International Union of Crystallography

Commission on Mathematical and Theoretical Crystallography

Symmetry Relationships between Crystal Structures with Applications to Structural and Magnetic Phase Transitions

Varanasi, India, 27-31 October 2014

international year of crystallography

SPACE-GROUP SYMMETRY

International Tables for Crystallography, Volume A

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

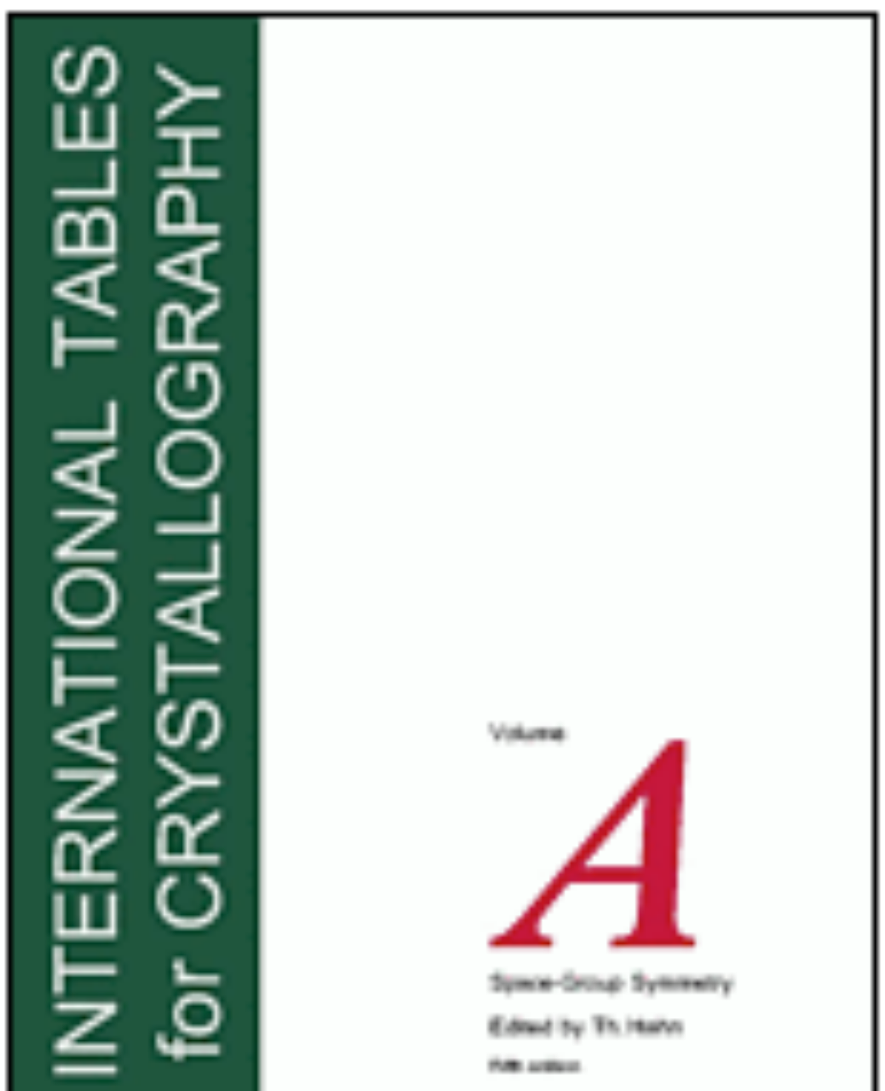
Translation subgroup $H \triangleleft G$: The infinite set of all translations that are symmetry operations of the crystal pattern

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 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;
- extensive subgroup and supergroup data

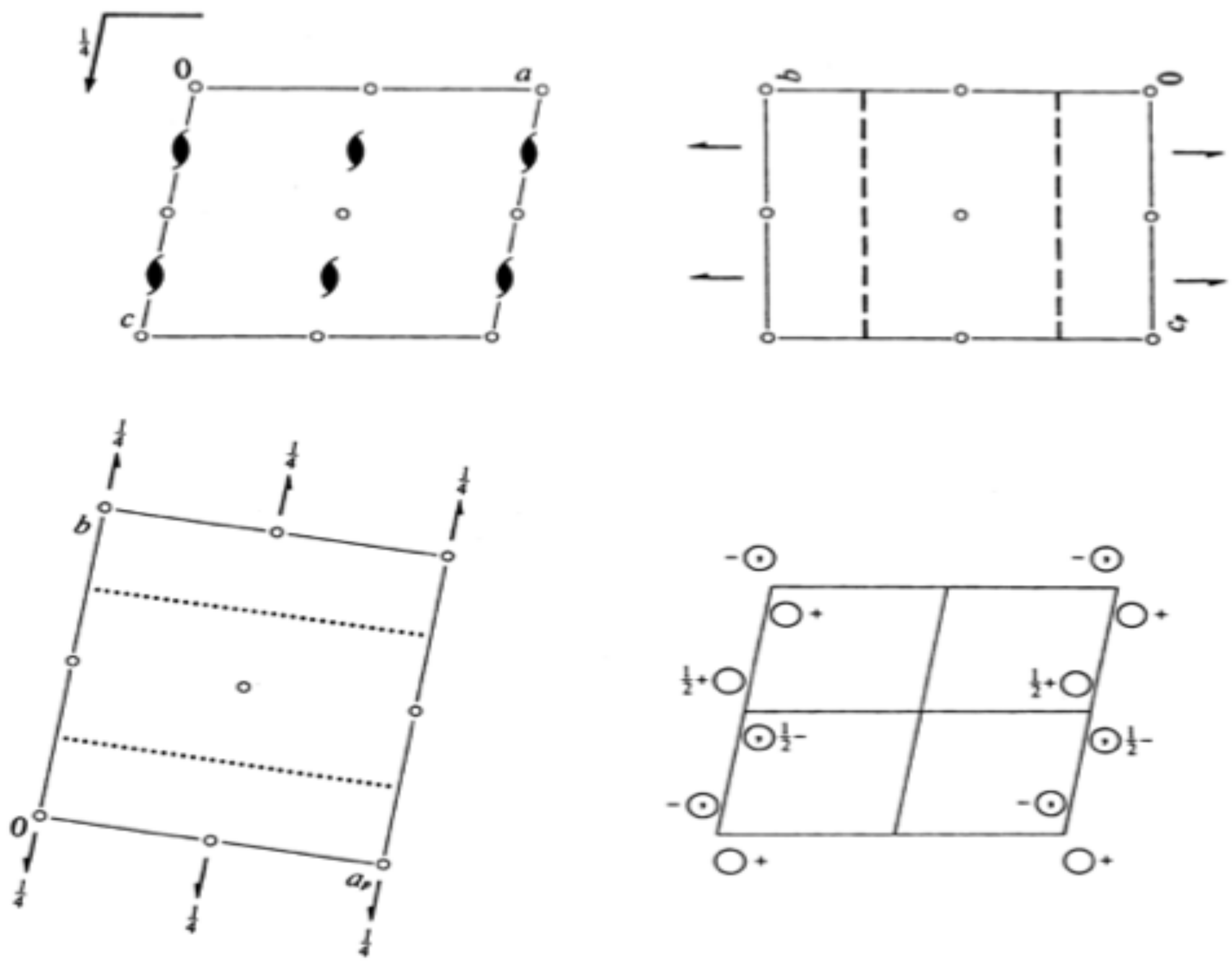
GENERAL LAYOUT: LEFT-HAND PAGE

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

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

No. 14 | $P1\,2_1/c\,1$ | Patterson symmetry $P1\,2/m\,1$

UNIQUE AXIS b, CELL CHOICE 1



Origin at $\bar{1}$

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

Symmetry operations

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

General Layout: Right-hand page

CONTINUED — No. 14 — $P2_1/c$

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 $0,y,0$

Maximal non-isomorphic subgroups

I [2] $P1c1$ (Pc, 7) 1; 4
[2] $P12_11$ ($P2_1$, 4) 1; 2
[2] $P\bar{1}$ (2) 1; 3

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [2] $P12_1/c1$ ($\mathbf{a}'=2\mathbf{a}$ or $\mathbf{a}'=2\mathbf{a}, \mathbf{c}'=2\mathbf{a}+\mathbf{c}$) ($P2_1/c$, 14); [3] $P12_1/c1$ ($\mathbf{b}'=3\mathbf{b}$) ($P2_1/c$, 14)

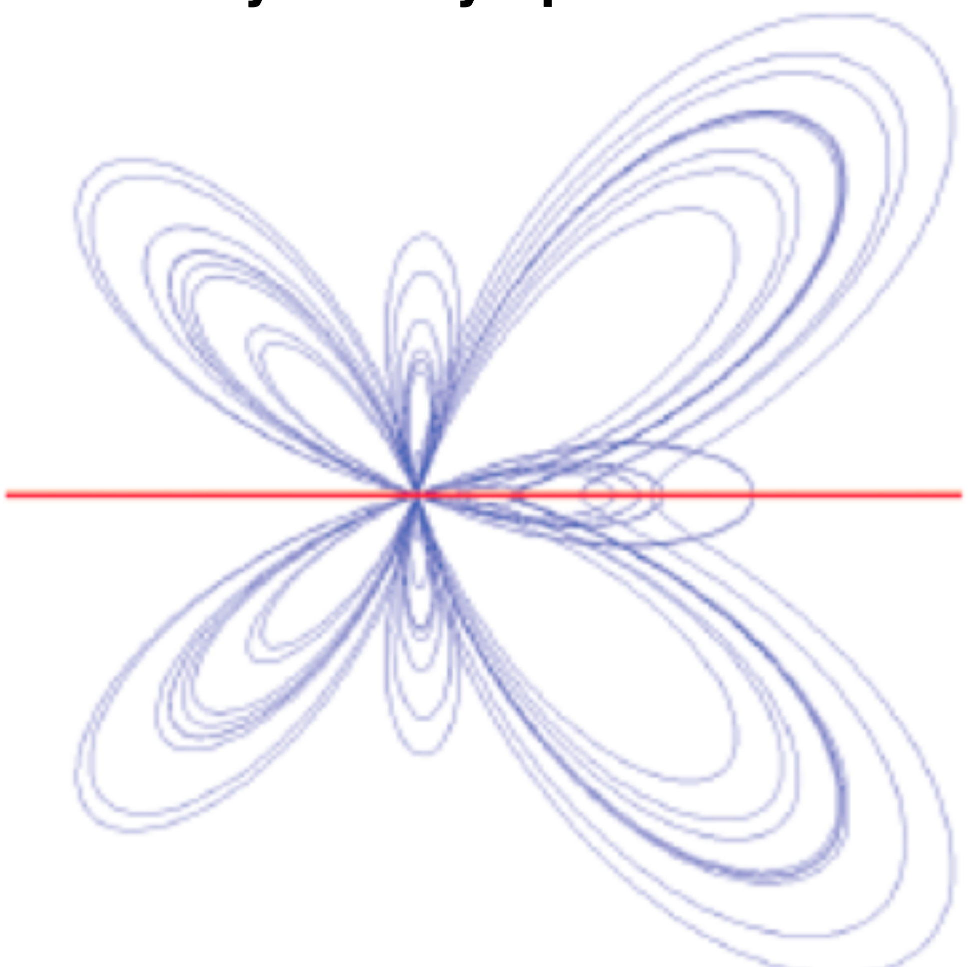
Minimal non-isomorphic supergroups

I [2] $Pnna$ (52); [2] $Pmna$ (53); [2] $Pcca$ (54); [2] $Pbam$ (55); [2] $Pccn$ (56); [2] $Pbcm$ (57); [2] $Pnnm$ (58); [2] $Pbcn$ (60);

SYMMETRY OPERATIONS
(revision)

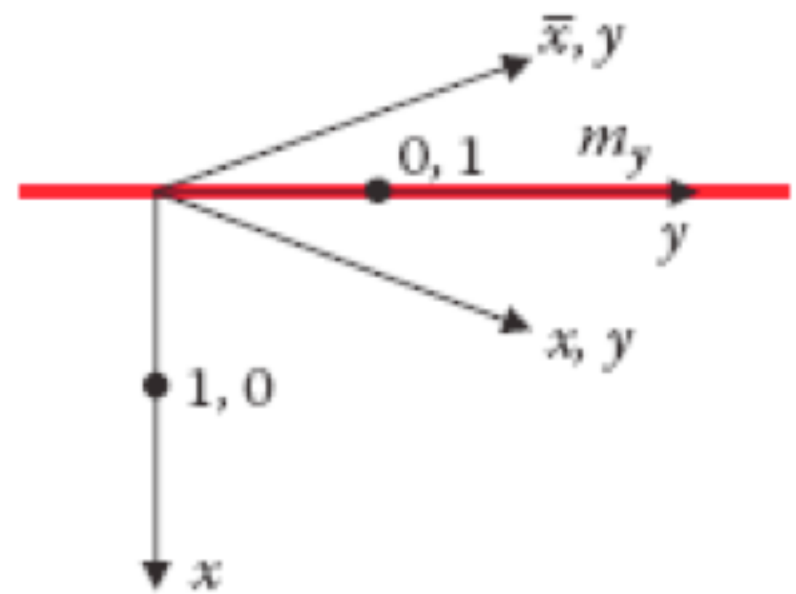
Example: Matrix presentation of symmetry operation

Mirror symmetry operation



drawing: M.M. Julian
Foundations of Crystallography

Mirror line m_y at 0,y



Matrix representation

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

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

Fixed points

$$m_y \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} x \\ y \end{pmatrix}$$

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

EXERCISES

Problem 2.14

Characterization of the symmetry operations:

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

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

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

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:

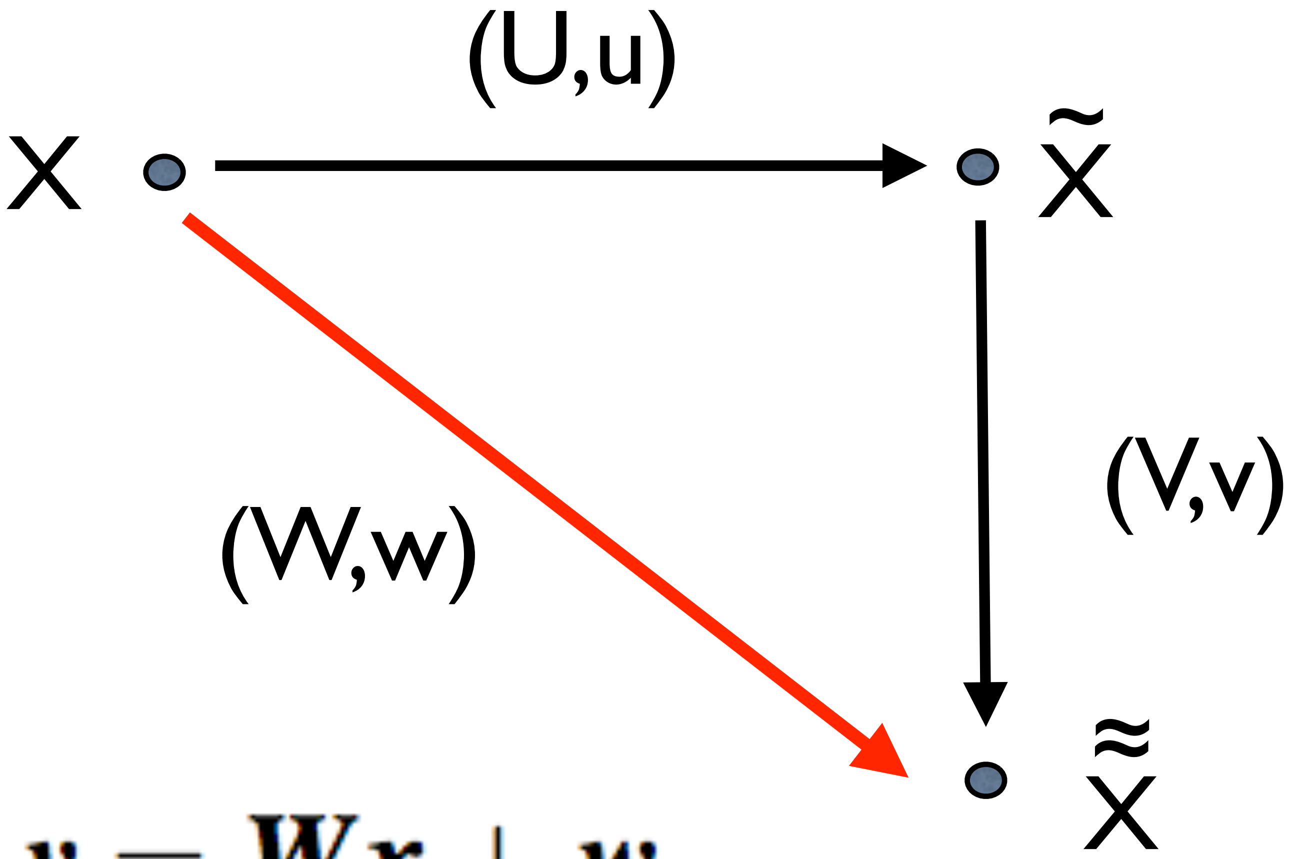
(1) x,y,z

(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

Problem 2.14(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:

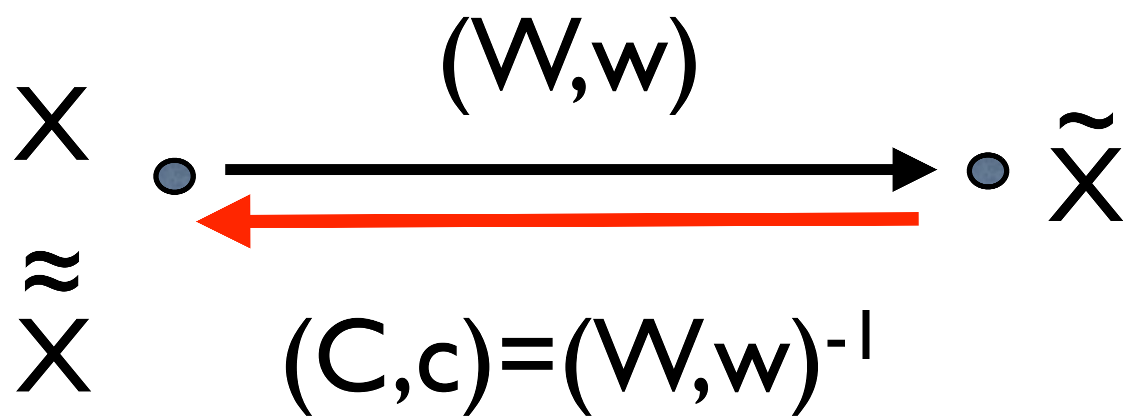
$$(W,w)=(W_1,w_1)(W_2,w_2)$$

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

combination of isometries:

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

Inverse isometries



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

$\boldsymbol{o}$ = zero translation column

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

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

$CW=\boldsymbol{I}$ → $C=W^{-1}$

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

EXERCISES

Problem 2.14(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:

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

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

SPACE-GROUP SYMMETRY OPERATIONS

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

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

Space Groups: infinite order

Coset decomposition G:T_G

General position

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

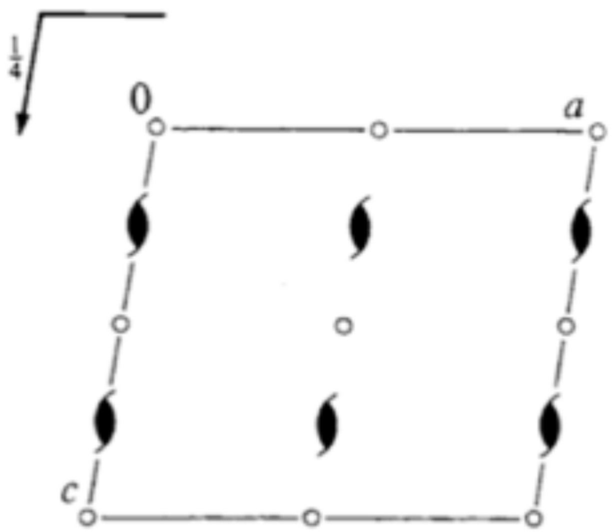
Factor group G/T_G

isomorphic to the point group P_G of G

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

EXAMPLE

Coset decomposition $P2_1/c$:T



General position

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

(I,0)	(2,0 ½ ½)	($\bar{1}$,0)	(m,0 ½ ½)
(I,t_1)	(2,0 ½ ½+t_1)	($\bar{1}$,t_1)	(m,0 ½ ½ +t_1)
(I,t_2)	(2,0 ½ ½ +t_2)	($\bar{1}$,t_2)	(m,0 ½ ½ +t_2)
...	... ...	...	... ...
(I,t_j)	(2,0 ½ ½ +t_j)	($\bar{1}$,t_j)	(m,0 ½ ½ +t_j)
...	... ...	...	... ...

inversion centers

($\bar{1}$,p q r): $\bar{1}$ at p/2,q/2,r/2

2_1screw axes

(2,u ½+v ½ +w) → (2,0 ½+v ½) ; (2,u ½ ½ +w)

EXAMPLE

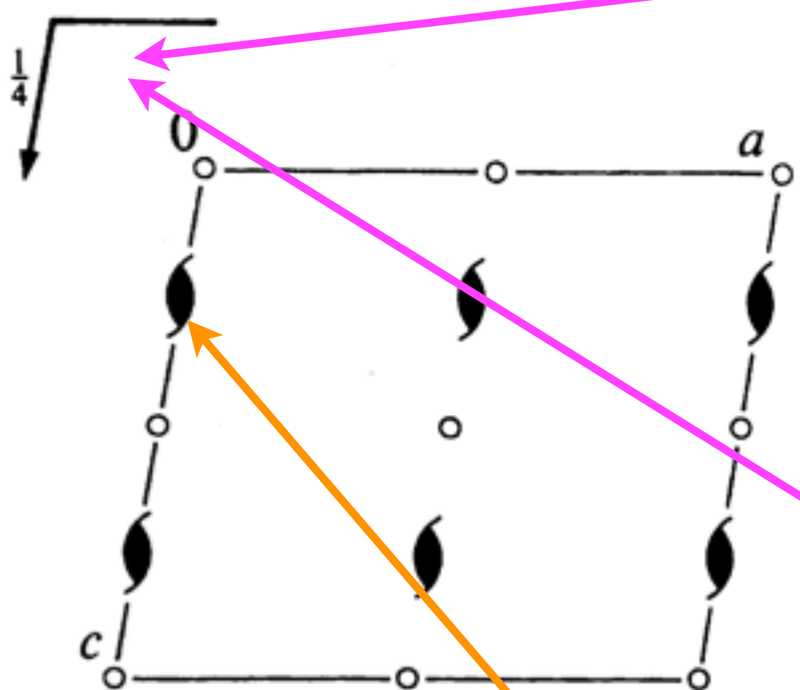
Space group $P2_1/c$ (No. 14)

Symmetry operations

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

Geometric interpretation

glide plane, **t**=1/2**c**
at y=1/4, ⊥**b**



Matrix-column presentation of symmetry operations

General Position

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

screw rotation, **t**=1/2**b**
at c=1/4, || **b**

FCT/ZTF

bilbao crystallographic server

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

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

Sections

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

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- How to cite the server
- Tutorials

Material from the ITOnline Workshop
(September 2011)

IT on 2011 bilbao

Material from the school on the server
(June 2009)

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

Space Groups Retrieval Tools

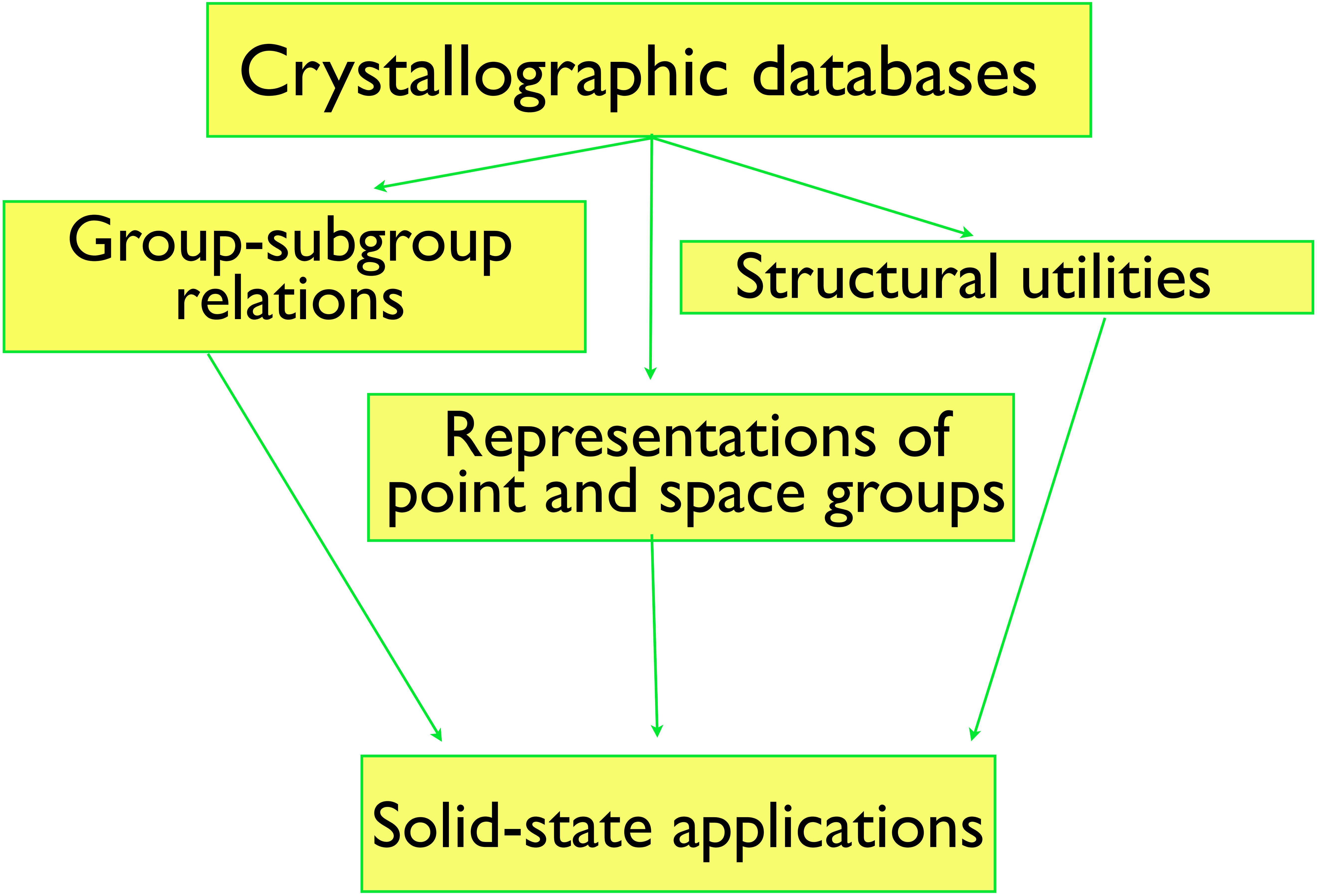
GENPOS	Generators and General Positions of Space Groups
WYCKPOS	Wyckoff Positions of Space Groups
HKLCOND	Reflection conditions of Space Groups
MAXSUB	Maximal Subgroups of Space Groups
SERIES	Series of Maximal Isomorphic Subgroups of Space Groups
WYCKSETS	Equivalent Sets of Wyckoff Positions
NORMALIZER	Normalizers of Space Groups
KVEC	The k-vector types and Brillouin zones of Space Groups
SYMMETRY OPERATIONS	Geometric interpretation of matrix column representations of symmetry operations

Magnetic Space Groups

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

Group - Subgroup Relations of Space Groups

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


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

Crystallographic Databases

International Tables for Crystallography

Bilbao Crystallographic Server

Problem: Matrix-column presentation
Geometrical interpretation

GENPOS

Generators and General Positions

space group

How to select the group

The space groups are specified by their sequential number as given in the *International Tables for Crystallography*, Vol. A. You can give this number, if you know it, or you can choose it from the table with the space group numbers and symbols if you click on the button [**choose it**].

To see the data in a non conventional setting click on [**Non conventional Setting**] or [**ITA Settings**] for checking the non

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

[choose it] 14

Show:

Generators only ○

All General Positions ⦿

[Standard/Default Setting] [Non Conventional Setting] [ITA Settings]

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

Space-group symmetryoperations

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

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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.

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.

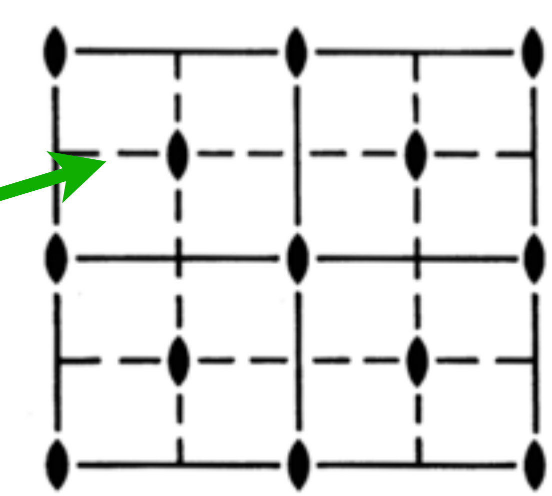
Introduce the crystal system	
Or enter the sequential number of group as given in the *International Tables for Crystallography*, Vol. A	choose it 35
Matrix column representation of symmetry operation	-x+1/2,y+1/2,z

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

Symmetry operation of the space group 35 (*Cmm2*)

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



EXERCISES

Problem 2.17 (b)

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.

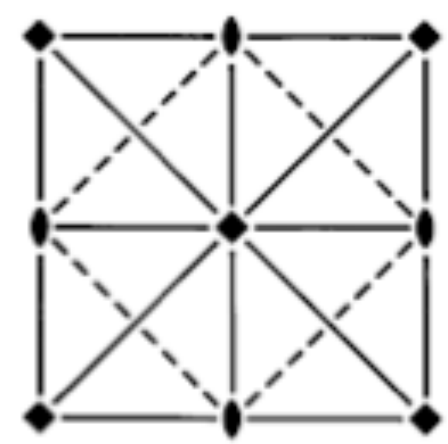
3. Compare your results with the results of the program SYMMETRY OPERATIONS

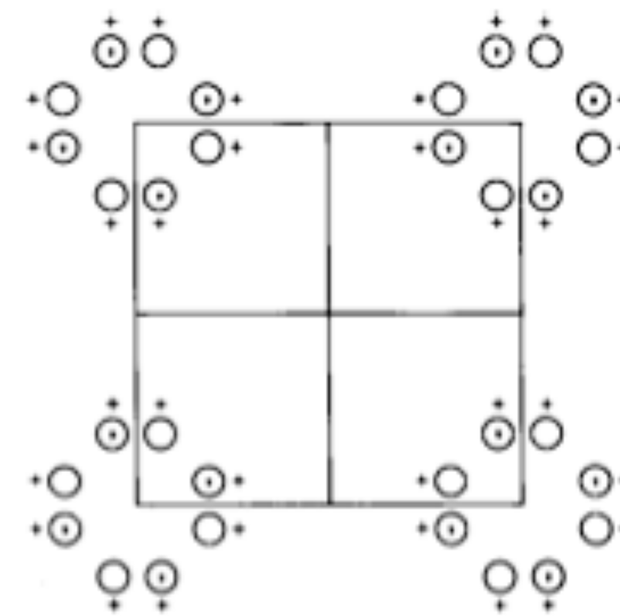
Problem 2.17(b)

SOLUTION

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

Geometric interpretation

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

Matrix-column presentation

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

General and special Wyckoff positions

Site-symmetry group S_o={(W,w)} of a point X_o

$$(W,w)X_o = X_o$$

$$\left(\begin{pmatrix} a & b & c \\ d & e & f \\ g & h & i \end{pmatrix} \begin{pmatrix} w1 \\ w2 \\ w3 \end{pmatrix} \right) \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

General position X_o

$$S=\{(I,\mathbf{o})\}\simeq \mathbf{1}$$

Special position X_o

$$S>\mathbf{1}=\{(I,\mathbf{o}),...,\}$$

Site-symmetry groups: oriented symbols

General position

(i) coordinate triplets of an image point $\tilde{X}$ of the original point X under (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

Coset decomposition $G:T_G$

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

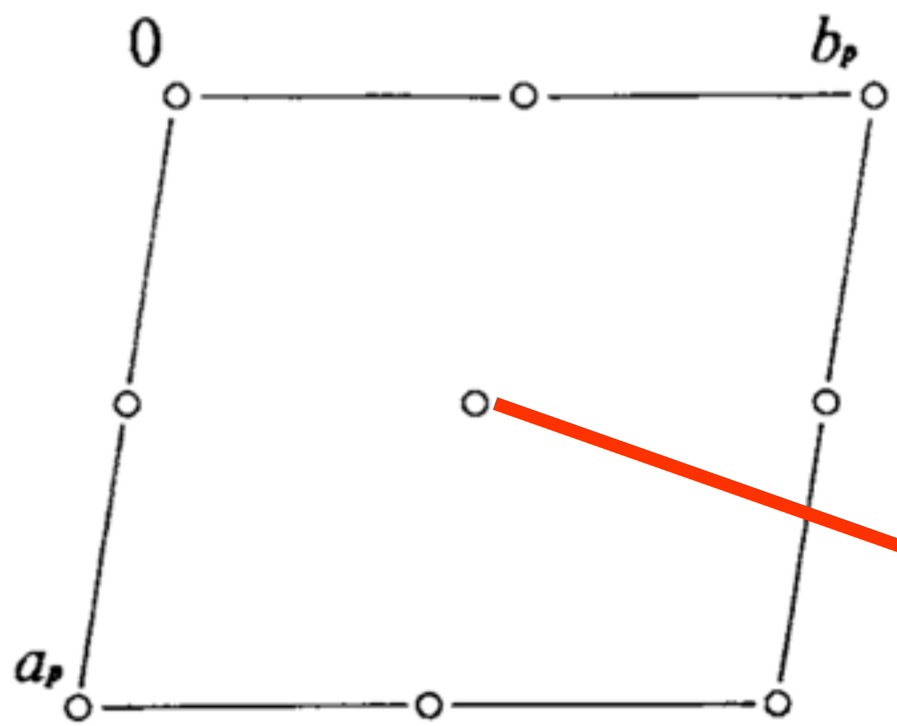
Factor group G/T_G

isomorphic to the point group P_G of G

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

Example: Calculation of the Site-symmetry groups

Group P-1



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

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

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

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

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates	
2	*i*	1	(1) x,y,z	(2) $\bar{x},\bar{y},\bar{z}$
1	*h*	$\bar{1}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	
1	*g*	$\bar{1}$	$0,\frac{1}{2},\frac{1}{2}$	
1	*f*	$\bar{1}$	$\frac{1}{2},0,\frac{1}{2}$	
1	*e*	$\bar{1}$	$\frac{1}{2},\frac{1}{2},0$	
1	*d*	$\bar{1}$	$\frac{1}{2},0,0$	
1	*c*	$\bar{1}$	$0,\frac{1}{2},0$	
1	*b*	$\bar{1}$	$0,0,\frac{1}{2}$	
1	*a*	$\bar{1}$	$0,0,0$	

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Problem: Wyckoff positions
Site-symmetry groups

WYCKPOS

Wyckoff Positions

space group

How to select the group

The space groups are specified by their number as given in the *International Tables for Crystallography*, Vol. A. You can give this number, if you know it, or you can choose it from the table with the space group numbers and symbols if you click on the link **choose it**.

If you are using this program in the preparation of a paper, please cite it in the following form:

Aroyo, *et. al. Zeitschrift fuer Kristallographie* (2006), **221**, 1, 15-27.

Please, enter the sequential number of group as given in *International Tables for Crystallography*, Vol. A or choose it: 68

Standard/Default Setting | Non Conventional Setting | ITA Settings

Wyckoff Positions of Group 68 (*Ccce*) [origin choice 2]

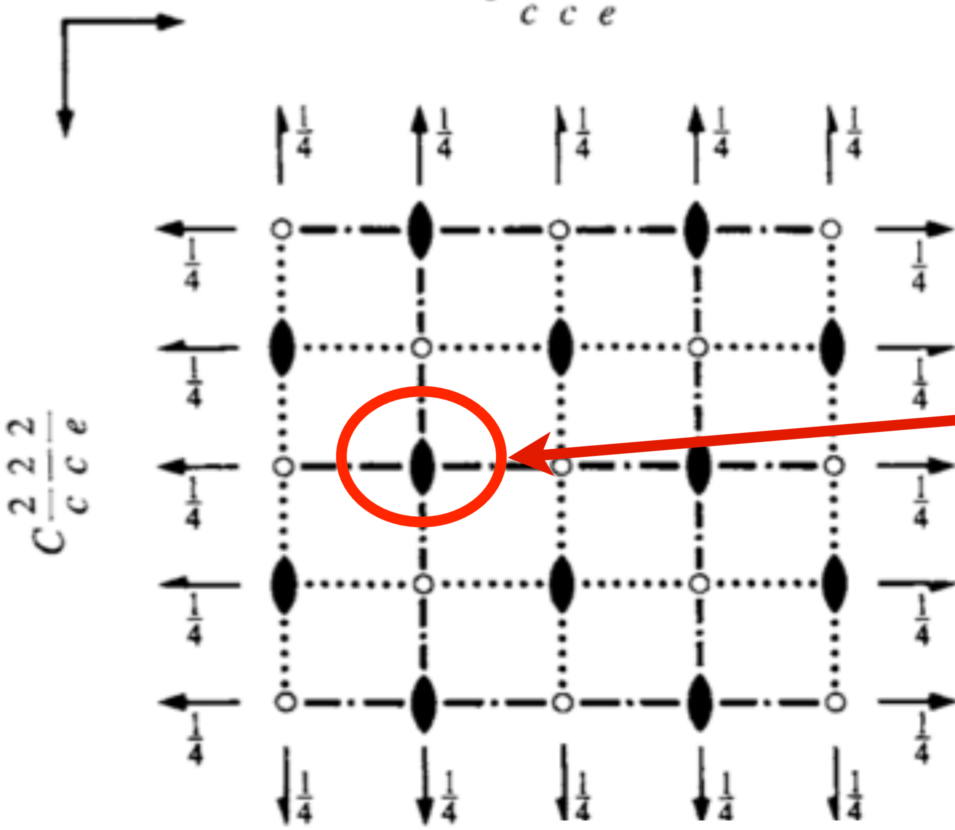
Multiplicity	Wyckoff letter	Site symmetry	Coordinates
			(0,0,0) + (1/2,1/2,0) +
16	i	1	(x,y,z) (-x+1/2,-y,z) (-x,y,-z+1/2) (x+1/2,-y,-z+1/2) (-x,-y,-z) (x+1/2,y,-z) (x,-y,z+1/2) (-x+1/2,y,z+1/2)
8	h	..2	(1/4,0,z) (3/4,0,-z+1/2) (3/4,0,-z) (1/4,0,z+1/2)
8	g	..2	(0,1/4,z) (0,1/4,-z+1/2) (0,3/4,-z) (0,3/4,z+1/2)
8	f	.2.	(0,y,1/4) (1/2,-y,1/4) (0,-y,3/4) (1/2,y,3/4)
8	e	2..	(x,1/4,1/4) (-x+1/2,3/4,1/4) (-x,3/4,3/4) (x+1/2,1/4,3/4)
8	d	-1	(0,0,0) (1/2,0,0) (0,0,1/2) (1/2,0,1/2)
8	c	-1	(1/4,3/4,0) (1/4,1/4,0) (3/4,3/4,1/2) (3/4,1/4,1/2)
4	b	222	(0,1/4,3/4) (0,3/4,1/4)
4	a	222	(0,1/4,1/4) (0,3/4,3/4)

Space Group : 68 (*Ccce*) [origin choice 2]
Point : (0,1/4,1/4)
Wyckoff Position : 4a

Site Symmetry Group 222

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

Example WYCKPOS: Wyckoff Positions Ccce (68)



2 1/2,y,1/4

2 x,1/4,1/4

Wyckoff position and site symmetry group of a specific point

Specify the point by its relative coordinates (in fractions or decimals)

Variable parameters (x,y,z) are also accepted

x = 1/2 y = 1/4 z = 1/4

Show

Space Group : 68 (*Ccce*) [origin choice 2]

Point : (1/2,1/4,1/4)

Wyckoff Position : 4b

Site Symmetry Group 222

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

EXERCISES

Problem 2.18

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

Determine the site-symmetry groups of Wyckoff positions *1a* and *1b*. 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.

Compare your results with the results of the program WYCKPOS.

Problem 2.18

SOLUTION

CONTINUED

Space group P4mm

No. 99

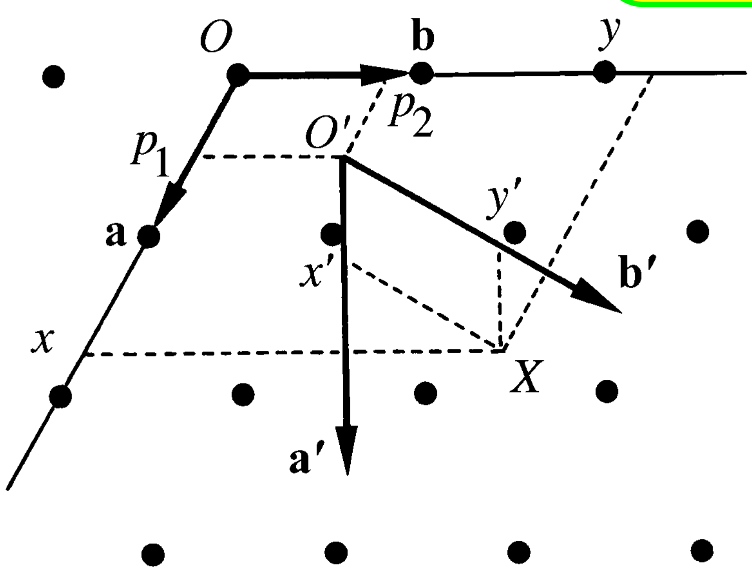
Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

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*	$\frac{1}{2},\frac{1}{2},z$			
1	*a*	4 *m m*	$0,0,z$			

CO-ORDINATE TRANSFORMATIONS IN CRYSTALLOGRAPHY

Co-ordinate transformation



3-dimensional space

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

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

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

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

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

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

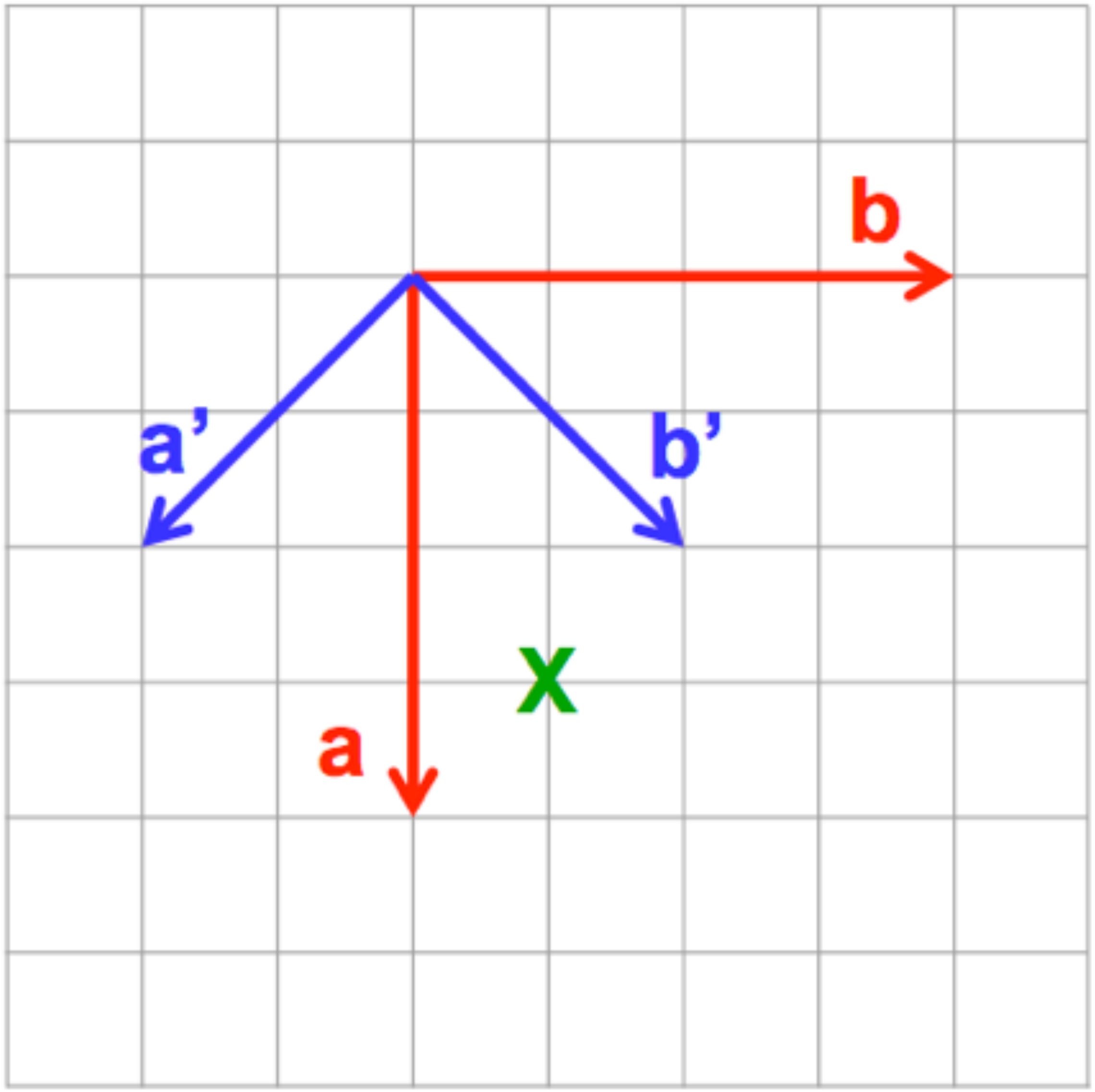
$$= (\mathbf{a}, \mathbf{b}, \mathbf{c}) \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix} = (P_{11}\mathbf{a} + P_{21}\mathbf{b} + P_{31}\mathbf{c}, \; P_{12}\mathbf{a} + P_{22}\mathbf{b} + P_{32}\mathbf{c}, \; P_{13}\mathbf{a} + P_{23}\mathbf{b}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

(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

EXAMPLE



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

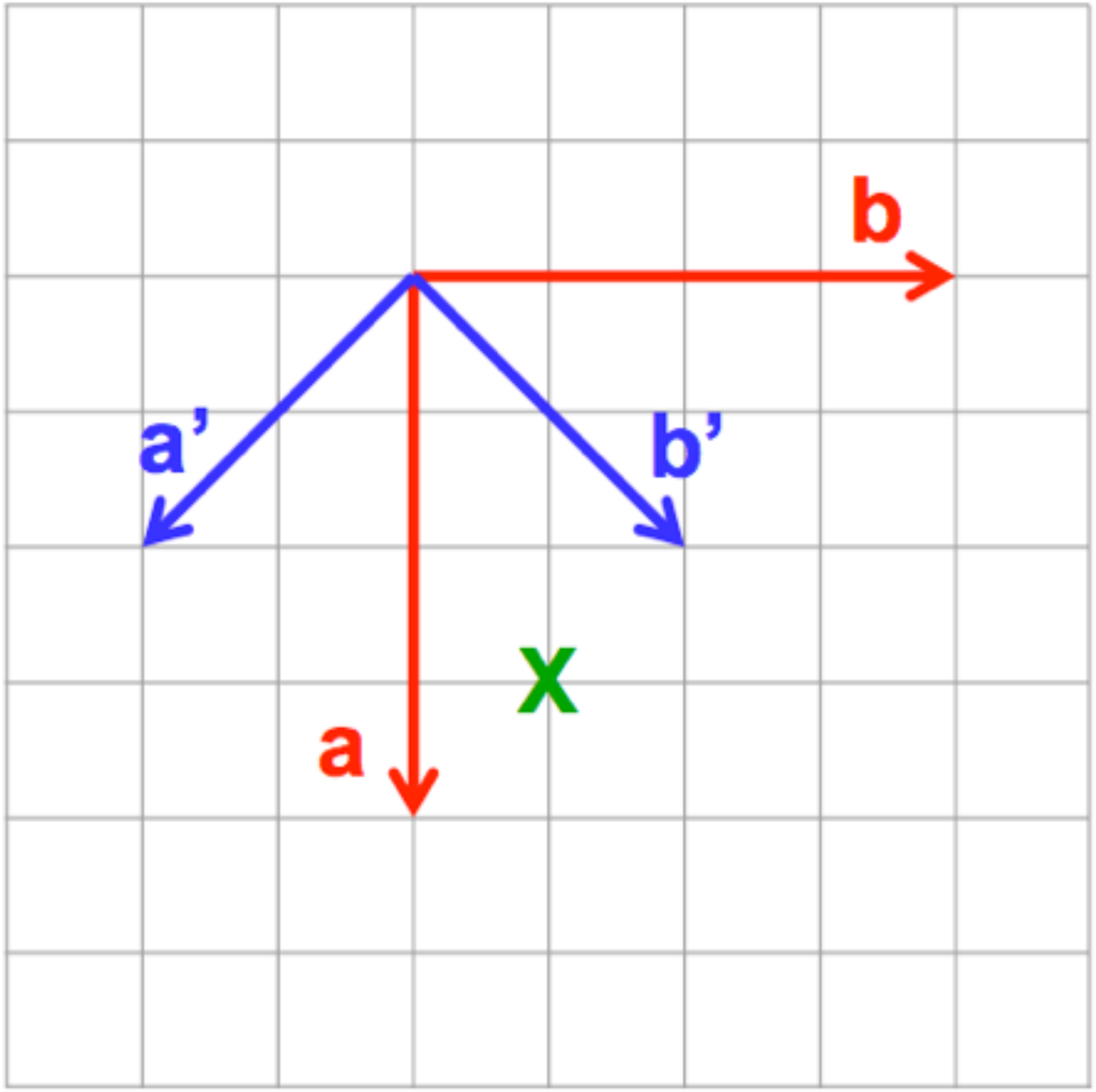
$$(a,b,c) = (a',b',c')\begin{pmatrix} ? \end{pmatrix}$$

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

$$X' = (?)$$

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

EXAMPLE



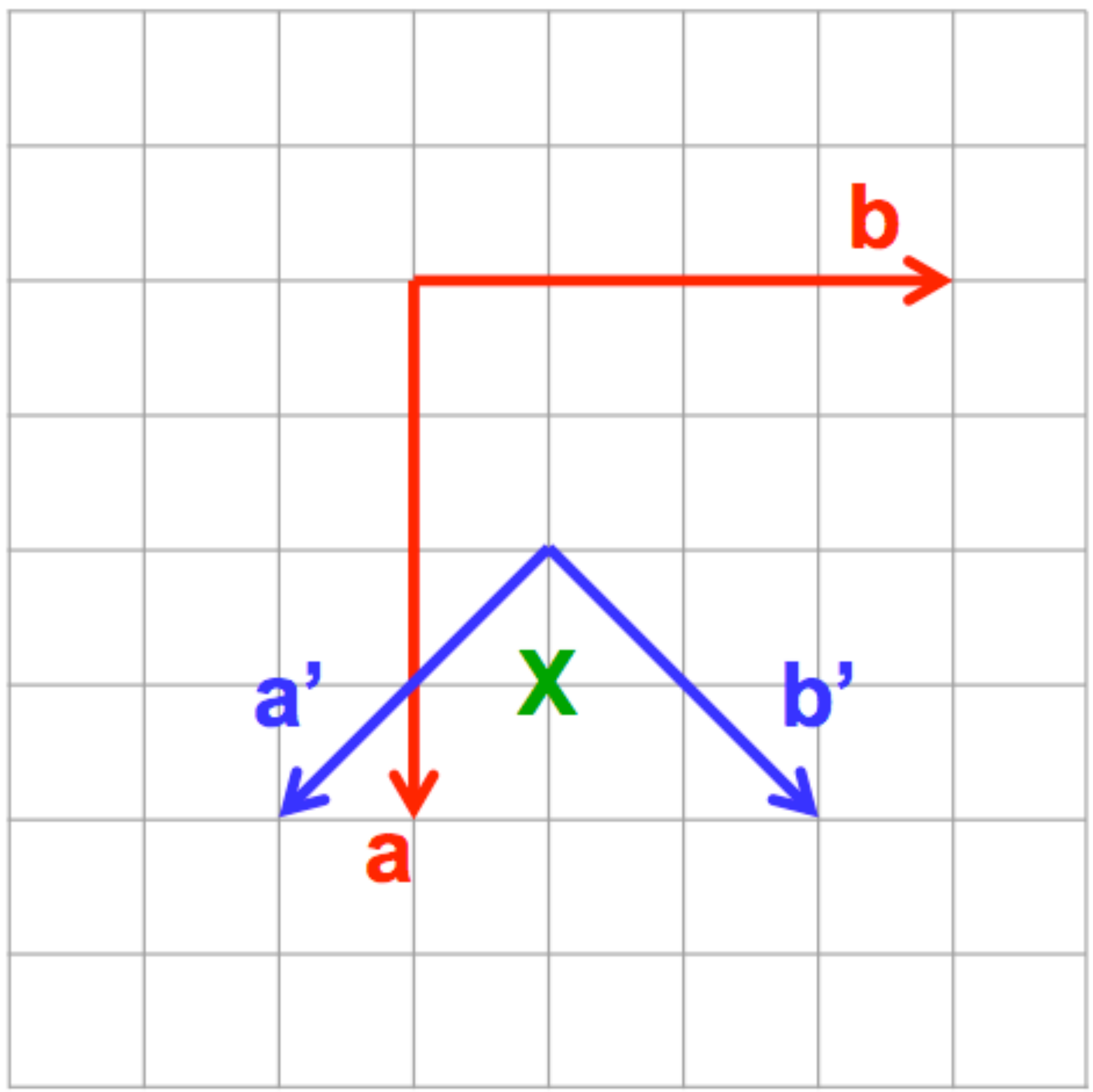
$$(\boldsymbol{a}',\boldsymbol{b}',\boldsymbol{c}') = (\boldsymbol{a},\boldsymbol{b},\boldsymbol{c})\begin{pmatrix} 1/2 & 1/2 & 0 \\ -1/2 & 1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$(\boldsymbol{a},\boldsymbol{b},\boldsymbol{c}) = (\boldsymbol{a}',\boldsymbol{b}',\boldsymbol{c}')\begin{pmatrix} 1 & -1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\boldsymbol{X} = (3/4, 1/4, 0)$$

$$\boldsymbol{X}' = (1/2, 1, 0)$$

EXAMPLE



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

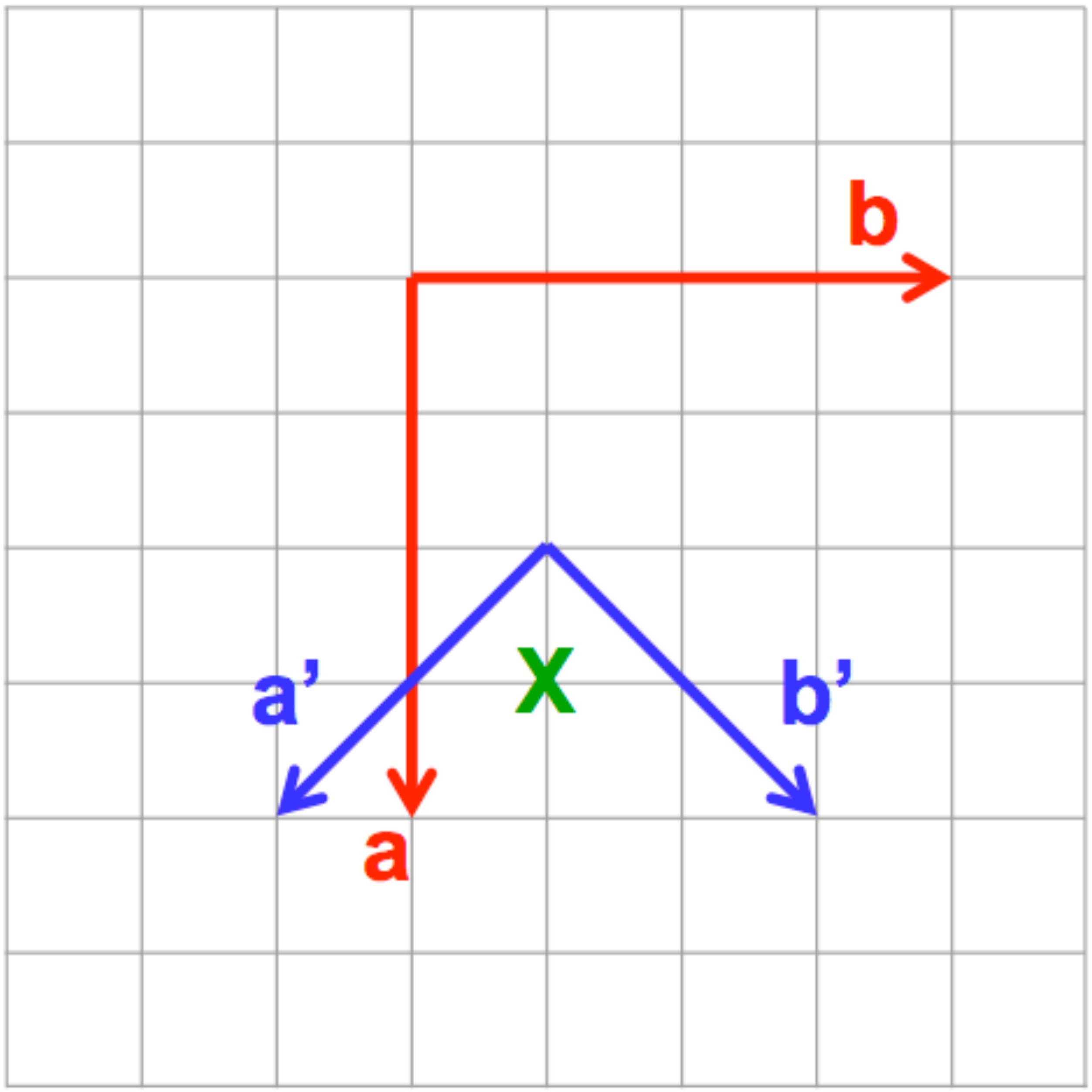
$$q = \begin{pmatrix} ? \end{pmatrix}$$

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

$$X' = (?)$$

Linear parts as before.

EXAMPLE



$$p = \begin{pmatrix} 1/2 \\ 1/4 \\ 0 \end{pmatrix}$$

$$q = \begin{pmatrix} -1/4 \\ -3/4 \\ 0 \end{pmatrix}$$

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

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

Linear parts as before.

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

$$(P,p)=\left(\begin{array}{ccc|c} 1/2 & 1/2 & 0 & 1/2 \\ -1/2 & 1/2 & 0 & 1/4 \\ 0 & 0 & 1 & 0 \end{array}\right)$$

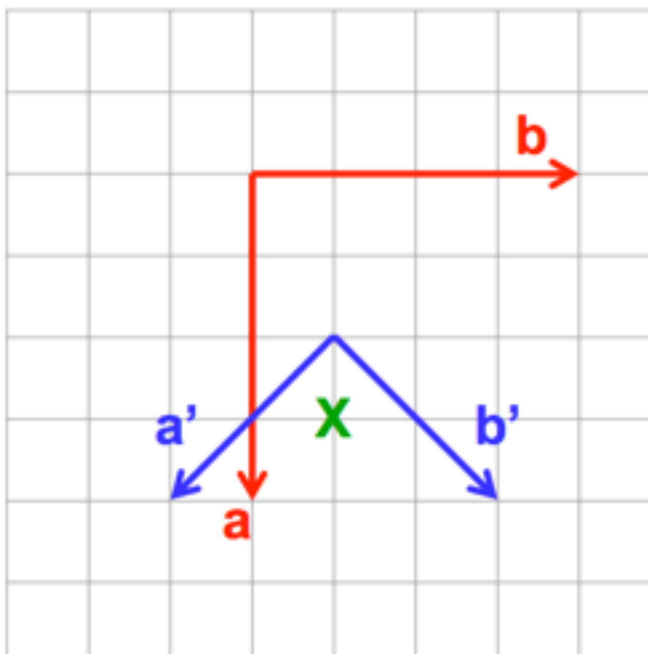
$$(P,p)^{-1}=\left(\begin{array}{ccc|c} 1 & -1 & 0 & -1/4 \\ 1 & 1 & 0 & -3/4 \\ 0 & 0 & 1 & 0 \end{array}\right)$$

a'=1/2a-1/2b

b'=1/2a+1/2b

c'=c

O'=O+ $\begin{pmatrix} 1/2 \\ 1/4 \\ 0 \end{pmatrix}$



a=a'+b'

b=-a'+b'

c=c'

O=O'+ $\begin{pmatrix} -1/4 \\ -3/4 \\ 0 \end{pmatrix}$

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

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

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \left(\begin{array}{ccc|c} P11 & P12 & P13 & p1 \\ P21 & P22 & P23 & p2 \\ P31 & P32 & P33 & p3 \end{array} \right)^{-1} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

special cases

-origin shift (***P*=*I***): $\boldsymbol{x}' = \boldsymbol{x} - \boldsymbol{p}$

-change of basis (***p*=o**) : $\boldsymbol{x}' = \boldsymbol{P}^{-1}\boldsymbol{x}$

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

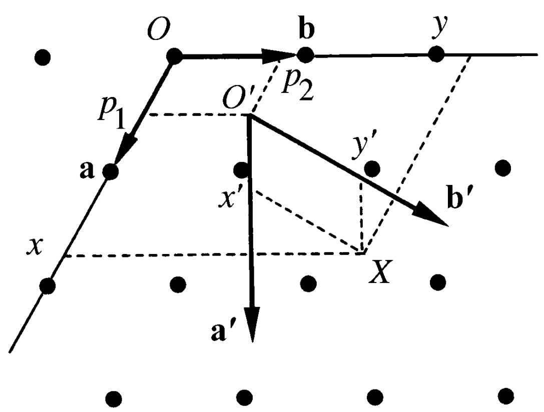
$$(W',w') = (P,p)^{-1}(W,w)(P,p)$$

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

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

Short-hand notation for the description of transformation matrices

Transformation matrix:



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

$$(P,p)=\left(\begin{array}{ccc|c} P11 & P12 & P13 & p1 \\ P21 & P22 & P23 & p \\ P31 & P32 & P33 & p \end{array}\right)$$

(**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

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$\underline{\bar{b}}$a	ab$\underline{c}$	ba$\underline{\bar{c}}$	$\underline{a}$bc	$\underline{\bar{a}}$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	$P2/m$	$P1\frac{2}{m}1$	$P1\frac{2}{m}1$	$P11\frac{2}{m}$	$P11\frac{2}{m}$	$P\frac{2}{m}11$	$P\frac{2}{m}11$	
11	C_{2h}^2	$P2_1/m$							

Monoclinic descriptions

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

Orthorhombic descriptions

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

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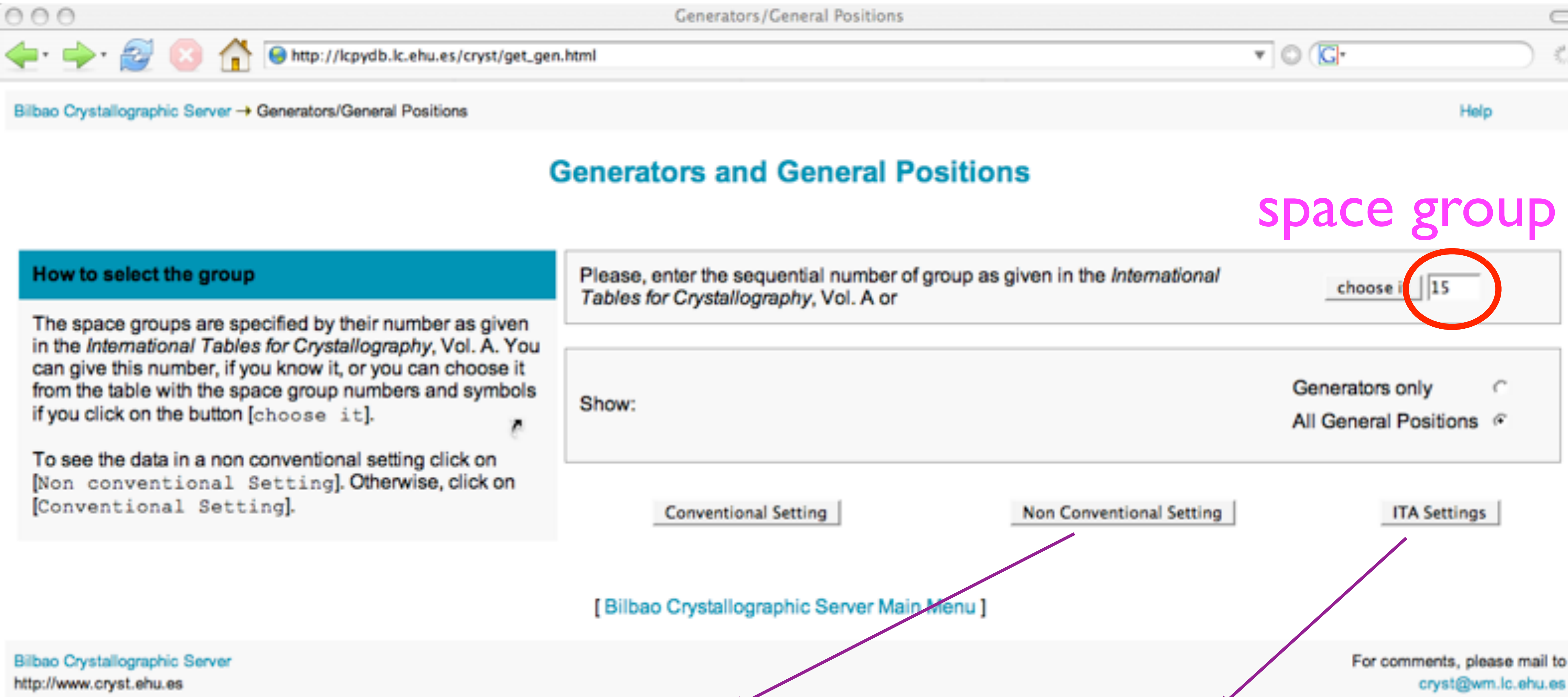
Problem: Coordinate transformations
Generators
General positions

GENPOS

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 *C2/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 **_A112/a_ setting**

Bilbao Crystallographic Server

Problem: Coordinate transformations Wyckoff positions — WYCKPOS

Wyckoff Positions

space group

How to select the group

The space groups are specified by their number as given in the *International Tables for Crystallography*, Vol. A. You can give this number, if you know it, or you can choose it from the table with the space group numbers and symbols if you click on the link **choose it**.

If you are using this program in the preparation of a paper, please cite it in the following form:

Aroyo, et. al. *Zeitschrift fuer Kristallographie* (2006), **221**, 1, 15-27.

Please, enter the sequential number of group as given in *International Tables for Crystallography*, Vol. A or choose it: 68

Standard/Default Setting | Non Conventional Setting | ITA Settings

Transformation of the basis

ITA settings

ITA-Settings for the Space Group 68

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

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

ITA number	Setting	P	P-1
68	*C c c e* [origin 1]	**a,b,c**	**a,b,c**
68	*A e a a* [origin 1]	**c,a,b**	**b,c,a**
68	*B b e b* [origin 1]	**b,c,a**	**c,a,b**
68	*C c c e* [origin 2]	**a,b,c**	**a,b,c**
68	*A e a a* [origin 2]	**c,a,b**	**b,c,a**
68	*B b e b* [origin 2]	**b,c,a**	**c,a,b**

EXERCISES

Problem 2.20

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 $\boldsymbol{P}$= c,a,b.

Use the retrieval tools GENPOS (generators and general positions) and WYCKPOS (Wyckoff positions) 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*.

EXERCISES

Problem 2.21

Use the retrieval tools GENPOS or *Generators* and *General positions*, WYCKPOS (or *Wyckoff 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**)