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

IUCr

Malvern Panalytical
a spectris company

CPQCOL
Consejo Profesional de Química Colombia

CRYSTALLOGRAPHIC SYMMETRY OPERATIONS

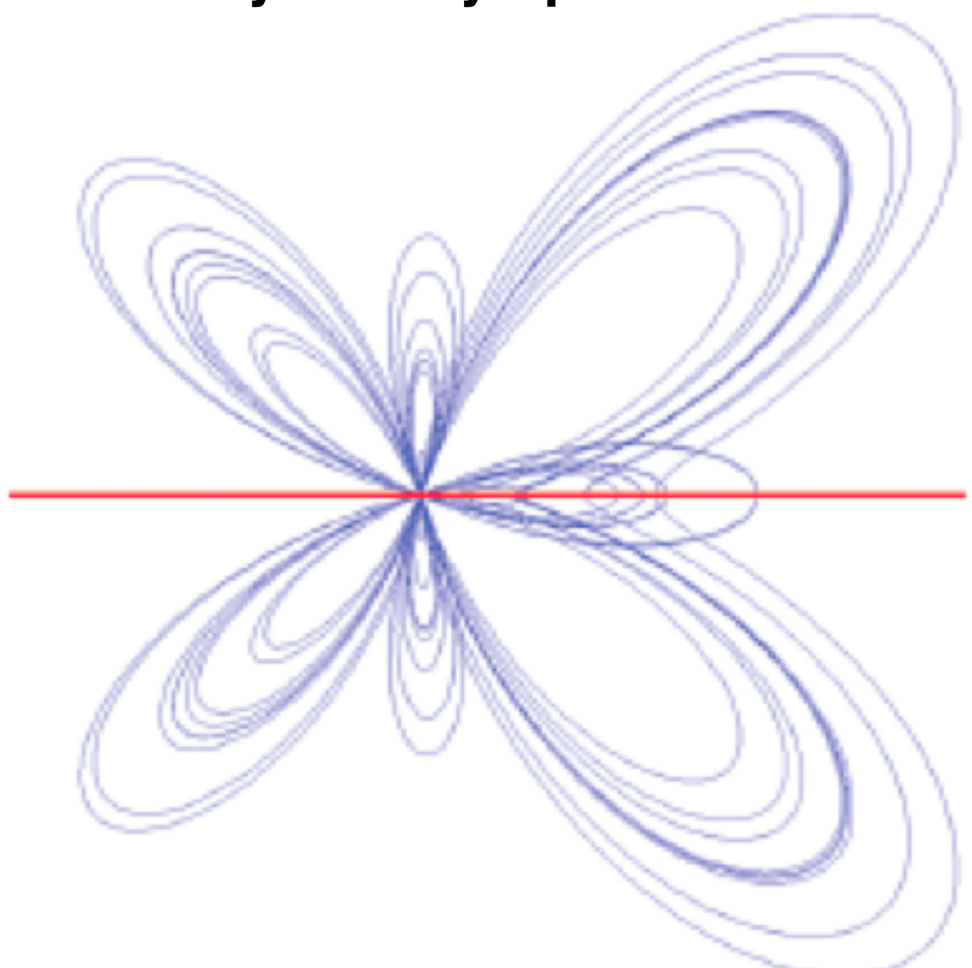
Mois I. Aroyo
Universidad del Pais Vasco, Bilbao, Spain

eman ta zabal zazu
Universidad del País Vasco
Euskal Herriko Unibertsitatea

SYMMETRY OPERATIONS AND THEIR MATRIX-COLUMN PRESENTATION

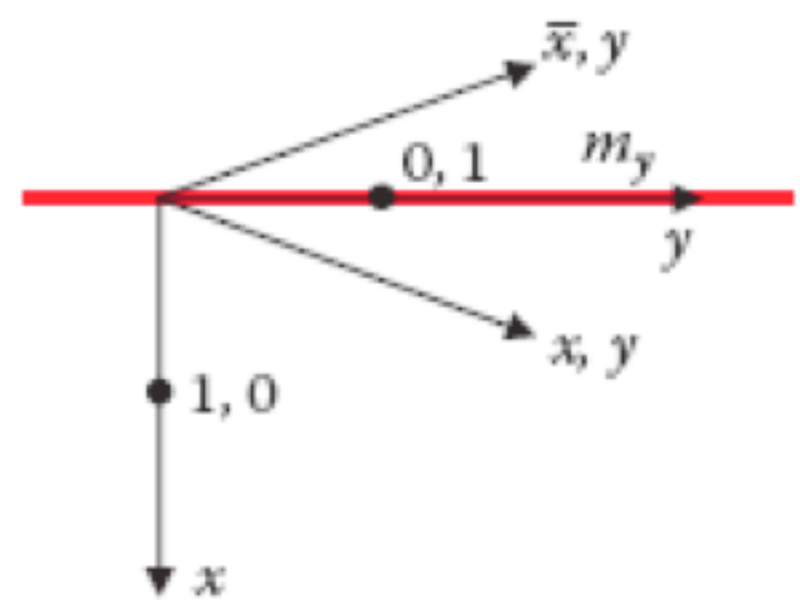
Example: Matrix presentation of symmetry operation

Mirror symmetry operation



drawing: M.M. Julian
Foundations of Crystallography

Mirror line m_y at 0,y



Matrix representation

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

$$\det \begin{pmatrix} -1 & \\ & 1 \end{pmatrix} = ? \quad \mathrm{tr} \begin{pmatrix} -1 & \\ & 1 \end{pmatrix} = ?$$

Fixed points

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

Description of isometries

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

isometry:

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

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

Matrix-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

EXERCISES

Problem 2.14

Referred to an 'orthorhombic' coordinated system ($a \neq b \neq c$; $\alpha=\beta=\gamma=90$) two symmetry operations are represented by the following matrix-column pairs:

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

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

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

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

And of (W_2,w_2)?

Hint:

A drawing could be rather helpful

Problem 2.14

Characterization of the symmetry operations:

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

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

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

Short-hand notation for the description of isometries

isometry:

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

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

notation rules:

-left-hand side: omitted

-coefficients 0, +1, -1

-different rows in one line

examples:

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

$\longrightarrow$ $\begin{cases} -x+1/2,\ y,\ -z+1/2 \\ \bar{x}+1/2,\ y,\ \bar{z}+1/2 \end{cases}$

EXERCISES

Problem 2.15

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

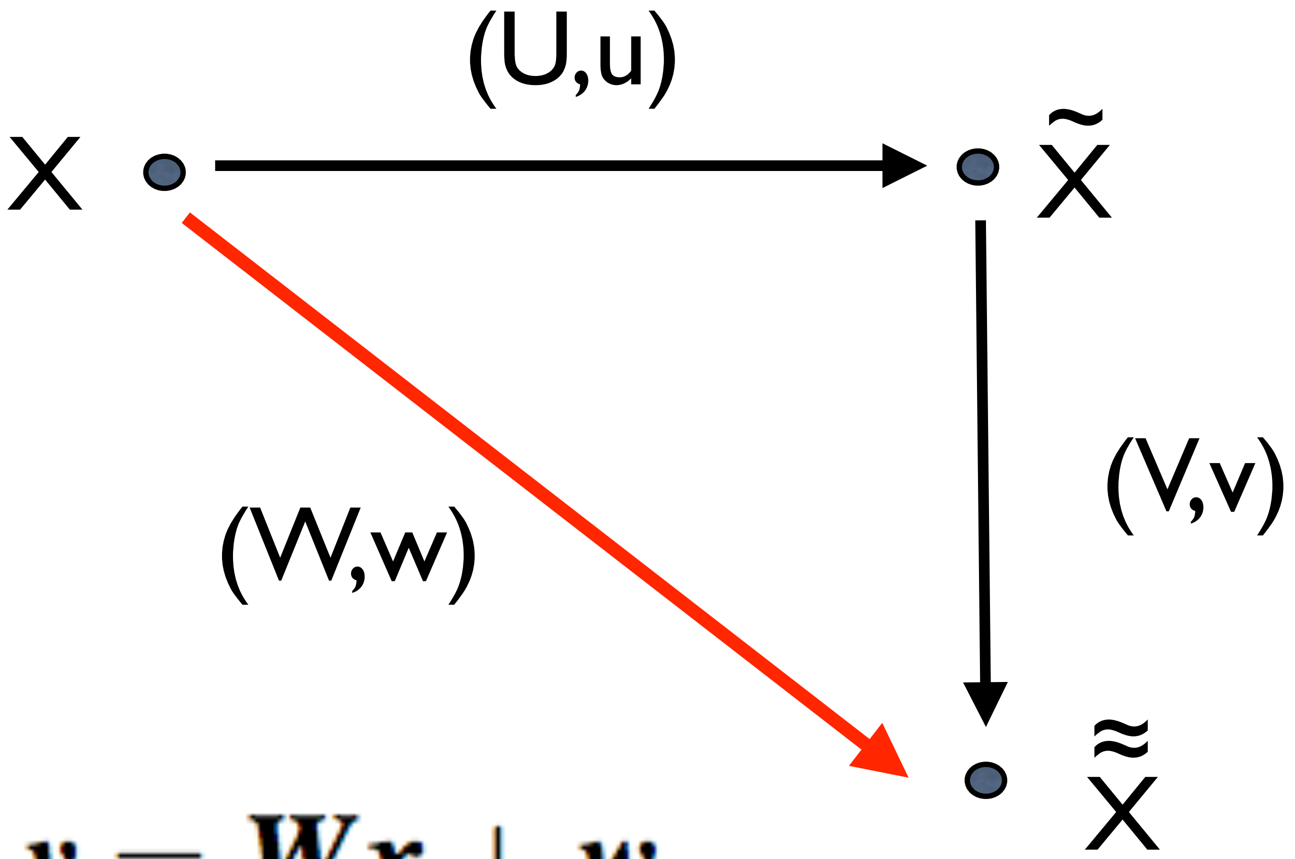
(1) x,y,z

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

(3) -x,-y,-z

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

Combination of isometries



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

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

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

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

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

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

EXERCISES

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

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

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

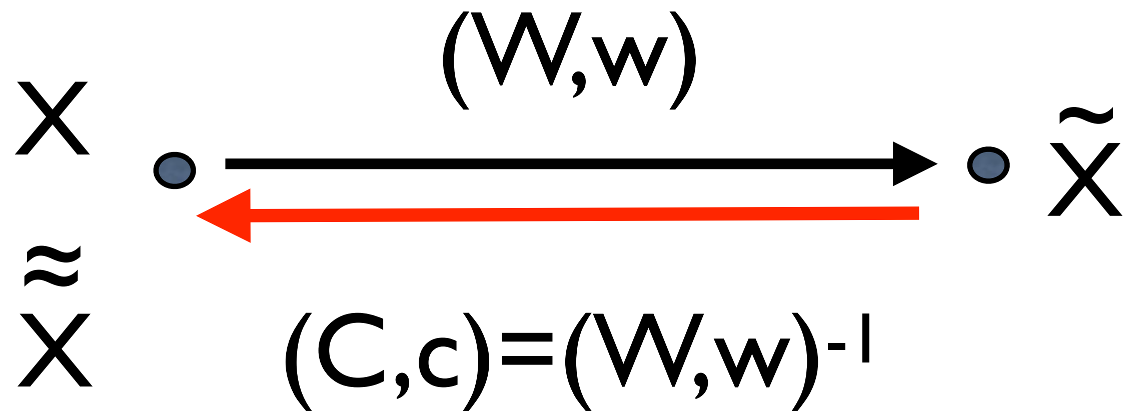
$$(W,w)=(W_1,w_1)(W_2,w_2)$$

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

combination of isometries:

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

Inverse isometries



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

$\boldsymbol{o}$ = zero translation column

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

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

$CW=\boldsymbol{I}$ → $C=W^{-1}$

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

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

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

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

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

inverse of isometries:

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

EXERCISES

Problem 2.14(cont)

Consider the matrix-column pairs

$$(\boldsymbol{A},\boldsymbol{a}) = \begin{pmatrix} 0\,1\,0 \\ 1\,0\,0 \\ 0\,0\,\bar{1} \end{pmatrix}, \begin{pmatrix} 1/2 \\ 1/2 \\ 1/2 \end{pmatrix} \text{ and } (\boldsymbol{B},\boldsymbol{b}) = \begin{pmatrix} 0\,1\,0 \\ 0\,0\,1 \\ 1\,0\,0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

(i) What is the matrix–column pair resulting from $(\boldsymbol{B},\,\boldsymbol{b})\,(\boldsymbol{A},\,\boldsymbol{a}) = (\boldsymbol{C},\boldsymbol{c})$, and $(\boldsymbol{A},\,\boldsymbol{a})\,(\boldsymbol{B},\,\boldsymbol{b}) = (\boldsymbol{D},\boldsymbol{d})$?

(ii) What is $(\boldsymbol{A},\boldsymbol{a})^{-1}$, $(\boldsymbol{B},\boldsymbol{b})^{-1}$, $(\boldsymbol{C},\boldsymbol{c})^{-1}$ and $(\boldsymbol{D},\boldsymbol{d})^{-1}$?

(iii) What is $(\boldsymbol{B},\boldsymbol{b})^{-1}\,(\boldsymbol{A},\,\boldsymbol{a})^{-1}$?

Matrix formalism: 4x4 matrices

$$\boldsymbol{x} \rightarrow \mathbb{x} = \begin{pmatrix} x \\ y \\ z \\ \hline 1 \end{pmatrix} ; \; \tilde{\boldsymbol{x}} \rightarrow \tilde{\mathbb{x}} = \begin{pmatrix} \tilde{x} \\ \tilde{y} \\ \tilde{z} \\ \hline 1 \end{pmatrix}$$

augmented matrices:

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

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

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

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

4x4 matrices: general formulae

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

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

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 2.15 (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

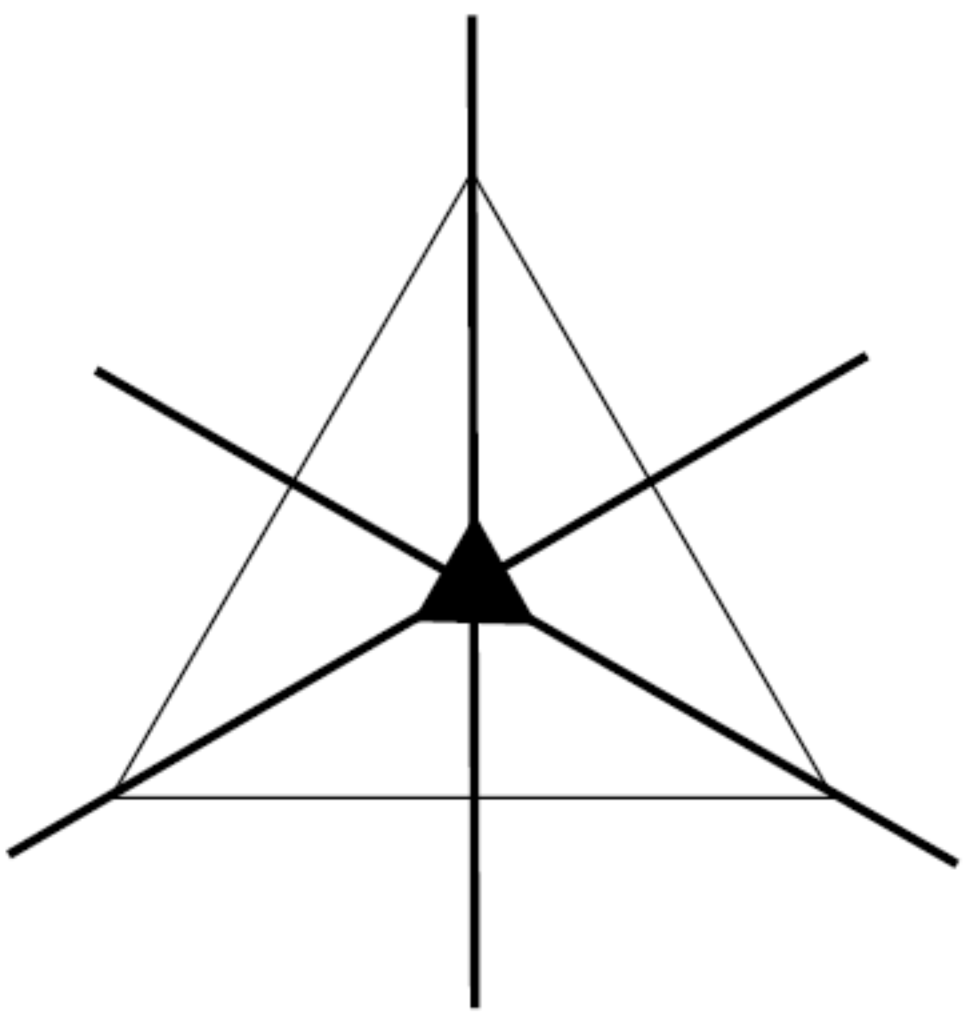
Crystallographic symmetry operations

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

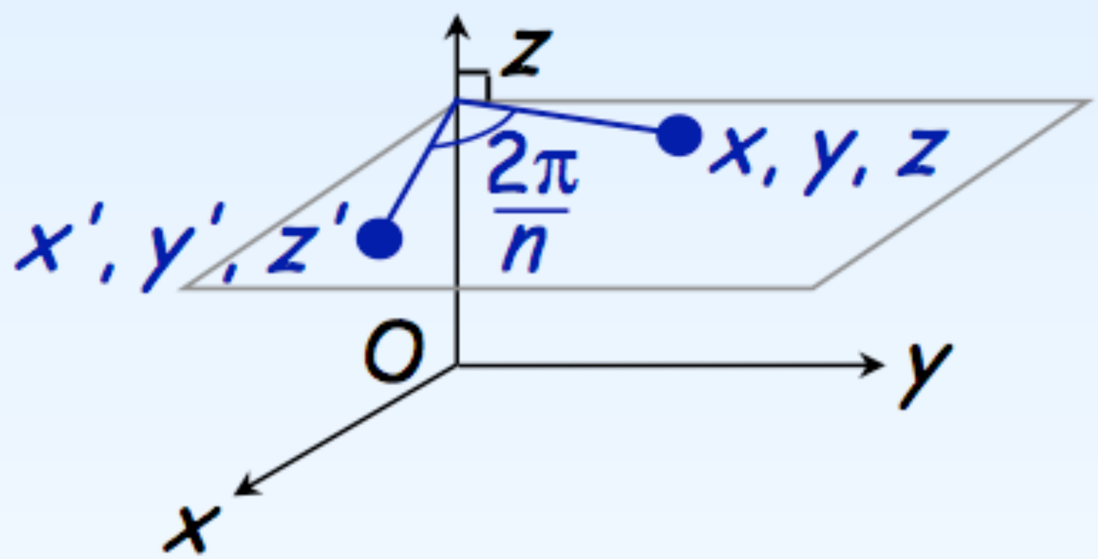
rotation: one line fixed, rotation axis $\phi = k \times 360^\circ / N$

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

Crystallographic symmetry operations

Rotation (around an axis)

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

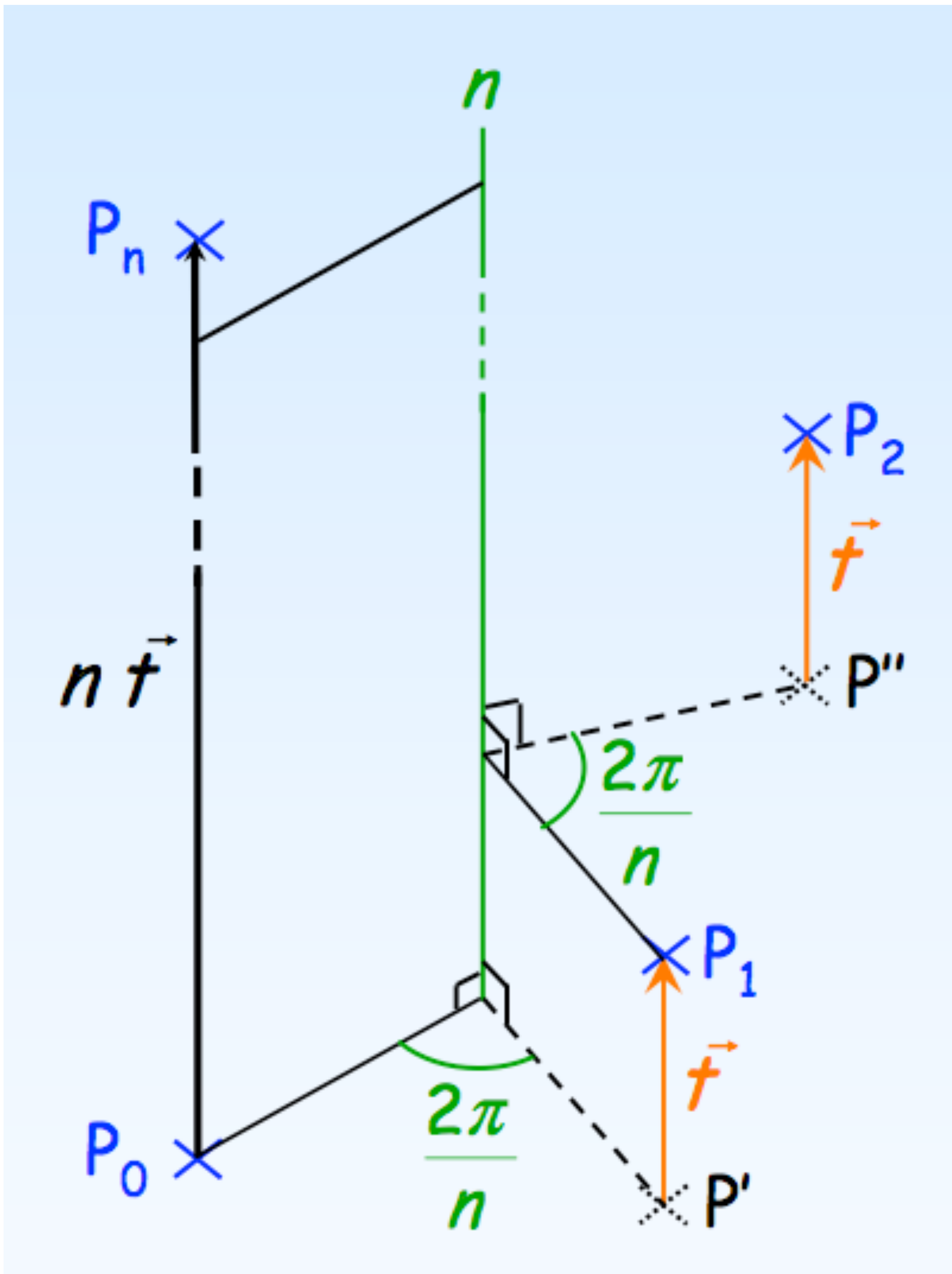


n

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

Det = +1

Screw rotation



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

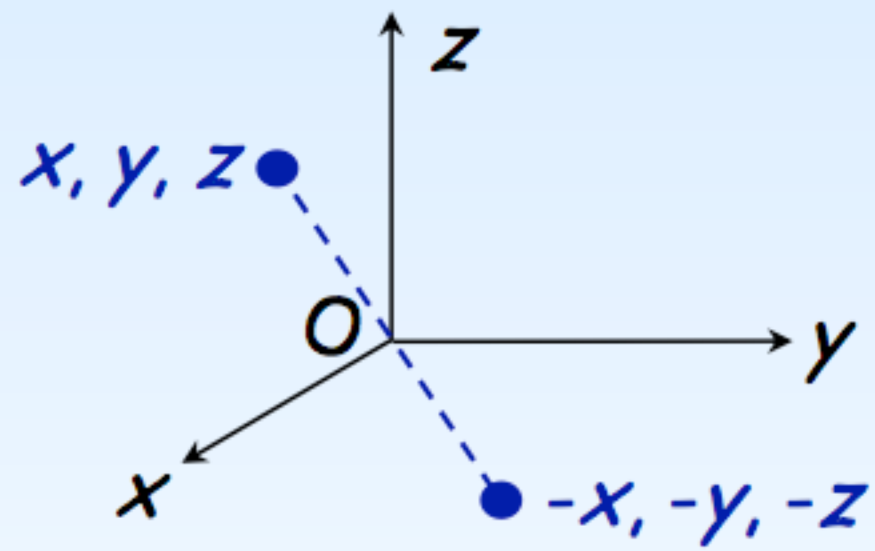
Its application *n* times results in a translation parallel to the rotation axis

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

Symmetry operations in 3D
Rotoinvertions

Inversion (through a point)



$\bar{1}$

a crystal which has the inversion symmetry is called centrosymmetrical.

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

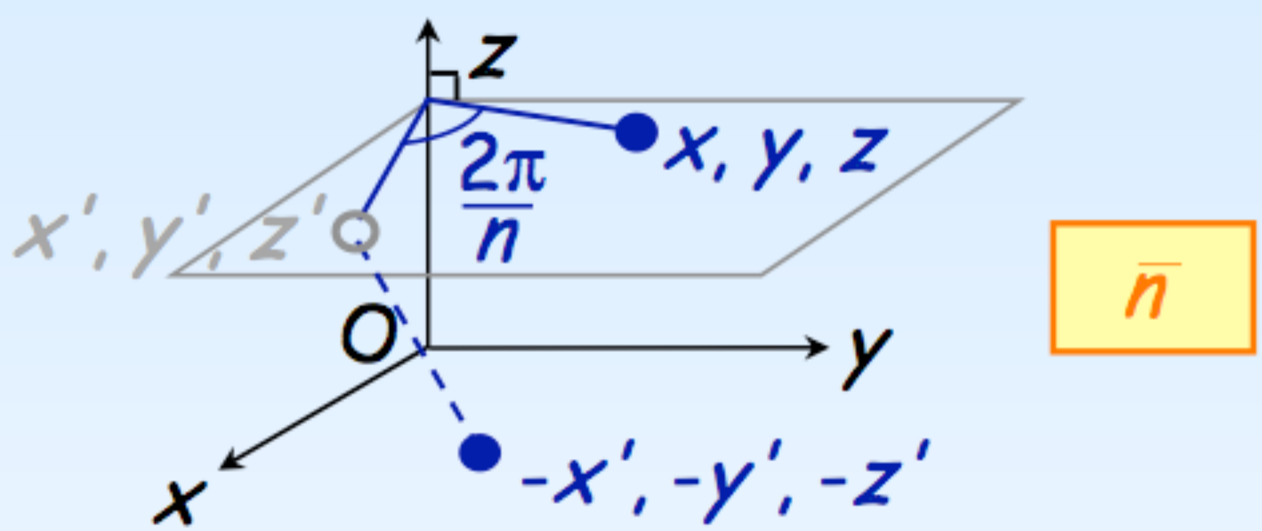
Det = -1

Symmetry operations in 3D
Rotoinvertions

Roto-inversion

(around an axis and through a point)

Rotation followed by an inversion

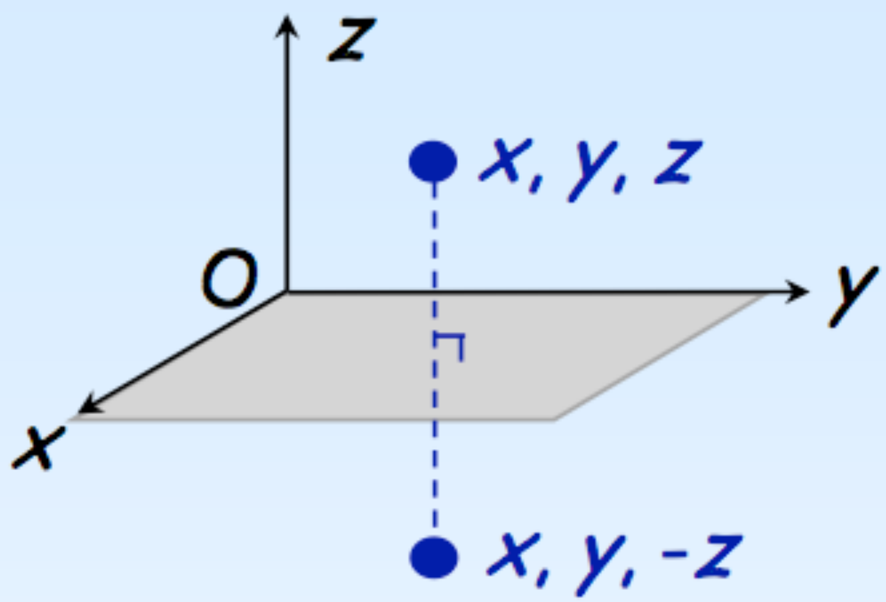


$$\alpha(\bar{n}) = \begin{pmatrix} -\cos\varphi & \sin\varphi & 0 \\ -\sin\varphi & -\cos\varphi & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

Det = -1

Symmetry operations in 3D
Rotoinvertions

Reflection (through a mirror plane)



m

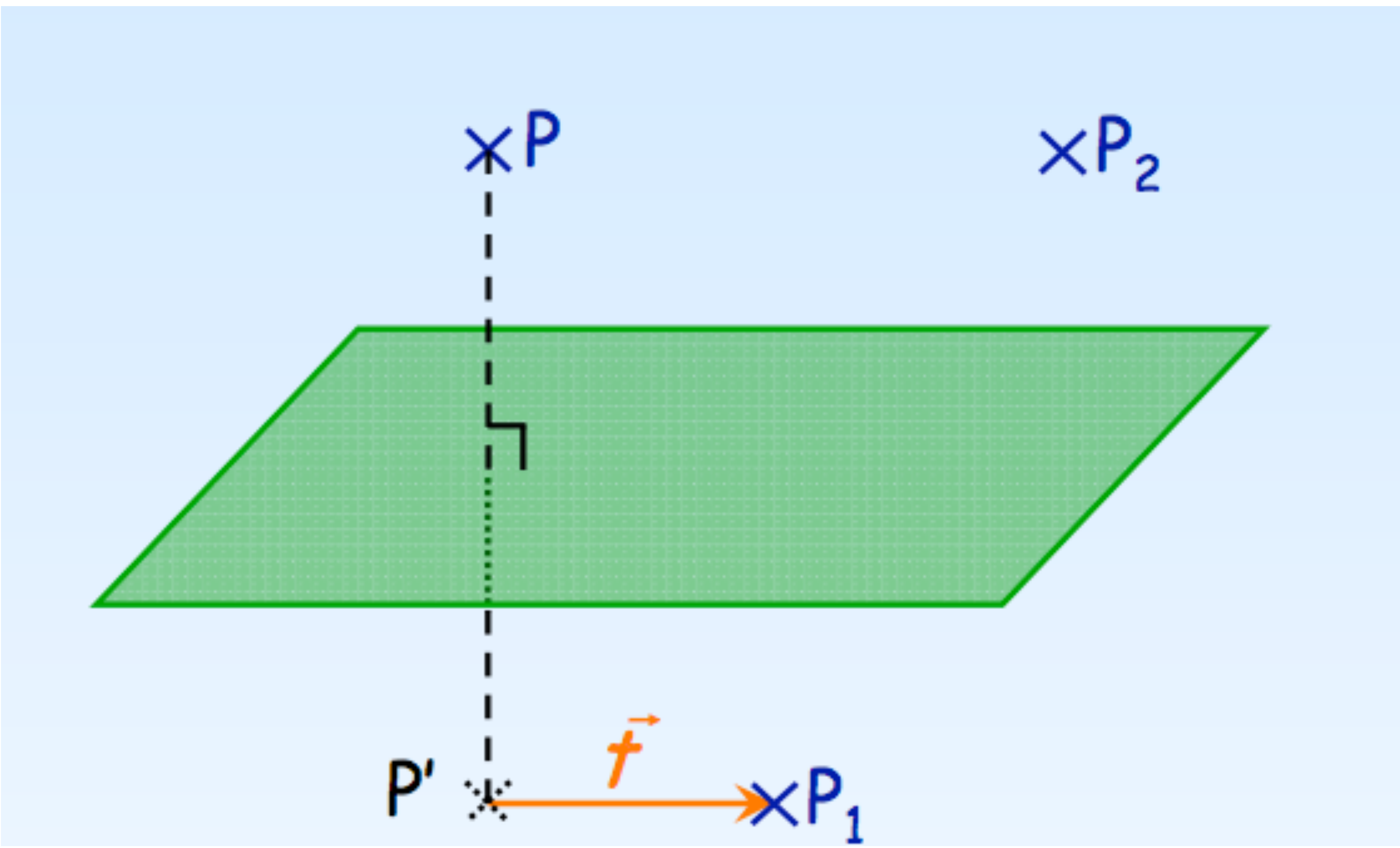
Note that: $m = \bar{2}$ *!*

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

Det = -1

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:

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

GEOMETRICAL INTERPRETATION OF MATRIX-COLUMN PRESENTATIONS OF SYMMETRY OPERATIONS

Geometric meaning of (W, w)

W information

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

EXERCISES

Problem 2.15 (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

EXERCISES

Problem 2.14(cont.)

Consider the matrix-column pairs

$$(\boldsymbol{A}, \boldsymbol{a}) = \begin{pmatrix} 0\,1\,0 \\ 1\,0\,0 \\ 0\,0\,\bar{1} \end{pmatrix}, \begin{pmatrix} 1/2 \\ 1/2 \\ 1/2 \end{pmatrix} \text{ and } (\boldsymbol{B}, \boldsymbol{b}) = \begin{pmatrix} 0\,1\,0 \\ 0\,0\,1 \\ 1\,0\,0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

(i) What is the matrix–column pair resulting from $(\boldsymbol{B},\ \boldsymbol{b})\,(\boldsymbol{A},\ \boldsymbol{a}) = (\boldsymbol{C}, \boldsymbol{c})$, and $(\boldsymbol{A},\ \boldsymbol{a})\,(\boldsymbol{B},\ \boldsymbol{b}) = (\boldsymbol{D}, \boldsymbol{d})$?

(ii) What is $(\boldsymbol{A}, \boldsymbol{a})^{-1}$, $(\boldsymbol{B}, \boldsymbol{b})^{-1}$, $(\boldsymbol{C}, \boldsymbol{c})^{-1}$ and $(\boldsymbol{D}, \boldsymbol{d})^{-1}$?

(iii) What is $(\boldsymbol{B}, \boldsymbol{b})^{-1}\,(\boldsymbol{A},\ \boldsymbol{a})^{-1}$?

Determine the type and order of isometries that are represented by the matrices ***A***, ***B***, ***C*** and ***D***:

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

Direction of rotation axis/normal

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=?

tr W=?

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

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

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

Problem 2.15 (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(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

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

solution:
point, line, plane or space

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

Fixed points?

NO solution:

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

translation part $\mathbf{w} = \begin{pmatrix} w1 \\ w2 \\ w3 \end{pmatrix}$

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

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

EXERCISES

Problem 2.15 (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: $\boldsymbol{t}/k = 1/k\ (\boldsymbol{W}^{k-1} + \ldots + \boldsymbol{W} + \boldsymbol{I})\boldsymbol{w}$

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

Fixed points of (W,w)

Location (fixed points x_F):

(B1) $t/k = 0$:

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

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

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

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

EXERCISES

Problem 2.15 (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: $(\boldsymbol{W}, \boldsymbol{w}_{lp})\boldsymbol{x}_F = \boldsymbol{x}_F$

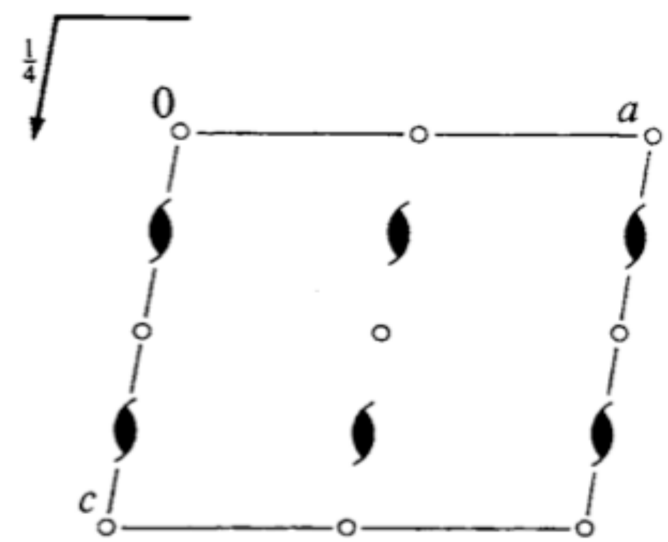
Space group $P2_1/c$ (No. 14)

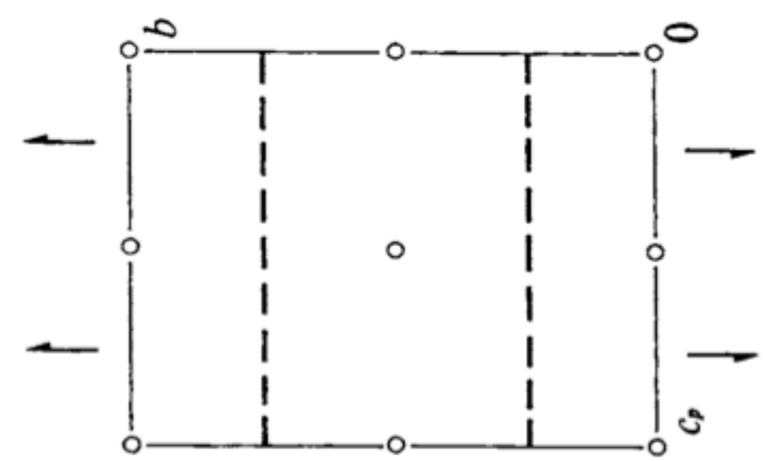
$P2_1/c$ C^5_{2h} $2/m$

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

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

bilbao crystallographic server

Contact us | About us | Publications | How to cite the server

Space-group symmetry

Magnetic Symmetry and Applications

Group-Subgroup Relations of Space Groups

Representations and Applications

Solid State Theory Applications

Structure Utilities

Subperiodic Groups: Layer, Rod and Frieze Groups

Structure Databases

Raman and Hyper-Raman scattering

Point-group symmetry

Plane-group symmetry

www.cryst.ehu.es

bilbao crystallographic server

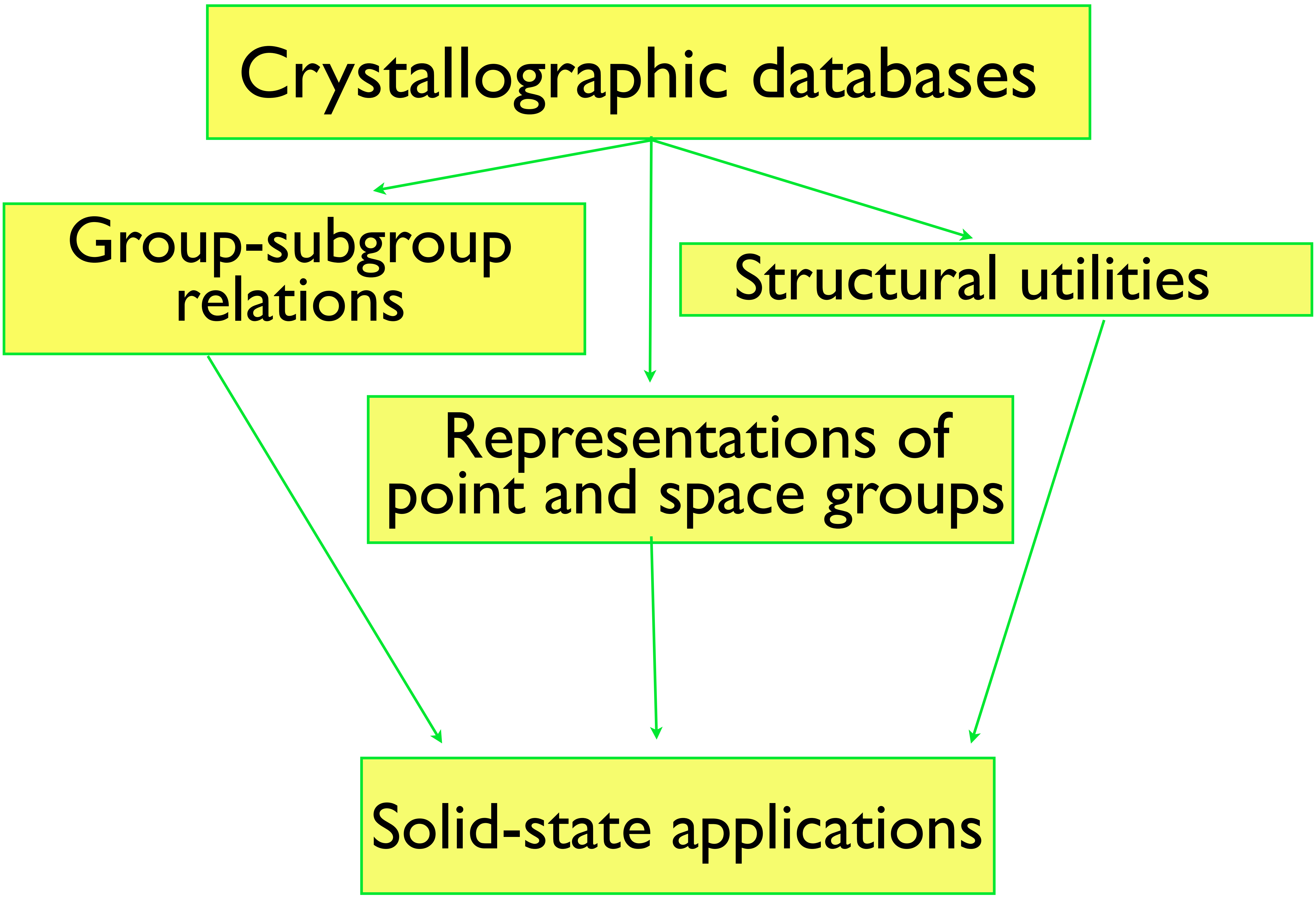
ECM31-Oviedo Satellite

rystallography online: workshop on the se and applications of the structural tools of the Bilbao Crystallographic Server

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**


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

Crystallographic Databases

International Tables for Crystallography

EXERCISES

Problem 2.15

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.

FCT/ZTF

bilbao crystallographic server

Contact us | About us | Publications | How to cite the server

bilbao crystallographic server

ECM31-Oviedo Satellite

Crystallography online: workshop on ...se and applications of the structural t... of the Bilbao Crystallographic Serve...

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

Symmetry Operation

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

Input:

i) The crystal system or the space group number.

ii) The matrix column representation of symmetry operation.

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

Output:

We obtain the geometric interpretation of the symmetry operation.

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

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

Standard/Default Setting | Non Conventional Setting | ITA Settings

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