THE BILBAO CRYSTALLOGRAPHIC SERVER:

CRYSTALLOGRAPHIC DATABASES AND COMPUTER PROGRAMS

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Bilbao Crystallographic Server

FCT/ZTF

bilbao crystallographic server

UPV/EHU

[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]

First announcement and pre-registration of a School in 2009 on

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

this server

Sections

Retrieval Tools
Group-Subgroup
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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

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.
COMMONSUBS	Common Subgroups of Space Groups
COMMONSUPER	Common Supergroups of Two Space Groups

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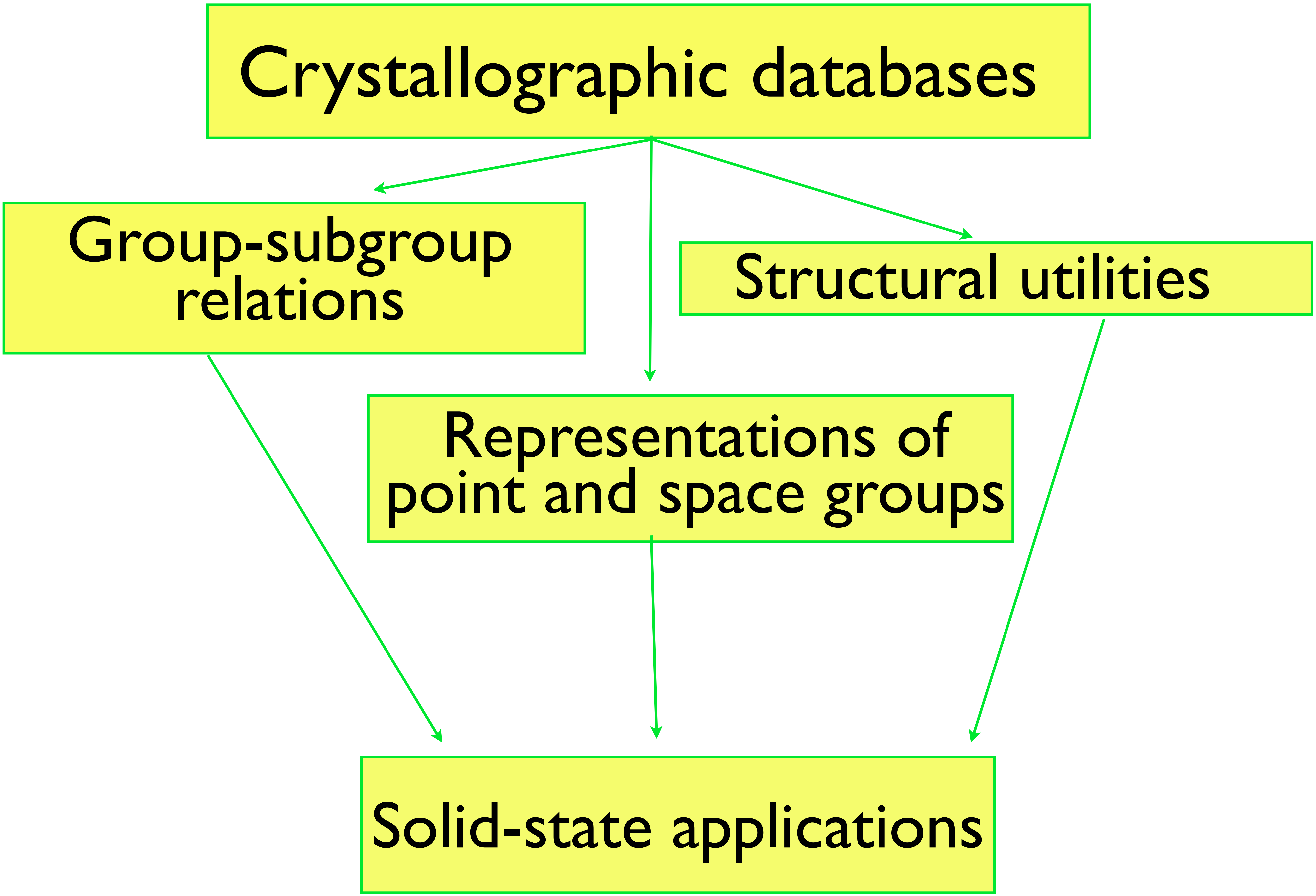
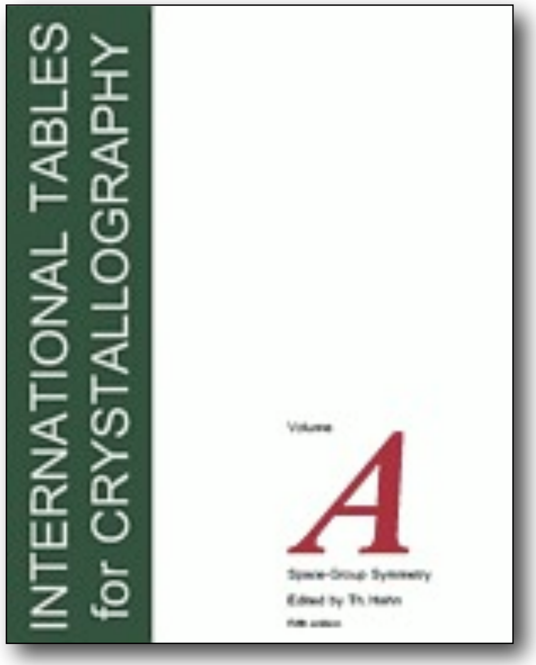

Crystallographic databases
Group-subgroup relations
Structural utilities
Representations of point and space groups
Solid-state applications

Crystallographic Databases

International Tables for Crystallography



Space-group Data

International Tables for Crystallography

Volume A: Space-group symmetry

generators
Wyckoff positions
Wyckoff sets
normalizers

Volume A1: Symmetry Relations between space groups

maximal subgroups of index 2,3 and 4
series of isomorphic subgroups

Retrieval tools

ITA space group $P4mm$

GENPOS

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

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	g	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$	no conditions
			(5) $x,\bar{y},z$	(6) $\bar{x},y,z$	(7) $\bar{y},\bar{x},z$	(8) y,x,z	
							Special:
4	f	$.m.$	$x,\frac{1}{2},z$	$\bar{x},\frac{1}{2},z$	$\frac{1}{2},x,z$	$\frac{1}{2},\bar{x},z$	no extra conditions
4	e	$.m.$	$x,0,z$	$\bar{x},0,z$	$0,x,z$	$0,\bar{x},z$	no extra conditions
4	d	$..m$	x,x,z	$\bar{x},\bar{x},z$	$\bar{x},x,z$	$x,\bar{x},z$	no extra conditions
2	c	$2mm.$	$\frac{1}{2},0,z$	$0,\frac{1}{2},z$			$hkl: h+k=2n$
1	b	$4mm$	$\frac{1}{2},\frac{1}{2},z$				no extra conditions
1	a	$4mm$	$0,0,z$				no extra conditions

WYCKPOS

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [110] $p1m1$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I [2]$P411$ ($P4$, 75) 1; 2; 3; 4
[2]$P21m$ ($Cmm2$, 35) 1; 2; 7; 8
[2]$P2m1$ ($Pmm2$, 25) 1; 2; 5; 6

IIa none

IIb [2]$P4_2mc$($\mathbf{c}'=2\mathbf{c}$)(105); [2]$P4cc$($\mathbf{c}'=2\mathbf{c}$)(103); [2]$P4_2cm$($\mathbf{c}'=2\mathbf{c}$)(101); [2]$C4md$($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$)($P4bm$, 100); [2]$F4mc$($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$)($I4cm$, 108); [2]$F4mm$($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b},\mathbf{c}'=2\mathbf{c}$)($I4mm$, 107)

MAXSUB

Maximal isomorphic subgroups of lowest index

IIc [2]$P4mm$($\mathbf{c}'=2\mathbf{c}$)(99); [2]$C4mm$($\mathbf{a}'=2\mathbf{a},\mathbf{b}'=2\mathbf{b}$)($P4mm$, 99)

SERIES

Minimal non-isomorphic supergroups

I [2]$P4/mmm$(123); [2]$P4/nmm$(129)

II [2]$I4mm$(107)

MINSUP

Generators/General Positions

http://lcpydb.lc.ehu.es/cryst/get_gen.html

Bilbao Crystallographic Server → Generators/General Positions   Help

Generators and General Positions

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 button [`choose it`].

To see the data in a non conventional setting click on [`Non conventional Setting`]. Otherwise, click on [`Conventional Setting`].

Please, enter the sequential number of group as given in the *International Tables for Crystallography*, Vol. A or   choose it   15

Show: Generators only   All General Positions

Conventional Setting   Non Conventional Setting   ITA Settings

[Bilbao Crystallographic Server Main Menu]

Bilbao Crystallographic Server
http://www.cryst.ehu.es

For comments, please mail to
cryst@wm.lc.ehu.es

Transformation of the basis

ITA-settings symmetry data

PRACTICAL EXERCISES

Bilbao Crystallographic Server

www.cryst.ehu.es

Bilbao Crystallographic Server - mirror site

http://158.227.0.68/

MATRIX-COLUMN PRESENTATION OF SYMMETRY OPERATIONS

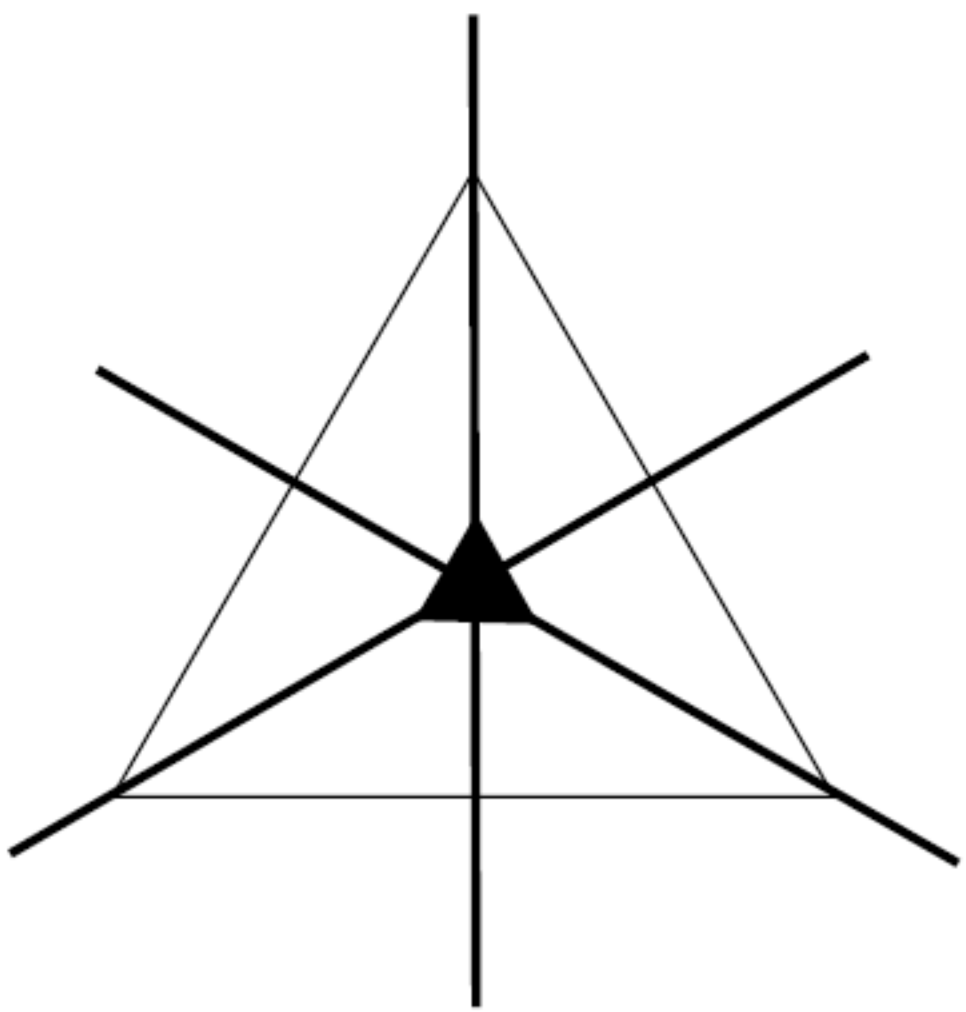
Crystallographic symmetry operations

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.

Description of isometries

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

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

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

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

Matrix formalism

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:

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

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:

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

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

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

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 1.1

Construct the matrix column pair (W,w) (and the corresponding (4x4) matrix) 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

GEOMETRIC MEANING OF MATRIX-COLUMN PAIRS (W,w)

Crystallographic symmetry operations

characteristics: fixed point of isometries $\tilde{P} = P$

Types of isometries preserve handedness

identity: the whole space fixed

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

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

screw rotation: no fixed point screw axis

screw vector

Types of isometries do not preserve handedness

roto-inversion: centre of roto-inversion fixed
roto-inversion axis

inversion: centre of inversion fixed

reflection: plane fixed
reflection/mirror plane

glide reflection: no fixed point
glide plane
glide vector

Geometric meaning of (W, w)

W information

(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

rotation angle

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

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

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 $\boldsymbol{u}$

Geometric meaning of (W, w)

w-information

(A) intrinsic translation part :

glide or screw component t/k

(A1) screw rotations:

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

(A2) glide reflections:

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

Geometric meaning of (W, w)

w-information

(B) 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 1.1(cont.)

Construct the matrix-column pairs (W,w) (and the corresponding (4x4) matrices) 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, *i.e.* determine (i) the type, (ii) glide (screw) components, (iii) fixed points, (iv) nature and location of the symmetry elements.

Problem 1.1

SOLUTION

(i)

$$\mathbb{W}(1)=\left(\begin{array}{ccc|c}1&0&0&0\\0&1&0&0\\0&0&1&0\\\hline 0&0&0&1\end{array}\right),\quad \mathbb{W}(2)=\left(\begin{array}{ccc|c}\bar{1}&0&0&0\\0&1&0&\frac{1}{2}\\0&0&\bar{1}&\frac{1}{2}\\\hline 0&0&0&1\end{array}\right)$$

$$\mathbb{W}(3)=\left(\begin{array}{ccc|c}\bar{1}&0&0&0\\0&\bar{1}&0&0\\0&0&\bar{1}&0\\\hline 0&0&0&1\end{array}\right),\quad \mathbb{W}(4)=\left(\begin{array}{ccc|c}1&0&0&0\\0&\bar{1}&0&\frac{1}{2}\\0&0&1&\frac{1}{2}\\\hline 0&0&0&1\end{array}\right)$$

(ii) *ITA* description: under **Symmetry operations**

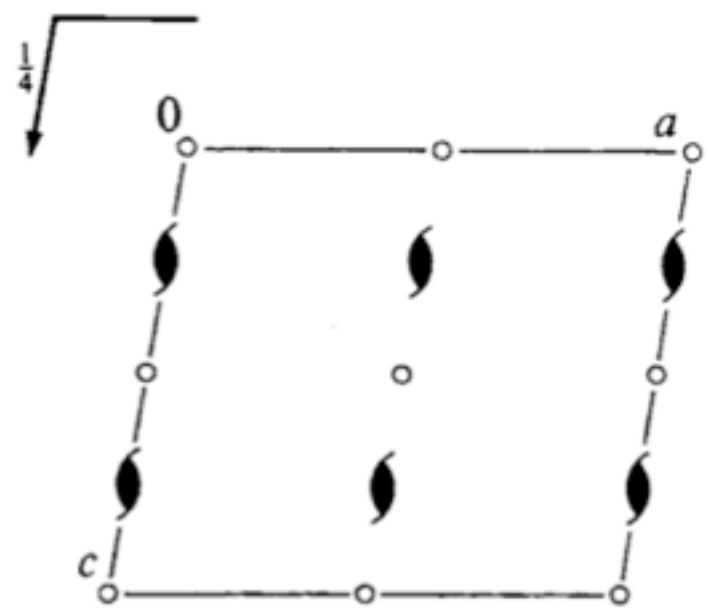
(1)	(2)	(3)	(4)
1	$2(0,\frac{1}{2},0)\ 0,y,\frac{1}{4}$	$\bar{1}\ 0,0,0$	$c\ x,\frac{1}{4},z$

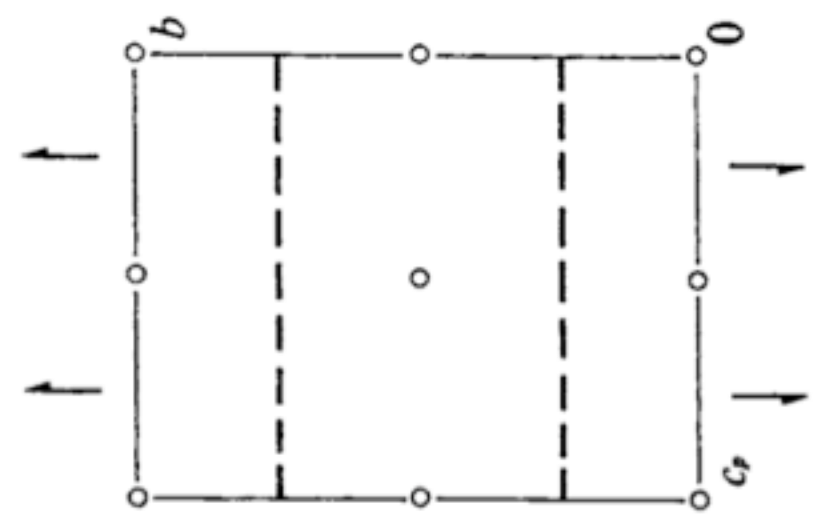
International Tables for Crystallography (2006). Vol. A, Space group 14, pp. 184–191.

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

No. 14 $\qquad$ $P\,1\,2_1/c\,1$ $\qquad$ 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

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

Symmetry operations

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

EXERCISES

Problem 1.2

Consider the matrices

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

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

(iv) The geometrical meaning of $(\boldsymbol{A}, \boldsymbol{a})$, $(\boldsymbol{B}, \boldsymbol{b})$, $(\boldsymbol{C}, \boldsymbol{c})$ and $(\boldsymbol{D}, \boldsymbol{d})$

Problem 1.2

SOLUTION

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

$\boldsymbol{B}\,\boldsymbol{a} + \boldsymbol{b} = \boldsymbol{B}\,\boldsymbol{a}$ for $\boldsymbol{b} = \boldsymbol{o}$.

Therefore, $(\boldsymbol{B}\,\boldsymbol{A}, \boldsymbol{B}\,\boldsymbol{a} + \boldsymbol{b}) = (\boldsymbol{C}, \boldsymbol{c}) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & \bar{1} \\ 0 & 1 & 0 \end{pmatrix}, \begin{pmatrix} 1/2 \\ 1/2 \\ 1/2 \end{pmatrix}$.

Analogously one calculates

$$(\boldsymbol{A}, \boldsymbol{a})\,(\boldsymbol{B}, \boldsymbol{b}) = (\boldsymbol{D}, \boldsymbol{d}) = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ \bar{1} & 0 & 0 \end{pmatrix}, \begin{pmatrix} 1/2 \\ 1/2 \\ 1/2 \end{pmatrix}.$$

Problem 1.2

SOLUTION

(ii) $(\boldsymbol{A},\boldsymbol{a})^{-1} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}, \begin{pmatrix} -1/2 \\ -1/2 \\ 1/2 \end{pmatrix}; (\boldsymbol{B},\boldsymbol{b})^{-1} = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}.$

$(\boldsymbol{C},\boldsymbol{c})^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & \bar{1} & 0 \end{pmatrix}, \begin{pmatrix} -1/2 \\ -1/2 \\ 1/2 \end{pmatrix}; (\boldsymbol{D},\boldsymbol{d})^{-1} = \begin{pmatrix} 0 & 0 & \bar{1} \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 1/2 \\ -1/2 \\ -1/2 \end{pmatrix}.$

(iii) $(\boldsymbol{B},\boldsymbol{b})^{-1}(\boldsymbol{A},\boldsymbol{a})^{-1} = \begin{pmatrix} 0 & 0 & \bar{1} \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 1/2 \\ -1/2 \\ -1/2 \end{pmatrix} = (\boldsymbol{D},\boldsymbol{d})^{-1} \neq (\boldsymbol{C},\boldsymbol{c})^{-1}.$

Note, that $(\boldsymbol{B},\boldsymbol{b})^{-1}(\boldsymbol{A},\boldsymbol{a})^{-1} = [(\boldsymbol{A},\boldsymbol{a})(\boldsymbol{B},\boldsymbol{b})]^{-1} = (\boldsymbol{D},\boldsymbol{d})^{-1}$.

Problem 1.2

SOLUTION

From the matrix parts the 'types' of the operations are determined by the determinants and traces:

	$\boldsymbol{A}$	$\boldsymbol{B}$	$\boldsymbol{C}$	$\boldsymbol{D}$
det	$+1$	$+1$	$+1$	$+1$
tr	$\bar{1}$	0	1	1
type	2	3	4	4

All the matrices are those of rotations. The directions [u v w] of the rotation axes are determined by applying either equation 1.4.11 or calculating the corresponding matrices $\boldsymbol{Y}(\boldsymbol{W})$:

$\boldsymbol{A}$	$\boldsymbol{B}$	$\boldsymbol{C}$	$\boldsymbol{D}$
$u = v$	$u = v$	$u = u$	$u = w$
$v = u$	$v = w$	$v = -w$	$v = v$
$w = -w$	$w = u$	$w = v$	$w = -u$
[1 1 0]	[1 1 1]	[1 0 0]	[0 1 0]

Problem 1.2

SOLUTION

The matrix-column pair $(\boldsymbol{A}, \boldsymbol{a})$: translation part

$$\frac{1}{2}\left[\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix} + \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}\right]\begin{pmatrix} 1/2 \\ 1/2 \\ 1/2 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1/2 \\ 1/2 \\ 1/2 \end{pmatrix} = \begin{pmatrix} 1/2 \\ 1/2 \\ 0 \end{pmatrix}$$

is the screw part of $(\boldsymbol{A}, \boldsymbol{a})$.

The reduced operation is $(\boldsymbol{A}, \boldsymbol{a}_{lp}) = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1/2 \end{pmatrix}$.

ITA description:

$(\boldsymbol{A}, \boldsymbol{a})$: screw rotation 2_1

screw rotation axis x,x,1/4

2(1/2,1/2,0) x,x,1/4

$(\boldsymbol{B}, \boldsymbol{b})$: rotation 3

rotation axis x,x,x

3^- x,x,x

Problem 1.2

SOLUTION

The matrix-column pair $(\boldsymbol{C}, \boldsymbol{c})$: translation part

$$\frac{\boldsymbol{t}}{4} = \frac{1}{4}\left[\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & \bar{1} & 0 \end{pmatrix} + \begin{pmatrix} 1 & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix} + \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & \bar{1} \\ 0 & 1 & 0 \end{pmatrix} + \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}\right]\begin{pmatrix} 1/2 \\ 1/2 \\ 1/2 \end{pmatrix} =$$

$$= \frac{1}{4}\begin{pmatrix} 4 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1/2 \\ 1/2 \\ 1/2 \end{pmatrix} = \begin{pmatrix} 1/2 \\ 0 \\ 0 \end{pmatrix}.$$

$(\boldsymbol{C}, \boldsymbol{c})$: screw rotation 4_2

screw rotation axis x,0,1/2

*IT*A description:

$4^+(1/2,0,0)$ x,0,1/2

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

Geometric Interpretation of Matrix Column Representation of 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.

Inpunt:

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 symmetry operation.

Please, introduce the crystal system	
Or please, enter the sequential number of group as given in the *International Tables for Crystallography*, Vol. A	choose it
Matrix column representation of symmetry operation	

	Rotational part			Traslation
In matrix form	1	0	0	0
	0	1	0	0
	0	0	1	0

Standard/Default Setting | Non Conventional Setting | ITA Settings

Problem 1.3

1. Solve the problems 1.1 and 1.2 applying the program SYMMETRY OPERATION

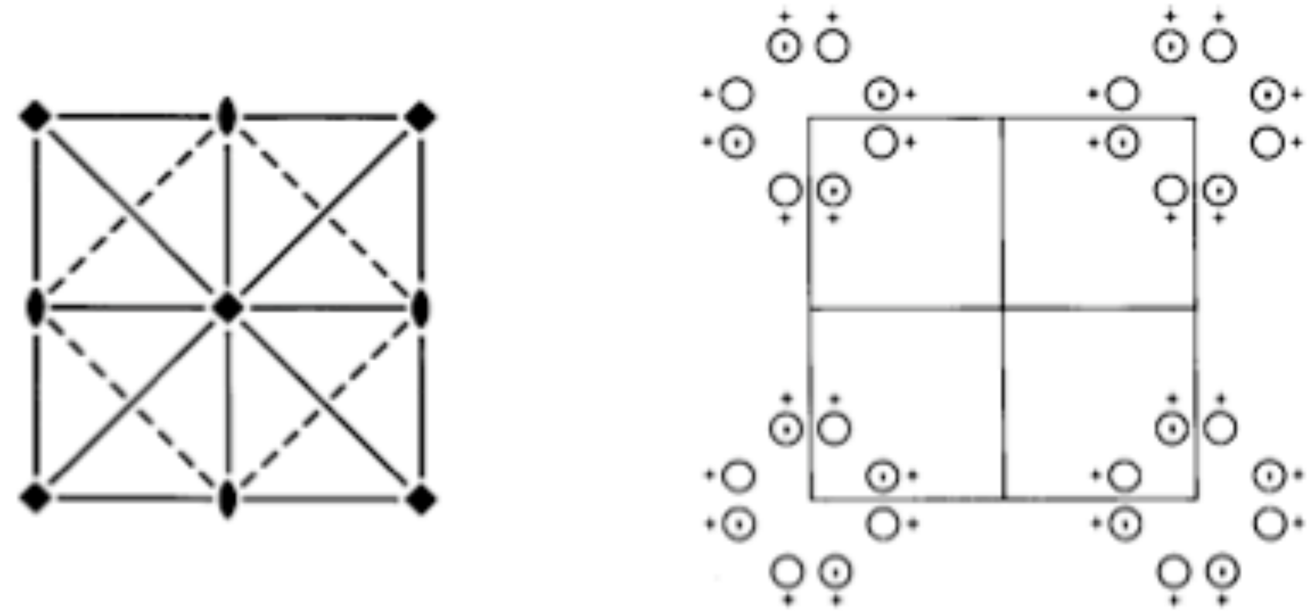
Problem 1.4

1. Characterize geometrically the matrix-column pairs listed under General position of the space group P4mm in ITA. Compare the results with the data listed under Symmetry operations.

2. Consider the diagram of the symmetry elements of P4mm. Try to determine the matrix-column pairs of the symmetry operations whose symmetry elements are indicated on the unit-cell diagram.

$P4mm$ C_{4v}^{1} $4mm$ Tetragonal

No. 99 $P4mm$ Patterson symmetry $P4/mmm$



Origin on $4mm$

Asymmetric unit $0 \leq x \leq \frac{1}{2}$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq 1$; $x \leq y$

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

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

Positions

Multiplicity, Wyckoff letter, Site symmetry — Coordinates

8	g	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$
			(5) $x,\bar{y},z$	(6) $\bar{x},y,z$	(7) $\bar{y},\bar{x},z$	(8) y,x,z

GENERATION
OF
SPACE GROUPS

Generators

Set of generators of a group is a set of space-group elements such that each element of the group can be obtained as an ordered product of the generators

$$W = G_h^{k_h} * G_{h-1}^{k_{h-1}} * \ldots * G_3^{k_3} * G_2^{k_2} * G_1$$

G_1 - identity

G_2, G_3, G_4 - primitive translations

G_5, G_6 - centring translations

G_7, G_8, ... - generate the rest of elements

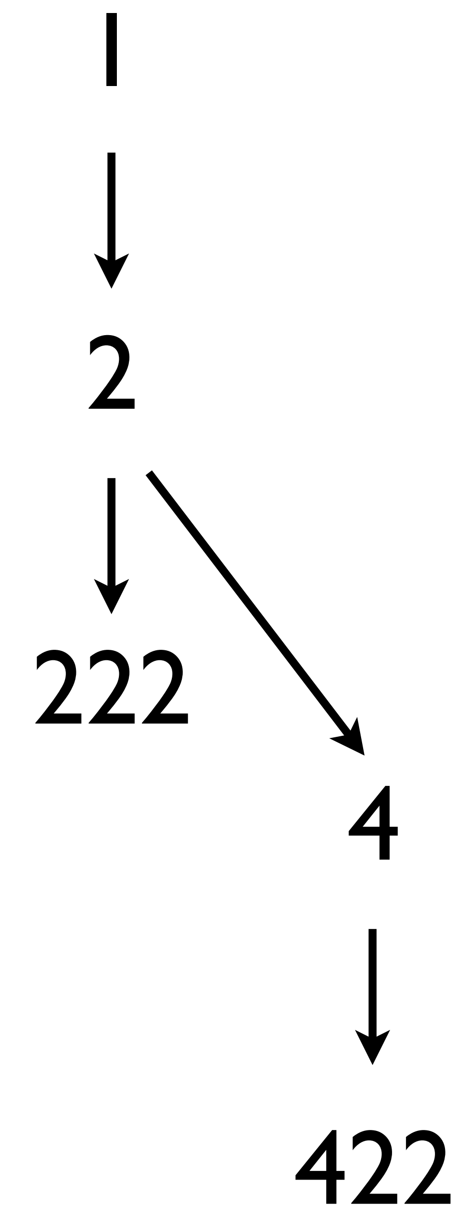
Generation of trigonal and hexagonal groups

3	3
$\bar{3}$	$3, \bar{1}$
321	$3, 2_{110}$
(rhombohedral coordinates	$3_{111}, 2_{10\bar{1}}$)
312	$3, 2_{1\bar{1}0}$
$3m1$	$3, m_{110}$
(rhombohedral coordinates	$3_{111}, m_{10\bar{1}}$)
$31m$	$3, m_{1\bar{1}0}$
$\bar{3}m1$	$3, 2_{110}, \bar{1}$
(rhombohedral coordinates	$3_{111}, 2_{10\bar{1}}, \bar{1}$)
$\bar{3}1m$	$3, 2_{1\bar{1}0}, \bar{1}$
6	$3, 2_z$
$\bar{6}$	$3, m_z$
$6/m$	$3, 2_z, \bar{1}$
622	$3, 2_z, 2_{110}$
$6mm$	$3, 2_z, m_{110}$
$\bar{6}m2$	$3, m_z, m_{110}$
$\bar{6}2m$	$3, m_z, 2_{110}$
$6/mmm$	$3, 2_z, 2_{110}, \bar{1}$

$$
\begin{tikzcd}
1 \arrow[d] & \\
3 \arrow[d] \arrow[rdd] & \\
32 & \\
 & 6 \arrow[d] \\
 & 622
\end{tikzcd}
$$

Generation of orthorhombic and tetragonal groups

Hermann–Mauguin symbol of crystal class	Generators G_i (sequence left to right)
1	1
$\bar{1}$	$\bar{1}$
2	2
m	m
$2/m$	$2, \bar{1}$
222	$2_z, 2_y$
$mm2$	$2_z, m_y$
mmm	$2_z, 2_y, \bar{1}$
4	$2_z, 4$
$\bar{4}$	$2_z, \bar{4}$
$4/m$	$2_z, 4, \bar{1}$
422	$2_z, 4, 2_y$
$4mm$	$2_z, 4, m_y$
$\bar{4}2m$	$2_z, \bar{4}, 2_y$
$\bar{4}m2$	$2_z, \bar{4}, m_y$
$4/mmm$	$2_z, 4, 2_y, \bar{1}$



EXERCISES

Problem 1.5

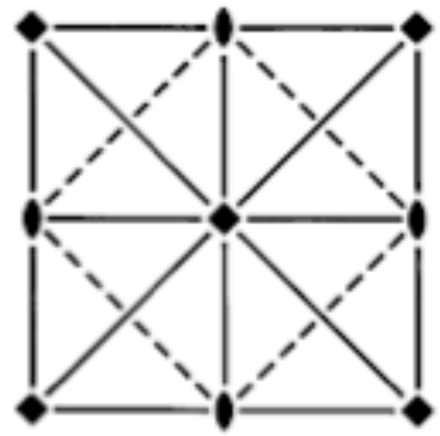
Generate the space group P4mm using the selected generators

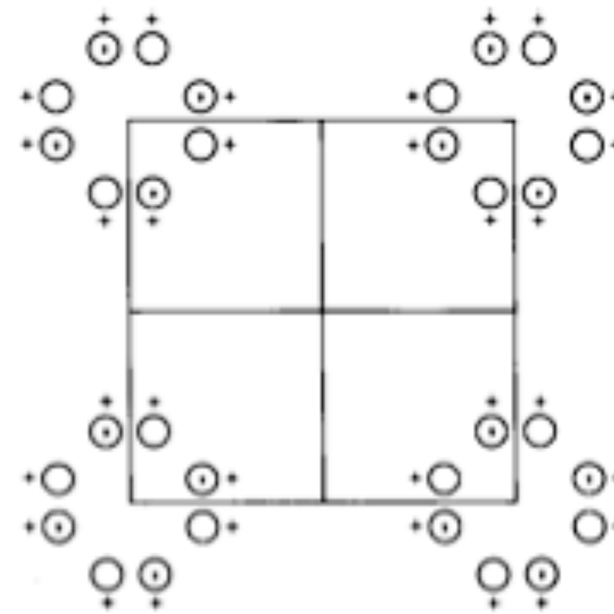
Compare the results of your calculation with the coordinate triplets listed under General position of the ITA data of P4mm

Compare the results of your calculations with the BCS data using the retrieval tools GENPOS (generators and general positions)

International Tables for Crystallography (2006). Vol. A, Space group 99, pp. 382–383.

$P4mm$	C_{4v}^{1}	$4mm$	Tetragonal
No. 99	$P4mm$		Patterson symmetry $P4/mmm$





Origin on $4mm$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le 1$; $x \le y$

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

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

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			
8 g 1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$
	(5) $x,\bar{y},z$	(6) $\bar{x},y,z$	(7) $\bar{y},\bar{x},z$	(8) y,x,z

SITE-SYMMETRY

GENERAL POSITION

SPECIAL WYCKOFF POSITIONS

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	$\bar{1}$	$\frac{1}{2},0,\frac{1}{2}$	

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

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

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

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

isomorphic

EXERCISES

Problem 1.6

Consider the special Wyckoff positions of the the space group P4mm.

Determine the site-symmetry groups of Wyckoff positions 1a and 2b. Compare the results with the listed ITA data

The coordinate triplets (x,1/2,z) and (1/2,x,z), belong to Wyckoff position 4f. Compare their site-symmetry groups.

Space group P4mm

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

Positions

Multiplicity, Wyckoff letter, Site symmetry — Coordinates

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

EXERCISES

Problem 1.7

Consider the data given in *ITA* for the space group $P4_2/mbc$, No. 135:

Generate the representatives of the *General Position* from the generators of the group. Starting from $\mathcal{T}_{\mathcal{G}}$, construct the chain of normal subgroups along which the space group $P4_2/mbc$ is step-wise generated;

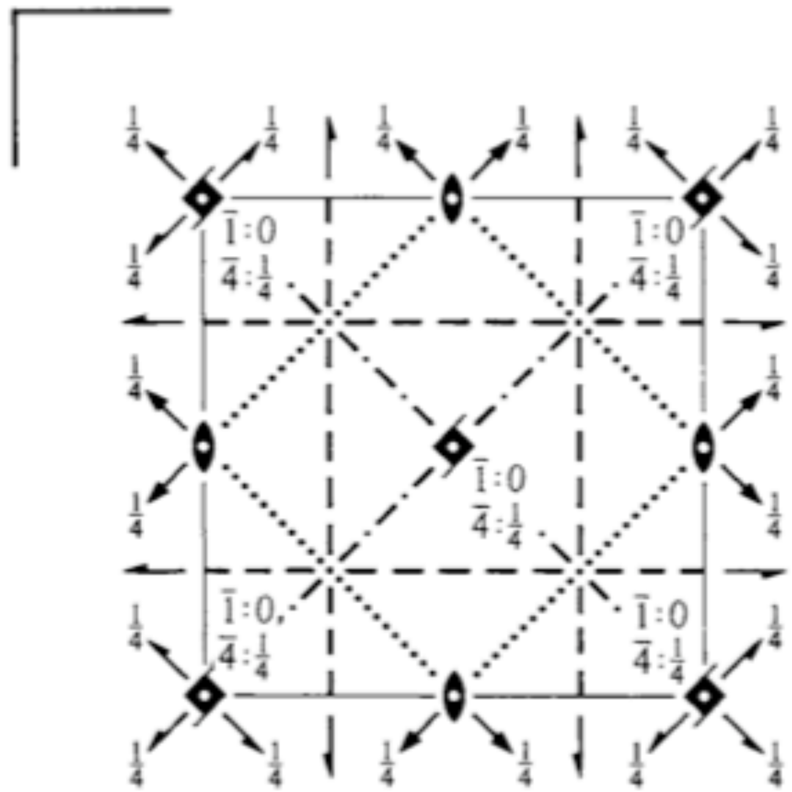
Determine the site-symmetry groups of the following *Wyckoff positions*: $4(a)$; $4(c)$; $4(d)$; $8(g)$. Construct the corresponding oriented site-symmetry symbols and compare them with those listed in *ITA*;

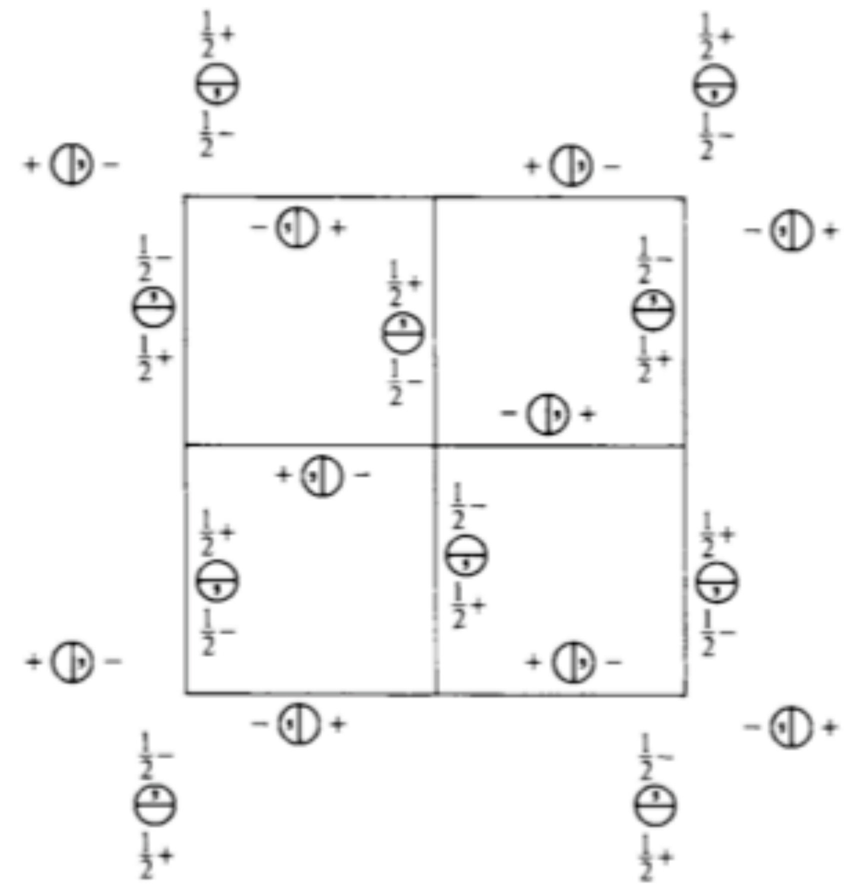
Characterize geometrically the isometries (3), (8), (12), (15) and (16) as listed under *General Position*. Compare the results with the corresponding geometric descriptions listed under *Symmetry operations* in *ITA*.

International Tables for Crystallography (2006). Vol. A, Space group 135, pp. 466–467.

$P4_2/mbc$ D_{4h}^{13} $4/mmm$ Tetragonal

No. 135 $P\ 4_2/m\ 2_1/b\ 2/c$ Patterson symmetry $P4/mmm$





Origin at centre $(2/m)$ at $4_2/m1n$

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

Symmetry operations

(1) 1	(2) $2\quad 0,0,z$	(3) $4^+(0,0,\frac{1}{2})\quad 0,0,z$	(4) $4^-(0,0,\frac{1}{2})\quad 0,0,z$
(5) $2(0,\frac{1}{2},0)\quad \frac{1}{4},y,0$	(6) $2(\frac{1}{2},0,0)\quad x,\frac{1}{4},0$	(7) $2(\frac{1}{2},\frac{1}{2},0)\quad x,x,\frac{1}{4}$	(8) $2\quad x,\bar{x}+\frac{1}{2},\frac{1}{4}$
(9) $\bar{1}\quad 0,0,0$	(10) $m\quad x,y,0$	(11) $\bar{4}^+\quad 0,0,z;\ 0,0,\frac{1}{4}$	(12) $\bar{4}^-\quad 0,0,z;\ 0,0,\frac{1}{4}$
(13) $a\quad x,\frac{1}{4},z$	(14) $b\quad \frac{1}{4},y,z$	(15) $c\quad x+\frac{1}{2},\bar{x},z$	(16) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})\quad x,x,z$

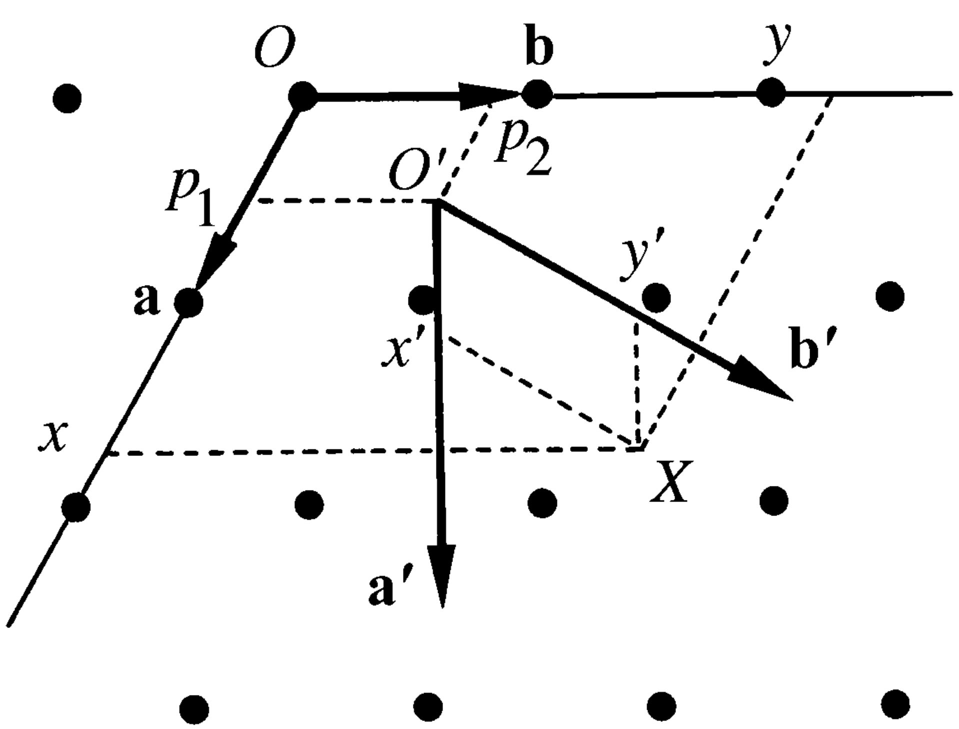
Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	i	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z+\frac{1}{2}$	(4) $y,\bar{x},z+\frac{1}{2}$	$0kl$: $k=2n$
			(5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	(7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	(8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	hhl : $l=2n$
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x,y,\bar{z}$	(11) $y,\bar{x},\bar{z}+\frac{1}{2}$	(12) $\bar{y},x,\bar{z}+\frac{1}{2}$	$00l$: $l=2n$
			(13) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(14) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	(15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(16) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	$h00$: $h=2n$
							Special: as above, plus
8	h	$m\,.\,.$	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{y},x,\frac{1}{2}$	$y,\bar{x},\frac{1}{2}$	no extra conditions
			$\bar{x}+\frac{1}{2},y+\frac{1}{2},0$	$x+\frac{1}{2},\bar{y}+\frac{1}{2},0$	$y+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	
8	g	$.\,.\,2$	$x,x+\frac{1}{2},\frac{1}{4}$	$\bar{x},\bar{x}+\frac{1}{2},\frac{1}{4}$	$\bar{x}+\frac{1}{2},x,\frac{3}{4}$	$x+\frac{1}{2},\bar{x},\frac{3}{4}$	hkl : $l=2n$
			$\bar{x},\bar{x}+\frac{1}{2},\frac{3}{4}$	$x,x+\frac{1}{2},\frac{3}{4}$	$x+\frac{1}{2},\bar{x},\frac{1}{4}$	$\bar{x}+\frac{1}{2},x,\frac{1}{4}$	
8	f	$2\,.\,.$	$0,\frac{1}{2},z$	$\frac{1}{2},0,z+\frac{1}{2}$	$\frac{1}{2},0,\bar{z}$	$0,\frac{1}{2},\bar{z}+\frac{1}{2}$	hkl : $h+k,l=2n$
			$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,\bar{z}+\frac{1}{2}$	$\frac{1}{2},0,z$	$0,\frac{1}{2},z+\frac{1}{2}$	
8	e	$2\,.\,.$	$0,0,z$	$0,0,z+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\bar{z}$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	hkl : $h+k,l=2n$
			$0,0,\bar{z}$	$0,0,\bar{z}+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	
4	d	$2\,.\,22$	$0,\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},0,\frac{3}{4}$	$0,\frac{1}{2},\frac{3}{4}$	$\frac{1}{2},0,\frac{1}{4}$	hkl : $h+k,l=2n$
4	c	$2/m\,.\,.$	$0,\frac{1}{2},0$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},\frac{1}{2}$	hkl : $h+k,l=2n$
4	b	$\bar{4}\,.\,.$	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$	$\frac{1}{2},\frac{1}{2},\frac{3}{4}$	$\frac{1}{2},\frac{1}{2},\frac{1}{4}$	hkl : $h+k,l=2n$
4	a	$2/m\,.\,.$	$0,0,0$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	hkl : $h+k,l=2n$

CO-ORDINATE TRANSFORMATIONS IN CRYSTALLOGRAPHY

General affine transformation

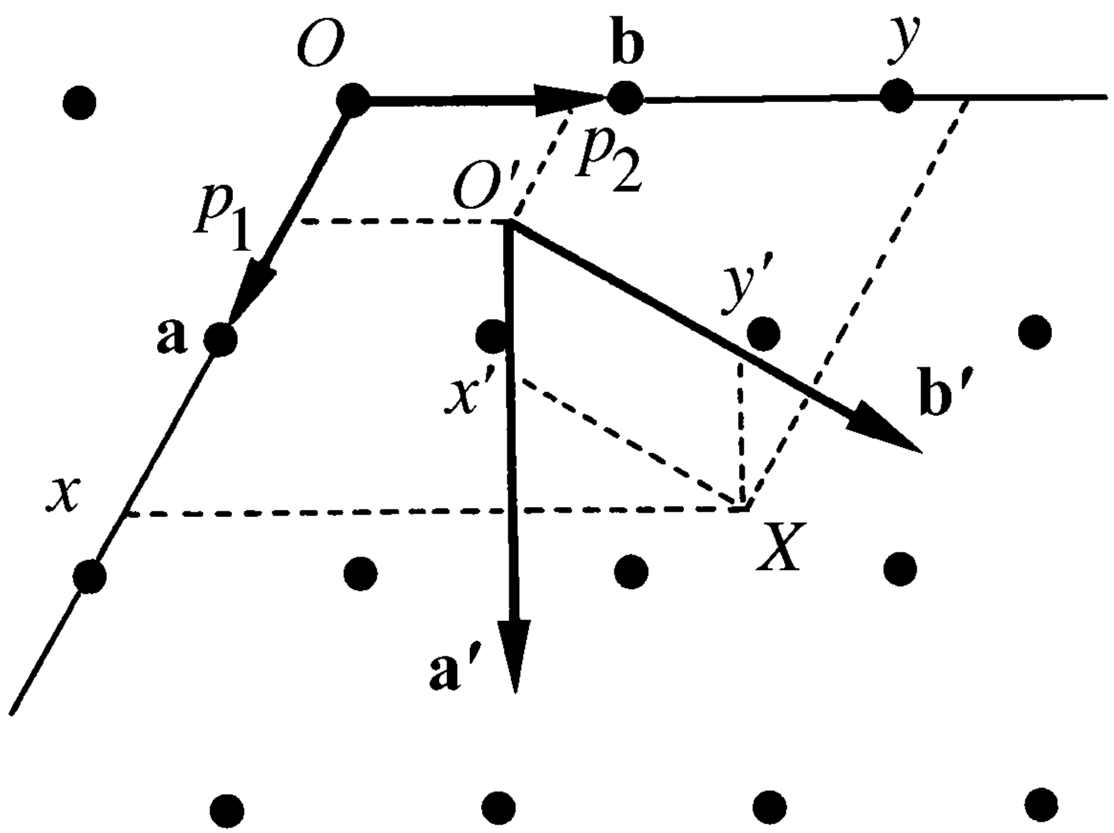


a change of basis from (**a**, **b**) to (**a’** , **b’**)

a shift of origin from O to O’ by a shift vector ***p*** with components p_1 and p_2

Change in the coordinates of the point X from (x, y) to (x’,y’)

Problem: BASIS TRANSFORMATION



3-dimensional space

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

$$\big\downarrow (P,p)$$

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

Transformation of symmetry operations (W,w):

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

3-dimensional space

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

$$\Big\downarrow{\scriptstyle (\boldsymbol{P},\boldsymbol{p})}$$

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

(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

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

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \boldsymbol{Q}\begin{pmatrix} x \\ y \\ z \end{pmatrix} + \boldsymbol{q}$$

with

$$\boldsymbol{Q} = \boldsymbol{P}^{-1}$$
$$\boldsymbol{q} = -\boldsymbol{P}^{-1}\boldsymbol{p}.$$

$$= \begin{pmatrix} Q_{11}x + Q_{12}y + Q_{13}z + q_1 \\ Q_{21}x + Q_{22}y + Q_{23}z + q_2 \\ Q_{31}x + Q_{32}y + Q_{33}z + q_3 \end{pmatrix}.$$

special cases

-origin shift: $\boxed{\boldsymbol{x}' = \boldsymbol{x} - \boldsymbol{p}}$

-change of basis : $\boxed{\boldsymbol{x}' = \boldsymbol{P}^{-1}\boldsymbol{x}}$

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

$$\begin{tikzcd}
 & \text{point} & & \text{image point} & \\
 & X & & \widetilde{X} & \\
x & \circ \arrow[rr, "(\boldsymbol{W},\boldsymbol{w})"] & & \circ & \tilde{x} \quad \text{old coordinates} \\
x' & \circ \arrow[u, "(\boldsymbol{P},\boldsymbol{p})"'] \arrow[rr, "(\boldsymbol{W}',\,\boldsymbol{w}')"] & & \circ \arrow[u, "(\boldsymbol{P},\boldsymbol{p})"] & \tilde{x}' \quad \text{new coordinates}
\end{tikzcd}$$

Mapping of mappings

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

Matrix formalism: 4x4 matrices

augmented matrices:

$$\mathbb{W} = \left(\begin{array}{ccc|c} W_{11} & W_{12} & W_{13} & w_1 \\ W_{21} & W_{22} & W_{23} & w_2 \\ W_{31} & W_{32} & W_{33} & w_3 \\ \hline 0 & 0 & 0 & 1 \end{array}\right), \quad \mathbb{x} = \begin{pmatrix} x \\ y \\ z \\ \hline 1 \end{pmatrix}; \quad \mathbb{x}' = \begin{pmatrix} x' \\ y' \\ z' \\ \hline 1 \end{pmatrix}$$

$$\mathbb{x}' = \mathbb{Q}\,\mathbb{x} = \mathbb{P}^{-1}\mathbb{x}$$

$$\mathbb{W}' = \mathbb{Q}\,\mathbb{W}\,\mathbb{P} = \mathbb{P}^{-1}\,\mathbb{W}\,\mathbb{P}$$

Problem: SYMMETRY DATA
ITA SETTINGS

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

4. SYNOPTIC TABLES OF SPACE-GROUP SYMBOLS

Table 4.3.1 (*cont.*)

MONOCLINIC SYSTEM

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

SYMMETRY DATA: ITA SETTINGS

Monoclinic descriptions

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

Orthorhombic descriptions

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

EXERCISES

Problem 2.1

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

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

CRYSTAL-STRUCTURE DESCRIPTIONS

Inorganic Crystal Structure Database

CC=45520 Details Bonds Pattern Structure Jmol

Title	Redetermination of the oxygen parameters in zircon (Zr Si O4).
Authors	Krstanovic, I.R.
Reference	Acta Crystallographica (1958) **11**, 896-897 **Link XRef SCOPUS SCIRUS Google**
Compound	**Zr (Si O4)** - **[Zircon]** Zirconium silicate **[ABX4] [tI24] [h b a] [ZrSiO4]**
Cell	6.6164(5), 6.6164, 6.0150(5), 90., 90., 90. **I41/AMDZ (141)** V=263.32
Remarks	R=0.070000 : PDC =01-073-6646 : PDF =6-266 : TYP =ZrSiO4 : XDS MIN =Zircon : At least one temperature factor missing in the paper. hk0- and 0kl-data, crystals not metamict

Atom (site) Oxid.			**x, y, z, B, Occupancy**				
Zr1	(4a)	4	0	0.75	0.125	0	1
Si1	(4b)	4	0	0.75	0.625	0	1
O1	(16h)	-2	0	0.067(3)	0.198(3)	0	1

lattice parameters

space group

asymmetric-unit data

EXERCISES

Problem 2.2

Print **2** entries selected.

CC=Collection Code: [AB2X4]=ANX Form: [cF56]=Pearson: [e d a]=Wyckoff Symbol: [Al2MgO4]=Structure Type:

Click the ANX, Pearson or Wyckoff Symbol to find structures with that symbol.

CC=45520 Details Bonds Pattern Structure Jmol

Title	Redetermination of the oxygen parameters in zircon (Zr Si O4).
Authors	Krstanovic, I.R.
Reference	Acta Crystallographica (1958) **11**, 896-897 **Link XRef SCOPUS SCIRUS Google**
Compound	**Zr (Si O4) - [Zircon]** Zirconium silicate **[ABX4] [tI24] [h b a] [ZrSiO4]**
Cell	6.6164(5), 6.6164, 6.0150(5), 90., 90., 90. **I41/AMDZ (141)** V=263.32
Remarks	R=0.070000 : PDC =01-073-6646 : PDF =6-266 : TYP =ZrSiO4 : XDS MIN =Zircon : At least one temperature factor missing in the paper. hk0- and 0kl-data, crystals not metamict

Atom (site) Oxid.			**x, y, z, B, Occupancy**				
Zr1	(4a)	4	0	0.75	0.125	0	1
Si1	(4b)	4	0	0.75	0.625	0	1
O1	(16h)	-2	0	0.067(3)	0.198(3)	0	1

CC=31101 Details Bonds Pattern Structure Jmol

Title	Die Kristallstruktur von Zirkon und die Kriterien fuer spezielle Lagen in tetragonalen Raumgruppen..
Authors	Wyckoff, R.W.G.;Hendricks, S.B.
Reference	Zeitschrift fuer Kristallographie, Kristallgeometrie, Kristallphysik, Kristallchemie (1927) **66**, 73-102 **Link XRef SCOPUS SCIRUS Google** **Also:** Philosophical Magazine, Serie (1926) **1**, 1151-1151
Compound	**Zr (Si O4) - [Zircon]** Zirconium silicate **[ABX4] [tI24] [h b a] [ZrSiO4]**
Cell	6.61, 6.61, 5.98, 90., 90., 90. **I41/AMDS (141)** V=261.28
Remarks	COR MIN =Zircon : PDF =6-266 : TYP =ZrSiO4 : XDS At least one temperature factor missing in the paper. No R value given in the paper. Revised data of 31084

Atom (site) Oxid.			**x, y, z, B, Occupancy**				
Zr1	(4a)	4	0	0	0	0	1
Si1	(4b)	4	0	0	0.5	0	1
O1	(16h)	-2	0	0.2(1)	0.34(2)	0	1

EXERCISES

Problem 2.2

Structure 1: Space group *I*4$_1$/*amd*, No. 141
origin choice 1 at $\bar{4}m2$
a=6.60 $\AA$ c=5.88 $\AA$

$$Zr:(a)\ 0,0,0;\ 0,\tfrac{1}{2},\tfrac{1}{4};\ \tfrac{1}{2},0,\tfrac{3}{4};\ \tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2};$$
$$Si:(b)\ 0,0,\tfrac{1}{2};\ 0,\tfrac{1}{2},\tfrac{3}{4};\ \tfrac{1}{2},0,\tfrac{1}{4};\ \tfrac{1}{2},\tfrac{1}{2},0;$$
$$O:(h)\ (0,u,v;\ 0,\bar{u},v;\ u,0,\bar{v};\ \bar{u},0,\bar{v};$$
$$\bar{u},\tfrac{1}{2},v+\tfrac{1}{4};\ u,\tfrac{1}{2},v+\tfrac{1}{4};)\ [\text{and t}$$

u=0.20; *v*=0.34

Problem 2.2

Structure 2: Space group $I4_1/amd$, No. 141

origin choice 2

at $2/m$ at 0,-1/4,1/8 from $\bar{4}m2$

a=6.6164 $\AA$ c=6.015 $\AA$

Coordinate transformation

Origin choice 1 $\longrightarrow$ Origin choice 2

$\boldsymbol{p}$=0,-1/4,1/8

(i) What are the new coordinates of the Zr atoms ?

(ii) What are the new coordinates of the Si atoms ?

(iii) What are the new coordinates of the O atom at $0, u, v$?

(iv) What are the new coordinates of the other O atoms ?

Problem 2.2

Coordinate transformation

primitive basis description

$$\mathbf{a}' = \mathbf{a};\ \mathbf{b}' = \mathbf{b};\ \mathbf{c}' = \frac{1}{2}(\mathbf{a} + \mathbf{b} + \mathbf{c})$$

(v) What are the new coordinates of the first Zr atom ?

(vi) What are the new coordinates of the first Si atom ?

(vii) What are the new coordinates of the O atom originally a

(viii) What are the lattice parameters of the primitive unit cell

Problem 2.2

SOLUTION

Origin 2 description $x' = x - p$

(i) $Zr:\ (a)\ \ 0, \frac{1}{4}, \frac{\bar{1}}{8} \sim \frac{7}{8};\ 0, \frac{3}{4}, \frac{1}{8};\ \frac{1}{2}, \frac{1}{4}, \frac{5}{8};\ \frac{1}{2}, \frac{3}{4}, \frac{3}{8};$

(ii) $Si:\ (b)\ \ 0, \frac{1}{4}, \frac{3}{8};\ 0, \frac{3}{4}, \frac{5}{8};\ \frac{1}{2}, \frac{1}{4}, \frac{1}{8};\ \frac{1}{2}, \frac{3}{4}, \frac{\bar{1}}{8} \sim \frac{7}{8};$

(iii) $O:\ (h)\ \ 0, 0.20 + 0.25, 0.34 - 0.125 = 0, 0.45, 0.215.$

the rest of oxygen atoms

0, 0.05, 0.215 0.20, 0.25, 0.535 0.80, 0.25, 0.535 0, 0.95, 0.785
0, 0.55, 0.785 0.80, 0.75, 0.465 0.20, 0.75, 0.465, all also with
$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$.

0, 0.0167, 0.198

Problem 2.2

SOLUTION

primitive basis description

$$\boldsymbol{P} = \begin{pmatrix} 1 & 0 & 1/2 \\ 0 & 1 & 1/2 \\ 0 & 0 & 1/2 \end{pmatrix} \qquad \boldsymbol{P}^{-1} = \begin{pmatrix} 1 & 0 & \bar{1} \\ 0 & 1 & \bar{1} \\ 0 & 0 & 2 \end{pmatrix}$$

$$\boldsymbol{x}' = \boldsymbol{P}^{-1}\boldsymbol{x}$$

(v) The new coordinates of the first Zr atom are
$0 - \frac{7}{8}, \frac{1}{4} - \frac{7}{8}, 2 \cdot \frac{7}{8} \ \sim \ \frac{1}{8}, \frac{3}{8}, \frac{3}{4}$.

(vi) The new coordinates of the first Si atom are
$0 - \frac{3}{8}, \frac{1}{4} - \frac{3}{8}, 2 \cdot \frac{3}{8} \ \sim \ \frac{5}{8}, \frac{7}{8}, \frac{3}{4}$.

(vii) The new coordinates of the first O atom are
$0 - 0.215, 0.45 - 0.215, 2 \cdot 0.215 \sim 0.785, 0.235, 0.430$.

Structure Utilities

Structure Utilities	
CELLTRAN	Transform Unit Cells
STRAIN	Strain Tensor Calculation
WPASSIGN	Assignment of Wyckoff Positions
TRANSTRU	Transform structures to lower symmetry Space Group basis.
SETSTRU	Alternative Settings for a given Crystal Structure
EQUIVSTRU	Equivalent Descriptions for a given Crystal Structure

Problem: ALTERNATIVE SETTINGS SETSTRU

ITA-settings for the space group C2/c (No.15)

Choose the initial and final space groups symbols

n matrices must be read by columns. **P** is the transformation from standard to non-

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

Initial	Final	Setting	P	P^{-1}
		C 1 2/*c* 1	a,b,c	a,b,c
		A 1 2/*n* 1	-a-c,b,a	c,b,-a-c
		I 1 2/*a* 1	c,b,-a-c	-a-c,b,a
		A 1 2/*a* 1	c,-b,a	c,-b,a
		C 1 2/*n* 1	a,-b,-a-c	a,-b,a-c
		I 1 2/*c* 1	-a-c,-b,c	-a-c,-b,c
		A 1 1 2/*a*	c,a,b	b,c,a
		B 1 1 2/*n*	a,-a-c,b	a,c,-a-b
		I 1 1 2/*b*	-a-c,c,b	-a-b,c,b
		B 1 1 2/*b*	a,c,-b	a,-c,b
		A 1 1 2/*n*	-a-c,a,-b	b,-c,-a-b
		I 1 1 2/*a*	c,-a-c,-b	-a-b,-c,a
		B 2/*b* 1 1	b,c,a	c,a,b

Problem: STRUCTURE TRANSFORMATION TRANSTRU

Transform Structure

Transform Structure

TRANSTRU can transform a structure in two ways:

- To a lower symmetry space group. The transformed structure is given in the low symmetry space group basis, taking care of all possible splittings of the Wyckoff positions.
- With an arbitrary matrix. The structure, including the cell parameters and the atoms in the unit cell, is transformed with an arbitrary matrix introduced by the user.

Structure Data [in CIF format] Examinar...

HINT: [The option for a given filename is preferential]

High Symmetry Structure

```
# Space Group ITA number
221
# Lattice parameters
5.0 5.0 5.0 90 90 90
# Number of independent atoms in the asymmetric unit
3
# [atom type] [number] [WP] [x] [y] [z]
Ba   1 1a 0.0 0.0 0
Ti   2 1b 0.5 0.5 0.5
O    3 3c 0.5 0.0 0.5
```

Transform structure to a subgroup basis ◉

Transform structure with an arbitrary matrix ○

Show

structure asymmetric unit

default settings

Problem: UNIT CELL TRANSFORMATION CELLTRAN

Transform Unit Cell

Transform Unit Cell

Given the cell parameters (separated with spaces), the centring and a transformation matrix the program calculates:

- The transformed unit cell.
- The primitive unit cell.
- The reduced unit cell.
- The metric tensors for each cell.
- The standard root tensor (transformation from the conventional to a cartesian basis)

Cell Parameters: 4 4 4 90 90 90 Centering F

Please, define the transformation matrix that relates the group and the subgroup bases

in abc form: Ex: c,a,b (read by columns)

or in matrix form:

Rotational part			Origin Shift
1	0	0	0
0	1	0	0
0	0	1	0

Show

EXERCISES

Problem 2.2 (cont)

Repeat the calculations of Problem 2.2 applying the corresposponding tools of the Bilbao Crystallographic server. Compare the results.

Problem: STRUCTURE VISUALIZATION VISUALIZE

Visualize with Jmol

Visualize structures with Jmol

Visualize structures using Jmol. Jmol is an open-source Java viewer for chemical structures in 3D. http://www.jmol.org/

Structure Data [in CIF format] Examinar...

HINT: [The option for a given filename is preferential]

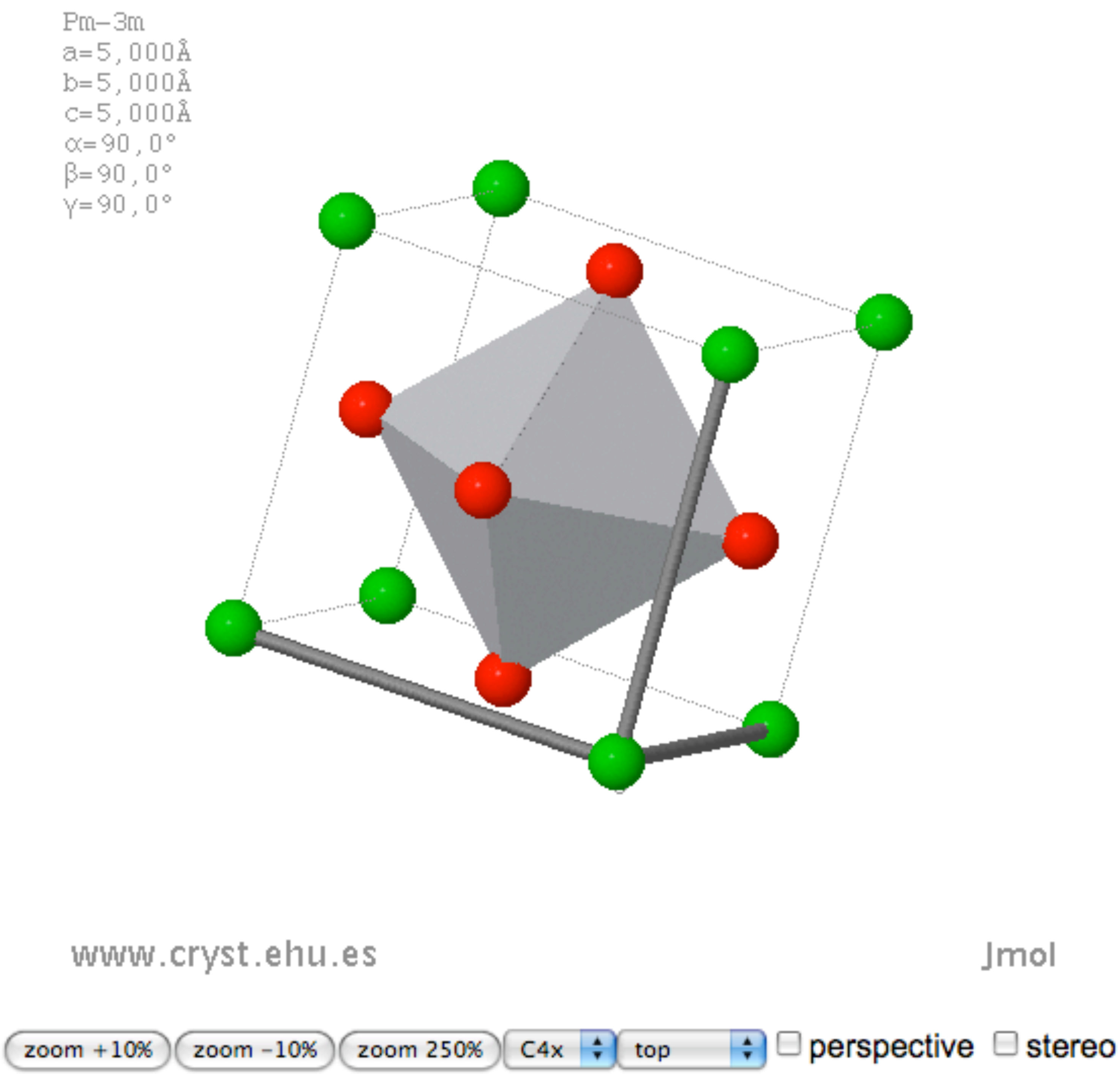
or fill the area

```
# Space Group ITA number
221
# Lattice parameters
5.0 5.0 5.0 90 90 90
# Number of independent atoms in the asymmetric unit
3
# [atom type] [number] [WP] [x] [y] [z]
Ba  1 - 0.0 0.0 0
Ti  2 - 0.5 0.5 0.5
O   3 - 0.5 0.0 0.5
```

Show

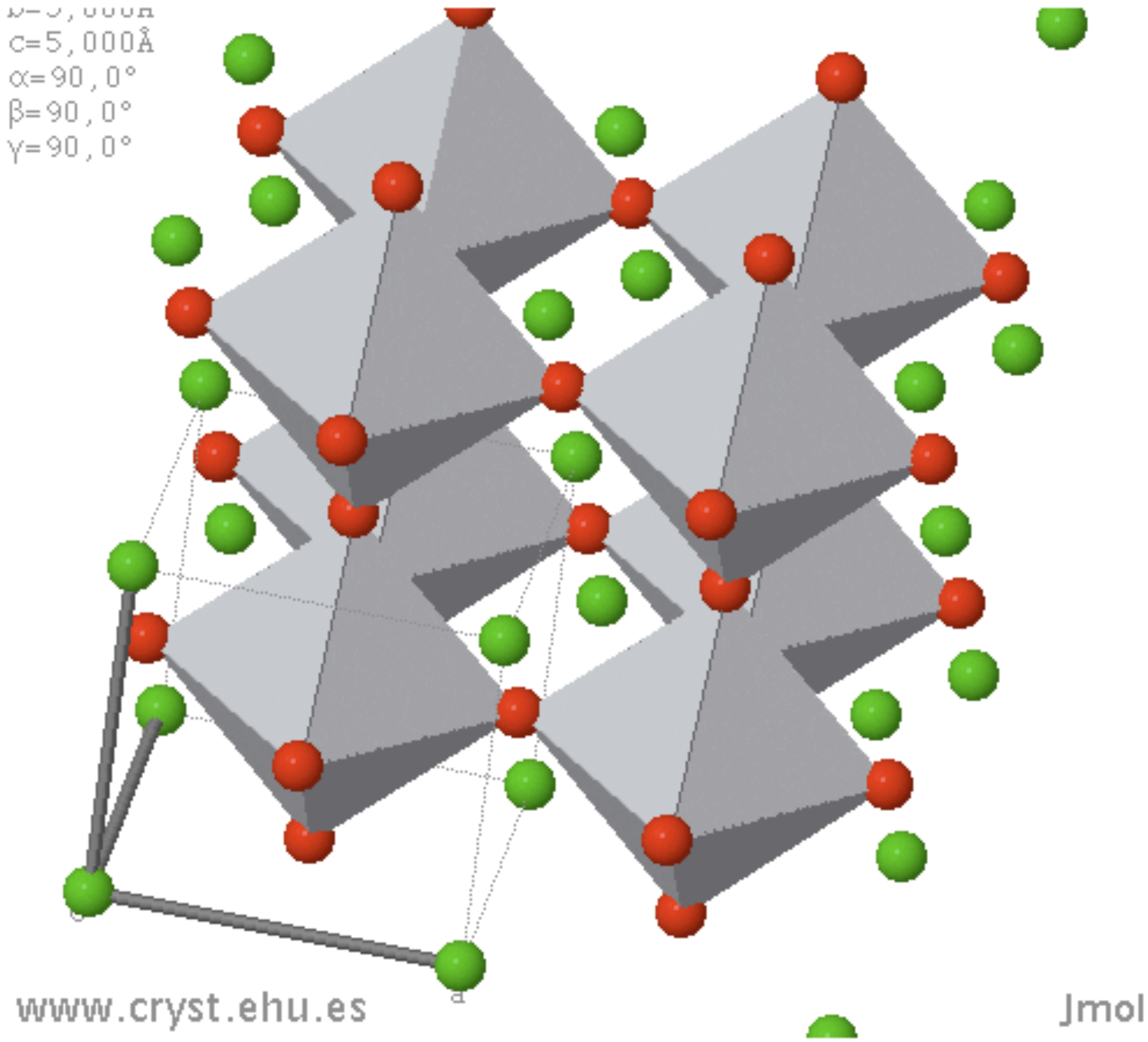
Structure visualization

View Structure (with Jmol applet)



Structure visualization

View Structure (with Jmol applet)



Subperiodic groups: rod and layer groups

Rod groups:	3dim groups with 1dim translations	polymeric molecules nanotubes uniform magnetic field to bulk crystals
Layer groups:	3dim groups with 2dim translations	bicrystals interfaces domain walls thin films

Databases for subperiodic groups

International Tables for Crystallography, Volume E: Subperiodic groups

generators
general postitions
Wyckoff positions

Data on maximal subgroups (Aroyo & Wondratschek)

maximal subgroups of index 2,3 and 4
series of isomorphic subgroups

Retrieval tools