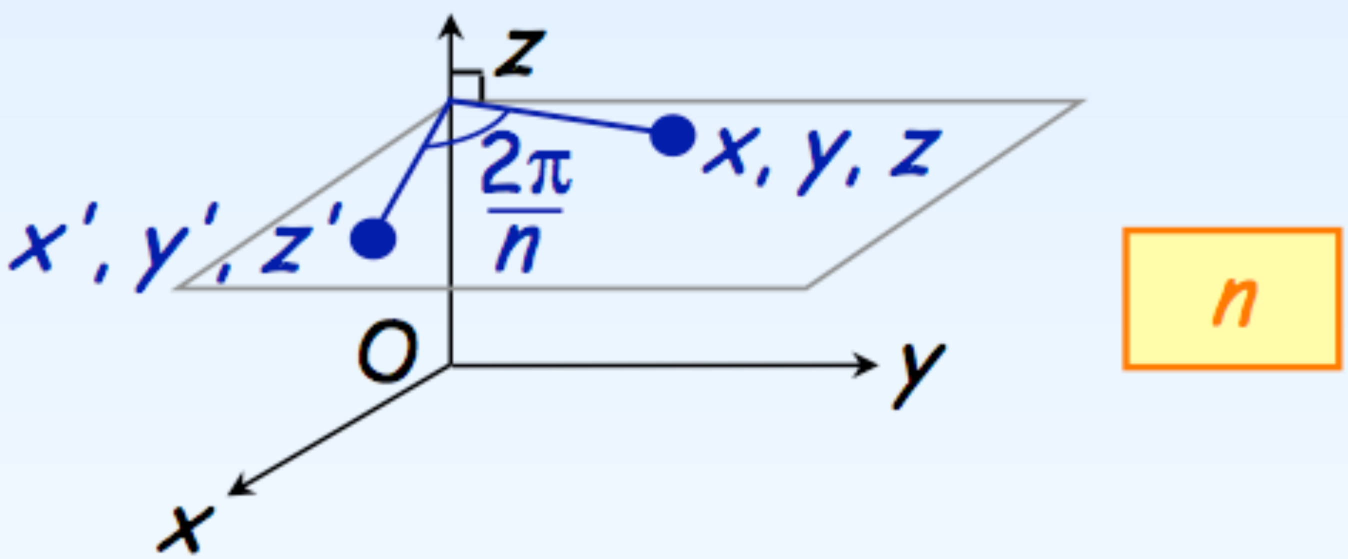
rotation: one line fixed
rotation axis $\phi = k \times 360^\circ/N$

screw rotation: no fixed point
screw axis
screw vector

Crystallographic symmetry operations

Rotation (around an axis)

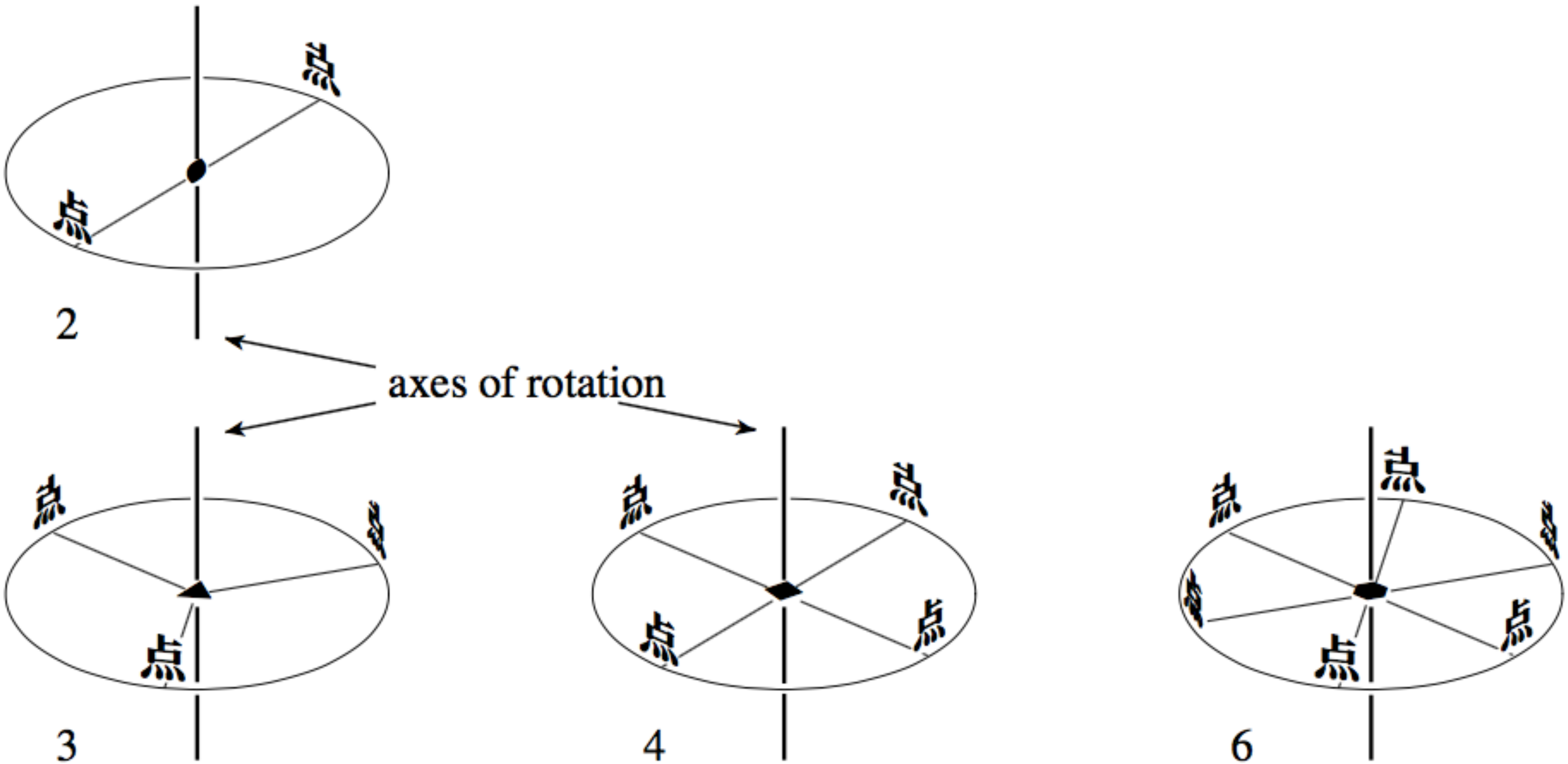
Rotation of order n = rotation by $\varphi = \frac{2\pi}{n}$



$$\alpha(n) = \begin{pmatrix} \cos\varphi & -\sin\varphi & 0 \\ \sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

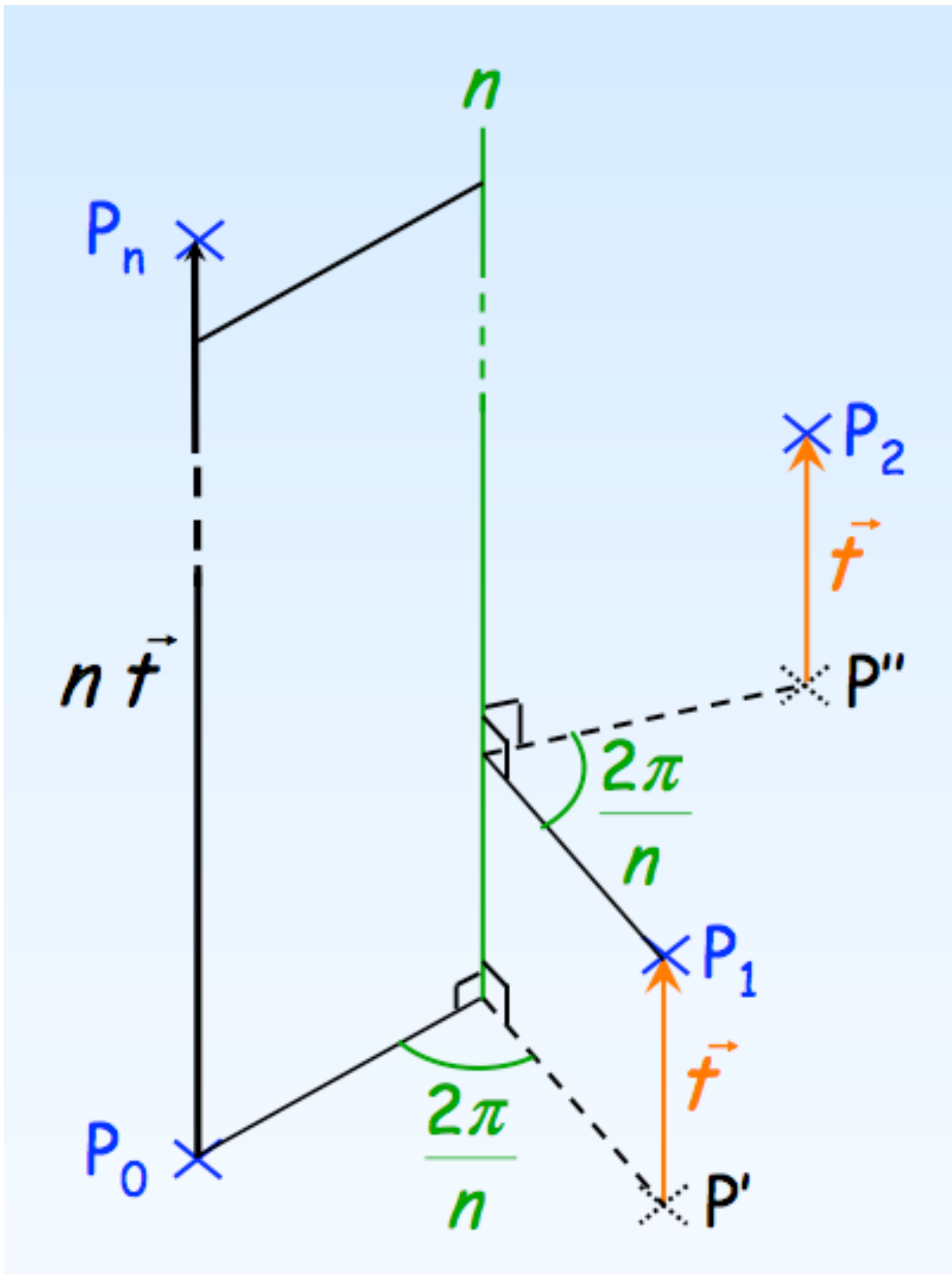
Det = +1

Rotations



Chinese symbol for point, pronounced
dia˘n in Chinese, hoshi in Japanese).

Screw rotation

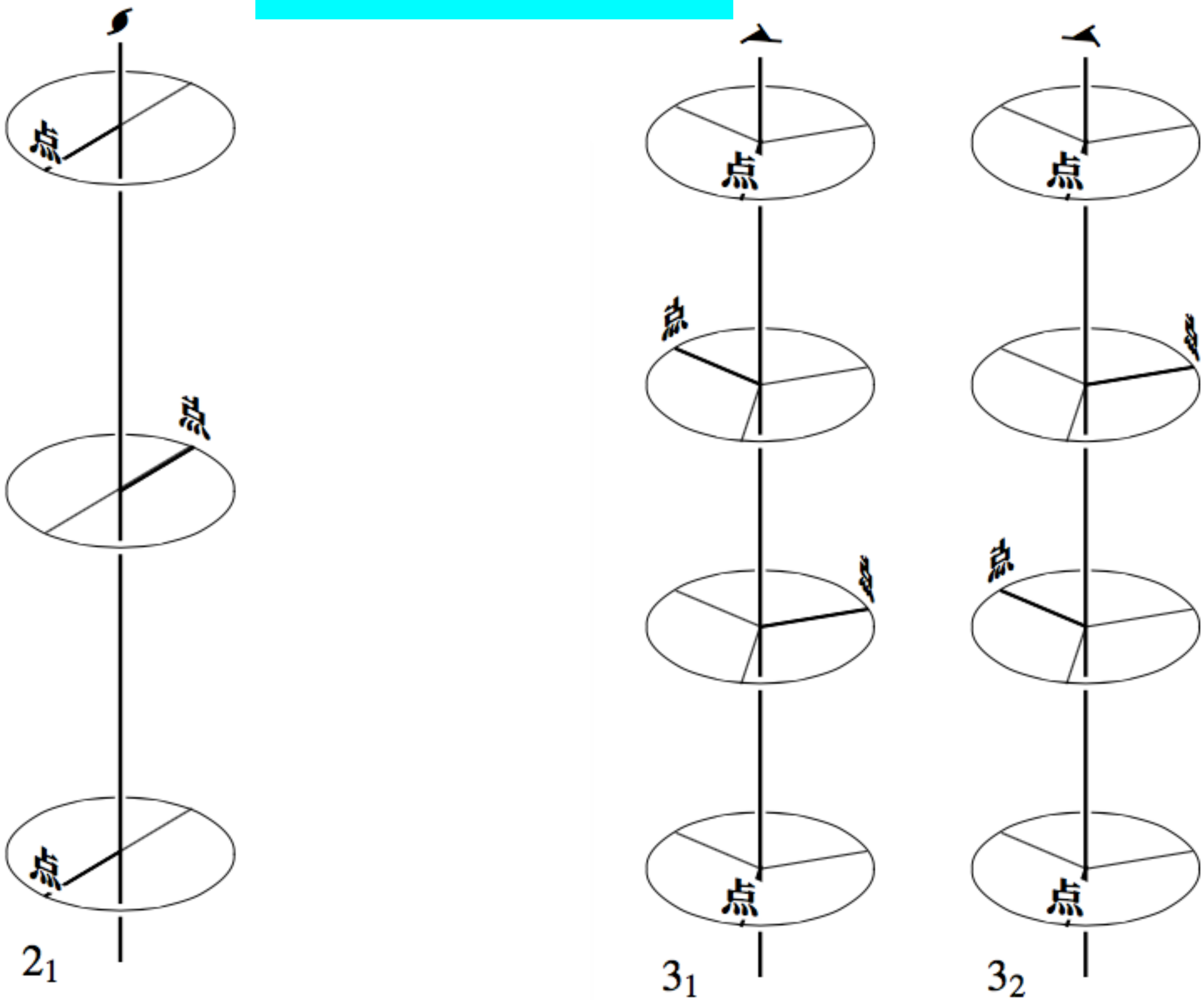


n-fold rotation followed by a fractional translation $\frac{p}{n}\mathbf{t}$ parallel to the rotation axis

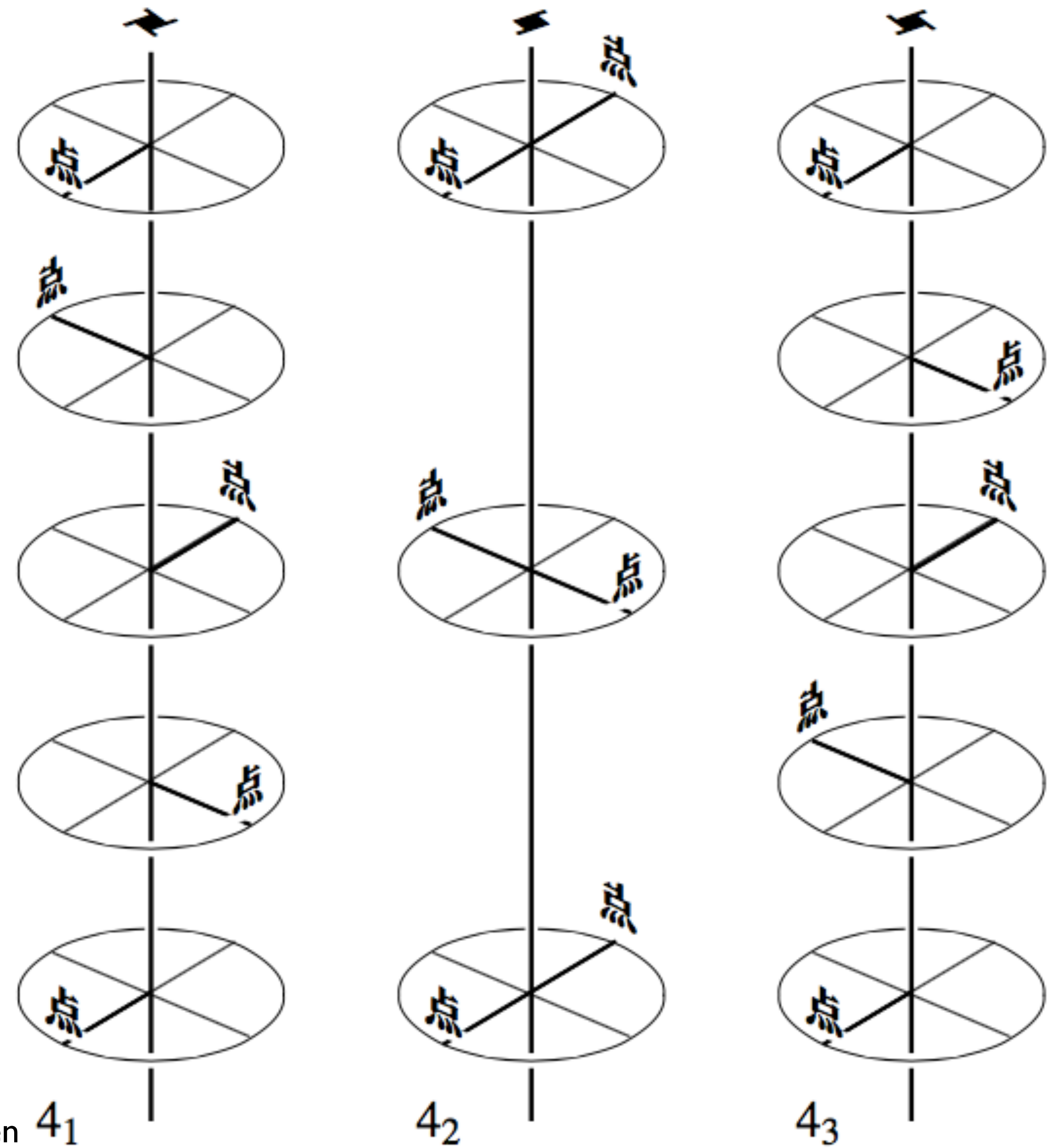
symbol: n_p

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

Screw rotations



Screw rotations



Types of isometries

DO NOT
preserve handedness

characteristics:

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

roto-inversion:

centre of roto-inversion fixed
roto-inversion axis

inversion:

centre of inversion fixed

reflection:

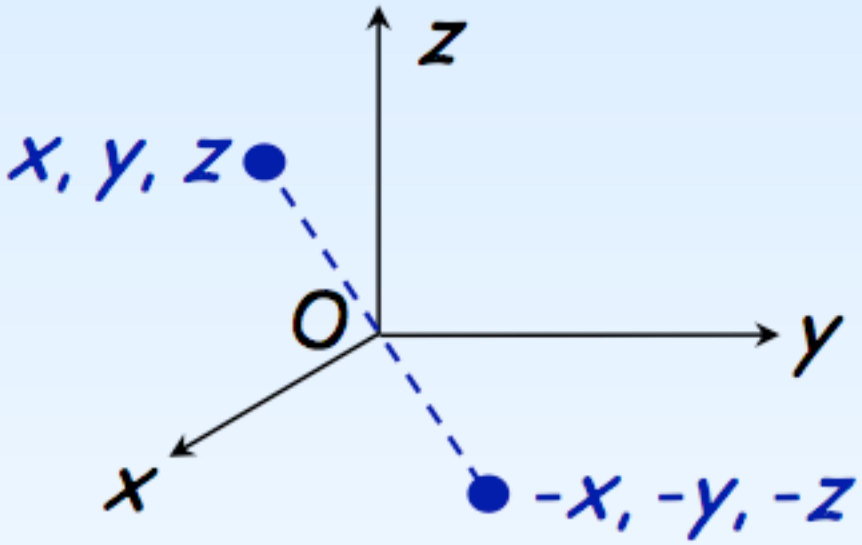
plane fixed
reflection/mirror plane

glide reflection:

no fixed point
glide plane
glide vector

Symmetry operations in 3D
Rotoinvertions

Inversion (through a point)



$\bar{1}$

a crystal which has the inversion symmetry is called centrosymmetrical.

$$\alpha(\bar{1}) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

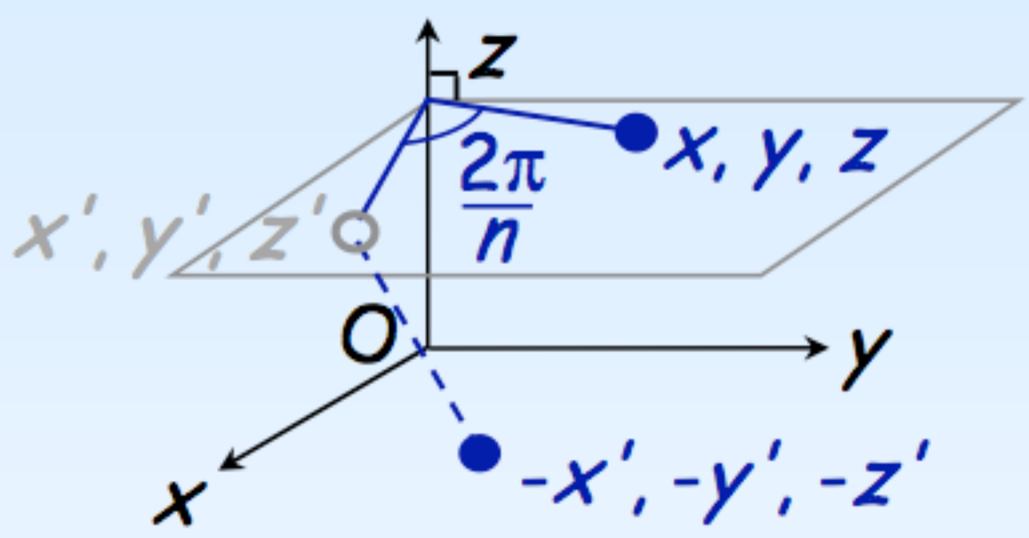
Det = -1

Symmetry operations in 3D
Rotoinvertions

Roto-inversion

(around an axis and through a point)

Rotation followed by an inversion

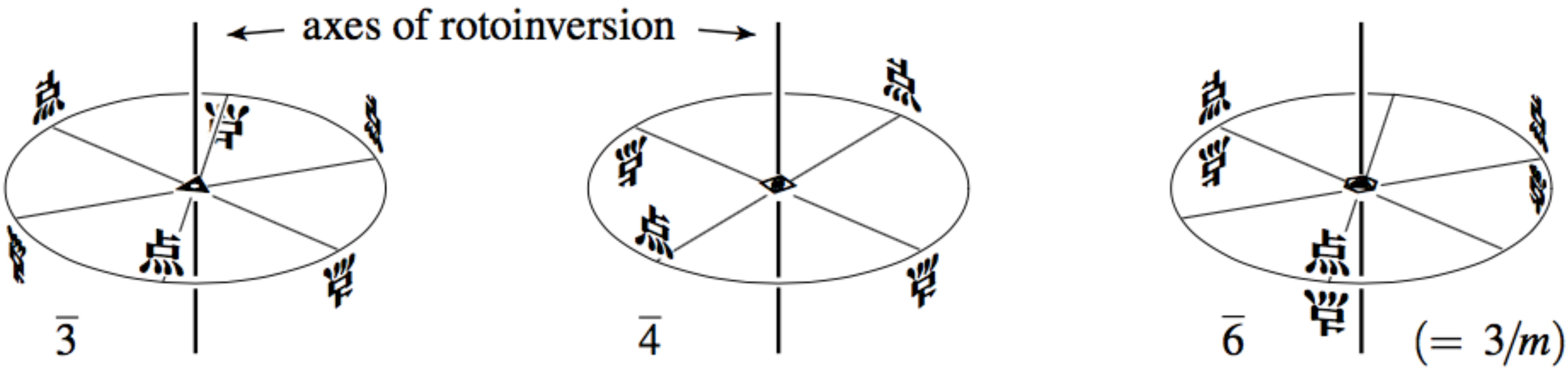


$\bar{n}$

$$\alpha(\bar{n}) = \begin{pmatrix} -\cos\varphi & \sin\varphi & 0 \\ -\sin\varphi & -\cos\varphi & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

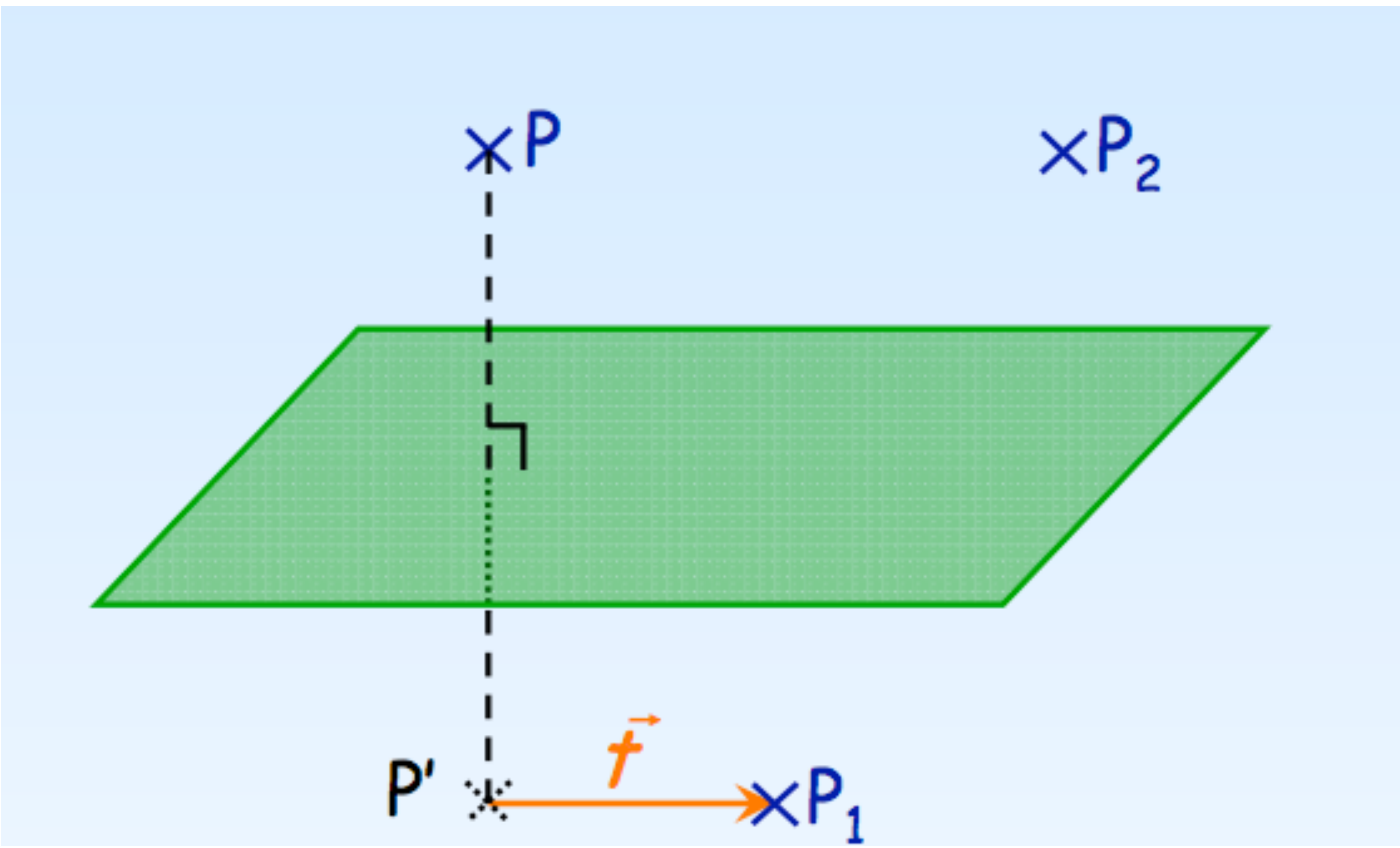
Det = -1

Rotoinversion



Crystallographic symmetry operations

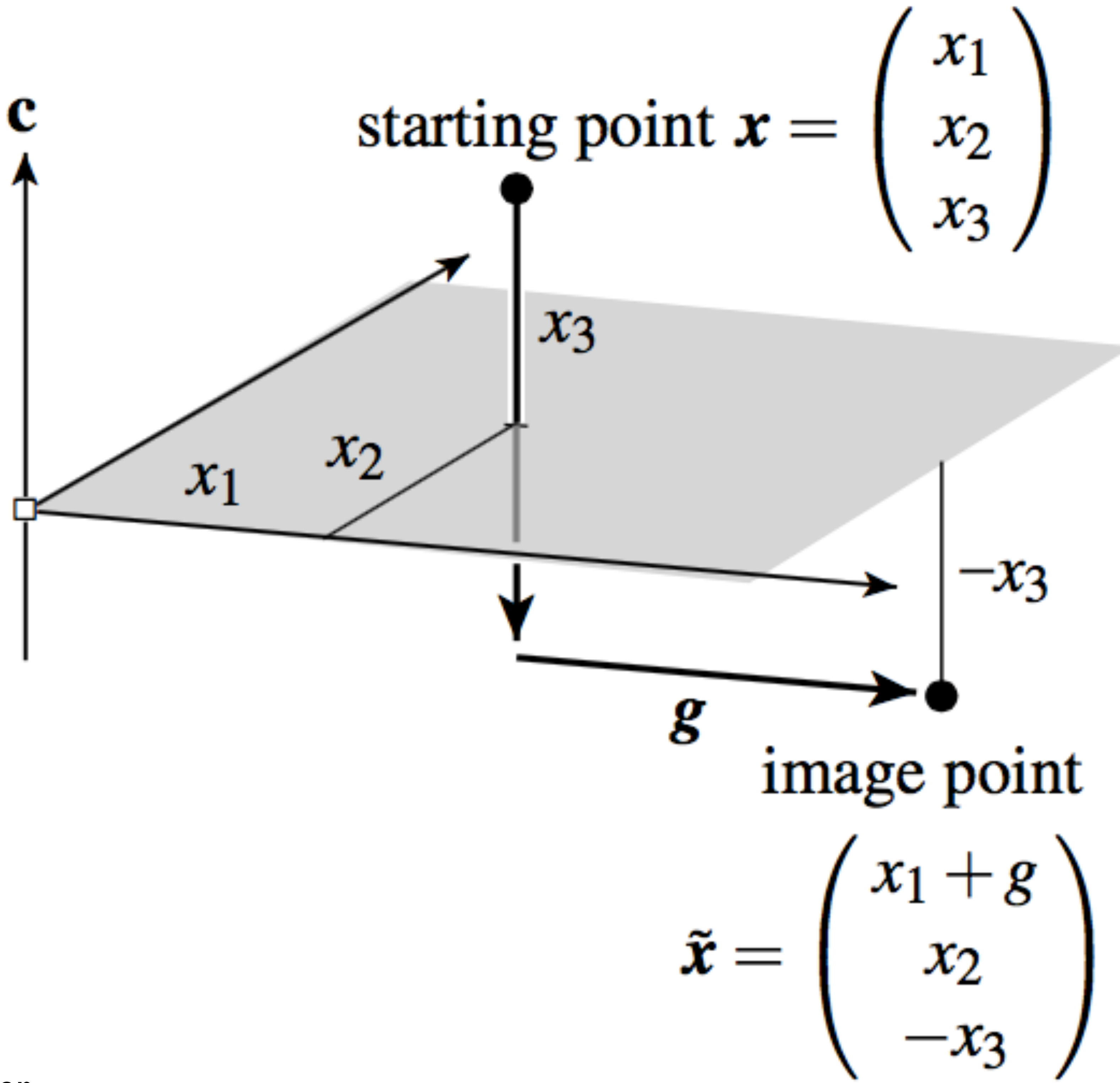
Glide plane



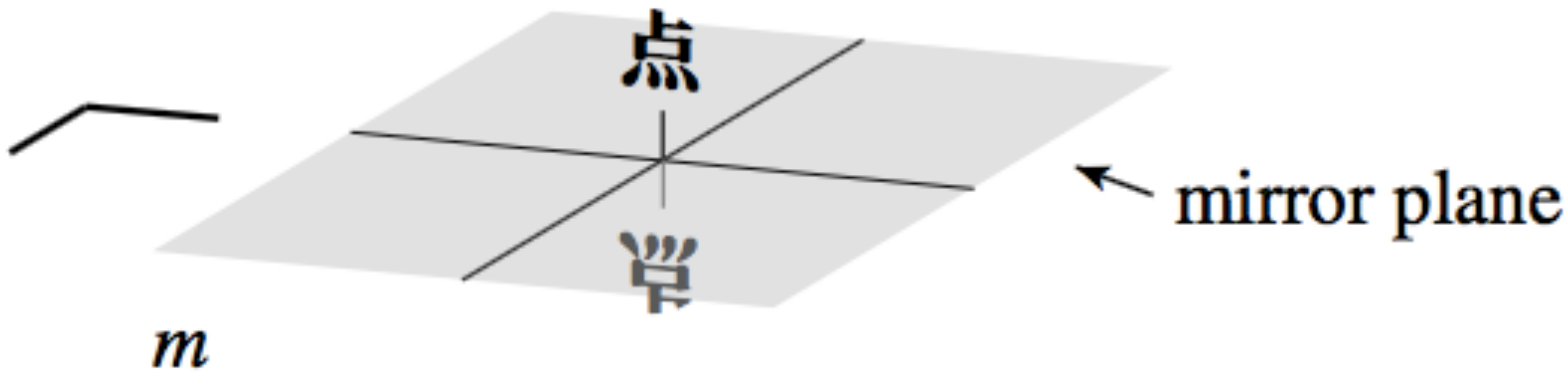
reflection followed by a fractional translation $\frac{1}{2}\mathbf{t}$ parallel to the plane

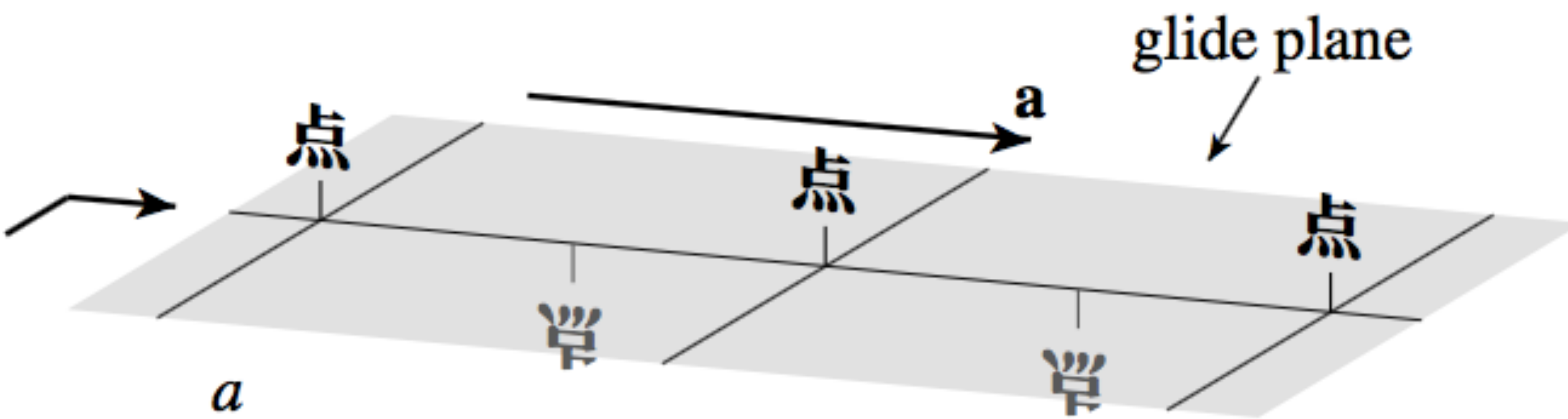
Its application 2 times results in a translation parallel to the plane

Glide reflection



Reflection and Glide reflection





Matrix-column presentation of some symmetry operations

Rotation or rotoinversion around the origin:

$$\left(\begin{array}{ccc|c} W_{11} & W_{12} & W_{13} & 0 \\ W_{21} & W_{22} & W_{23} & 0 \\ W_{31} & W_{32} & W_{33} & 0 \end{array} \right) \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

Translation:

$$\left(\begin{array}{ccc|c} 1 & & & w1 \\ & 1 & & w2 \\ & & 1 & w3 \end{array} \right) \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} x+w1 \\ y+w2 \\ z+w3 \end{pmatrix}$$

Inversion through the origin:

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

Symmetry Operations Block

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

KIND and TYPE of the symmetry operation

ORIENTATION of the geometric element

SCREW/GLIDE component

LOCATION of the geometric element

Geometric meaning of (W, w)

W information

(a) KIND and TYPE of isometry

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

order: $\boldsymbol{W}^n = \boldsymbol{I}$

rotation angle $\cos\varphi = (\pm\mathrm{tr}(\boldsymbol{W}) - 1)/2$

Example

(a) Determine the type and order of isometries that are represented by the following matrix-column pairs:

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

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

(b) The same for:

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

(a) type of isometry

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

Geometric meaning of (W, w)
W information

(b) axis or normal direction $\boldsymbol{u}$: $\boldsymbol{W}\boldsymbol{u} = \pm\boldsymbol{u}$

(b1) rotations: **u = *Y*(*W*)v** **v=** $\begin{bmatrix} v1 \\ v2 \\ v3 \end{bmatrix}$

$$\boldsymbol{Y}(\boldsymbol{W}) = \boldsymbol{W}^{k-1} + \boldsymbol{W}^{k-2} + \ldots + \boldsymbol{W} + \boldsymbol{I}$$

(b2) roto-inversions: $\boldsymbol{Y}(-\boldsymbol{W})$

reflections: $\boldsymbol{Y}(-\boldsymbol{W}) = -\boldsymbol{W} + \boldsymbol{I}$

Direction of rotation axis/normal

Example:

$$(W,w)=\left(\begin{array}{|c|c|c|}\hline 0 & 1 & 0 \\ \hline -1 & 0 & 0 \\ \hline 0 & 0 & 1 \\ \hline\end{array}\ \begin{array}{|c|}\hline 0 \\ \hline 1/2 \\ \hline 1/2 \\ \hline\end{array}\right)$$

det W=?
tr W=?

What is the type and order of the isometry?
Determine its rotation axis?

$$\boxed{\boldsymbol{Y(W) = W^{k-1} + W^{k-2} + \ldots + W + I}}$$

$$Y(W)=\underbrace{\begin{array}{|c|c|c|}\hline 0 & -1 & 0 \\ \hline 1 & 0 & 0 \\ \hline 0 & 0 & 1 \\ \hline\end{array}}_{W^3}+\underbrace{\begin{array}{|c|c|c|}\hline -1 & 0 & 0 \\ \hline 0 & -1 & 0 \\ \hline 0 & 0 & 1 \\ \hline\end{array}}_{W^2}+\underbrace{\begin{array}{|c|c|c|}\hline 0 & 1 & 0 \\ \hline -1 & 0 & 0 \\ \hline 0 & 0 & 1 \\ \hline\end{array}}_{W}+\underbrace{\begin{array}{|c|c|c|}\hline 1 & 0 & 0 \\ \hline 0 & 1 & 0 \\ \hline 0 & 0 & 1 \\ \hline\end{array}}_{I}=\begin{array}{|c|c|c|}\hline 0 & 0 & 0 \\ \hline 0 & 0 & 0 \\ \hline 0 & 0 & 4 \\ \hline\end{array}$$

Example

(a) Determine the rotation or rotoinversion axes (or normals in case of reflections) of the following symmetry operations

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

(b) The same for:

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

rotations: $\boldsymbol{Y(W) = W^{k-1} + W^{k-2} + \ldots + W + I}$

reflections: $\boldsymbol{Y(-W) = -W + I}$

Geometric meaning of (W, w)

W information

(c) sense of rotation:

for rotations or
rotoinversions with k>2

det$(\boldsymbol{Z})$: $\boldsymbol{Z} = [\boldsymbol{u}|\boldsymbol{x}|(\det \boldsymbol{W})\boldsymbol{W}\boldsymbol{x}]$

$\boldsymbol{x}$ non-parallel to $\boldsymbol{u}$

Sense of rotation

Example:

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

det W=1 tr W=1

$W=4_{001}$

What is its sense of rotation ?

$$\det(Z): \quad \boldsymbol{Z} = [\boldsymbol{u}|\boldsymbol{x}|(\det \boldsymbol{W})\,\boldsymbol{W}\,\boldsymbol{x}]$$

det Z=?

$$\mathbf{u}=\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \quad \mathbf{x}=\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \quad \mathbf{Wx}=\begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \quad \mathbf{Z}=\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & -1 \\ 1 & 0 & 0 \end{pmatrix}$$

What is the sense of rotation of the operation

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

Fixed points of isometries

$$(W,w)X_f = X_f$$

Fixed points?

$$\left(\begin{array}{|c|c|c|}\hline -1 & 0 & 0 \\ \hline 0 & 1 & 0 \\ \hline 0 & 0 & -1 \\ \hline \end{array} \; \begin{array}{|c|}\hline 0 \\ \hline 0 \\ \hline 1/2 \\ \hline \end{array} \right) \begin{array}{|c|}\hline x \\ \hline y \\ \hline z \\ \hline \end{array} = \begin{array}{|c|}\hline x \\ \hline y \\ \hline z \\ \hline \end{array}$$

solution:

point, line, plane or space

$$\left(\begin{array}{|c|c|c|}\hline -1 & 0 & 0 \\ \hline 0 & 1 & 0 \\ \hline 0 & 0 & -1 \\ \hline \end{array} \; \begin{array}{|c|}\hline 0 \\ \hline 1/2 \\ \hline 1/2 \\ \hline \end{array} \right) \begin{array}{|c|}\hline x \\ \hline y \\ \hline z \\ \hline \end{array} = \begin{array}{|c|}\hline x \\ \hline y \\ \hline z \\ \hline \end{array}$$

NO solution:

translation part **w**= $\begin{array}{|c|}\hline w1 \\ \hline w2 \\ \hline w3 \\ \hline \end{array}$

intrinsic
(screw, glide)

location

Glide or **Screw** component (intrinsic translation part)

$$(\boldsymbol{W},\boldsymbol{w})^k = (\boldsymbol{W},\boldsymbol{w}).\,(\boldsymbol{W},\boldsymbol{w}).\,\ldots\,.(\boldsymbol{W},\boldsymbol{w}) = (\boldsymbol{I},\boldsymbol{t})$$

$$(\boldsymbol{W},\boldsymbol{w})^k = (\boldsymbol{W}^k,(\boldsymbol{W}^{k-1}+\ldots+\boldsymbol{W}+\boldsymbol{I})\boldsymbol{w}) = (\boldsymbol{I},\boldsymbol{t})$$

screw rotations : $\boxed{\boldsymbol{t}/k = 1/k\,(\boldsymbol{W}^{k-1}+\ldots+\boldsymbol{W}+\boldsymbol{I})\boldsymbol{w}}$

glide reflections: $\boldsymbol{t}/k = \frac{1}{2}(\boldsymbol{W}+\boldsymbol{I})w$

Determine the glide/screw component of the operations (if relevant)

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

Fixed points of (W,w)

Location (fixed points x_F):

(B1) $t/k = 0$:

$$(\boldsymbol{W}, \boldsymbol{w})\boldsymbol{x}_F = \boldsymbol{x}_F$$

(B2) $t/k \neq 0$:

$$(\boldsymbol{W}, \boldsymbol{w}_{lp})\boldsymbol{x}_F = \boldsymbol{x}_F$$

$$\boldsymbol{w}_{lp} = \boldsymbol{w} - \boldsymbol{t}/k$$

Determine the fixed points of the operations

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

SYMMETRY OPERATIONS AND THEIR MATRIX-COLUMN PRESENTATION in ITA

Space group $Cmm2$ (No. 35)

How are the symmetry operations represented in ITA ?

Diagram of symmetry elements

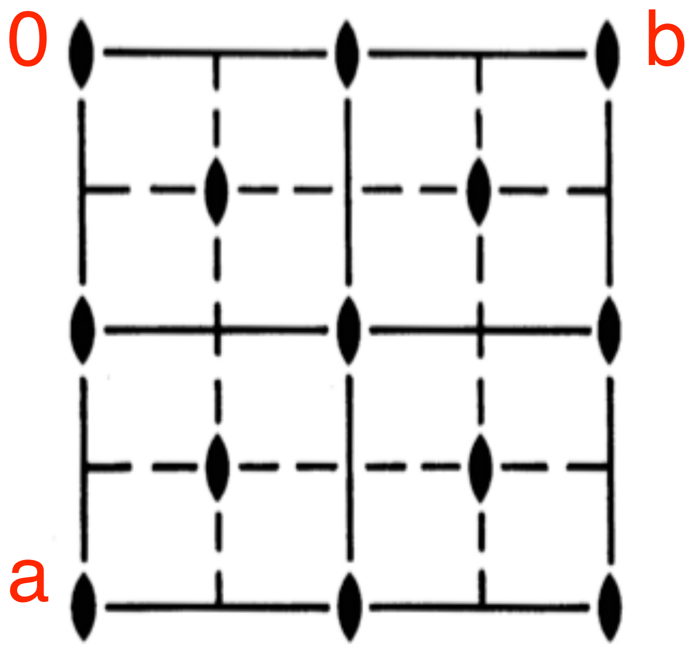
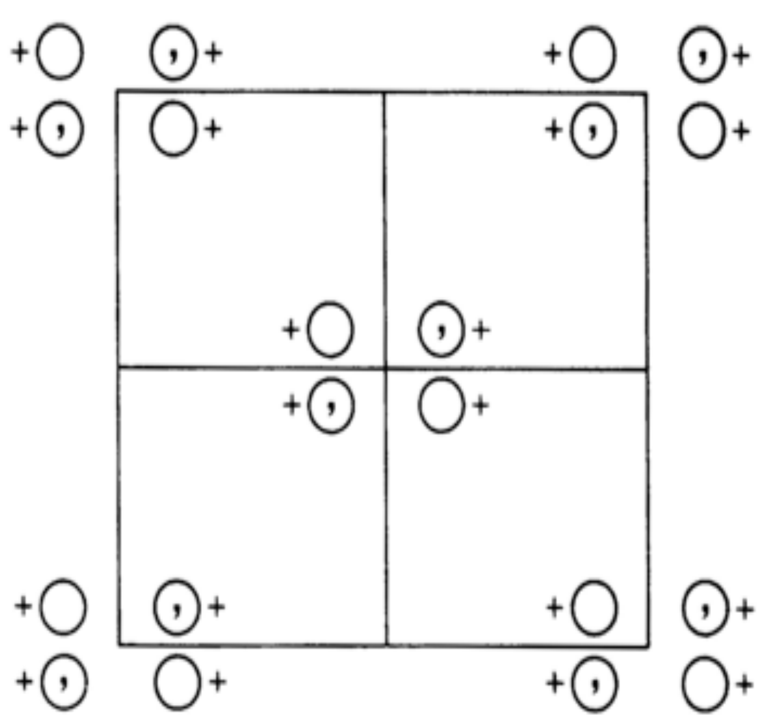


Diagram of
general position points



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

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

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

General position

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

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

(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

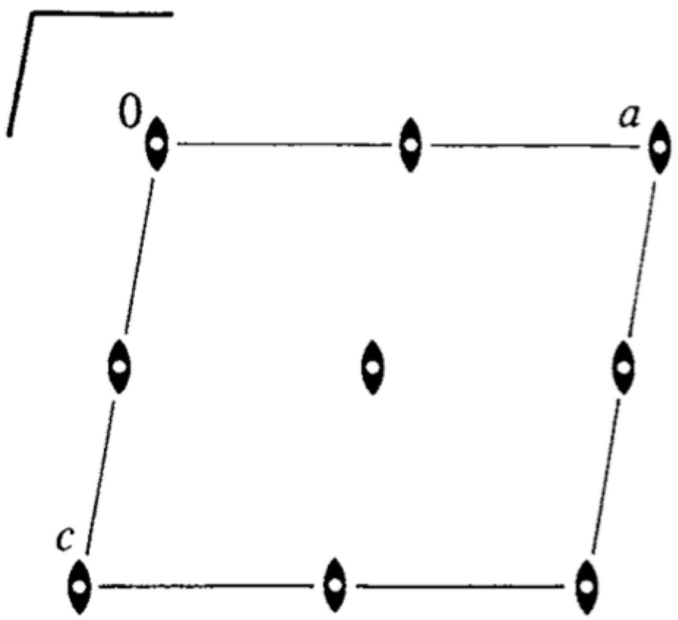
isomorphic to the point group P_G of G

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

Example: P12/m1

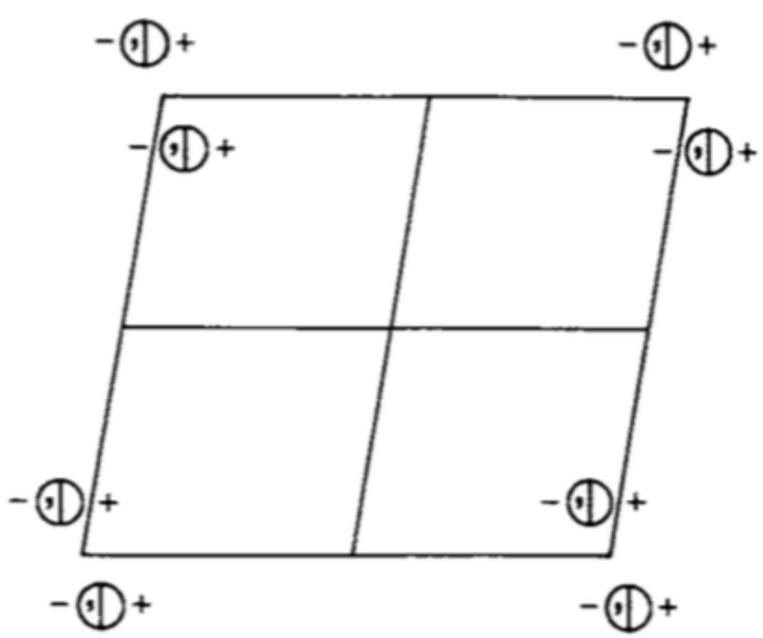
Coset decomposition $G:T_G$

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



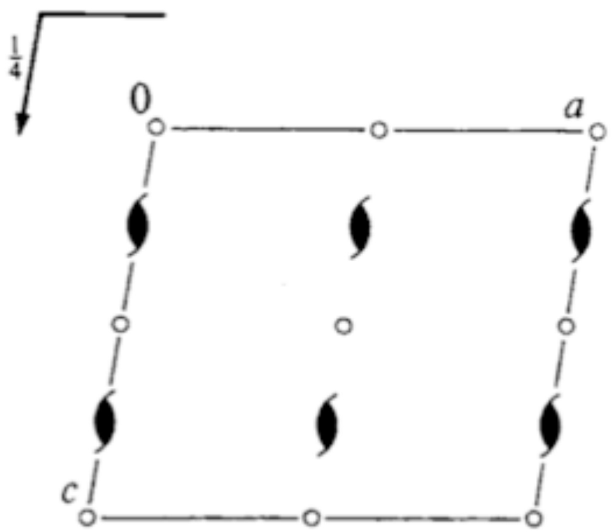
inversion centres $(\bar{1},t)$:

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

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_1screw axes

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

$\rightarrow$ $(2,u\ \frac{1}{2}\ \frac{1}{2}+w)$

Example: Cmm2

Diagram of symmetry elements

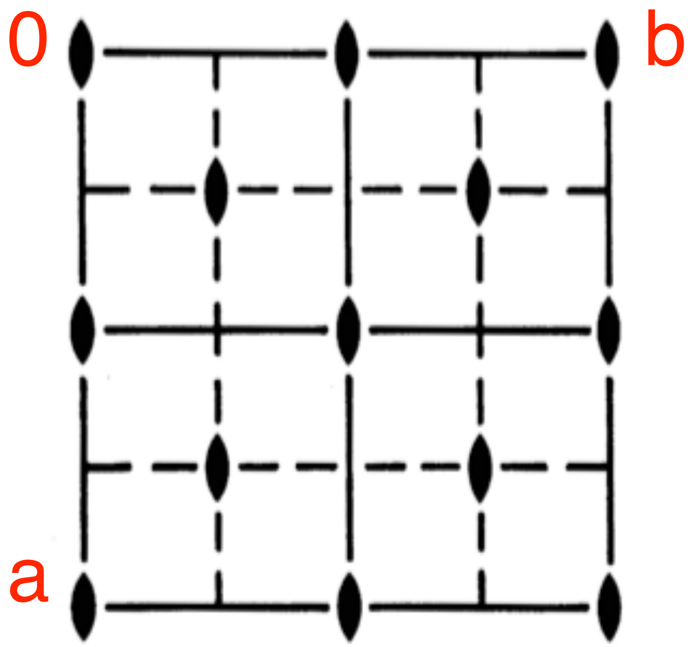
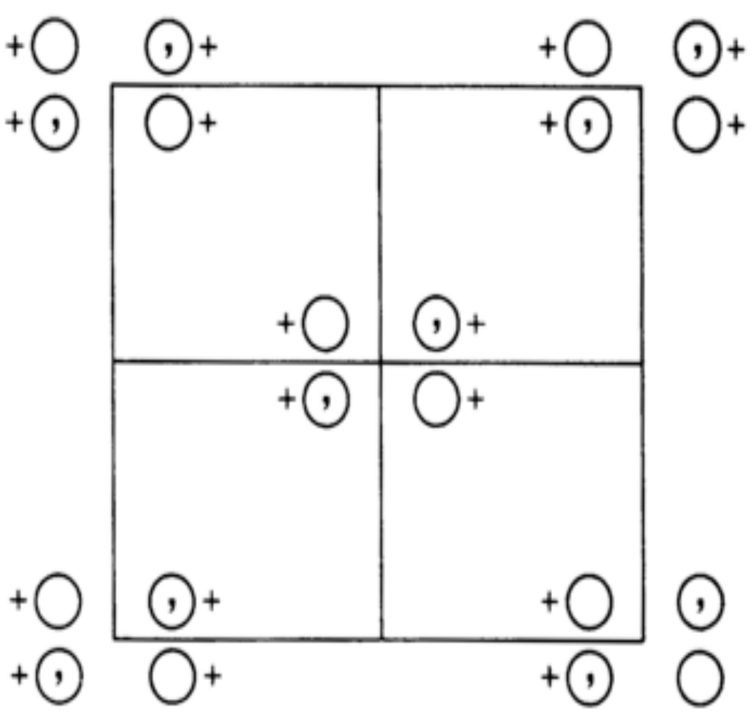


Diagram of
general position points



Coordinates

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

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	$T_G\,2$	$T_G\,m_y$	$T_G\,m_x$
$(I,0)$	$(2,0)$	$(m_y,0)$	$(m_x,0)$
(I,t_1)	$(2,t_1)$	(m_y,t_1)	(m_x, t_1)
(I,t_2)	$(2,t_2)$	(m_y,t_2)	(m_x,t_2)
...	...	...	...
(I,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 $\frac{1}{4},y,z$

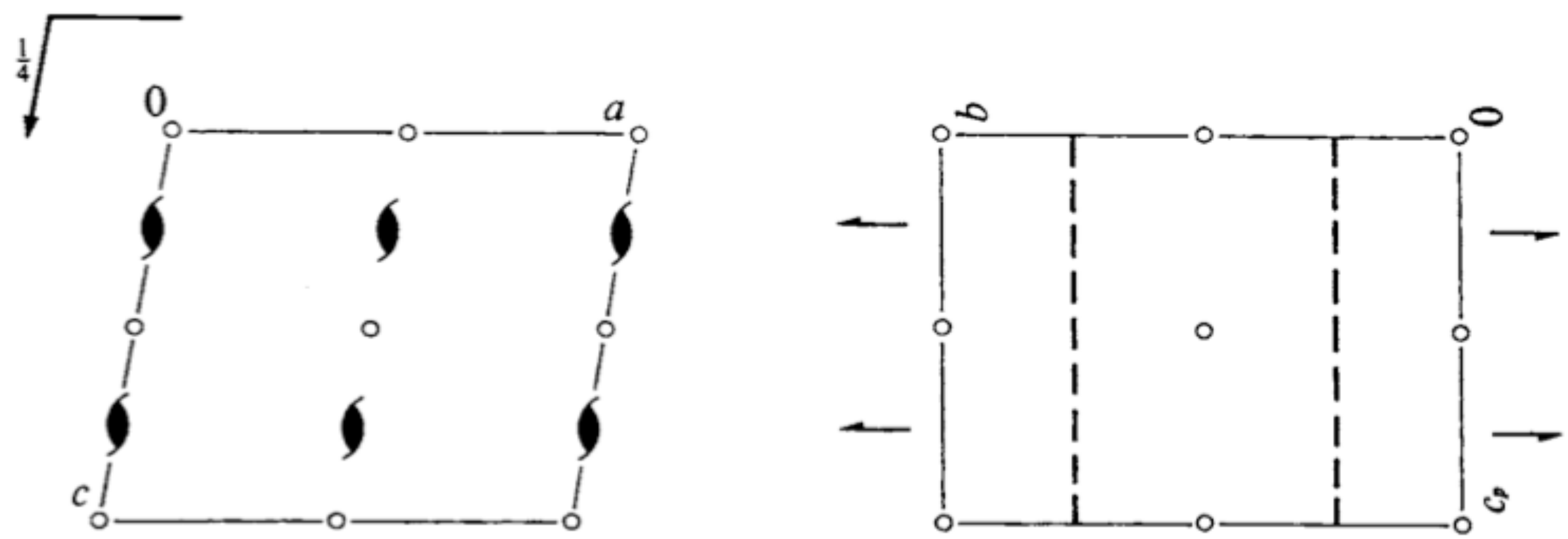
Space group $P2_1/c$ (No. 14)

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

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

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: Space group $P2_1/c$ (14)

BCS: GENPOS

Space-group symmetry operations

short-hand notation

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

Geometric interpretation

Seitz symbols

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

Click here to get the general positions in text format

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

ITA data

General positions

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

Symmetry operations

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

SEITZ SYMBOLS FOR SYMMETRY OPERATIONS

Seitz symbols { R | t }

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

rotation (or linear) part R

- specify the type and the order of the symmetry operation;
- orientation of the symmetry element by the direction of the axis for rotations and rotoinversions, or the direction of the normal to reflection planes.

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

translation part t

translation parts of the coordinate triplets of the *General position* blocks

EXAMPLE

Seitz symbols for symmetry operations of hexagonal and trigonal crystal systems

ITA description				Seitz symbol
No.	coord. triplet	type	orien-tation	
1)	x, y, z	1		1
2)	$\bar{y}, x-y, z$	3^+	$0, 0, z$	3^+_{001}
3)	$\bar{x}+y, \bar{x}, z$	3^-	$0, 0, z$	3^-_{001}
4)	$\bar{x}, \bar{y}, z$	2	$0, 0, z$	2_{001}
5)	$y, \bar{x}+y, z$	6^-	$0, 0, z$	6^-_{001}
6)	$x-y, x, z$	6^+	$0, 0, z$	6^+_{001}
7)	$y, x, \bar{z}$	2	$x, x, 0$	2_{110}
8)	$x-y, \bar{y}, \bar{z}$	2	$x, 0, 0$	2_{100}
9)	$\bar{x}, \bar{x}+y, \bar{z}$	2	$0, y, 0$	2_{010}
10)	$\bar{y}, \bar{x}, \bar{z}$	2	$x, \bar{x}, 0$	$2_{1\bar{1}0}$
11)	$\bar{x}+y, y, \bar{z}$	2	$x, 2x, 0$	2_{120}
12)	$x, x-y, \bar{z}$	2	$2x, x, 0$	2_{210}

ITA description				Seitz symbol
No.	coord. triplet	type	orien-tation	
13)	$\bar{x}, \bar{y}, \bar{z}$	$\bar{1}$		$\bar{1}$
14)	$y, \bar{x}+y, \bar{z}$	$\bar{3}^+$	$0, 0, z$	$\bar{3}^+_{001}$
15)	$x-y, x, \bar{z}$	$\bar{3}^-$	$0, 0, z$	$\bar{3}^-_{001}$
16)	$x, y, \bar{z}$	m	$x, y, 0$	m_{001}
17)	$\bar{y}, x-y, \bar{z}$	$\bar{6}^-$	$0, 0, z$	$\bar{6}^-_{001}$
18)	$\bar{x}+y, \bar{x}, \bar{z}$	$\bar{6}^+$	$0, 0, z$	$\bar{6}^+_{001}$
19)	$\bar{y}, \bar{x}, z$	m	$x, \bar{x}, z$	m_{110}
20)	$\bar{x}+y, y, z$	m	$x, 2x, z$	m_{100}
21)	$x, x-y, z$	m	$2x, x, z$	m_{010}
22)	y, x, z	m	x, x, z	$m_{1\bar{1}0}$
23)	$x-y, \bar{y}, z$	m	$x, 0, z$	m_{120}
24)	$\bar{x}, \bar{x}+y, z$	m	$0, y, z$	m_{210}

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

EXAMPLE

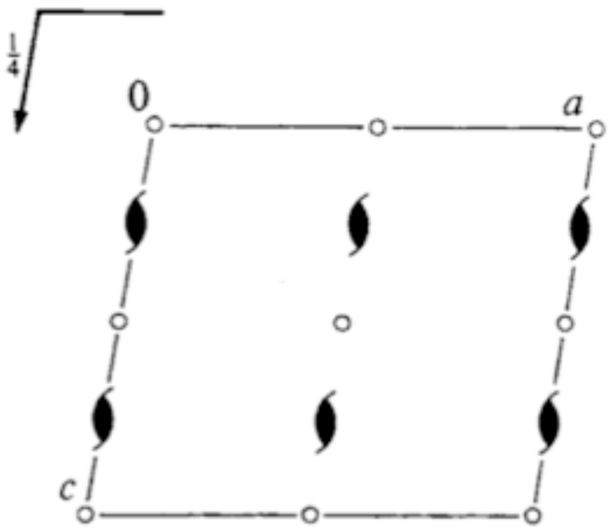
International Tables for Crystallography (2006). Vol. A, Space gro

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

$P2_1/c$ C_{2h}^5 $2/m$ $\bar{1}$

No. 14 $P\,1\,2_1/c\,1$ 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) $\{m_{010}|0\,1/2\,1/2\}$

NOT in ITA

SPACE-GROUPS DIAGRAMS

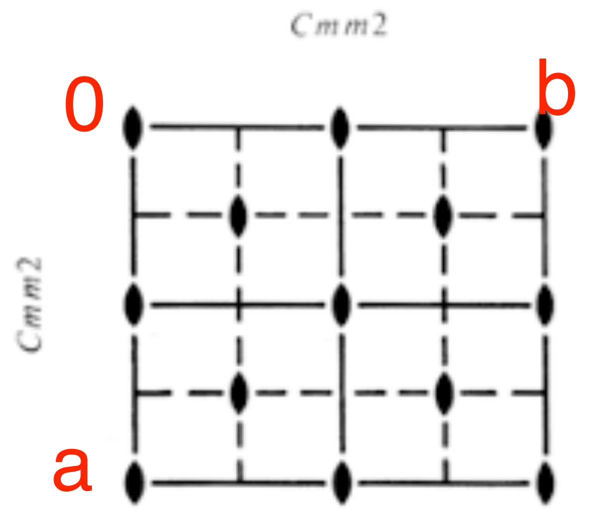
SYMMETRY ELEMENTS

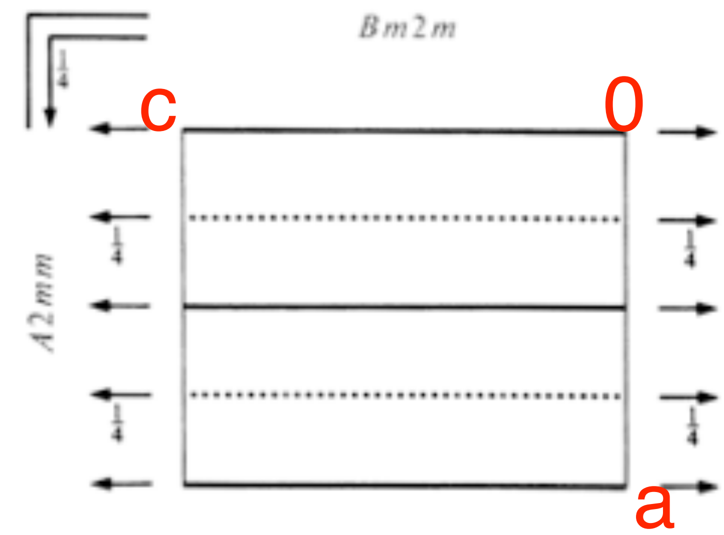
*Cmm*2 (No. 35)

Space-group diagrams

Symmetry-element diagrams

three different projections





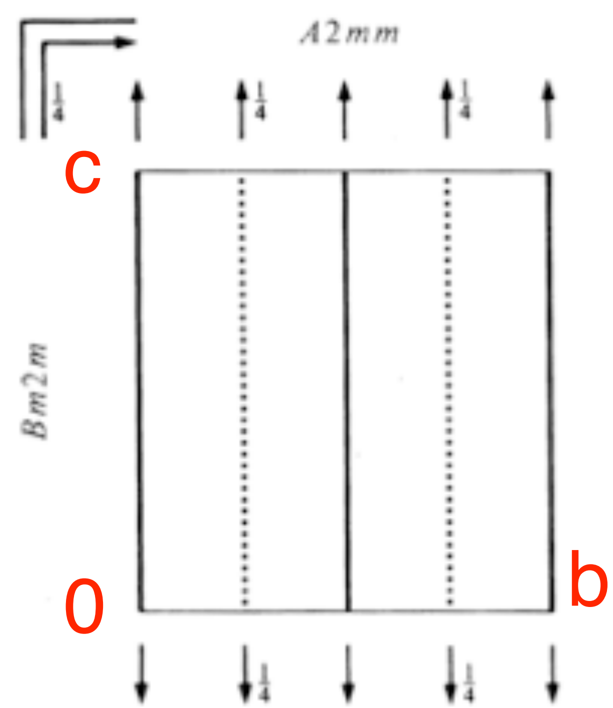
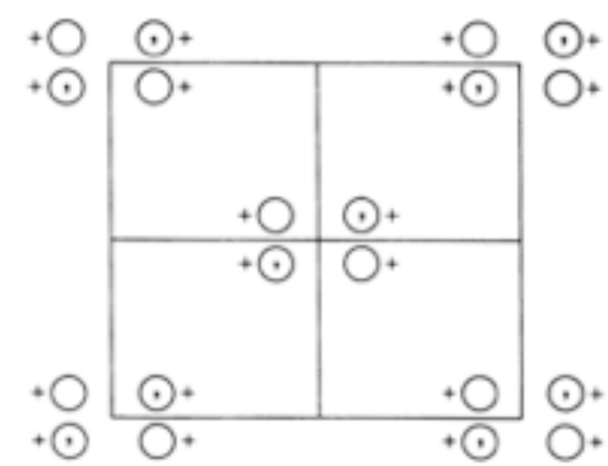


Diagram of general position points



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

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

EXAMPLE

Space group *Cmm*2 (No. 35)

Geometric interpretation

(6) Symmetry operations

For (0,0,0)+ set

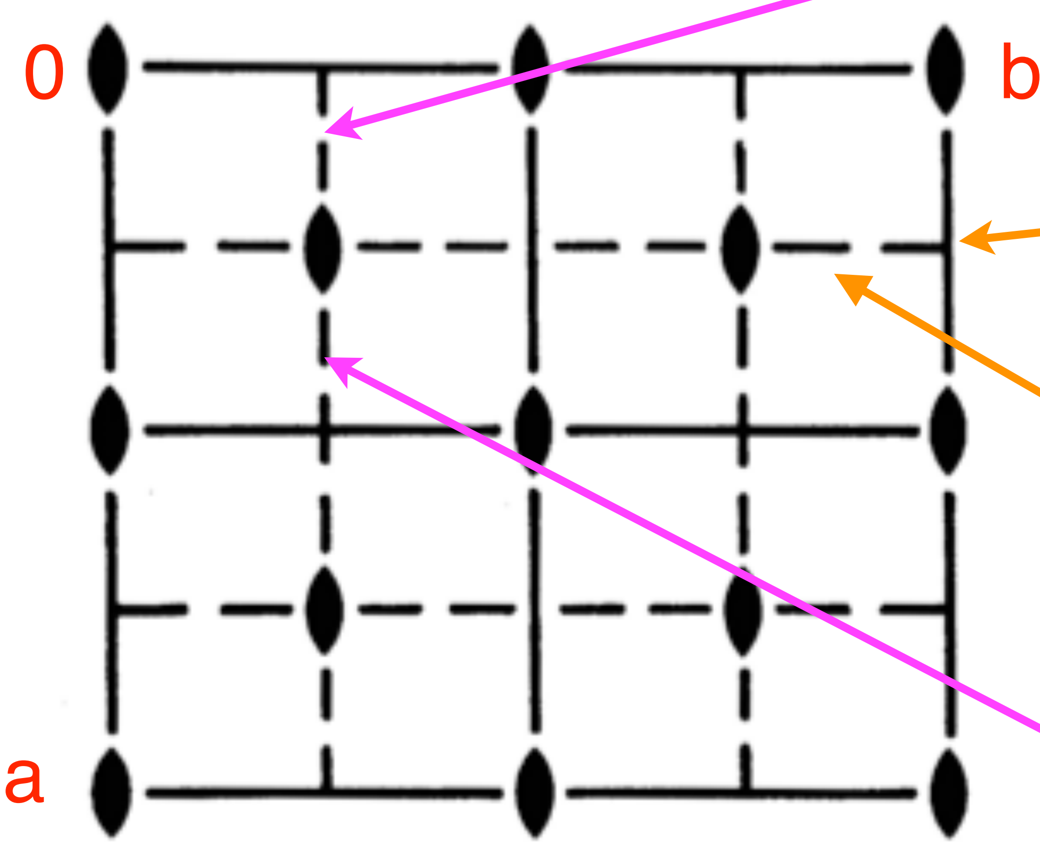
(1) 1 (2) 2 0,0,z (3) m x,0,z (4) m 0,y,z

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)+

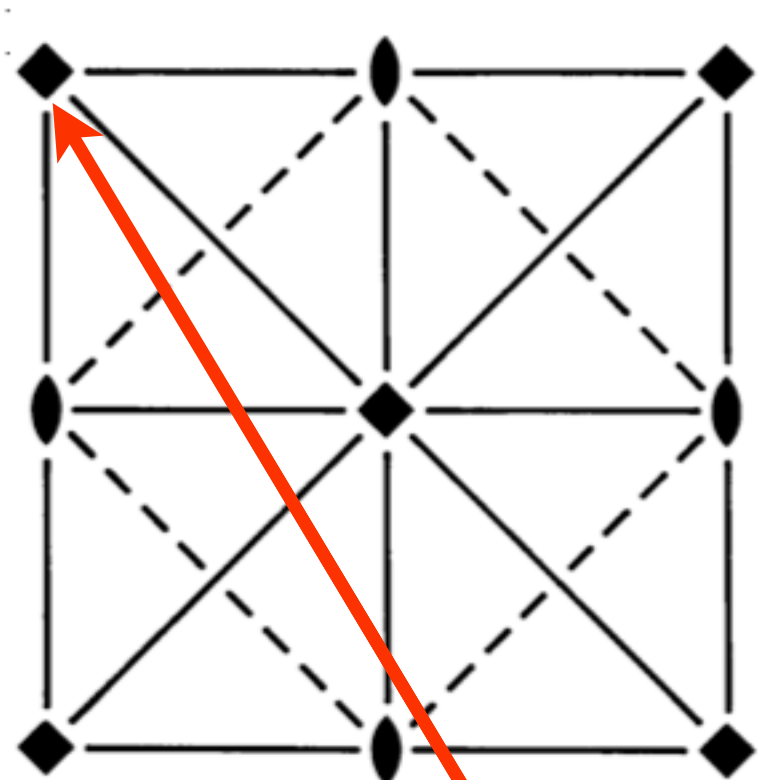
8 f 1 (1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $x,\bar{y},z$ (4) $\bar{x},y,z$

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

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

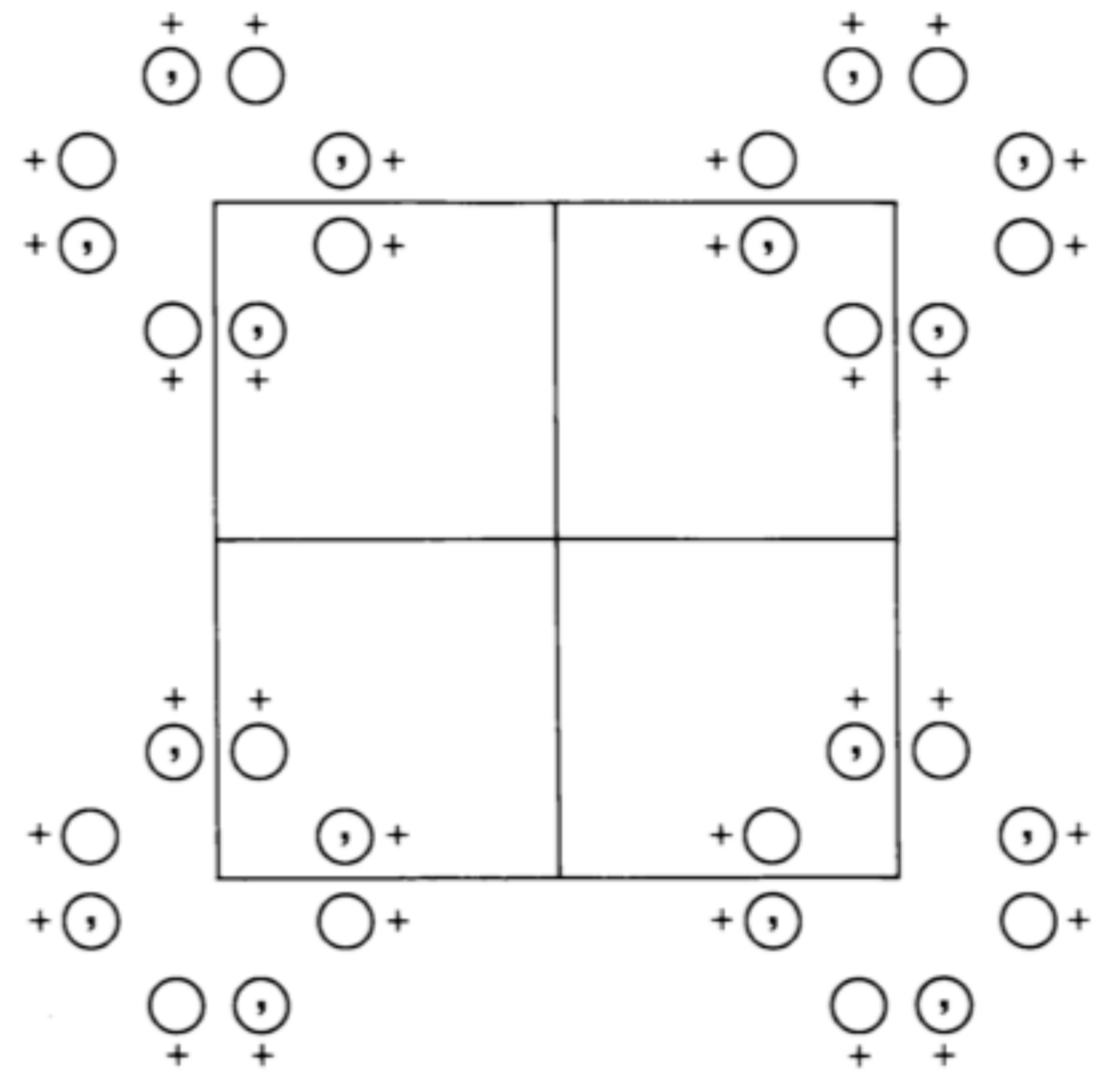
Example: P4mm

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 + 1^{st}, ..., $(n-1)^{th}$ 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

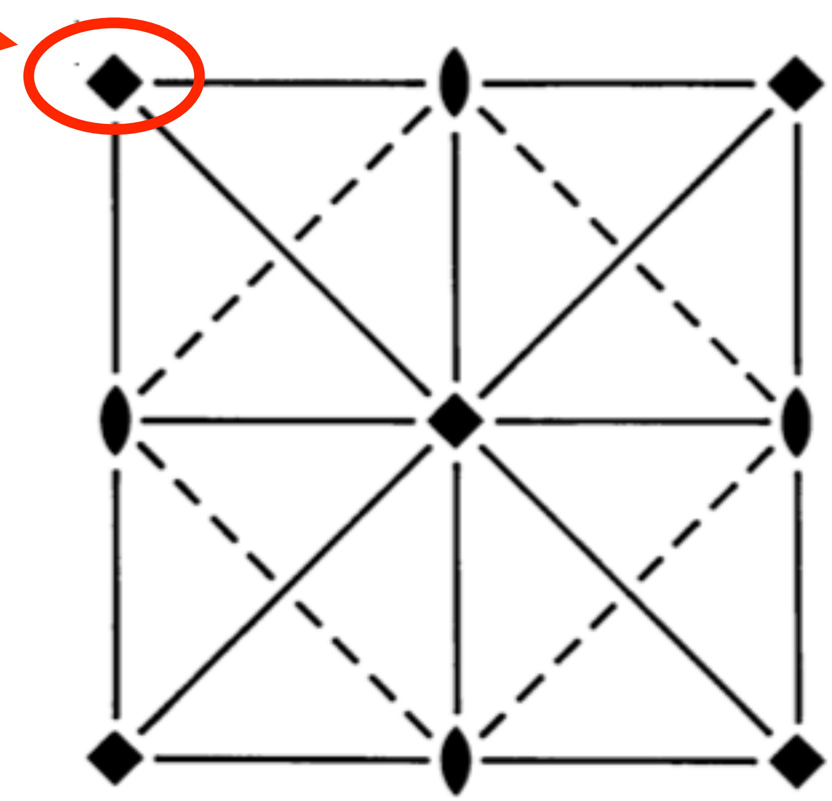
Diagram of symmetry elements

Symmetry operations that share (0,0,z) as geometric element } 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**
...	**...**

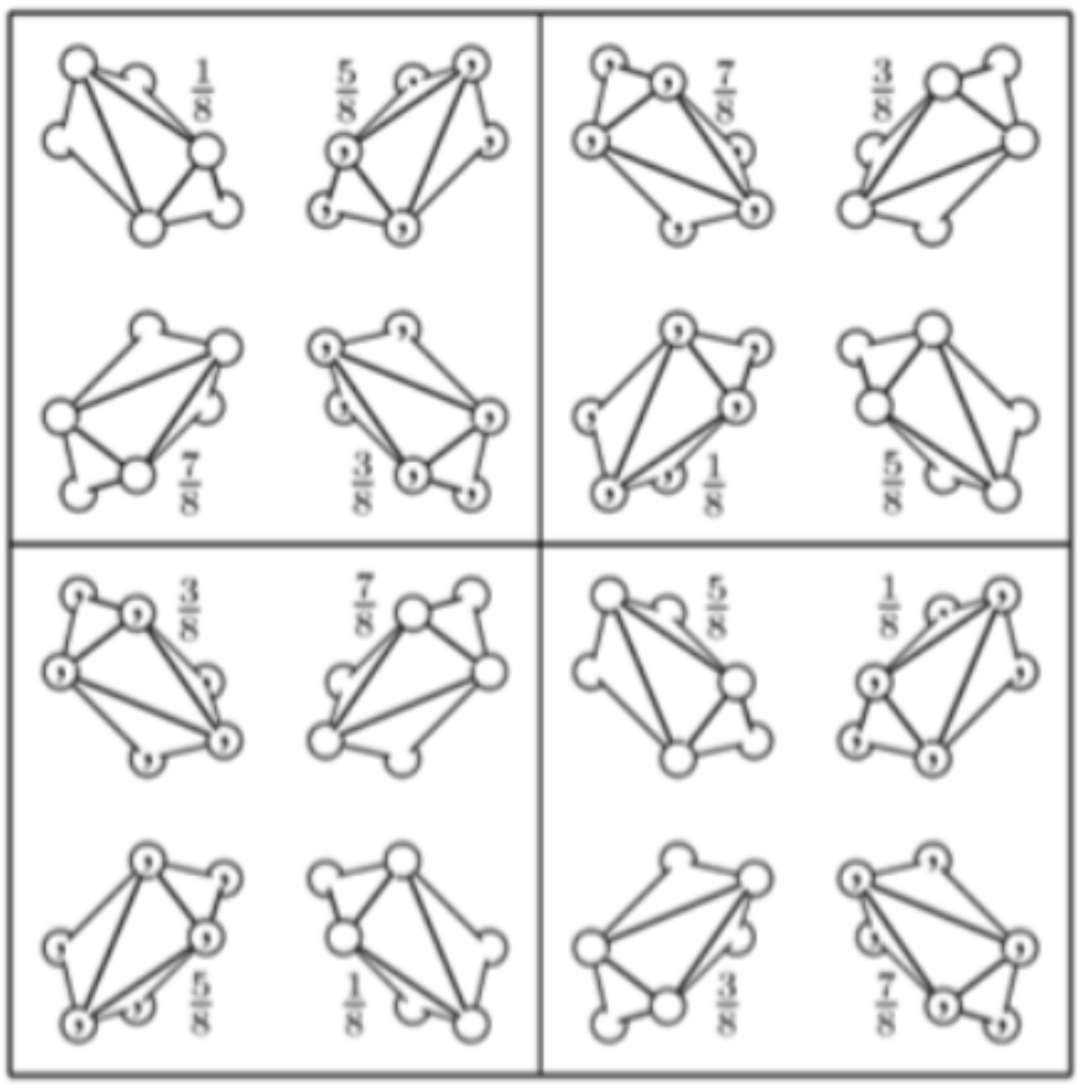


Example: $Ia\bar{3}d$ (No. 230)

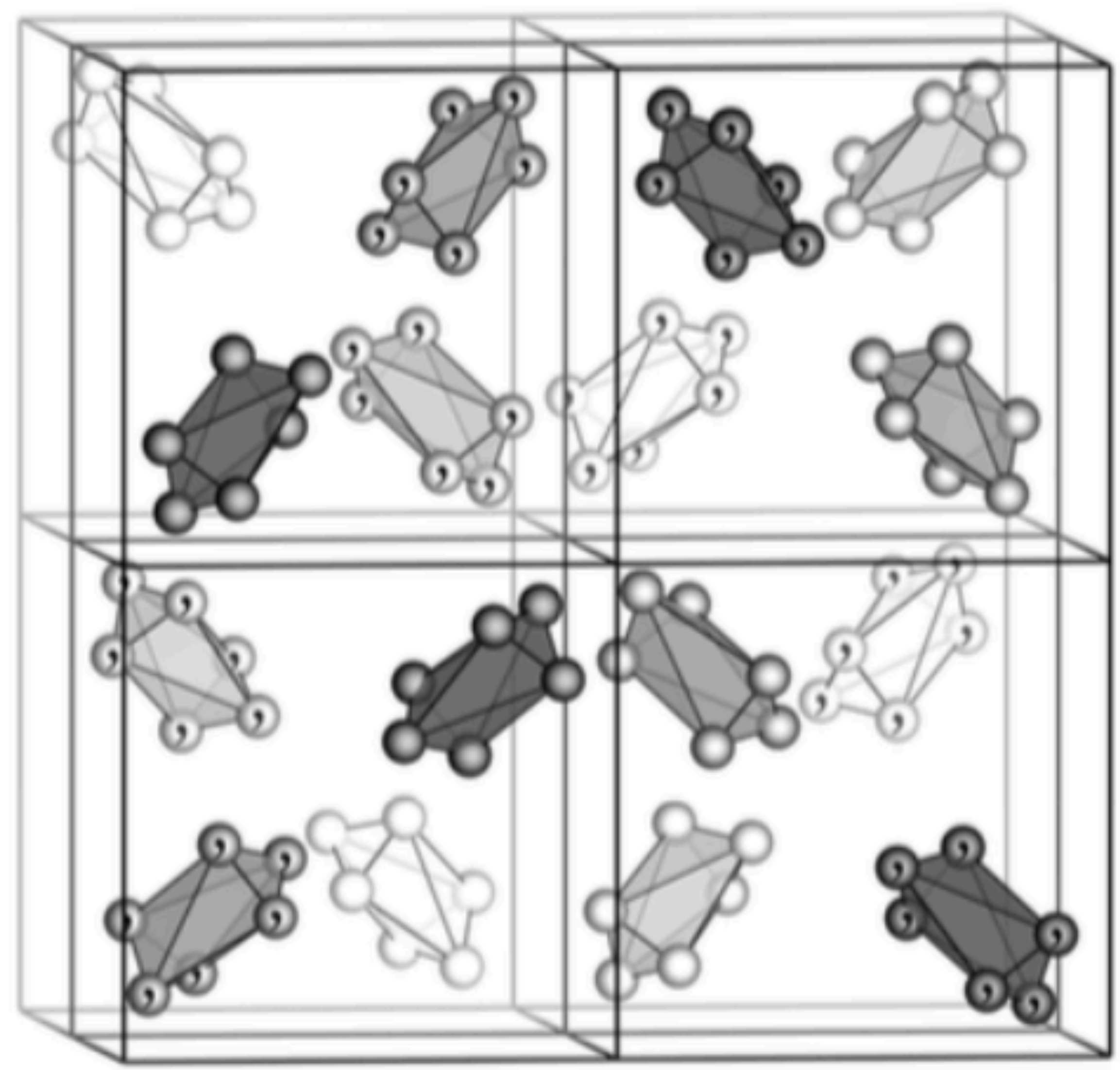
Diagrams of general position points

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

orthogonal projection



perspective projection

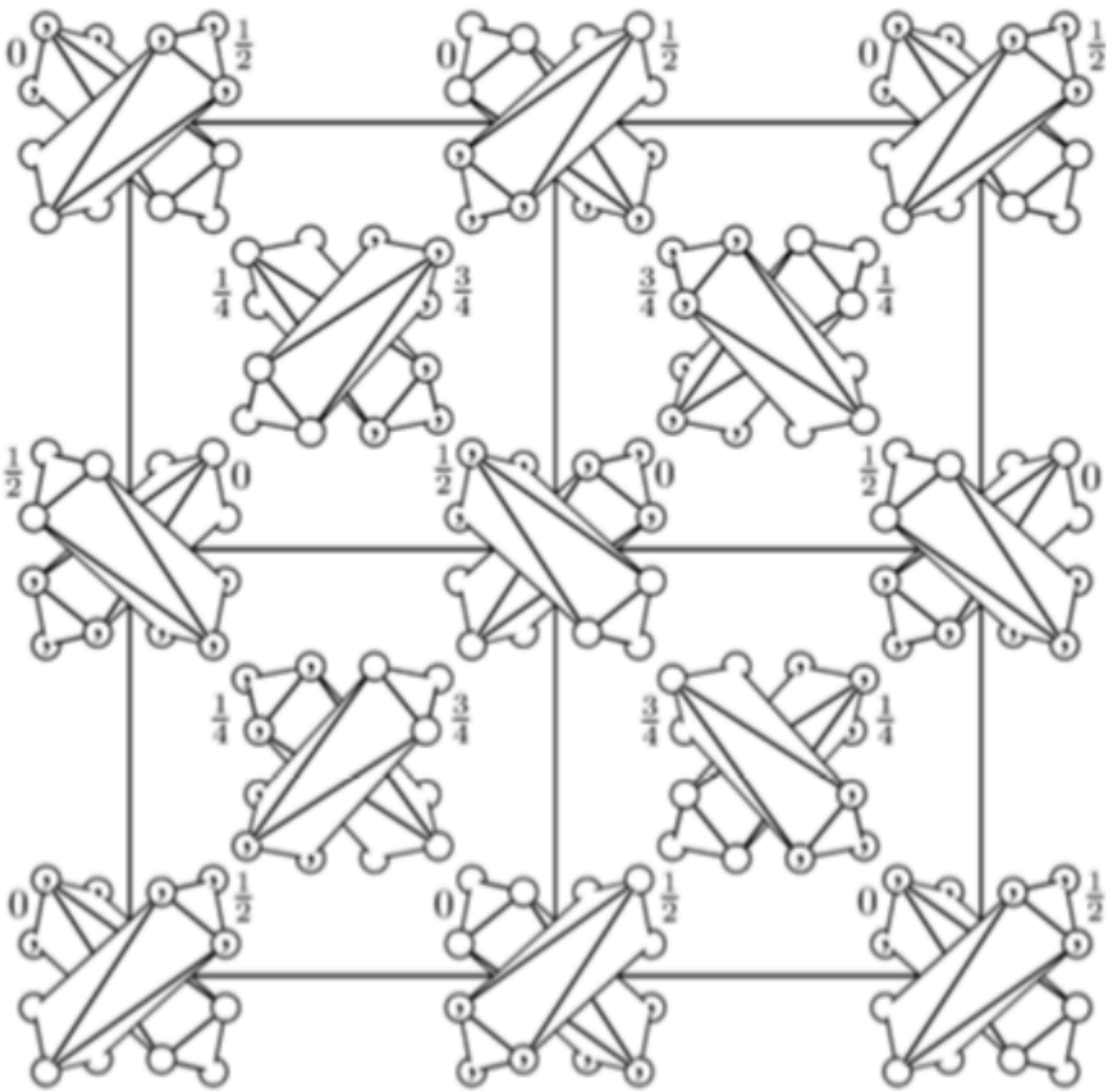


polyhedra (twisted trigonal antiprism) centres at (1/8,1/8,1/8) and its equivalent points, site symmetry .32.

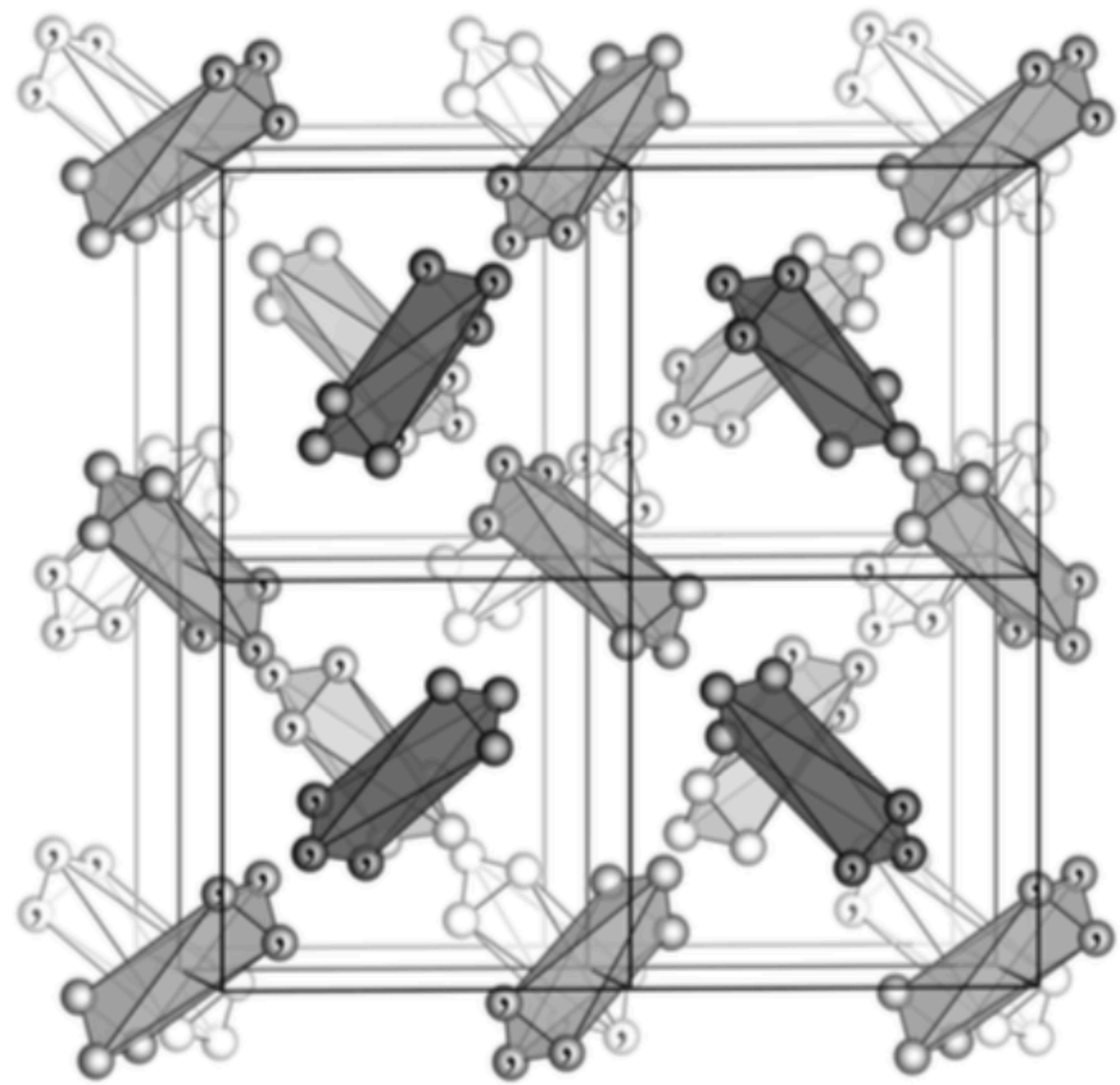
Example: I$a\bar{3}d$ (No. 230)

Diagrams of general position points

orthogonal projection



perspective projection

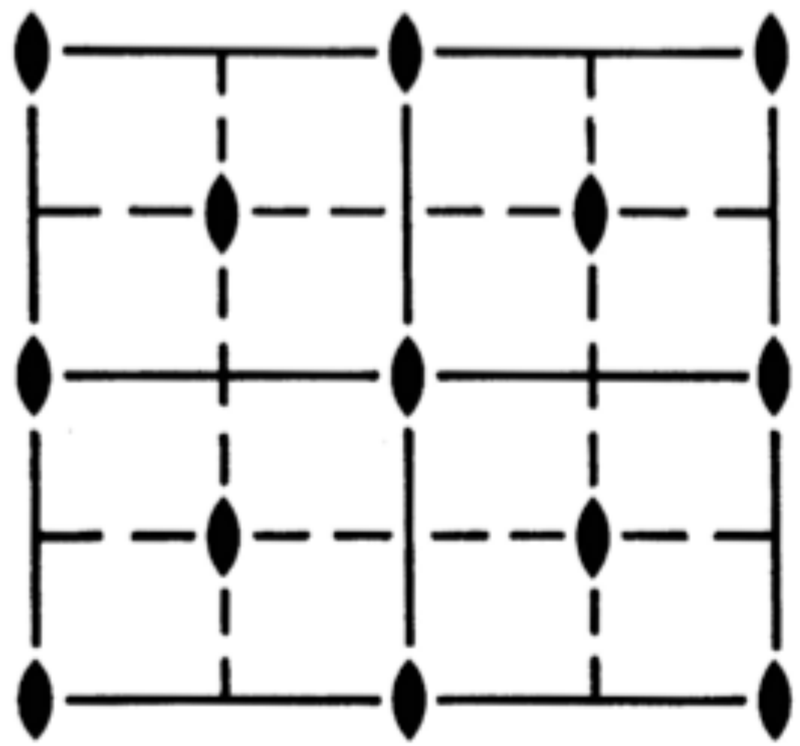


polyhedra (twisted trigonal antiprism) centres at (0,0,0) and its equivalent points, site symmetry .-3.

ORIGINS AND ASYMMETRIC UNITS

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

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



Origin on $mm2$

Origin statement

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

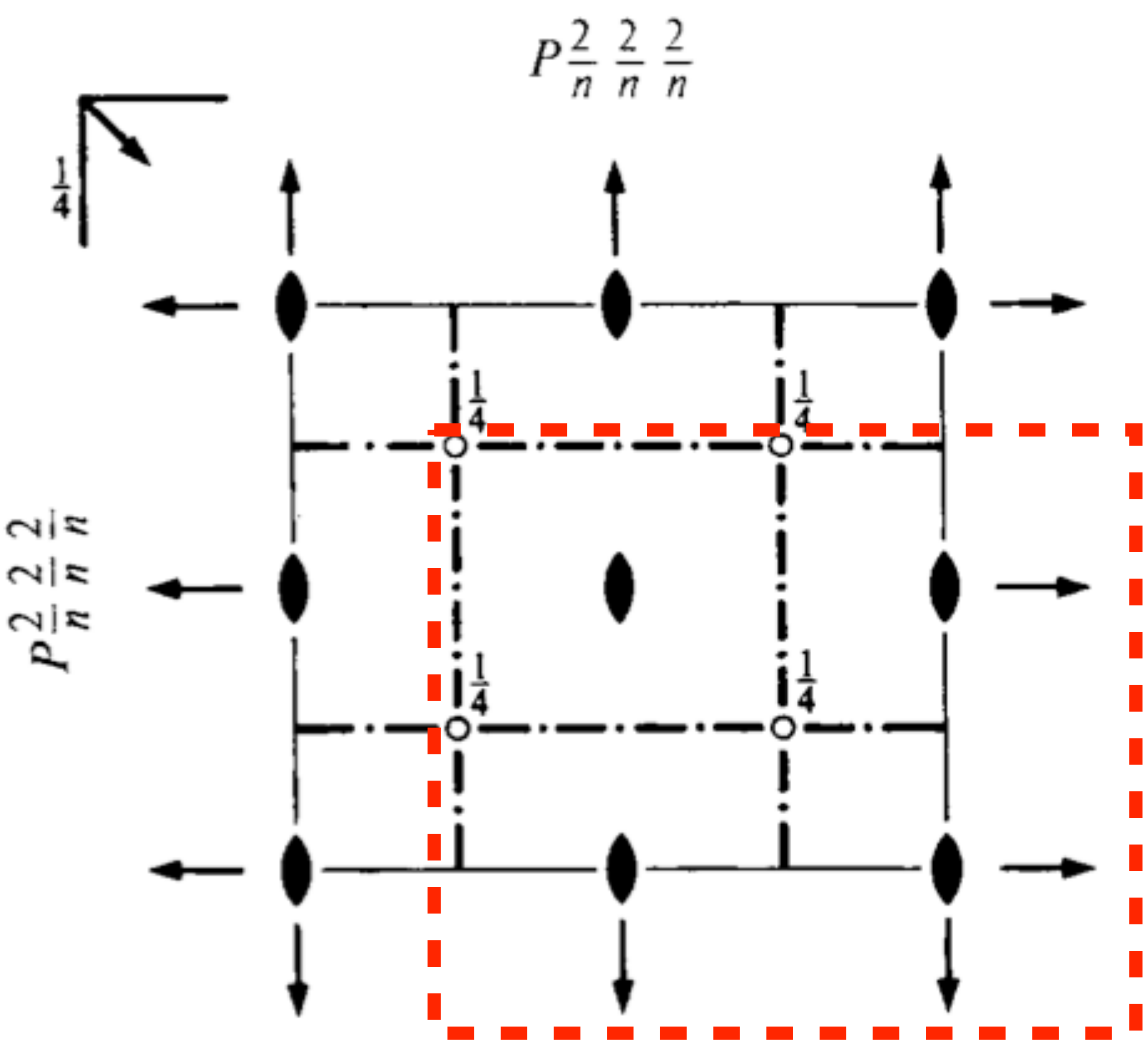
Space groups with two origins

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

Example: Different origins for *Pnnn*

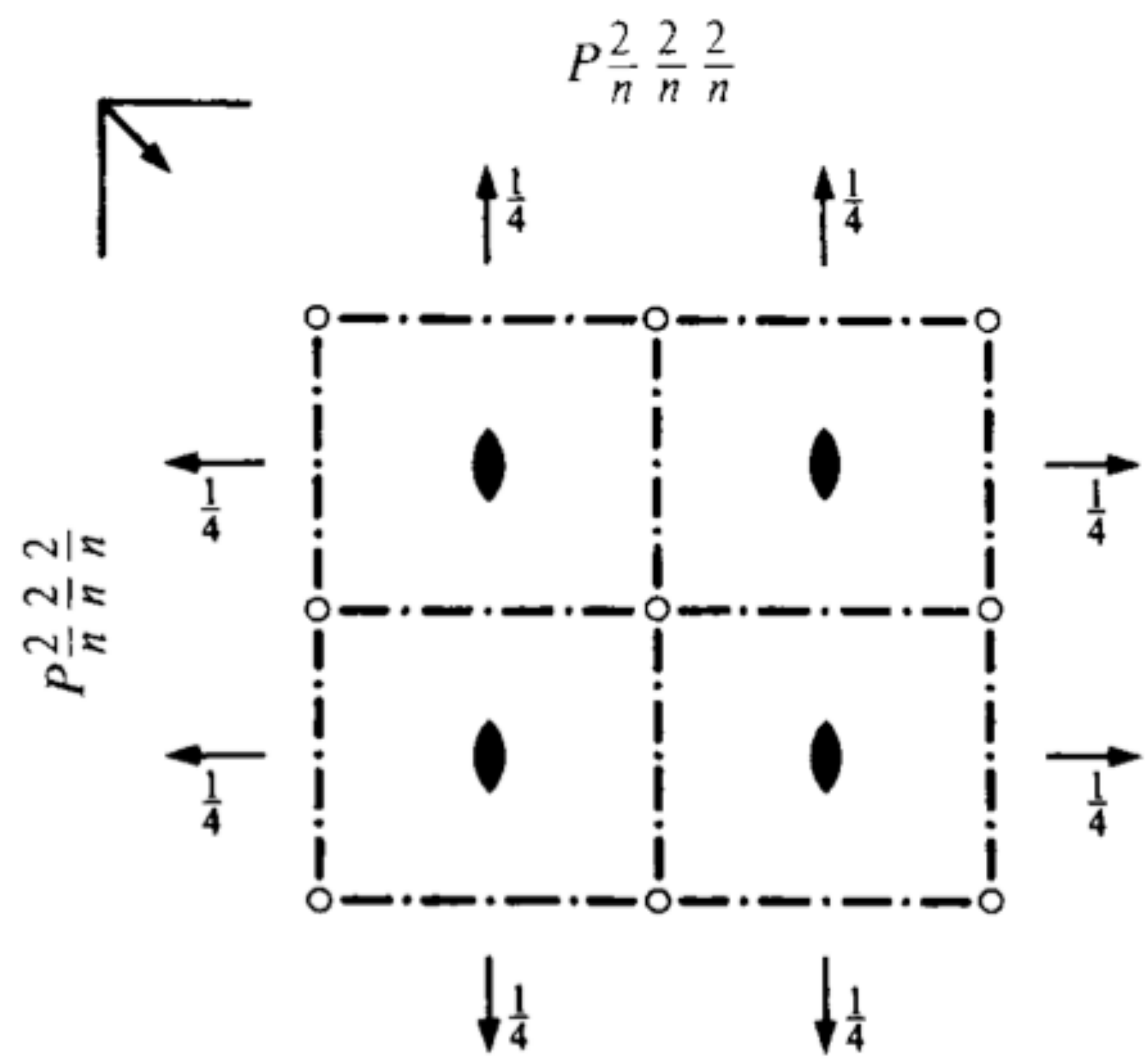
$Pnnn$	D_{2h}^{2}	mmm	Orthorhombic
No. 48	$P\ 2/n\ 2/n\ 2/n$		Patterson symmetry $Pmmm$

ORIGIN CHOICE 1



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

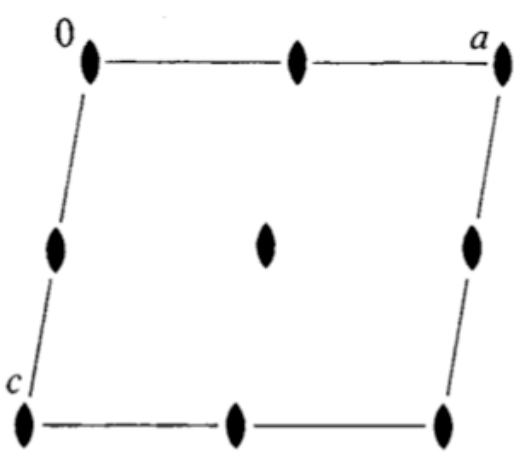
ORIGIN CHOICE 2

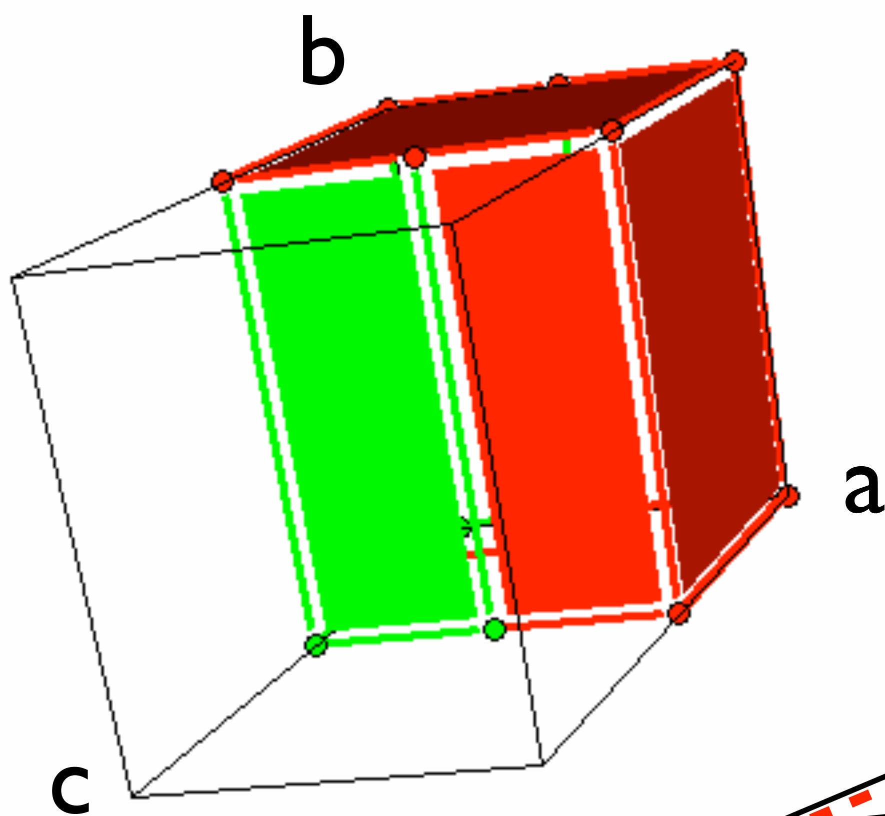


Origin at $\bar{1}$ at nnn, at $-\frac{1}{4},-\frac{1}{4},-\frac{1}{4}$ from 222

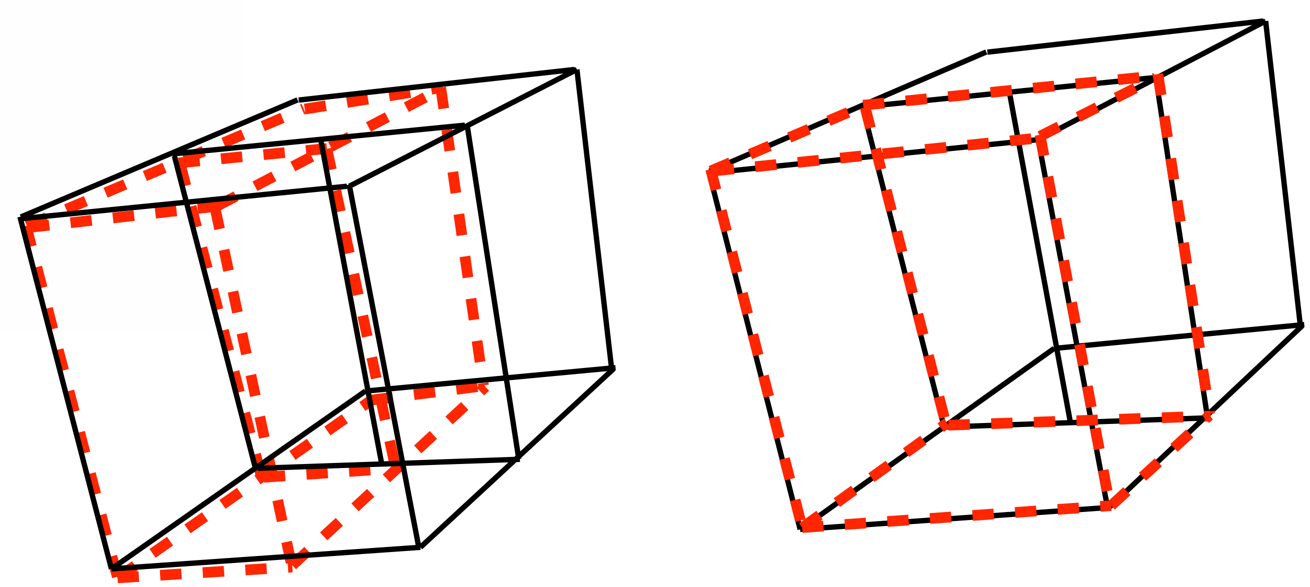
Example: Asymmetric units for the space group P121

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.





non-uniqueness

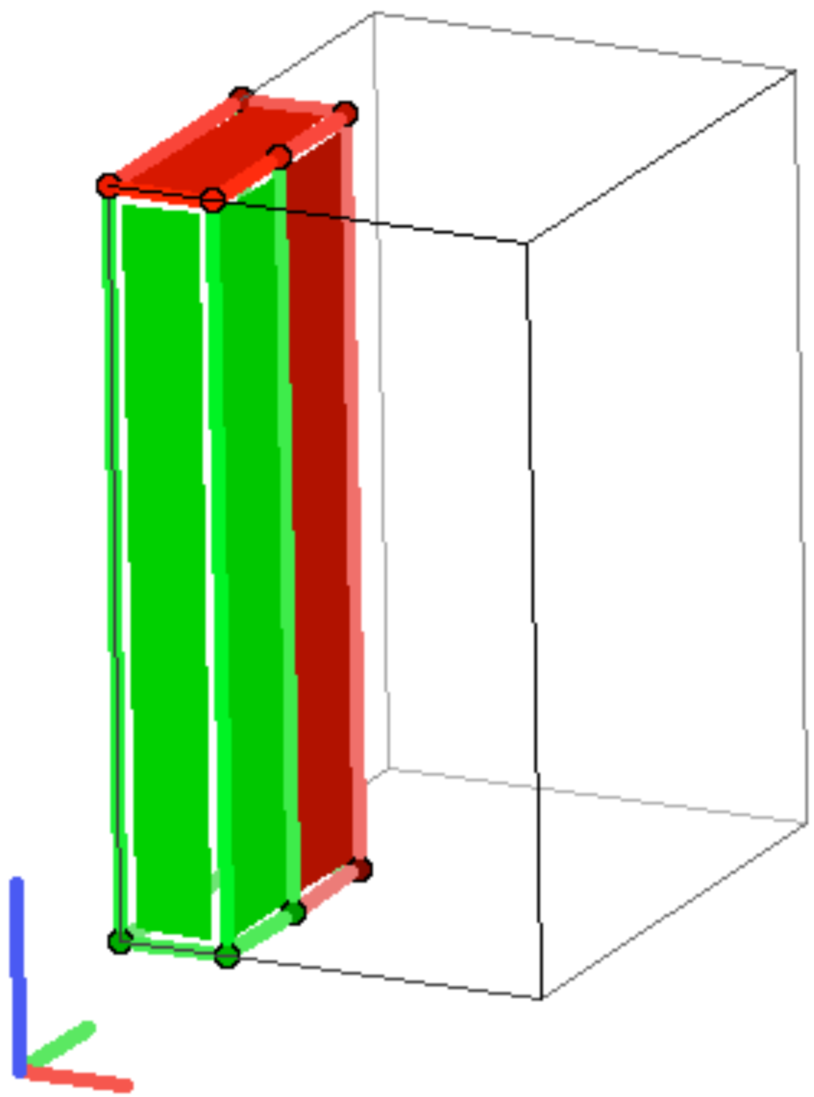


Number of vertices: 8	Number of facets: 6
0, 1, 1/2	x>=0
1, 1, 0	x<1
1, 0, 0	y>=0
0, 0, 1/2	y<1
1, 0, 1/2	z>=0 [x<=1/2]
0, 0, 0	z<=1/2 [x<=1/2]
0, 1, 0	
1, 1, 1/2	[Guide to notation]

(output cctbx: Ralf Grosse-Kustelve)

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

(output cctbx: Ralf Grosse-Kustelve)

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

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: $|P|/|S_o|$

Oriented symbols of site-symmetry groups

General position

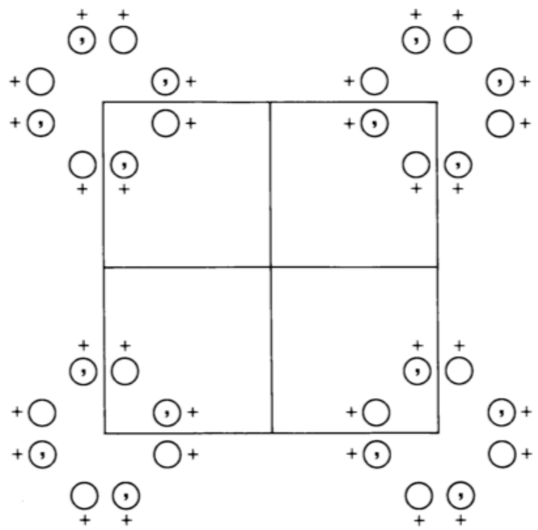
(i) **coordinate triplets** of an image point $\tilde{X}$ of the original point $X = \begin{bmatrix} x \\ y \\ z \end{bmatrix}$ under (W,w) of G

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

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

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

General Position of Space groups



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

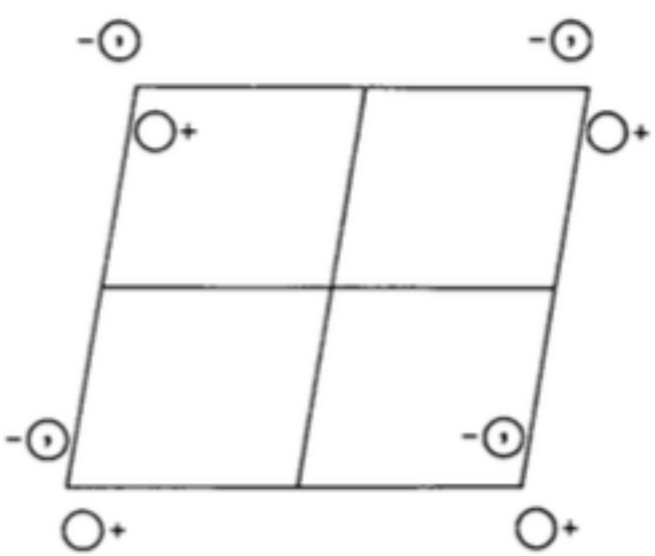
- presentation of infinite image points $\tilde{X}$ of X under the action of (W,w) of G: $0 \leq x_i < 1$

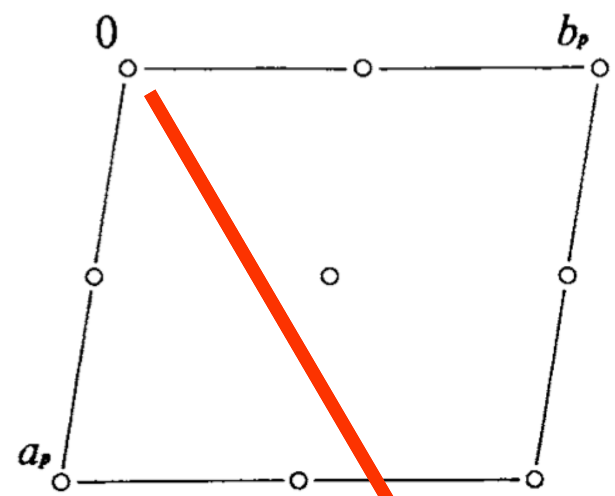
General position

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

Example: Calculation of the Site-symmetry groups

Group P-1





Positions

Multiplicity, Wyckoff letter, Site symmetry			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	$\bar{1}$	$0,0,0$	

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

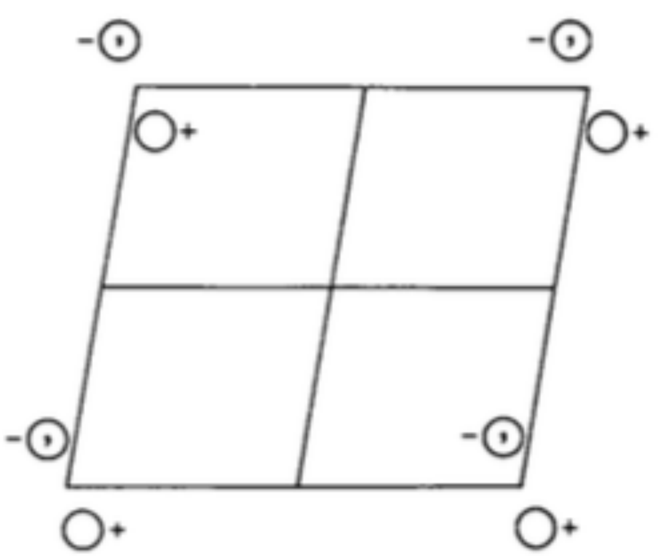
$$\left(\begin{array}{ccc|c} -1 & & & 0 \\ & -1 & & 0 \\ & & -1 & 0 \end{array}\right)\begin{pmatrix}0\\0\\0\end{pmatrix} = \begin{pmatrix}0\\0\\0\end{pmatrix}$$

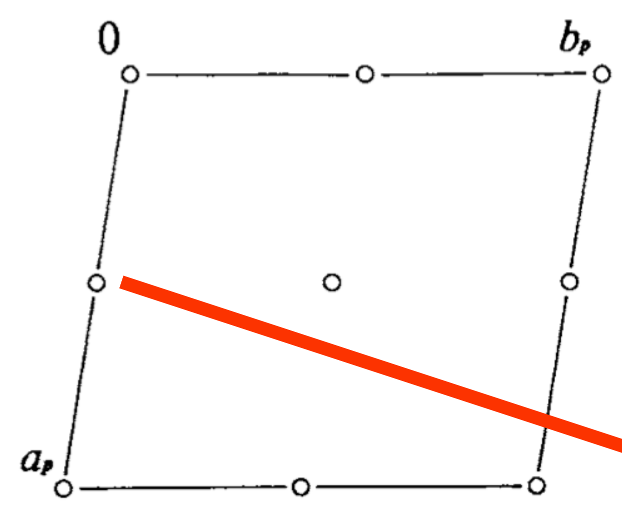
$S_f=\{(1,0),\ (-1,000)X_f = X_f\}$

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

QUIZ: Calculation of the Site-symmetry groups

Group P-1





Positions

Multiplicity, Wyckoff letter, Site symmetry			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*	$\bar{1}$	$0,0,0$	

Determine the site symmetry group of the point

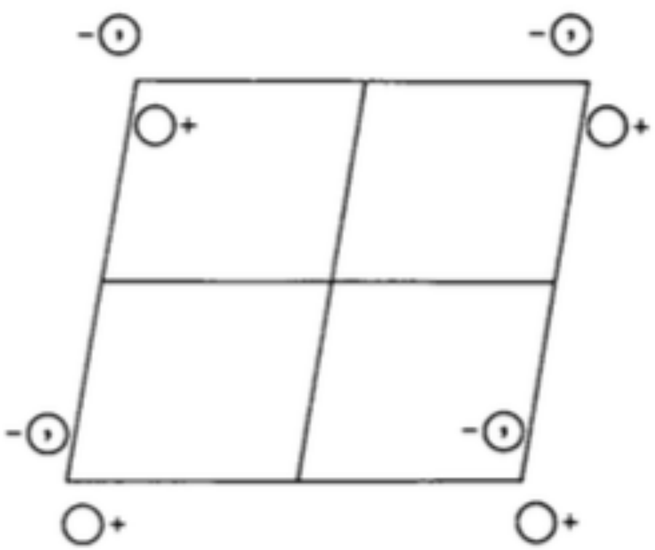
$$X_o = \begin{bmatrix} 1/2 \\ 0 \\ 1/2 \end{bmatrix}$$

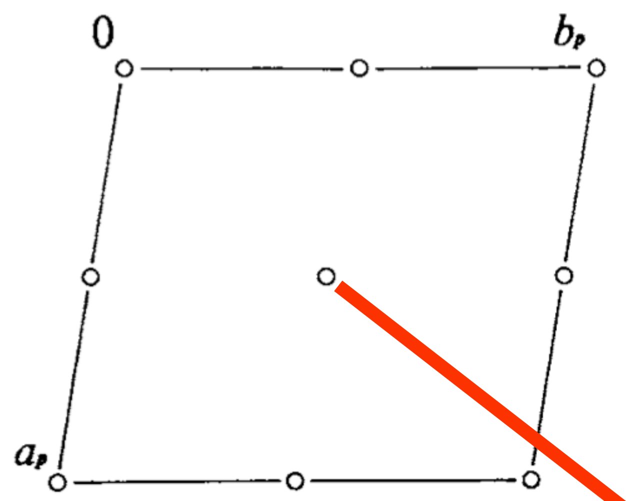
Hint: $\boxed{S=\{(W,w),\ (W,w)X_o = X_o\}}$

QUIZ: Calculation of the Site-symmetry groups

Group P-1

Solution





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

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

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

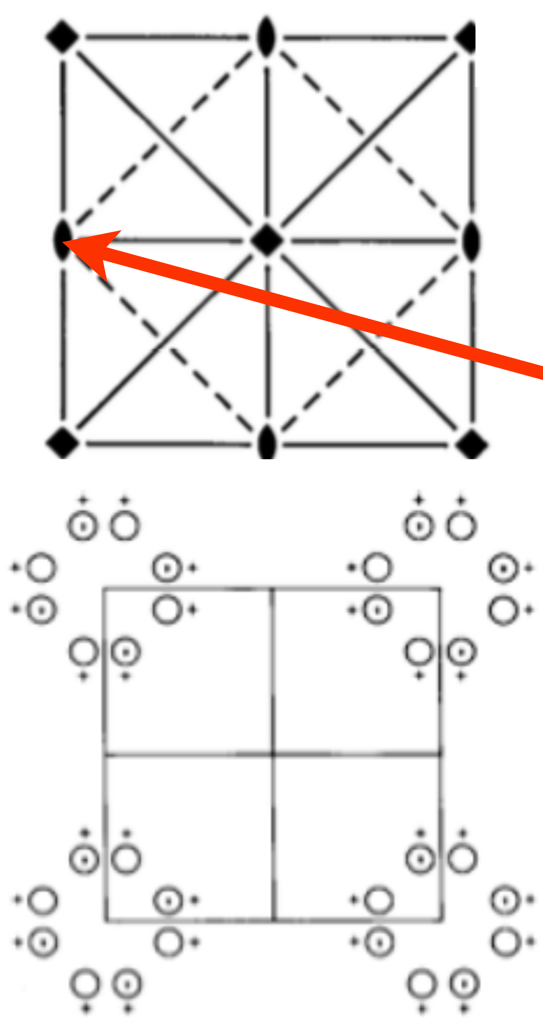
$$S_f=\{(1,0),\ (-1,101)X_f = X_f\}$$

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

EXAMPLE

Space group P4mm

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) $m\ \ x,x,z$

FCT/ZTF

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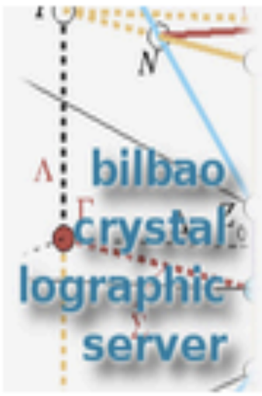

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20-21 August 2018

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

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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

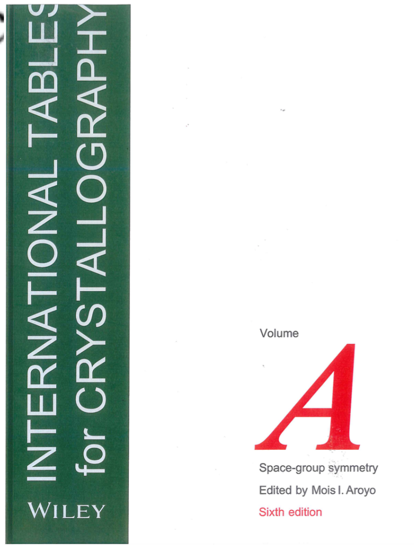
ces must be read by columns. **P** is the transformation f

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

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**

$Ccce$	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

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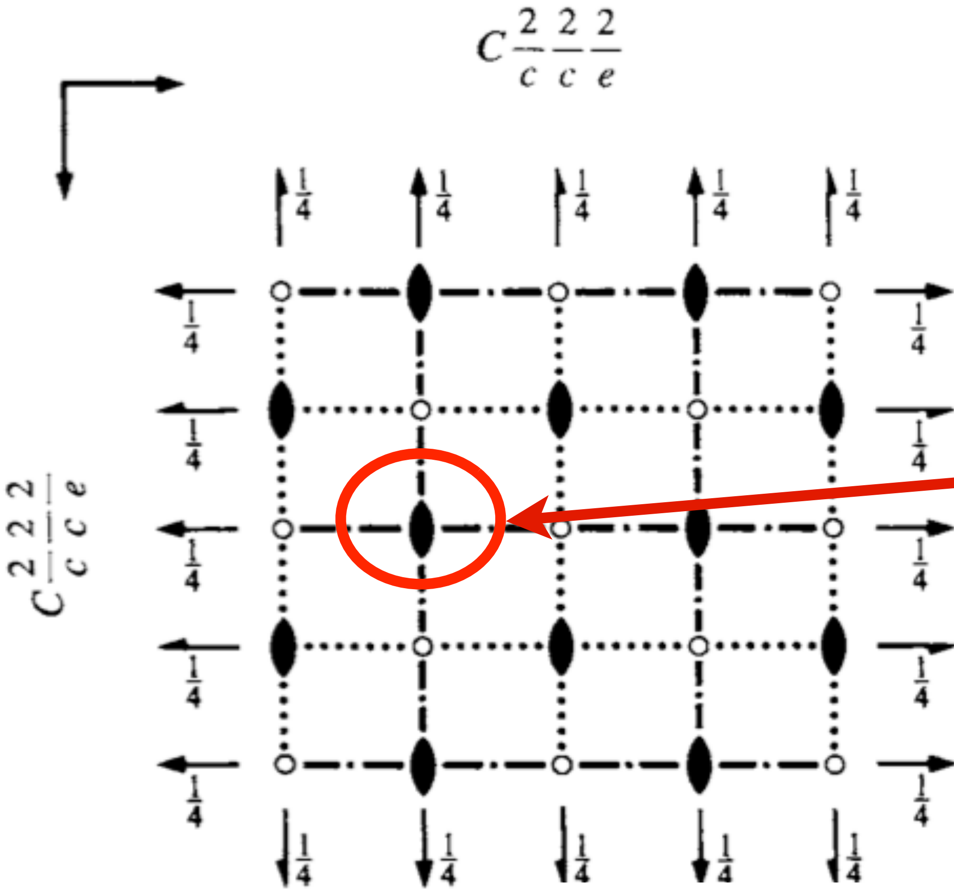
Example WYCKPOS: Wyckoff Positions Ccce (68)



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