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Introduction to International Tables for Crystallography, Vol. A: Space-group symmetry and Vol. A1Symmetry relations between space groups

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CRYSTALLOGRAPHIC SYMMETRY OPERATIONS

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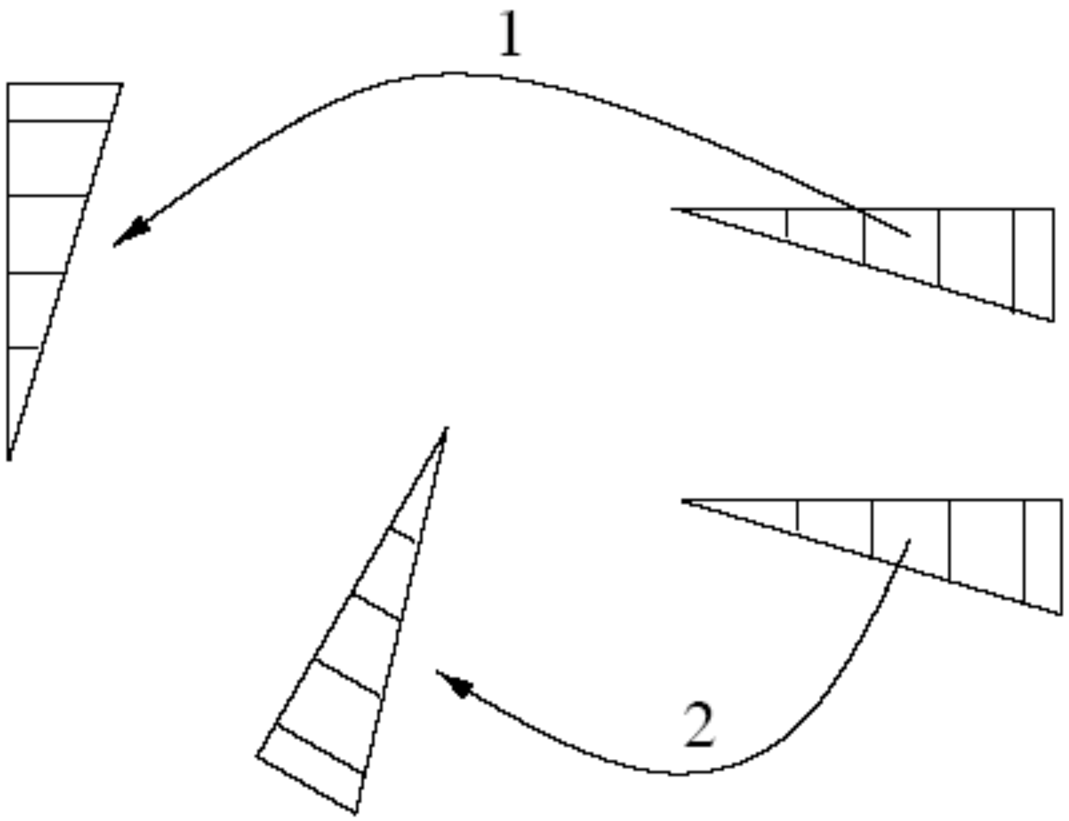
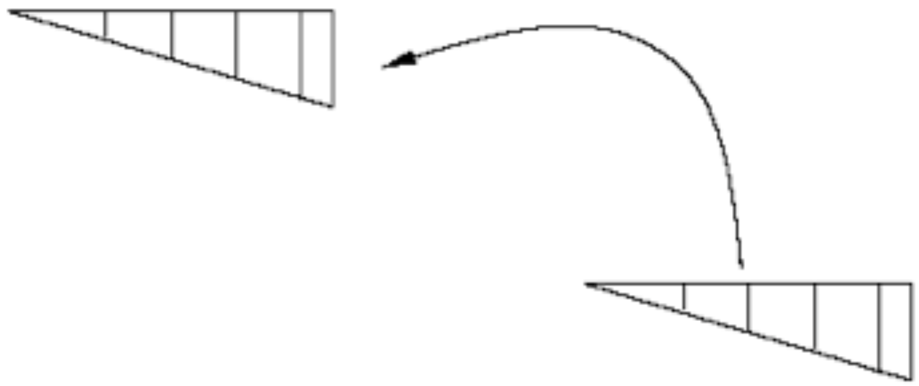
SYMMETRY OPERATIONS AND THEIR MATRIX-COLUMN PRESENTATION

Mappings and symmetry operations

Definition: A **mapping** of a set $\boldsymbol{A}$ into a set $\boldsymbol{B}$ is a relation such that for each element $\boldsymbol{a} \in \boldsymbol{A}$ there is a unique element $\boldsymbol{b} \in \boldsymbol{B}$ which is assigned to $\boldsymbol{a}$. The element $\boldsymbol{b}$ is called the *image* of $\boldsymbol{a}$.



An **isometry** leaves all distances and angles invariant. An ‘isometry of the first kind’, preserving the counter–clockwise sequence of the edges ‘short–middle–long’ of the triangle is displayed in the upper mapping. An ‘isometry of the second kind’, changing the counter–clockwise sequence of the edges of the triangle to a clockwise one is seen in the lower mapping.



A parallel shift of the triangle is called a **translation**. Translations are special isometries. They play a distinguished role in crystallography.

Description of isometries

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

isometry:

$\tilde{x} = F_1(x,y,z)$

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

Matrix-column presentation of isometries

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

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

Short-hand notation for the description of isometries

isometry:

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

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

notation rules:

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

examples:

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

→ -x+1/2, y, -z+1/2

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

EXERCISES

Problem 2.19

Construct the matrix-column pair (W,w) of the following coordinate triplets:

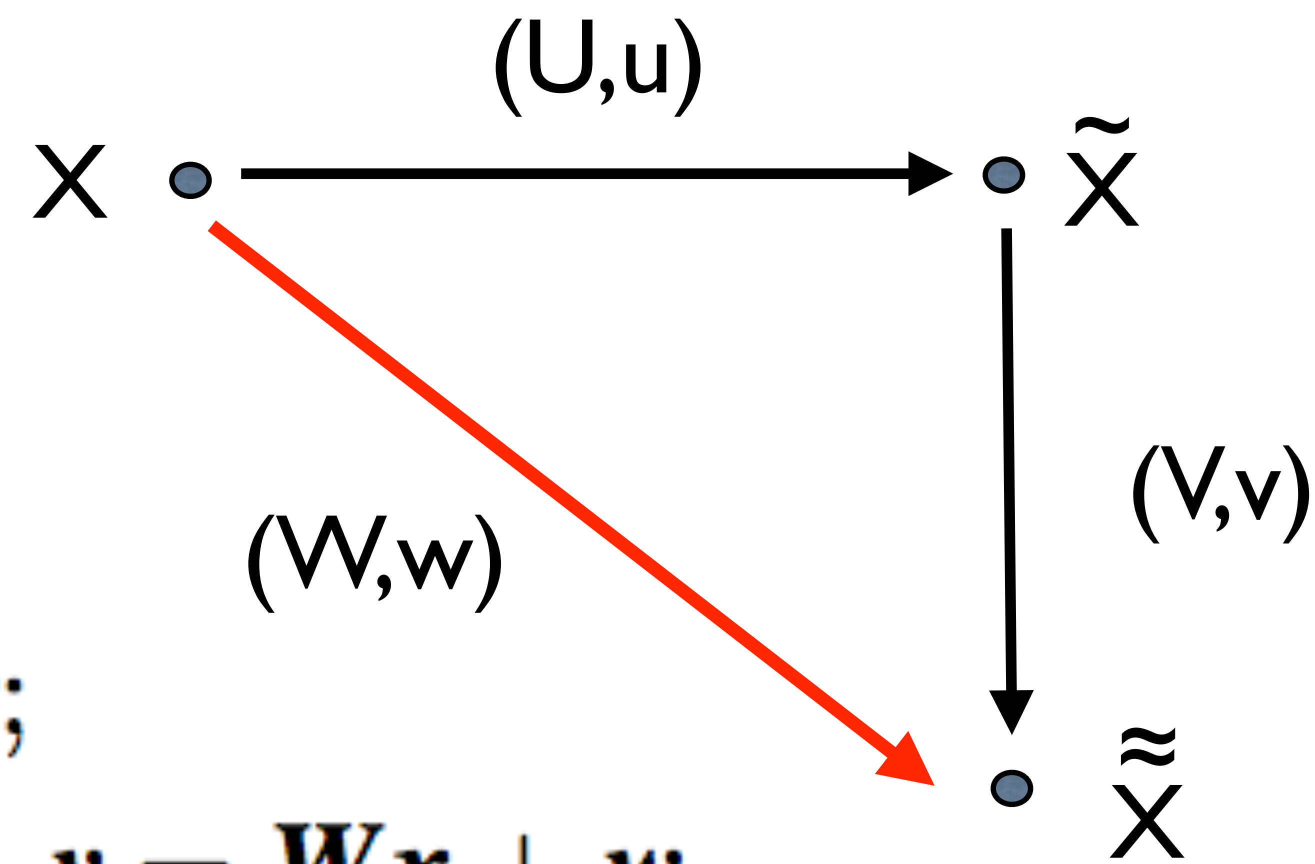
(1) x,y,z

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

(3) -x,-y,-z

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

Combination of isometries



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

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

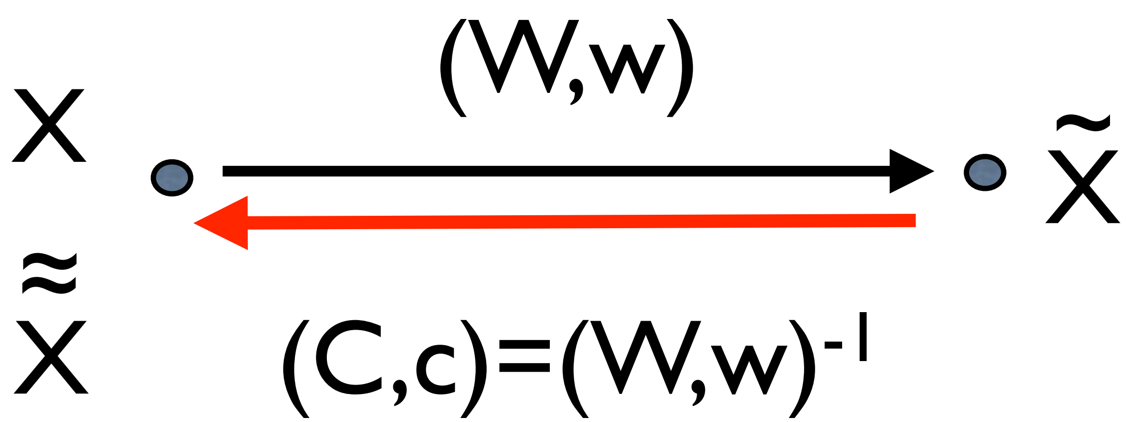
$$\tilde{\tilde{\boldsymbol{x}}} = \boldsymbol{V}(\boldsymbol{U}\boldsymbol{x} + \boldsymbol{u}) + \boldsymbol{v};$$

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

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

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

Inverse isometries



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

$\boldsymbol{o}$ = zero translation column

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

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

$CW=\boldsymbol{I}$ → $C=W^{-1}$

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

Matrix formalism: 4x4 matrices

$$\boldsymbol{x} \rightarrow \mathbb{x} = \left(\begin{array}{c} x \\ y \\ z \\ \hline 1 \end{array}\right) \; ; \; \tilde{\boldsymbol{x}} \rightarrow \tilde{\mathbb{x}} = \left(\begin{array}{c} \tilde{x} \\ \tilde{y} \\ \tilde{z} \\ \hline 1 \end{array}\right)$$

augmented matrices:

$$(\boldsymbol{W}, \boldsymbol{w}) \rightarrow \mathbb{W} = \left(\begin{array}{ccc|c} & \boldsymbol{W} & & \boldsymbol{w} \\ \hline 0 & 0 & 0 & 1 \end{array}\right)$$

$$\text{point } X \longrightarrow \text{point } \tilde{X} :$$

$$\tilde{\mathbb{x}} = \mathbb{W}\,\mathbb{x}$$

$$\left(\begin{array}{c} \tilde{x} \\ \tilde{y} \\ \tilde{z} \\ \hline 1 \end{array}\right) = \left(\begin{array}{ccc|c} & \boldsymbol{W} & & \boldsymbol{w} \\ \hline 0 & 0 & 0 & 1 \end{array}\right) \left(\begin{array}{c} x \\ y \\ z \\ \hline 1 \end{array}\right)$$

4x4 matrices: general formulae

point $X \longrightarrow$ point $\tilde{X}$:

$$\tilde{\mathbb{x}} = \mathbb{W}\,\mathbb{x} \qquad \left(\begin{array}{c} \tilde{x} \\ \tilde{y} \\ \tilde{z} \\ \hline 1 \end{array}\right) = \left(\begin{array}{ccc|c} & \boldsymbol{W} & & \boldsymbol{w} \\ \hline 0 & 0 & 0 & 1 \end{array}\right) \left(\begin{array}{c} x \\ y \\ z \\ \hline 1 \end{array}\right)$$

combination and inverse of isometries:

$$(\mathbb{W})^{-1} = (\mathbb{W}^{-1}) \qquad \mathbb{W}^{-1} = \left(\begin{array}{ccc|c} & \boldsymbol{W}^{-1} & & -\boldsymbol{W}^{-1}\boldsymbol{w} \\ \hline 0 & 0 & 0 & 1 \end{array}\right)$$

$$\mathbb{W}_3 = \mathbb{W}_2\,\mathbb{W}_1$$

EXERCISES

Problem 2.19 (cont.)

Construct the (4x4) matrix-presentation 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

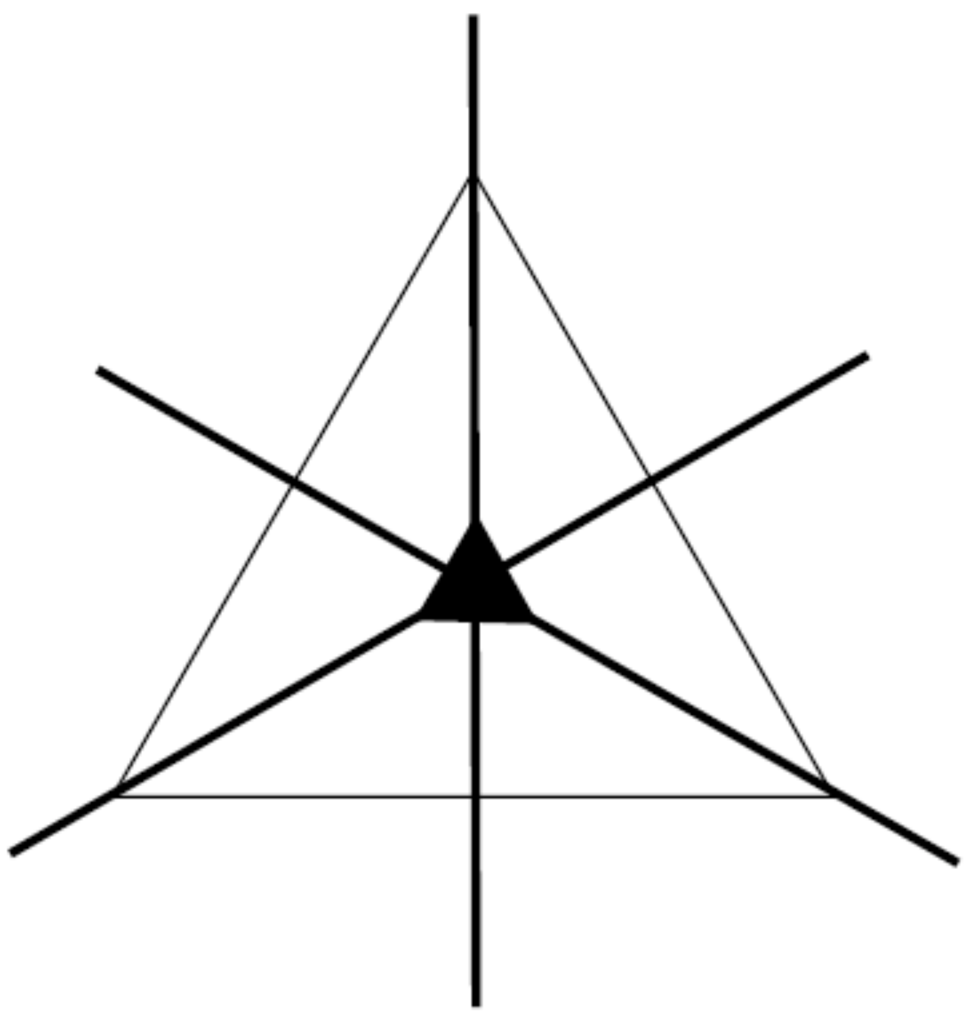
Crystallographic symmetry operations

Symmetry operations of an object

The isometries which map the object onto itself are called *symmetry operations of this object*. The *symmetry* of the object is the set of all its symmetry operations.

Crystallographic symmetry operations

If the object is a crystal pattern, representing a real crystal, its symmetry operations are called *crystallographic symmetry operations*.



The equilateral triangle allows six symmetry operations: rotations by 120 and 240 around its centre, reflections through the three thick lines intersecting the centre, and the identity operation.

Crystallographic symmetry operations

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

geometric elements

Types of isometries — preserve handedness

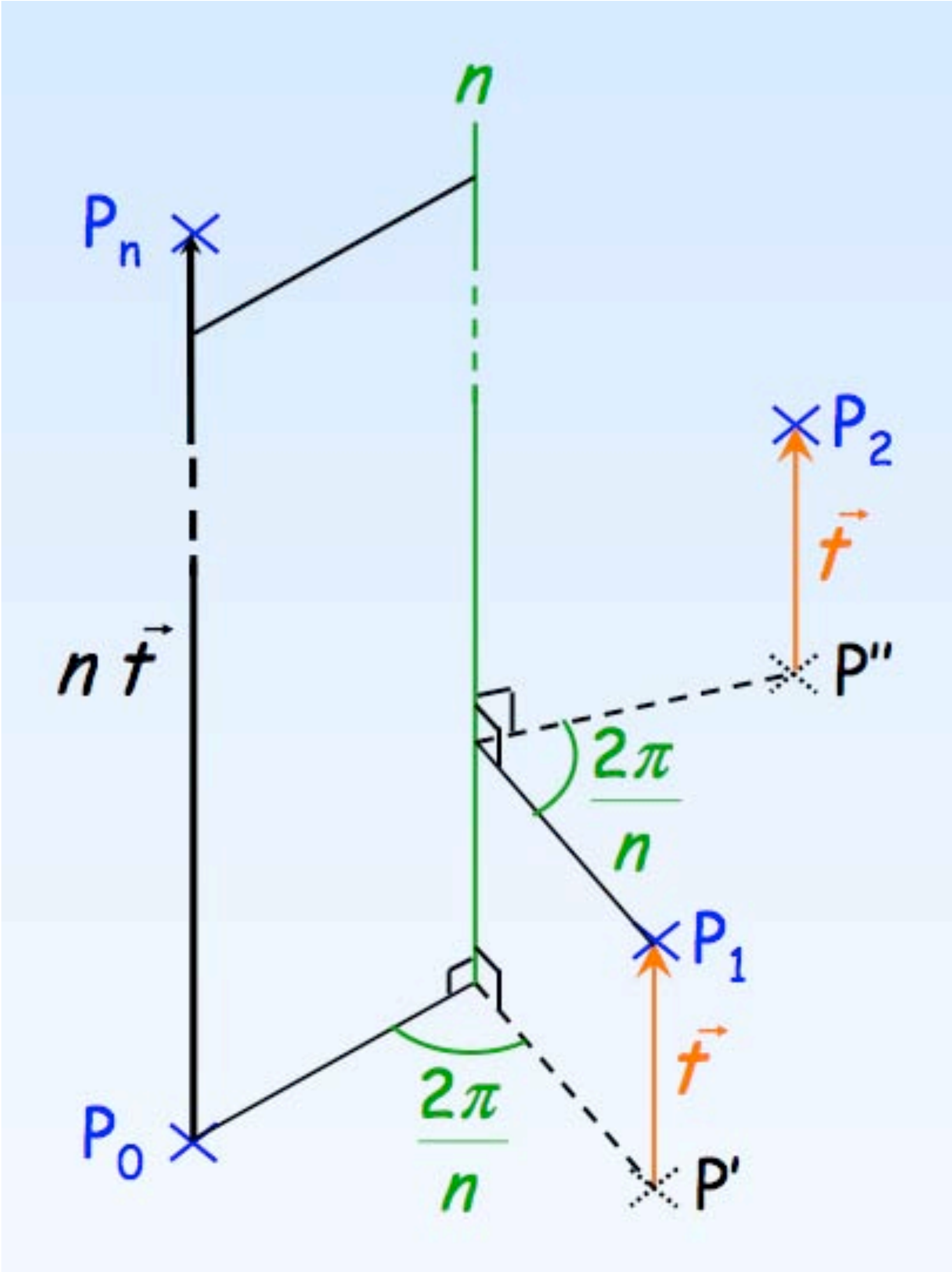
identity: the whole space fixed

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

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

screw rotation: no fixed point, screw axis — screw vector

Screw rotation



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

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

Types of isometries — do not preserve handedness

roto-inversion:

centre of roto-inversion fixed
roto-inversion axis

inversion:

centre of inversion fixed

reflection:

plane fixed
reflection/mirror plane

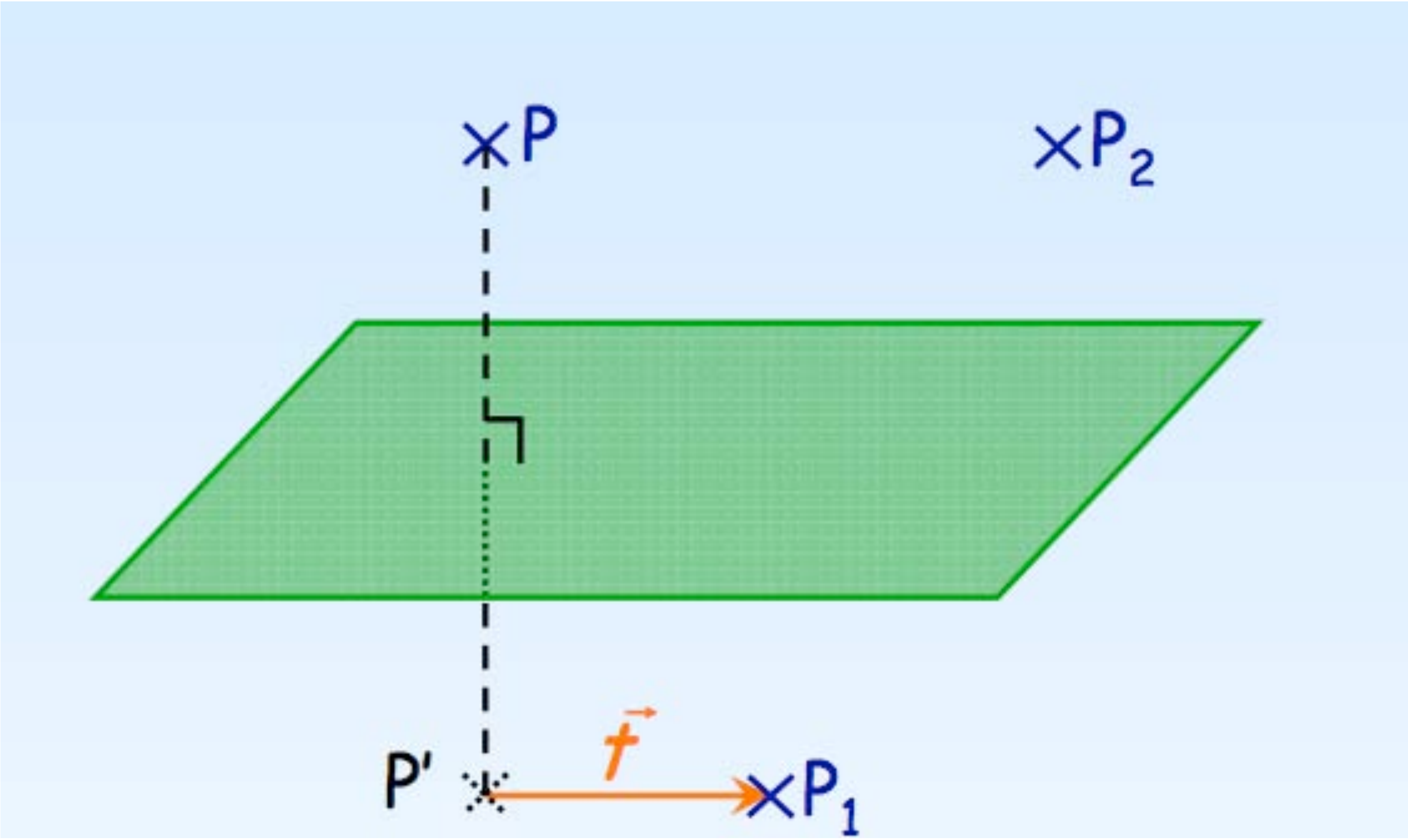
glide reflection:

no fixed point
glide plane

glide vector

Crystallographic symmetry operations

Glide plane



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

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

Matrix-column presentation of some symmetry operations

Rotation or roto-inversion 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:

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

Geometric meaning of (W, w)

W information

(a) type of isometry

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

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

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

EXERCISES

Problem 2.19 (cont.)

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

(a) type of isometry

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

Geometric meaning of (W, w)

W information

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

(b1) rotations:

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

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

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

EXERCISES

Problem 2.19 (cont)

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

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 $\boldsymbol{u}$

Fixed points of isometries

$(W,w)X_f = X_f$ → solution: point, line, plane or space

→ no solution

Examples:

solution:
$$\left(\begin{array}{ccc|c} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1/2 \end{array}\right)\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

What are the fixed points of this isometry?

NO solution:
$$\left(\begin{array}{ccc|c} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1/2 \\ 0 & 0 & -1 & 1/2 \end{array}\right)\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

Geometric meaning of (W,w)

$(\boldsymbol{W},\boldsymbol{w})^n=(\boldsymbol{I},\boldsymbol{t})$

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

(A) intrinsic translation part :

glide or screw component $\boldsymbol{t}/k$

(A1) screw rotations:

$$\boldsymbol{t}/k=\frac{1}{k}\boldsymbol{Y}\boldsymbol{w},\ \text{where}\ \boldsymbol{W}^k=\boldsymbol{I}$$

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

(A2) glide reflections:

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

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 :

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

glide reflections:

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

EXERCISES

Problem 2.20 (cont.)

Determine the intrinsic translation parts (if relevant) of the following symmetry operations

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

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

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

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

Fixed points of (W,w)

Location (fixed points x_F):

(B1) $\boldsymbol{t}/k = \mathbf{0}$:

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

(B2) $\boldsymbol{t}/k \neq \mathbf{0}$:

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

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

EXERCISES

Problem 2.19 (cont.)

Determine the fixed points of the following symmetry operations:

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

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

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

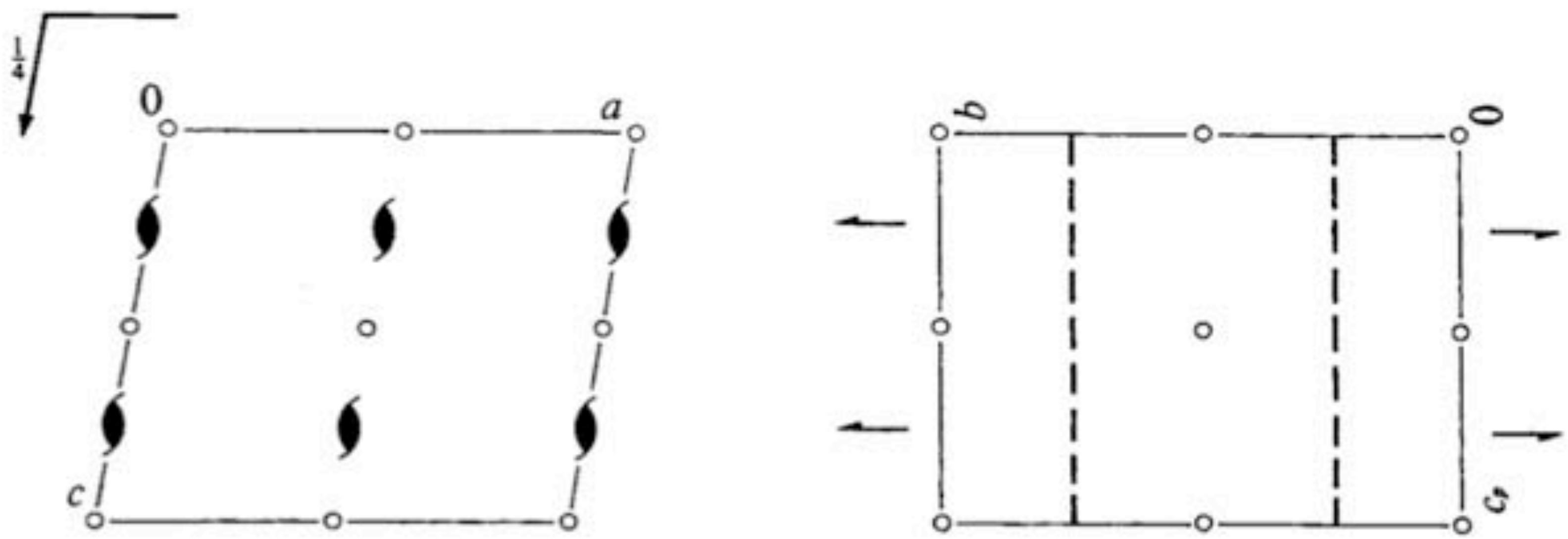
Space group $P2_1/c$ (No. 14)

$P2_1/c$ 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

bilbao crystallographic server

[The crystallographic site at the Condensed Matter Physics Dept. of the University of the Basque Country]

[Space Groups] [Layer Groups] [Rod Groups] [Frieze Groups] [Wyckoff Sets]

Sections

- Retrieval Tools
- Group-Subgroup
- Representations
- Solid State
- Structure Utilities
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- Incommensurate Structures Database

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Material from the ITOnline Workshop (September 2011)

Material from the school on the server (June 2009)

CrystallographyOnline: International School on the Use and Applications of the Bilbao Crystallographic

Space Groups Retrieval Tools

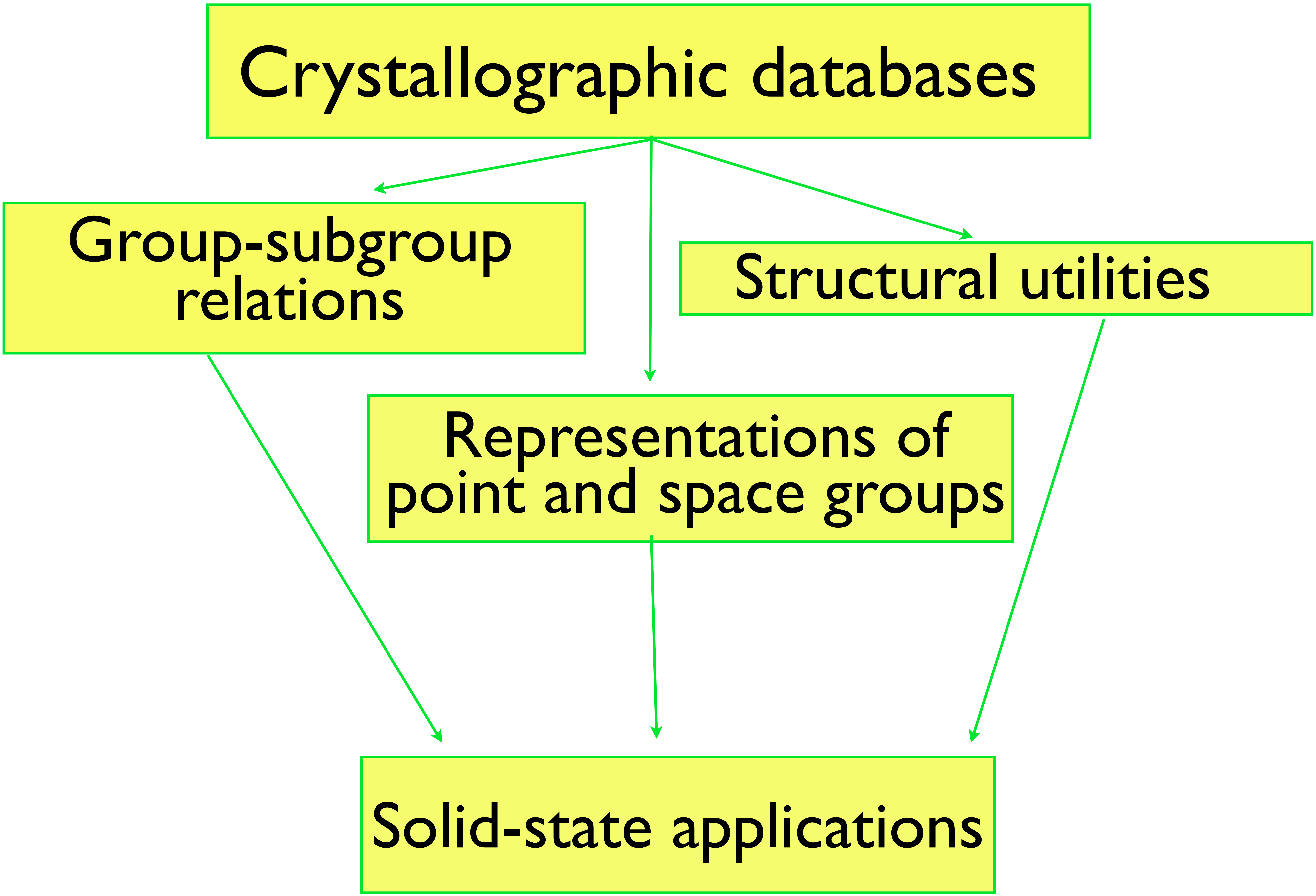
GENPOS	Generators and General Positions of Space Groups
WYCKPOS	Wyckoff Positions of Space Groups
HKLCOND	Reflection conditions of Space Groups
MAXSUB	Maximal Subgroups of Space Groups
SERIES	Series of Maximal Isomorphic Subgroups of Space Groups
WYCKSETS	Equivalent Sets of Wyckoff Positions
NORMALIZER	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

Magnetic Space Groups

MGENPOS	General Positions of Magnetic Space Groups
MWYCKPOS	Wyckoff Positions of Magnetic Space Groups
MAGNEXT	Extinction Rules of Magnetic Space Groups

Group - Subgroup Relations of Space Groups

SUBGROUPGRAPH	Lattice of Maximal Subgroups
HERMANN	Distribution of subgroups in conjugated classes
COSETS	Coset decomposition for a group-subgroup pair
WYCKSPLIT	The splitting of the Wyckoff Positions
MINSUP	Minimal Supergroups of Space Groups
SUPERGROUPS	Supergroups of Space Groups
CELLSUB	List of subgroups for a given k-index.
CELLSUPER	List of supergroups for a given k-index.
NONCHAR	Non Characteristic orbits.
COMMONSUBS	Common Subgroups of Space Groups
COMMONSUPER	Common Supergroups of Two Space Groups


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

Crystallographic Databases

International Tables for Crystallography

EXERCISES

Problem 2.19

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

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

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

Characterize geometrically these matrix-column pairs taking into account that they refer to a monoclinic basis with unique axis b,

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

Bilbao Crystallographic Server

Problem: Geometric Interpretation of (W,w) — SYMMETRY OPERATION

Symmetry Operation

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

Input:

i) The crystal system or the space group number.

ii) The matrix column representation of symmetry operation.

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

Output:

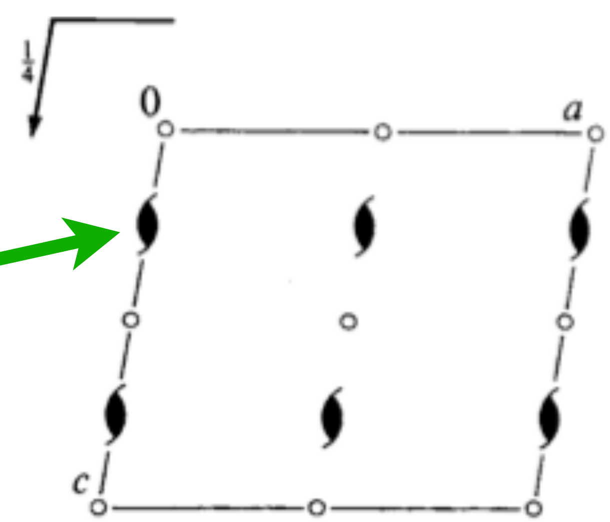
We obtain the geometric interpretation of the symmetry operation.

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

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

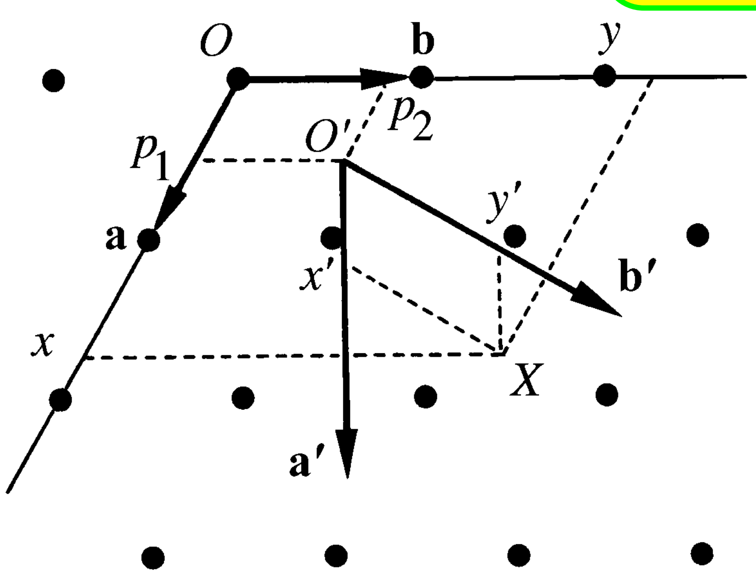
Standard/Default Setting | Non Conventional Setting | ITA Settings

-x,y+1/2,-z+1/2	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1/2 \\ 0 & 0 & -1 & 1/2 \end{pmatrix}$	2 (0,1/2,0) 0,y,1/4



CO-ORDINATE TRANSFORMATIONS IN CRYSTALLOGRAPHY

Co-ordinate transformation



3-dimensional space

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

(P,p) ↓

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

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

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

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

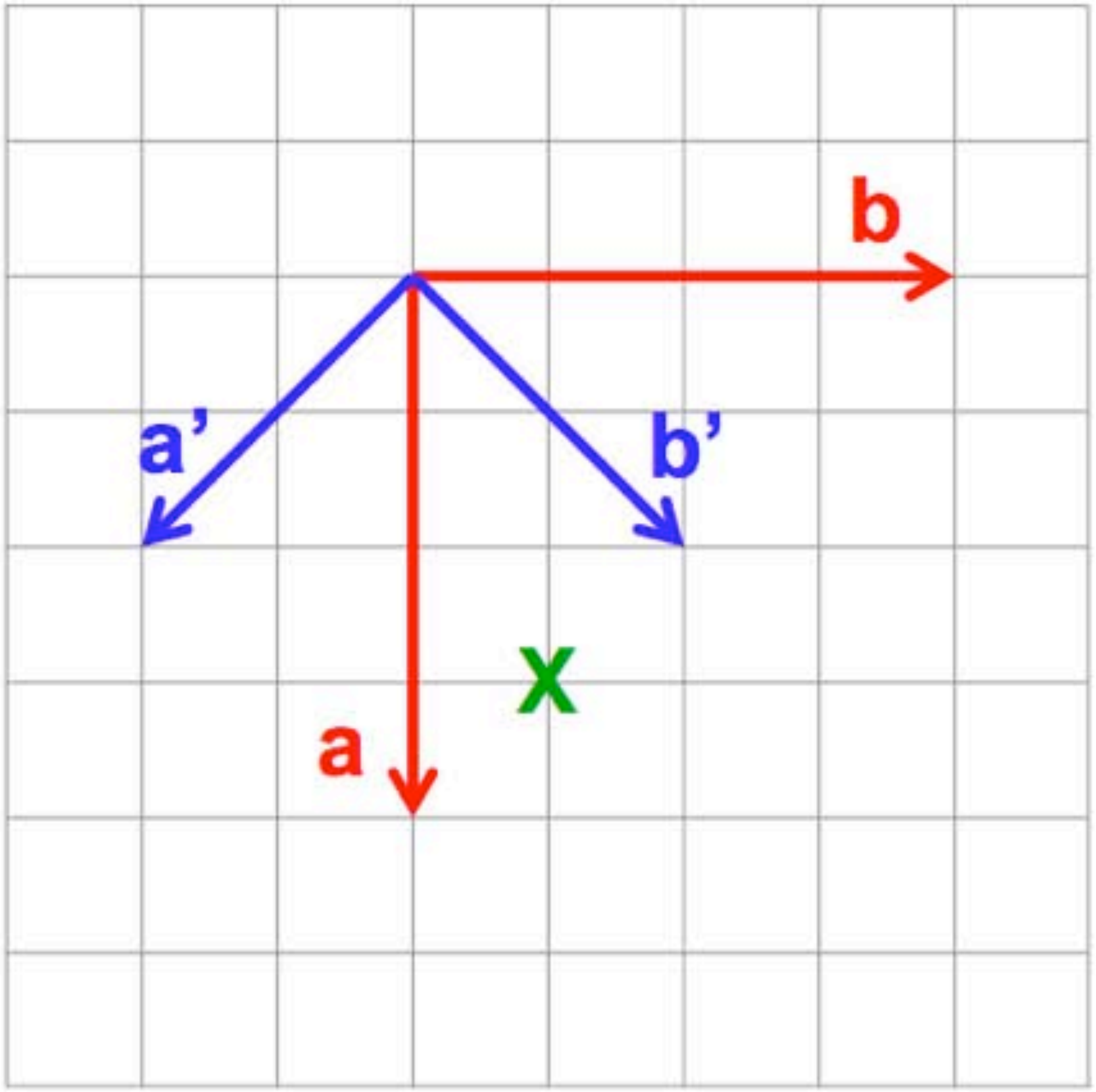
$$= (\mathbf{a}, \mathbf{b}, \mathbf{c}) \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix} = (P_{11}\mathbf{a} + P_{21}\mathbf{b} + P_{31}\mathbf{c}, \; P_{12}\mathbf{a} + P_{22}\mathbf{b} + P_{32}\mathbf{c}, \; P_{13}\mathbf{a} + P_{23}\mathbf{b}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

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

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

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

EXAMPLE



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

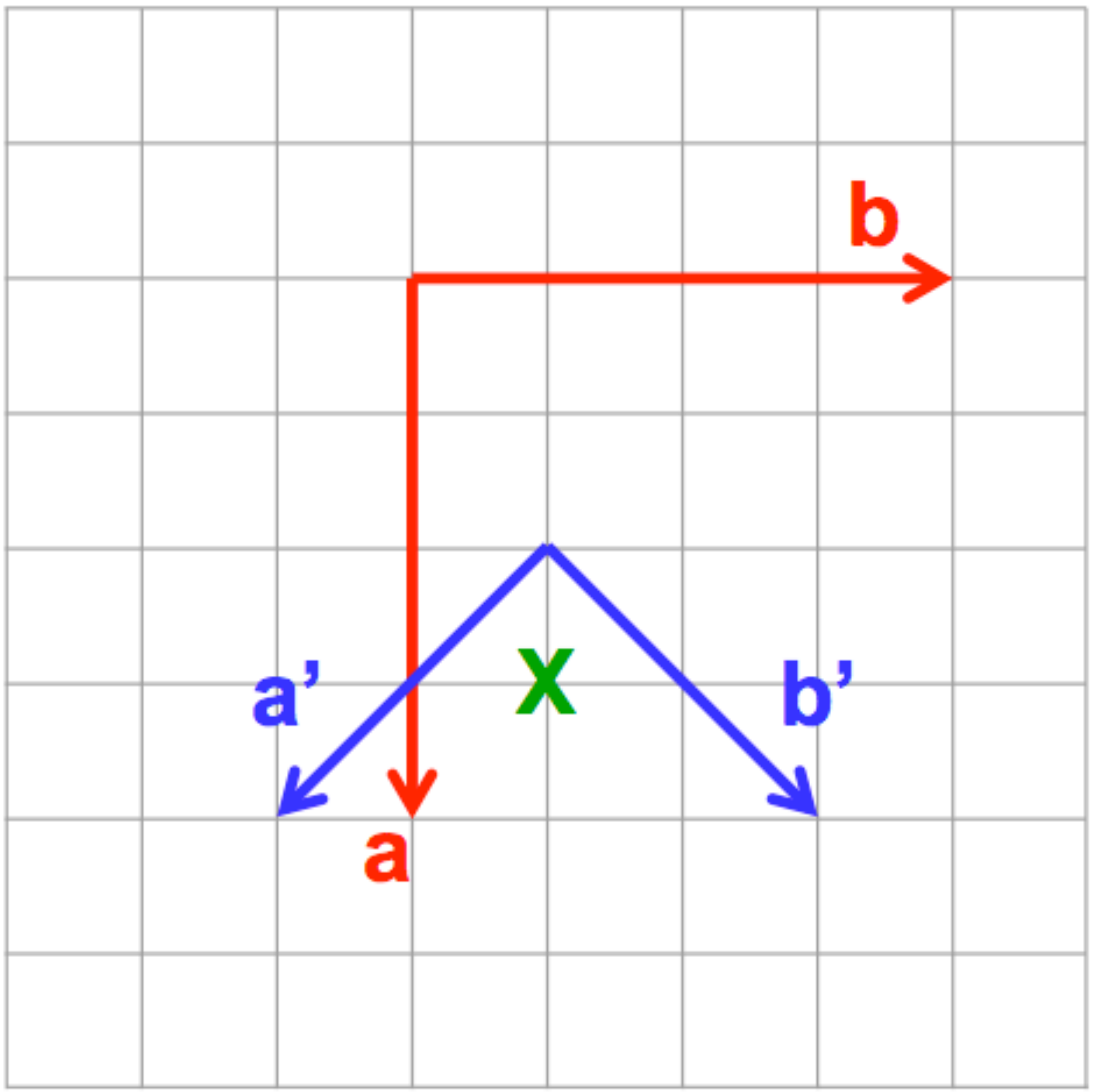
$$(a,b,c) = (a',b',c')\begin{pmatrix} ? \end{pmatrix}$$

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

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

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

EXAMPLE



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

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

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

$X' = (?)$

Linear parts as before.

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

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

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} P_{11} & P_{12} & P_{13} & p1 \\ P_{21} & P_{22} & P_{23} & p2 \\ P_{31} & P_{32} & P_{33} & p3 \end{pmatrix}^{-1} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

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*):

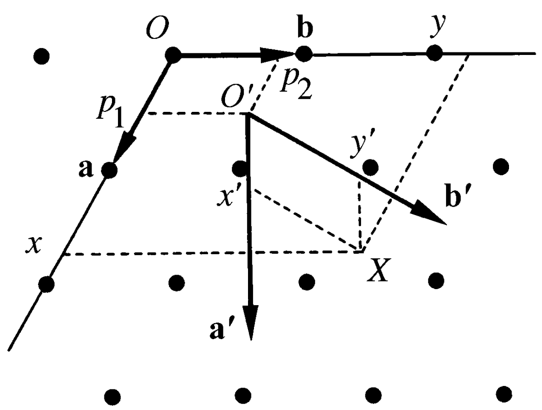
$$(W',w')=(P,p)^{-1}(W,w)(P,p)$$

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

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

Short-hand notation for the description of transformation matrices

Transformation matrix:



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

$$(P,p)=\left(\begin{array}{ccc|c} P_{11} & P_{12} & P_{13} & p1 \\ P_{21} & P_{22} & P_{23} & p_2 \\ P_{31} & P_{32} & P_{33} & p_3 \end{array}\right)$$

(**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

EXERCISES

Problem 2.20

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

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

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

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

0,70
0,31
0,95