CRYSTALLOGRAPHY ONLINE: WORKSHOP ON THE USE AND APPLICATIONS OF THE BILBAO CRYSTALLOGRAPHIC SERVER

20-21 August 2018

ECM31
31st European Crystallographic Meeting

CRYSTALLOGRAPHY ONLINE: BILBAO CRYSTALLOGRAPHIC SERVER

SPACE-GROUP SYMMETRY

SYMMETRY DATABASES OF BILBAO CRYSTALLOGRAPHIC SERVER

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SPACE GROUPS

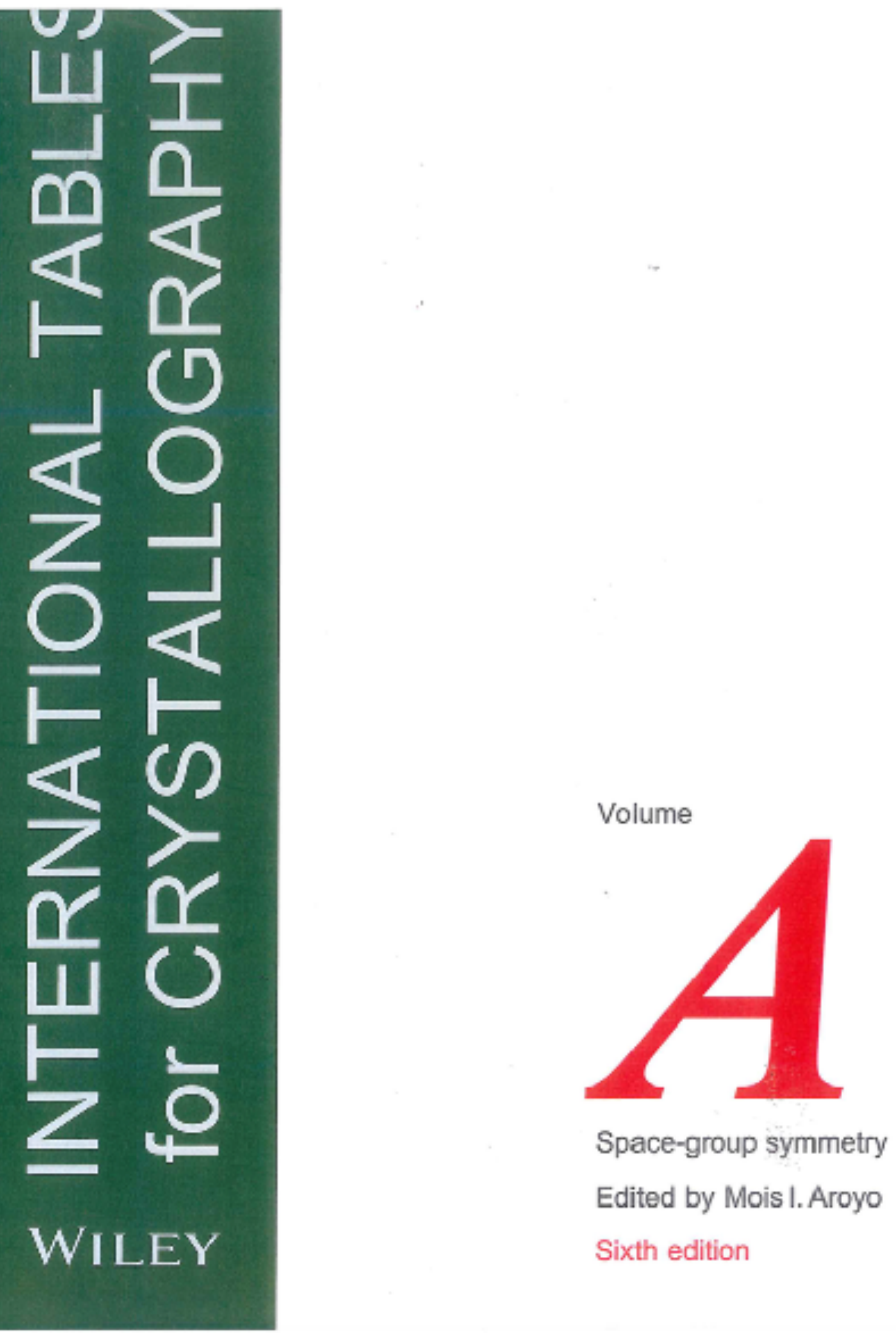
Crystal pattern: infinite, idealized crystal structure (without disorder, dislocations, impurities, etc.)

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

Translation subgroup $H \triangleleft G$: The infinite set of all translations that are symmetry operations of the crystal pattern

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

INTERNATIONAL TABLES FOR CRYSTALLOGRAPHY
VOLUME A: SPACE-GROUP SYMMETRY

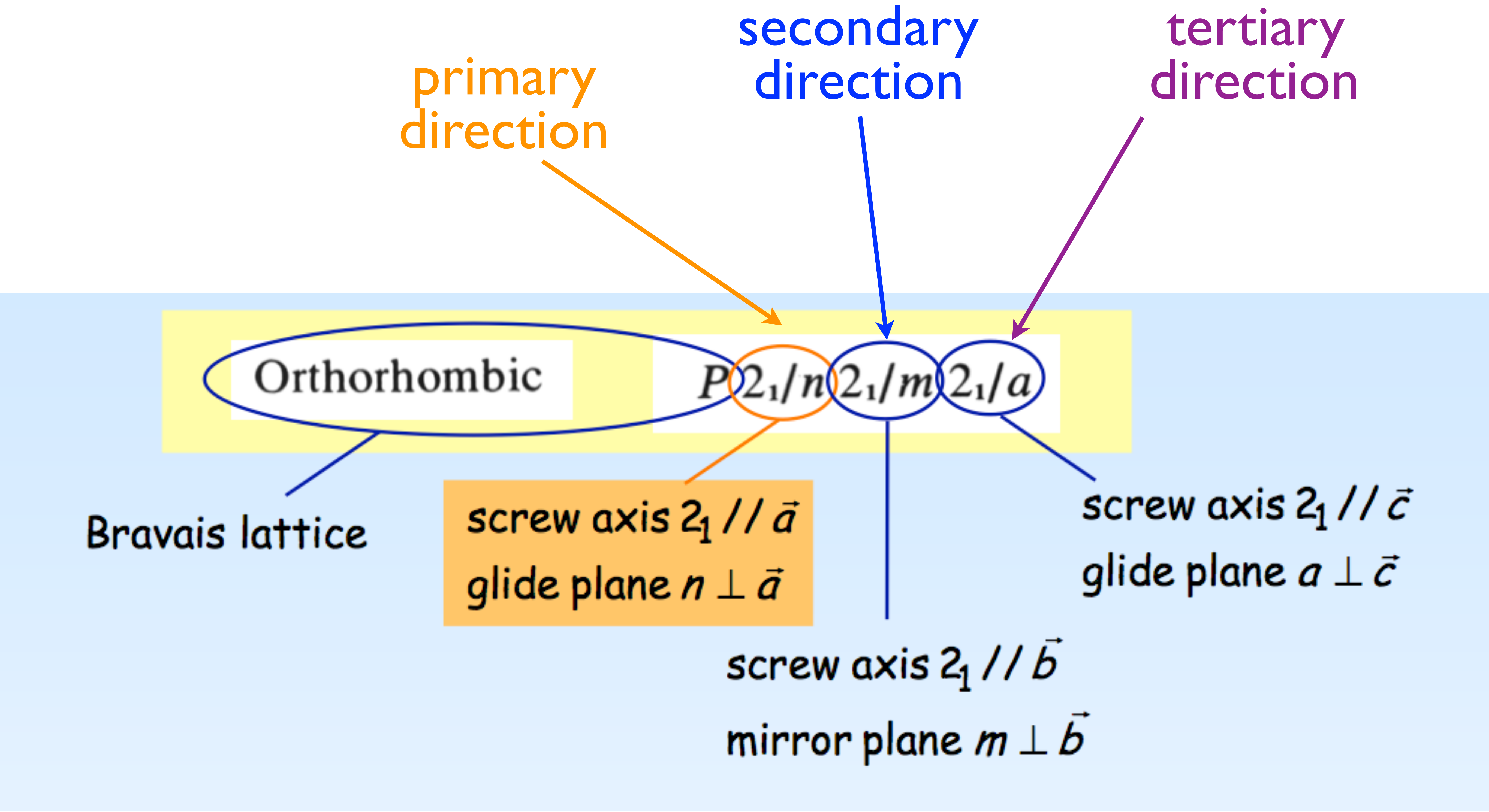


Extensive tabulations and illustrations of the 17 plane groups and of the 230 space groups

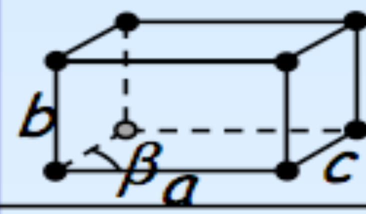
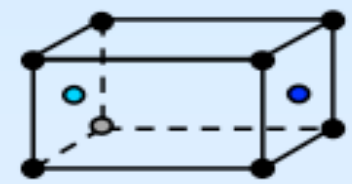
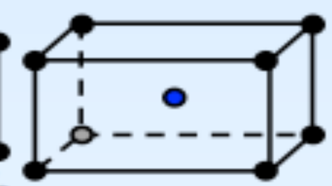
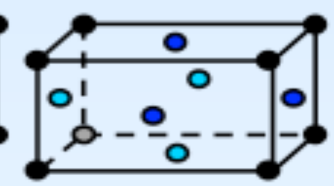
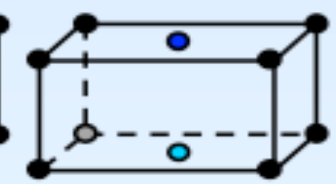
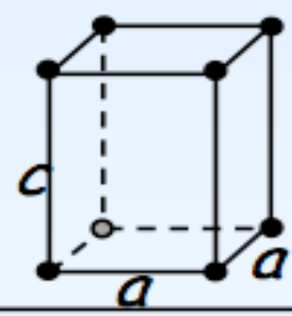
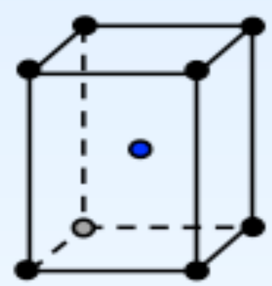
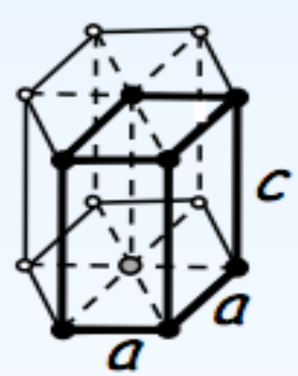
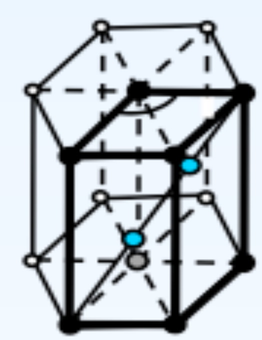
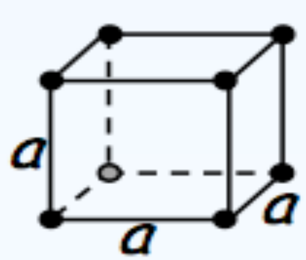
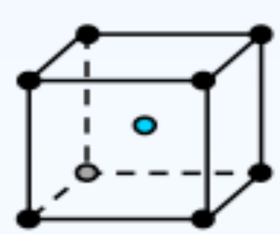
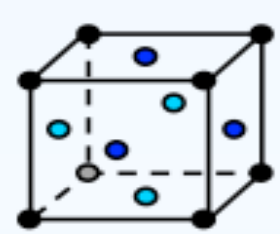
- headline with the relevant group symbols;
- diagrams of the symmetry elements and of the general position;
- specification of the origin and the asymmetric unit;
- list of symmetry operations;
- generators;
- general and special positions with multiplicities, site symmetries, coordinates and reflection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

HERMANN-MAUGUIN SYMBOLISM

Hermann-Mauguin symbols for space groups



14 Bravais Lattices

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

Hermann-Mauguin symbols for space groups

Directions that belong to the same set of equivalent symmetry directions are collected between braces. The first entry in each set is taken as the representative of that set.

Lattice	Symmetry direction (position in Hermann–Mauguin symbol)		
	Primary	Secondary	Tertiary
Triclinic	None		
Monoclinic*	[010] ('unique axis *b*') [001] ('unique axis *c*')		
Orthorhombic	[100]	[010]	[001]
Tetragonal	[001]	{ [100] [010] }	{ $[1\bar{1}0]$ [110] }
Hexagonal	[001]	{ [100] [010] $[\bar{1}\bar{1}0]$ }	{ $[1\bar{1}0]$ [120] $[\bar{2}\bar{1}0]$ }
Rhombohedral (hexagonal axes)	[001]	{ [100] [010] $[\bar{1}\bar{1}0]$ }	
Rhombohedral (rhombohedral axes)	[111]	{ $[1\bar{1}0]$ $[01\bar{1}]$ $[\bar{1}01]$ }	
Cubic	{ [100] [010] [001] }	{ [111] $[1\bar{1}\bar{1}]$ $[\bar{1}1\bar{1}]$ $[\bar{1}\bar{1}1]$ }	{ $[1\bar{1}0]$ [110] $[01\bar{1}]$ [011] $[\bar{1}01]$ [101] }

SPACE-GROUP SYMMETRY OPERATIONS

Symmetry Operations Characteristics

TYPE of the symmetry operation

preserve or not ***handedness***

SCREW/GLIDE component

GEOMETRIC ELEMENT

ORIENTATION of the geometric element

LOCATION of the geometric element

Crystallographic symmetry operations

characteristics:

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

geometric elements

Types of isometries preserve handedness

identity: the whole space fixed

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

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

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

Types of isometries do not preserve handedness

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

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

inversion: centre of inversion fixed

reflection: plane fixed
reflection/mirror plane

glide reflection: no fixed point
glide plane
glide vector

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 1.1

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 1.1(cont)

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:

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

EXERCISES

Problem 1.1(cont)

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:

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

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

$\longrightarrow$ $\left\{ \begin{array}{l} -x+1/2,\ y,\ -z+1/2 \\ \bar{x}+1/2,\ y,\ \bar{z}+1/2 \end{array} \right.$

EXERCISES

Problem 1.2

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

Matrix formalism: 4x4 matrices

augmented matrices:

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

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

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

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

4x4 matrices: general formulae

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

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

combination and inverse of isometries:

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

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

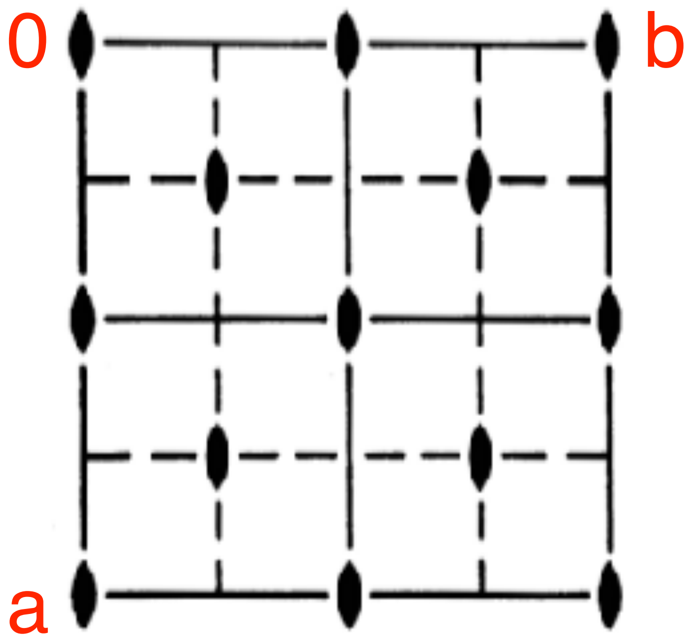
PRESENTATION OF SPACE-GROUP SYMMETRY OPERATIONS

IN INTERNATIONAL TABLES FOR CRYSTALLOGRAPHY, VOL. A

Space group *Cmm*2 (No. 35)

How are the symmetry operations represented in ITA ?

Diagram of symmetry elements



Symmetry operations

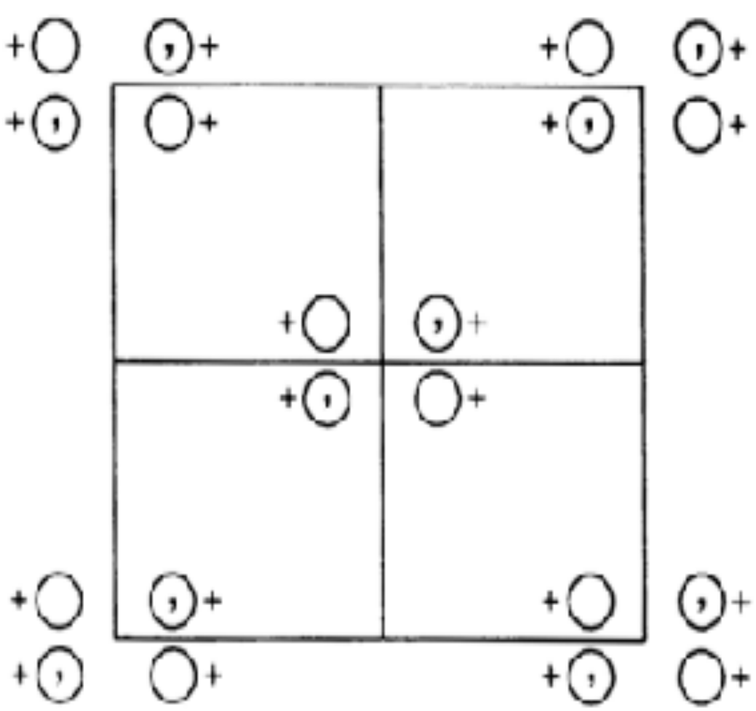
For (0,0,0)+ set

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

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

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

Diagram of general position points



General Position

Coordinates

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

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

General position

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

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

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

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

General Position of Space groups (infinite order)

Coset decomposition $G:T_G$

General position

Symmetry operations expressed in x,y,z notation

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

Factor group G/T_G

isomorphic to the point group P_G of G

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

Symmetry Operations Block

TYPE of the symmetry operation

ORIENTATION of the geometric element

SCREW/GLIDE component

LOCATION of the geometric element

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

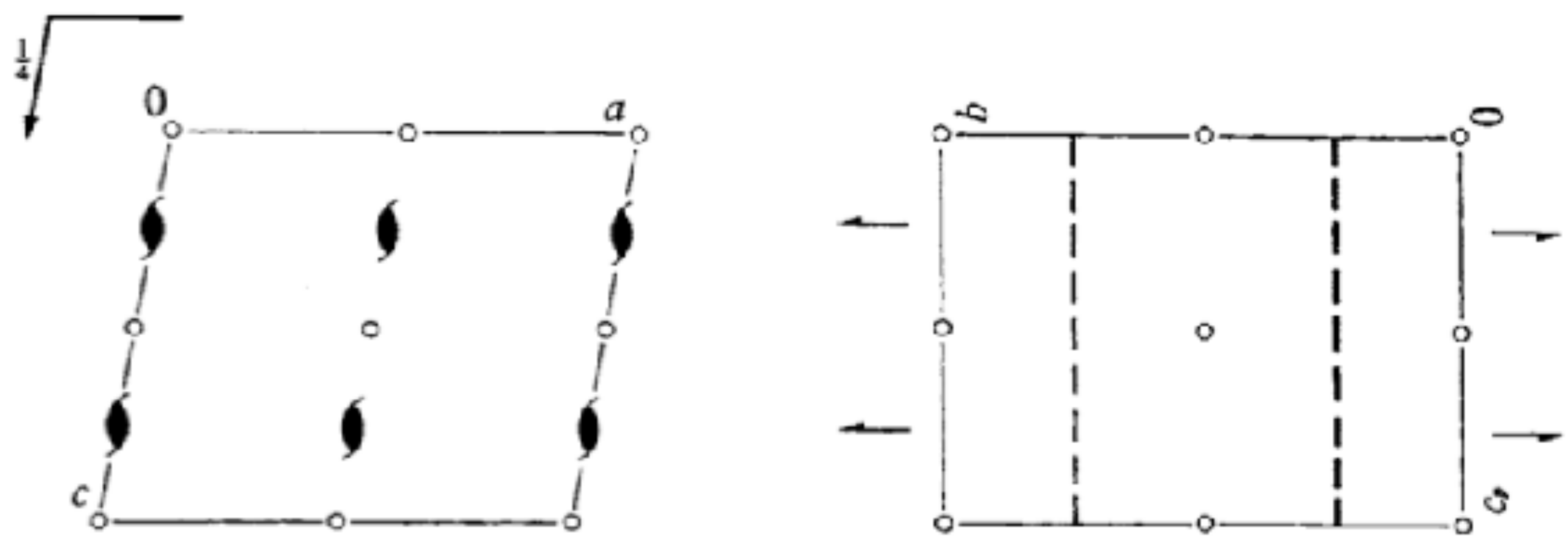
Space group $P2_1/c$ (No. 14)

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

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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

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Crystallography online: workshop on the use and applications of the structural tools of the Bilbao Crystallographic Server

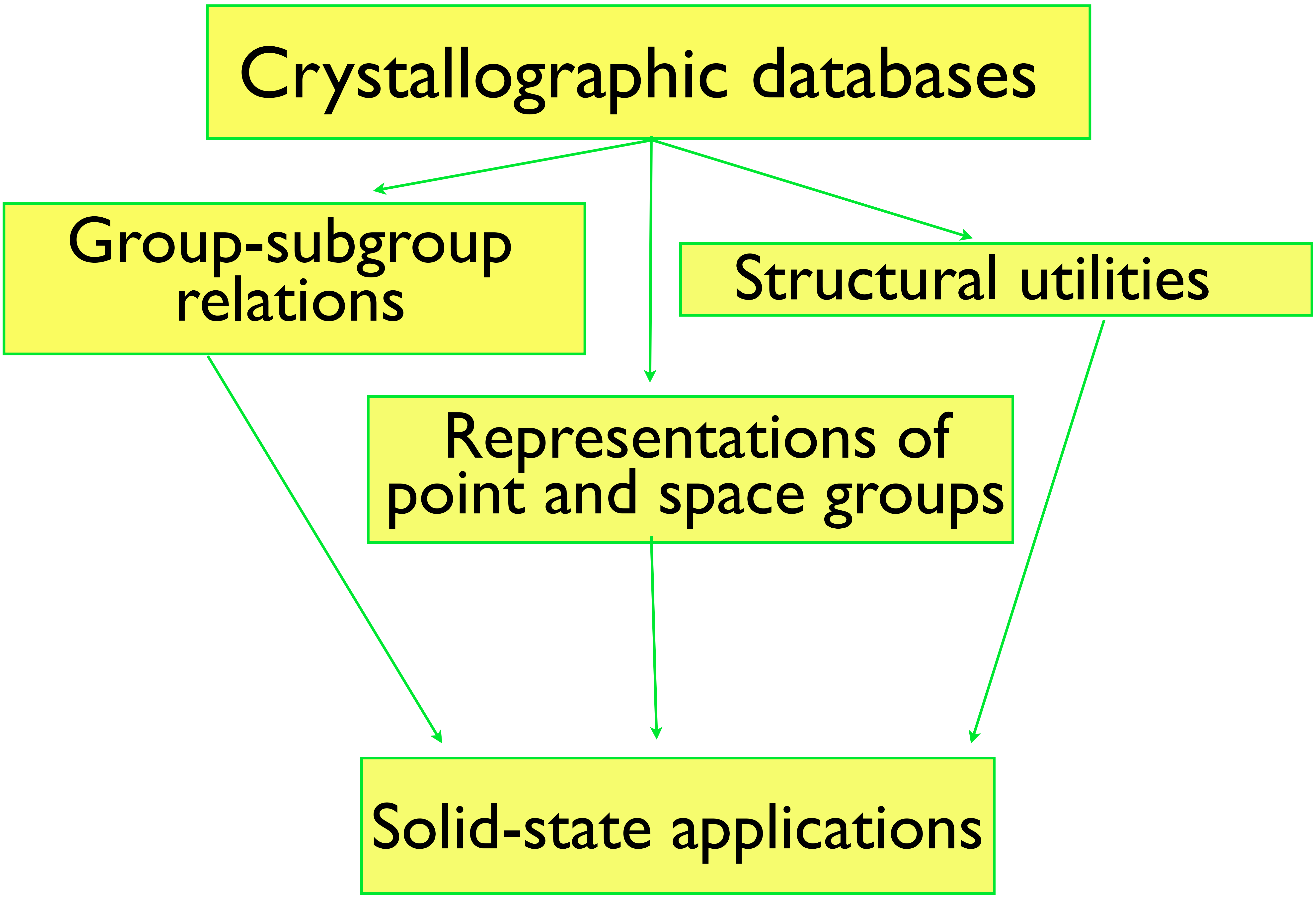
20-21 August 2018

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**
    04/2017: Irreducible representations of

Crystallographic Databases

International Tables for Crystallography


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

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20-21 August 2018

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    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

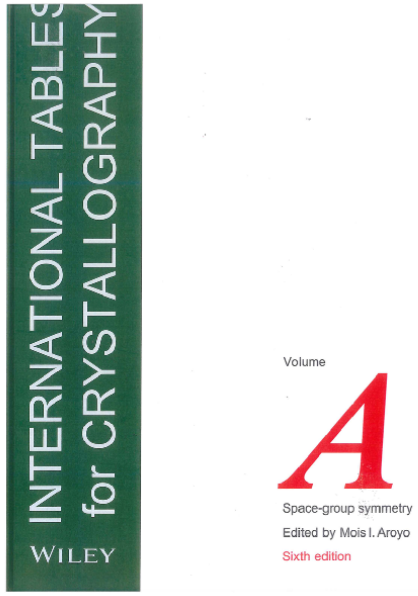
Subperiodic Groups: Layer, Rod and Frieze Groups

Structure Databases

Raman and Hyper-Raman scattering

Point-group symmetry

Plane-group symmetry

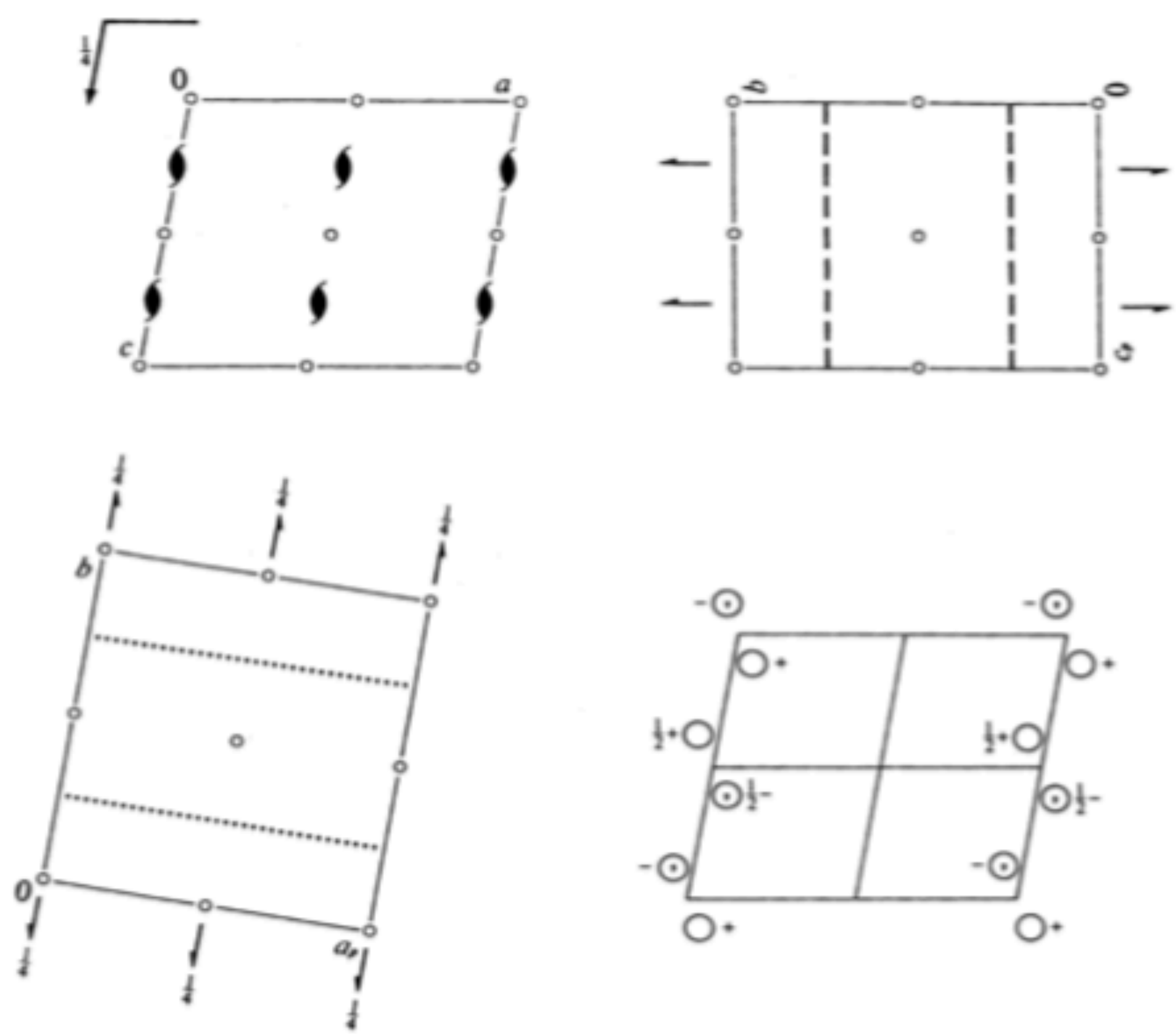


International Tables for Crystallography (2016). Vol. A, Space group 14, pp. 252–259.

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

No. 14 $\quad P\,1\,2_1/c\,1$ $\quad$ Patterson symmetry $P\,1\,2/m\,1$

UNIQUE AXIS *b*, CELL CHOICE 1



Origin at $\bar{1}$

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

Symmetry operations

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

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

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
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) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	$h0l$: $l=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
2	*d*	$\bar{1}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			hkl: $k+l=2n$
2	*c*	$\bar{1}$	$0,0,\frac{1}{2}$	$0,\frac{1}{2},0$			hkl: $k+l=2n$
2	*b*	$\bar{1}$	$\frac{1}{2},0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $k+l=2n$
2	*a*	$\bar{1}$	$0,0,0$	$0,\frac{1}{2},\frac{1}{2}$			hkl: $k+l=2n$

Symmetry of special projections

Along [001] $p2gm$
$\mathbf{a}'=\mathbf{a}_p$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2gg$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}_p$
Origin at $x,0,0$

Along [010] $p2$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

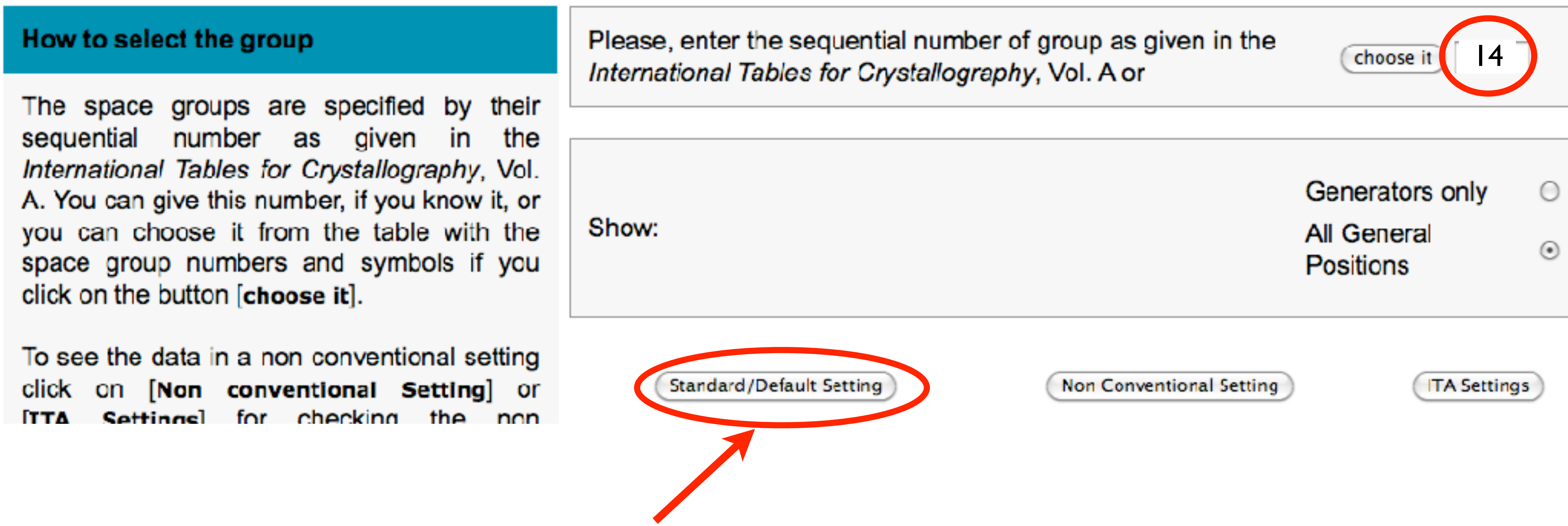
Bilbao Crystallographic Server

Problem: Matrix-column presentation
Geometrical interpretation

GENPOS

Generators and General Positions

space group



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

Space-group symmetry operations

short-hand notation

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

Geometric interpretation

Seitz symbols

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

Click here to get the general positions in text format

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

ITA data

General positions

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

Symmetry operations

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

SEITZ SYMBOLS FOR SYMMETRY OPERATIONS

Seitz symbols { R | t }

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

rotation (or linear) part R

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

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

translation part t

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

EXAMPLE

Seitz symbols for symmetry operations of hexagonal and trigonal crystal systems

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

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

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

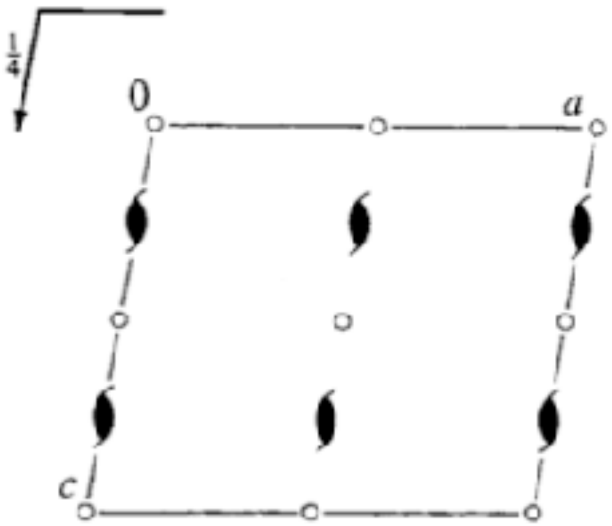
EXAMPLE

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

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

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

No. 14 $\qquad$ $P12_1/c1$ $\qquad$ 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

Matrix-column presentation

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

Symmetry operations

Geometric interpretation

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

Seitz symbols

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

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]

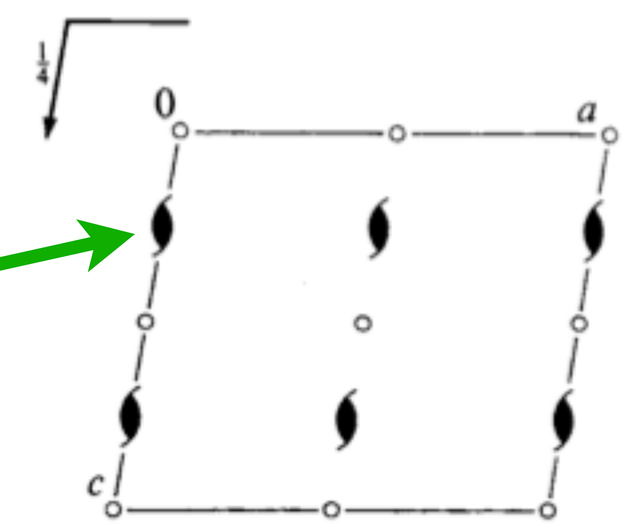
Or enter the sequential number of group as given in the *International Tables for Crystallography*, Vol. A [choose it]

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



Problem 1.2 (cont.)

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 (type of operation, glide/screw component, location of the symmetry operation).

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

EXERCISES

Problem 1.3

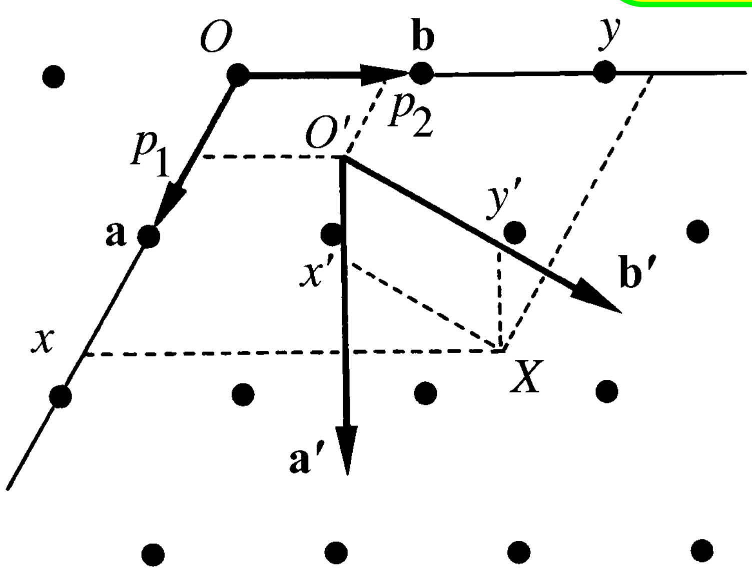
1. Characterize geometrically the matrix-column pairs listed under *General position* of the space group *P4mm* in ITA.

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

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

CO-ORDINATE TRANSFORMATIONS IN CRYSTALLOGRAPHY

Co-ordinate transformation



3-dimensional space

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

$\downarrow$ **(*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:

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

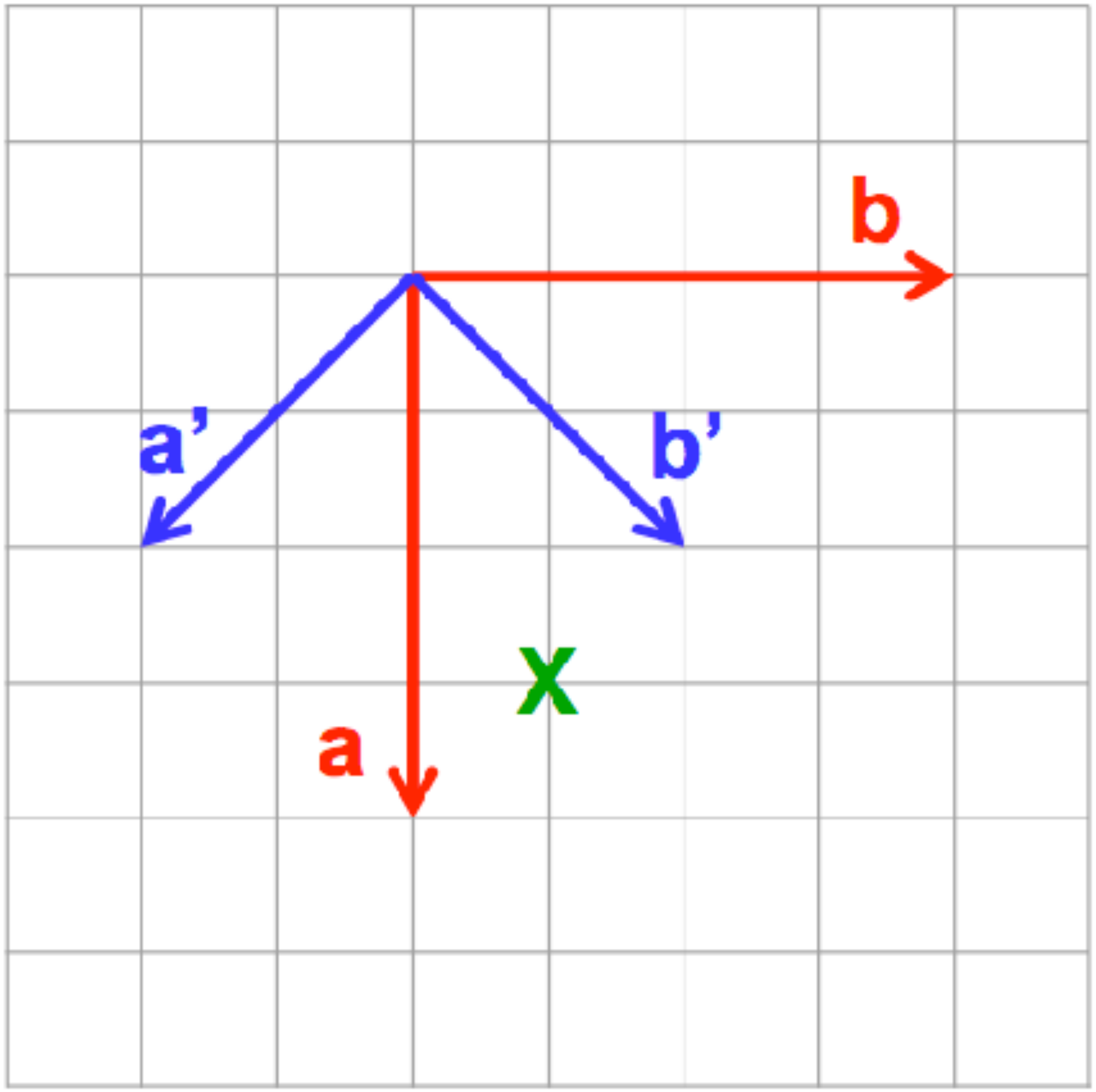
$$= (\mathbf{a}, \mathbf{b}, \mathbf{c}) \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix} = (P_{11}\mathbf{a} + P_{21}\mathbf{b} + P_{31}\mathbf{c}, \; P_{12}\mathbf{a} + P_{22}\mathbf{b} + P_{32}\mathbf{c}, \; P_{13}\mathbf{a} + P_{23}\mathbf{b}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

(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



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

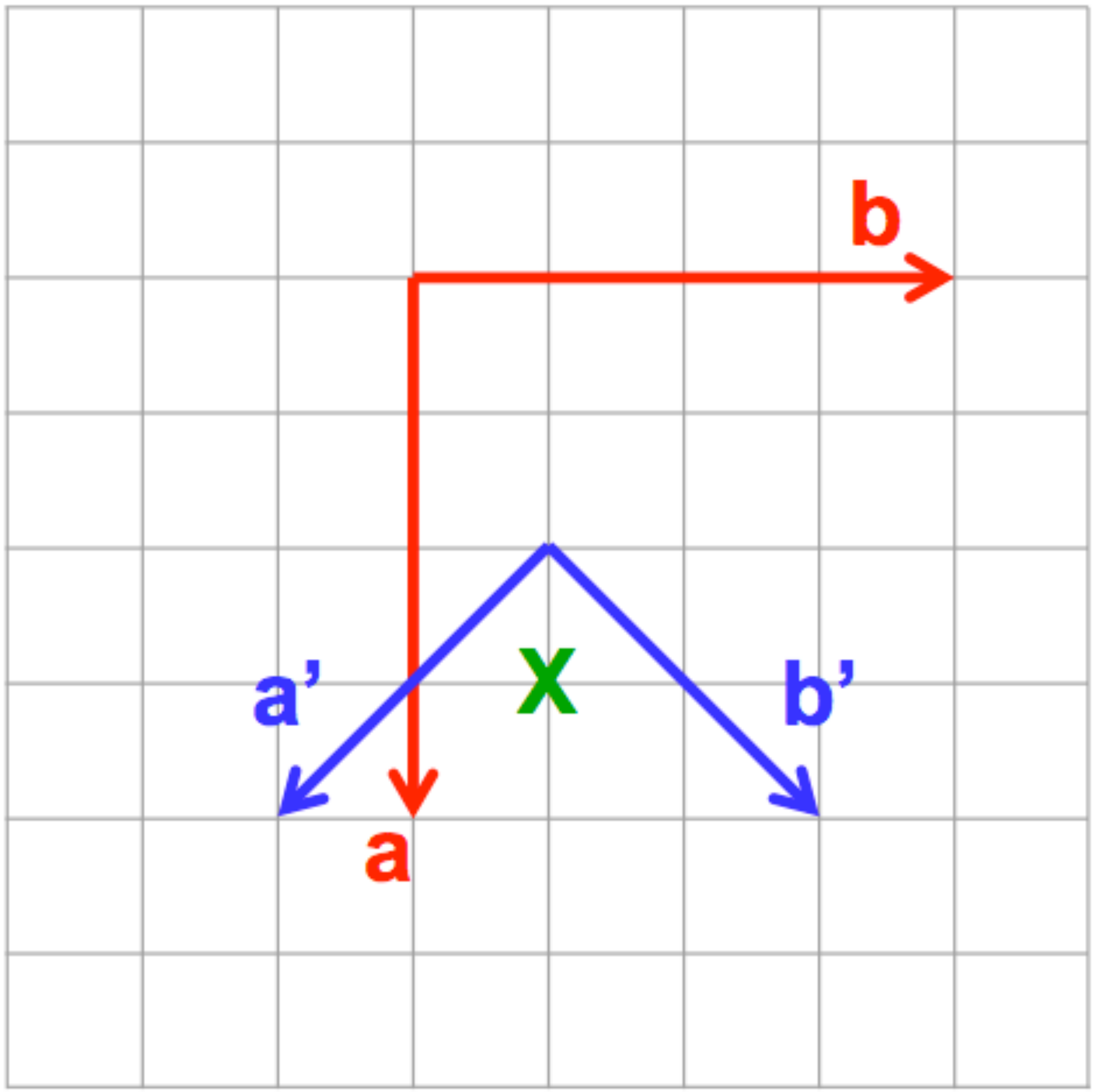
$$(a,b,c) = (a',b',c')\begin{pmatrix} ? \end{pmatrix}$$

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

$$X' = (?)$$

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

EXAMPLE



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

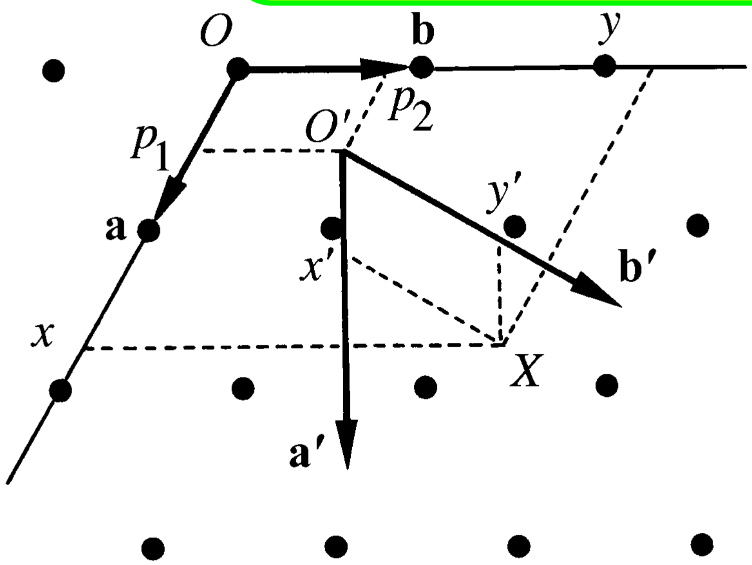
$q = \begin{pmatrix} ? \end{pmatrix}$

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

$X' = (\ ?\ )$

Linear parts as before.

Co-ordinate transformations in crystallography



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 $\boldsymbol{p}(p_1,p_2,p_3)$:

$$O' = O + p$$

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

Co-ordinate transformations in crystallography

Transformation of space-group operations (W,w) by $(\boldsymbol{P},\boldsymbol{p})$:

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

Structure-description transformation by $(\boldsymbol{P},\boldsymbol{p})$

unit cell parameters:

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

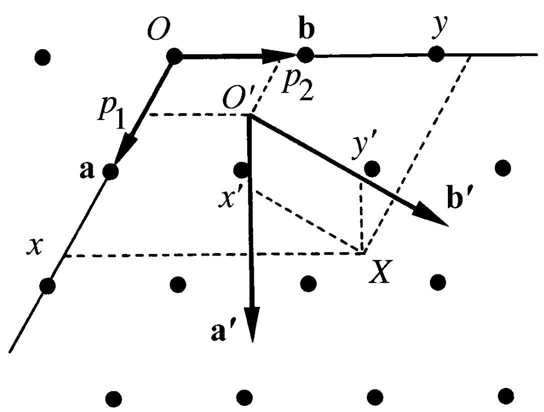
atomic coordinates X(x,y,z):

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

$$\begin{pmatrix} x' \\ y' \\ z \end{pmatrix} = \begin{pmatrix} P11 & P12 & P13 & p1 \\ P21 & P22 & P23 & p2 \\ P31 & P32 & P33 & p3 \end{pmatrix}^{-1} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

Short-hand notation for the description of transformation matrices

Transformation matrix:



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

$$(P,p)=\left(\begin{array}{ccc|c} P_{11} & P_{12} & P_{13} & p1 \\ P_{21} & P_{22} & P_{23} & p2 \\ P_{31} & P_{32} & P_{33} & p3 \end{array}\right)$$

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

notation rules:

-written by columns

-coefficients 0, +1, -1

-different columns in one line

-origin shift

example:

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

→ { a+b, -a+b, c;-1/4,-3/4,0

EXERCISES

Problem 1.4

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

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

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

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

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

0,70
0,31
0,95

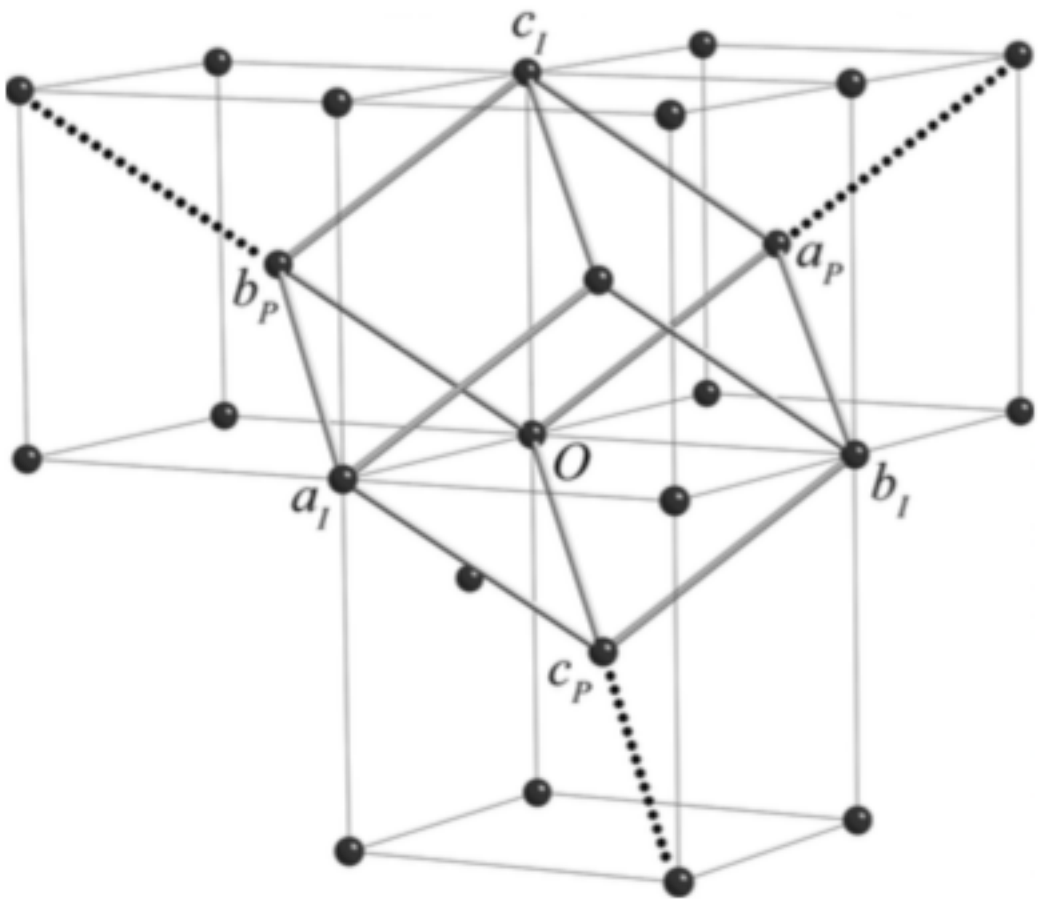
Hints

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

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

EXERCISES

Problem 1.5(a)



A body-centred cubic lattice (*cI*) has as its conventional basis the conventional basis ($\mathbf{a_P}$,$\mathbf{b_P}$,$\mathbf{c_P}$) of a primitive cubic lattice, but the lattice also contains the centring vector $1/2\mathbf{a_P}+1/2\mathbf{b_P}+1/2\mathbf{c_P}$ which points to the centre of the conventional cell.

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

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

(ii) for the primitive basis:

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

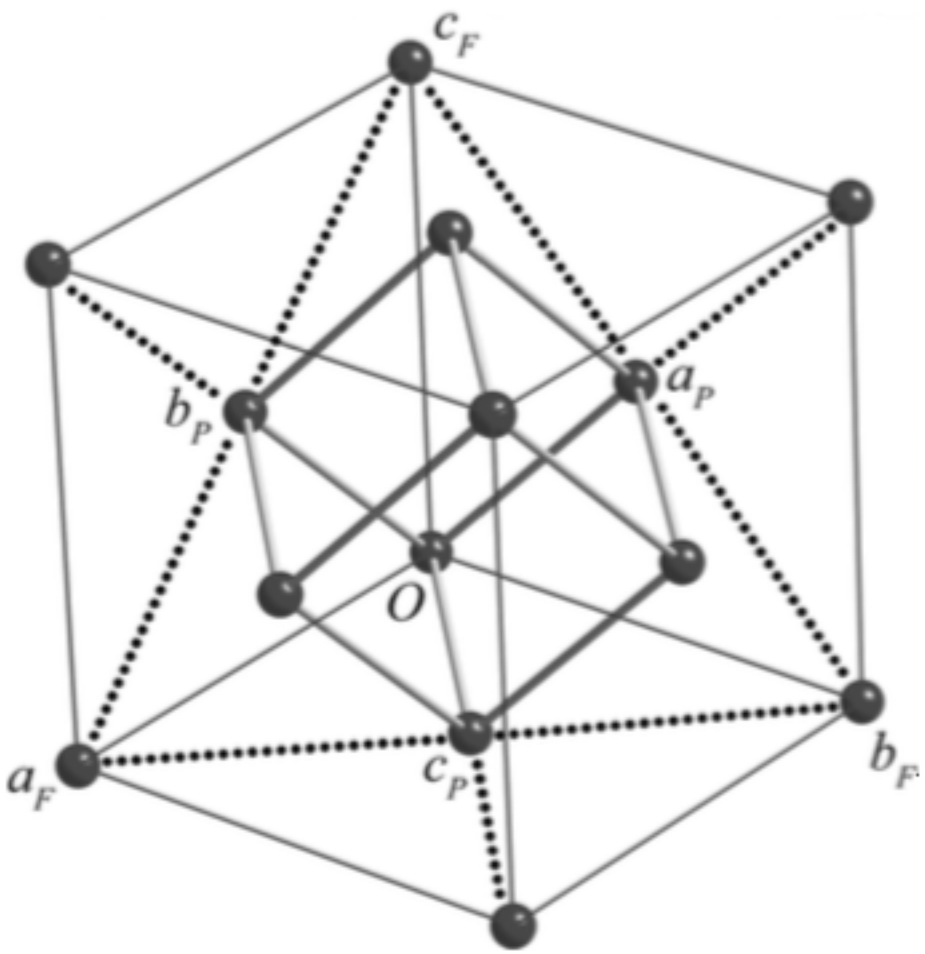
(iii) determine the lattice parameters of the primitive cell if a_P=4 Å

Hint

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

EXERCISES

Problem 1.5(b)



A face-centred cubic lattice (*cF*) has as its conventional basis the conventional basis (**a**$_P$,**b**$_P$,**c**$_P$) of a primitive cubic lattice, but the lattice also contains the centring vectors 1/2**b**$_P$+1/2**c**$_P$, 1/2**a**$_P$+1/2**c**$_P$, 1/2**a**$_P$+1/2**b**$_P$, which point to the centres of the faces of the conventional cell.

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

(i) for the conventional basis (**a**$_P$,**b**$_P$,**c**$_P$);

(ii) for the primitive basis:

a$_F$=1/2(**b**$_P$+**c**$_P$), **b**$_F$=1/2(**a**$_P$+**c**$_P$), **c**$_F$=1/2(**a**$_P$+**b**$_P$)

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

Problem: **ITA SETTINGS**

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

Monoclinic descriptions

	Transf.	**abc**	**c$\bar{\text{b}}$a**	**abc**	**ba$\bar{\text{c}}$**	**abc**	**$\bar{\text{a}}$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

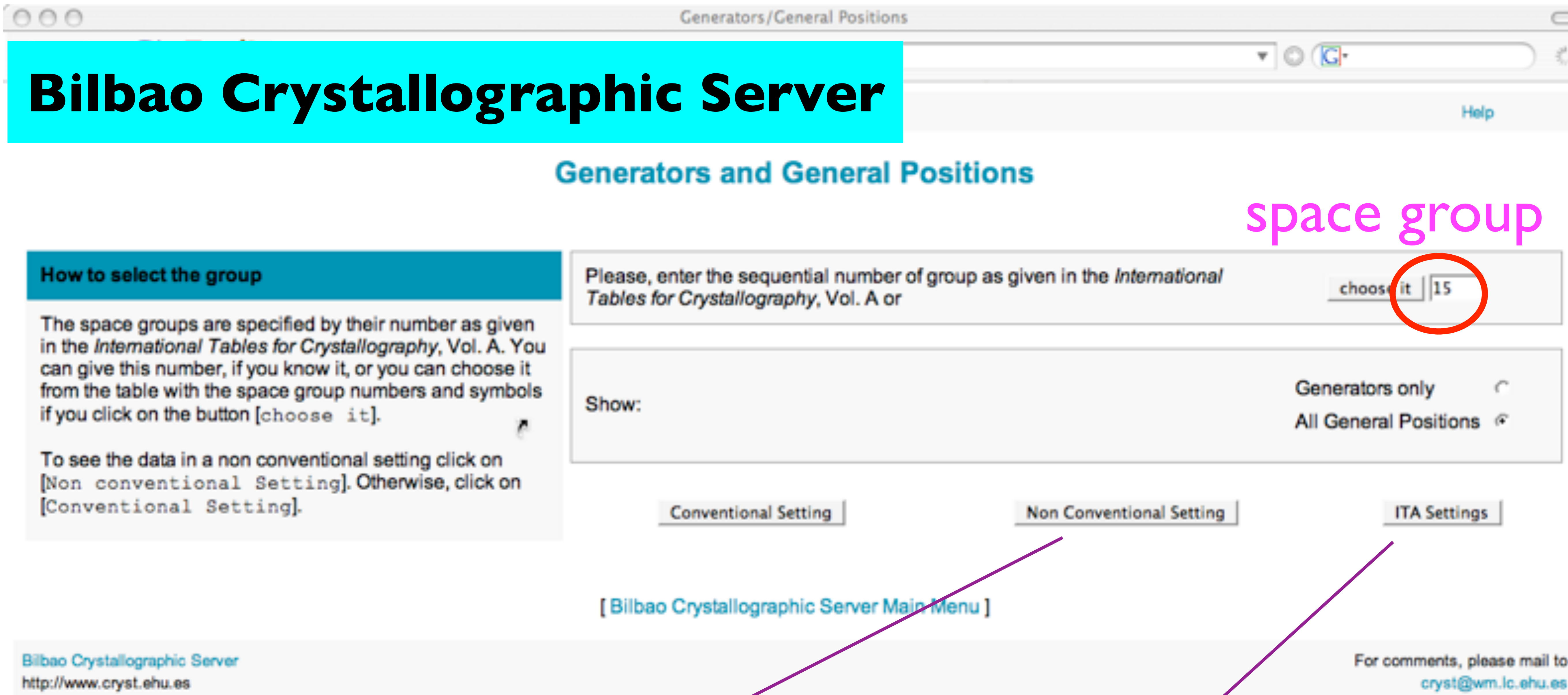
No.	HM	**abc**	**ba$\bar{\text{c}}$**	**cab**	**$\bar{\text{c}}$ba**	**bca**	**a$\bar{\text{c}}$b**
33	$Pna2_1$	$Pna2_1$	$Pbn2_1$	$P2_1nb$	$P2_1cn$	$Pc2_1n$	$Pn2_1a$

Problem: Co-ordinate transformations in crystallography

Generators
General positions

GENPOS

Bilbao Crystallographic Server



space group

Transformation of the basis

ITA-settings symmetry data

Example **GENPOS**:

default setting C12/c1

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

final setting A112/a

ITA-Settings for the Space Group 15

Note: The transformation matrices must be read by columns. **P** is the transformation from standard to the ITA-setting.

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

ITA number	Setting	P	P^{-1}
15	*C* 1 2/*c* 1	a,b,c	a,b,c
15	*A* 1 2/*n* 1	-a-c,b,a	c,b,-a-c
15	*I* 1 2/*a* 1	c,b,-a-c	-a-c,b,a
15	*A* 1 2/*a* 1	c,-b,a	c,-b,a
15	*C* 1 2/*n* 1	a,-b,-a-c	a,-b,a-c
15	*I* 1 2/*c* 1	-a-c,-b,c	-a-c,-b,c
15	*A* 1 1 2/*a*	c,a,b	b,c,a
15	*B* 1 1 2/*n*	a,-a-c,b	a,c,-a-b
15	*I* 1 1 2/*b*	-a-c,c,b	-a-b,c,b
15	*B* 1 1 2/*b*	a,c,-b	a,-c,b
15	*A* 1 1 2/*n*	-a-c,a,-b	b,-c,-a-b
15	*I* 1 1 2/*a*	c,-a-c,-b	-a-b,-c,a
15	*B* 2/*b* 1 1	b,c,a	c,a,b
15	*C* 2/*n* 1 1	b,a,-a-c	b,a,-b-c
15	*I* 2/*c* 1 1	b,-a-c,c	-b-c,a,c
15	*C* 2/*c* 1 1	-b,a,c	b,-a,c
15	*B* 2/*n* 1 1	-b,-a-c,a	c,-a,-b-c
15	*I* 2/*b* 1 1	-b,c,-a-c	-b-c,-a,b

Example **GENPOS**: ITA settings of C2/c(15)

The general positions of the group 15 (*A* 1 1 2/*a*)

N	Standard/Default Setting *C*2/*c*			ITA-Setting *A* 1 1 2/*a*		
	(x,y,z) form	matrix form	symmetry operation	(x,y,z) form	matrix form	symmetry operation
1	x, y, z	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	1	x, y, z	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	1
2	-x, y, -z+1/2	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1/2 \end{pmatrix}$	2 0,y,1/4	-x+1/2, -y, z	$\begin{pmatrix} -1 & 0 & 0 & 1/2 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	2 1/4,0,z
3	-x, -y, -z	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{pmatrix}$	-1 0,0,0	-x, -y, -z	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{pmatrix}$	-1 0,0,0
4	x, -y, z+1/2	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 1/2 \end{pmatrix}$	c x,0,z	x+1/2, y, -z	$\begin{pmatrix} 1 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{pmatrix}$	a x,y,0
5	x+1/2, y+1/2, z	$\begin{pmatrix} 1 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 1/2 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	t (1/2,1/2,0)	x, y+1/2, z+1/2	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1/2 \\ 0 & 0 & 1 & 1/2 \end{pmatrix}$	t (0,1/2,1/2)
6	-x+1/2, y+1/2, -z+1/2	$\begin{pmatrix} -1 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 1/2 \\ 0 & 0 & -1 & 1/2 \end{pmatrix}$	2 (0,1/2,0) 1/4,y,1/4	-x+1/2, -y+1/2, z+1/2	$\begin{pmatrix} -1 & 0 & 0 & 1/2 \\ 0 & -1 & 0 & 1/2 \\ 0 & 0 & 1 & 1/2 \end{pmatrix}$	2 (0,0,1/2) 1/4,1/4,z
7	-x+1/2, -y+1/2, -z	$\begin{pmatrix} -1 & 0 & 0 & 1/2 \\ 0 & -1 & 0 & 1/2 \\ 0 & 0 & -1 & 0 \end{pmatrix}$	-1 1/4,1/4,0	-x, -y+1/2, -z+1/2	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 1/2 \\ 0 & 0 & -1 & 1/2 \end{pmatrix}$	-1 0,1/4,1/4
8	x+1/2, -y+1/2, z+1/2	$\begin{pmatrix} 1 & 0 & 0 & 1/2 \\ 0 & -1 & 0 & 1/2 \\ 0 & 0 & 1 & 1/2 \end{pmatrix}$	n (1/2,0,1/2) x,1/4,z	x+1/2, y+1/2, -z+1/2	$\begin{pmatrix} 1 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 1/2 \\ 0 & 0 & -1 & 1/2 \end{pmatrix}$	n (1/2,1/2,0) x,y,1/4

default setting

***A*1 1 2/*a* setting**

EXERCISES

Problem 1.6

Consider the space group $P2_1/c$ (No. 14). Show that the relation between the *General* and *Special* position data of $P112_1/a$ (setting *unique axis c*) can be obtained from the data $P12_1/c1$ (setting *unique axis b*) applying the transformation $(\mathbf{a'},\mathbf{b'},\mathbf{c'})_\mathbf{c} = (\mathbf{a},\mathbf{b},\mathbf{c})_\mathbf{b}\boldsymbol{P}$, with $\boldsymbol{P} = \boldsymbol{c},\boldsymbol{a},\boldsymbol{b}$.

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

EXERCISES

Problem 1.7

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

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