AIC Commission on Crystallographic Teaching

AIC International Crystallography School 2019

CRYSTALLOGRAPHIC
INFORMATION
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www.cristallografia.org/aicschool2019

30 August
3 September
2019
Naples, Italy
SPACE-GROUP SYMMETRY

International Tables for Crystallography, Volume A

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Real crystal

Real crystals are finite objects in physical space which due to static (impurities and structural imperfections like disorder, dislocations, etc) or dynamic (phonons) defects are not perfectly symmetric.

Ideal crystal (ideal crystal structures)

Infinite periodic spatial arrangement of the atoms (ions, molecules) with no static or dynamic defects.

Crystal pattern:

A model of the ideal crystal (crystal structure) in point space consisting of a strictly 3-dimensional periodic set of points.

An abstraction of the atomic nature of the ideal structure, perfectly periodic.
Space group G:
The set of all symmetry operations (isometries) of a crystal pattern

Translation subgroup $T$: $T \triangleleft G$
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 $T$: $P_G ≅ G/H$

$(W,w)→W \quad P_G=\{W|(W,w)\in G\}$
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;
1. $C_{mm2}$  
2. No. 35  

3. $C_{2v}$  

4. Origin on $mm2$  

5. Asymmetric unit $0 \leq x \leq \frac{1}{4}; \quad 0 \leq y \leq \frac{1}{4}; \quad 0 \leq z \leq 1$  

6. Symmetry operations  
   For $(0,0,0) + \text{set}$  
   (1) 1  
   (2) 2 0,0,z  
   (3) $m \ x, 0, z$  
   (4) $m \ 0, y, z$  

$C_{mm2}$  

$C_{2v}$  

$mm2$ Orthorhombic  

Patterson symmetry $C_{mmm}$  

$B_{2m}$  

$A_{2mm}$  

$B_{mm2}$
CONTINUED

No. 35

Cmm2

Generators selected
(1) \( t(1,0,0); t(0,1,0); t(0,0,1); t(\frac{1}{3},0); \) (2); (3)

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site symmetry</th>
<th>Coordinates</th>
<th>Reflection conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>( f ) 1</td>
<td>(1) ( x,y,z ) (2) ( x,\bar{y},z ) (3) ( x,\bar{y},z ) (4) ( \bar{x},y,z )</td>
</tr>
</tbody>
</table>

| 4  | \( e \) m . . | 0,\( y,z \) 0,\( \bar{y},z \) |
| 4  | \( d \) . m . | \( x,0,z \) \( \bar{x},0,z \) |
| 4  | \( c \) . . 2 | \( \frac{1}{4},\frac{1}{4},z \) \( \frac{1}{4},\frac{1}{4},z \) |
| 2  | \( b \) m m 2 | 0,\( \frac{1}{2},z \) |
| 2  | \( a \) m m 2 | 0,0,\( z \) |

Symmetry of special projections

Along [001] \( c2mm \) \( a' = a \quad b' = b \)
Origin at 0,0,\( z \)

Along [100] \( p1m1 \) \( a' = \frac{1}{2}b \quad b' = c \)
Origin at \( x,0,0 \)

Along [010] \( p1 1m \) \( a' = c \quad b' = \frac{1}{2}a \)
Origin at 0,\( y,0 \)
<table>
<thead>
<tr>
<th>Number of space group</th>
<th>Full Hermann-Mauguin symbol</th>
<th>Schoenflies symbol</th>
<th>Crystal class (point group)</th>
<th>Crystal system</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Cmm2</strong></td>
<td>$C^{11}_{2v}$</td>
<td>$C_{2v}$</td>
<td><strong>mm2</strong></td>
<td>Orthorhombic</td>
</tr>
<tr>
<td><strong>No. 35</strong></td>
<td><strong>Cmm2</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Patterson symmetry $Cmmm$
HERMANN-MAUGUIN
SYMBOLISM FOR SPACE GROUPS
Hermann-Mauguin symbols for space groups

The Hermann–Mauguin symbol for a space group consists of a sequence of letters and numbers, here called the constituents of the HM symbol.

(i) The first constituent is always a symbol for the conventional cell of the translation lattice of the space group.

(ii) The second part of the full HM symbol of a space group consists of one position for each of up to three representative symmetry directions. To each position belong the generating symmetry operations of their representative symmetry direction. The position is thus occupied either by a rotation, screw rotation or rotoinversion and/or by a reflection or glide reflection.

(iii) Simplest-operation rule:

- pure rotations > screw rotations;
- pure rotations > rotoinversions
- reflection m > a; b; c > n

‘>’ means ‘has priority’
## 14 Bravais Lattices

<table>
<thead>
<tr>
<th>Crystal Family</th>
<th>Lattice Types</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Triclinic</strong></td>
<td><img src="image1.png" alt="Image" /></td>
</tr>
<tr>
<td><strong>Monoclinic</strong></td>
<td><img src="image2.png" alt="Image" /></td>
</tr>
<tr>
<td><strong>Orthorhombic</strong></td>
<td><img src="image3.png" alt="Image" /></td>
</tr>
<tr>
<td><strong>Tetragonal</strong></td>
<td><img src="image4.png" alt="Image" /></td>
</tr>
<tr>
<td><strong>Hexagonal</strong></td>
<td><img src="image5.png" alt="Image" /></td>
</tr>
<tr>
<td><strong>Cubic</strong></td>
<td><img src="image6.png" alt="Image" /></td>
</tr>
</tbody>
</table>
A direction is called a **symmetry direction** of a crystal structure if it is parallel to an axis of rotation, screw rotation or rotoinversion or if it is parallel to the normal of a reflection or glide-reflection plane. A symmetry direction is thus the direction of the geometric element of a symmetry operation, when the normal of a symmetry plane is used for the description of its orientation.
## 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.

<table>
<thead>
<tr>
<th>Lattice</th>
<th>Symmetry direction (position in Hermann–Mauguin symbol)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Primary</td>
</tr>
<tr>
<td>Triclinic</td>
<td>None</td>
</tr>
<tr>
<td>Monoclinic*</td>
<td>[010] (‘unique axis b’)</td>
</tr>
<tr>
<td>Orthorhombic</td>
<td>[100]</td>
</tr>
<tr>
<td>Tetragonal</td>
<td>[001]</td>
</tr>
<tr>
<td>Hexagonal</td>
<td>[001]</td>
</tr>
<tr>
<td>Rhombohedral (hexagonal axes)</td>
<td>[001]</td>
</tr>
<tr>
<td>Rhombohedral (rhombohedral axes)</td>
<td>[111]</td>
</tr>
<tr>
<td>Cubic</td>
<td>{ [100] [010] [001] }</td>
</tr>
</tbody>
</table>
Hermann-Mauguin symbols for space groups

Example:

- **Orthorhombic**
  - Bravais lattice
  - Screw axis $2_1 // \vec{a}$
  - Glide plane $n \perp \vec{a}$
  - Mirror plane $m \perp \vec{b}$

- **Secondary direction**
  - Screw axis $2_1 // \vec{b}$

- **Tertiary direction**
  - Screw axis $2_1 // \vec{c}$
  - Glide plane $a \perp \vec{c}$
Symmetry Operations

- KIND of the symmetry operation
- TYPE of the symmetry operation
- SCREW/GLIDE component
- ORIENTATION of the geometric element
- LOCATION of the geometric element
Kinds of Symmetry Operations

Symmetry operations of 1st kind (proper):

chirality (handedness)
- preserving

Symmetry operations of 2nd kind (improper):

chirality (handedness)
- non-preserving

**Chirality** is the geometric property of a rigid object of being non-superposable on its mirror image. An object displaying chirality is called **chiral**; the opposite term is **achiral**.
Crystallographic symmetry operations

Crystallographic restriction theorem

The rotational symmetries of a crystal pattern are limited to 2-fold, 3-fold, 4-fold, and 6-fold.

Matrix proof:

Rotation with respect to orthonormal basis

\[
R = \begin{pmatrix}
\cos\theta & -\sin\theta \\
\sin\theta & \cos\theta
\end{pmatrix}
\]

Rotation with respect to lattice basis

\[R: \text{integer matrix}\]

In a lattice basis, because the rotation must map lattice points to lattice points, each matrix entry — and hence the trace — must be an integer.

\[\text{Tr } R = 2\cos\theta = \text{integer}\]

<table>
<thead>
<tr>
<th>(m)</th>
<th>(m/2 = \cos\theta)</th>
<th>(\theta (^\circ))</th>
<th>(n = 360^\circ/\theta)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>90</td>
<td>Fourfold</td>
</tr>
<tr>
<td>1</td>
<td>1/2</td>
<td>60</td>
<td>Sixfold</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>0 = 360</td>
<td>Identity (onefold)</td>
</tr>
<tr>
<td>-1</td>
<td>-1/2</td>
<td>120</td>
<td>Threefold</td>
</tr>
<tr>
<td>-2</td>
<td>-1</td>
<td>180</td>
<td>Twofold</td>
</tr>
</tbody>
</table>
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 \(\tilde{x} = x + t\)

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

\[
(W_1, w_1) = \begin{pmatrix}
-1 & 0 \\
1 & 0 \\
-1 & 0 \\
0 & 1
\end{pmatrix}
\]

\[
(W_2, w_2) = \begin{pmatrix}
-1 & 1/2 \\
1 & 0 \\
-1 & 1/2 \\
0 & 1
\end{pmatrix}
\]

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.
Characterization of the symmetry operations:

\[
\begin{pmatrix}
-1 & 0 \\
0 & -1 \\
\end{pmatrix}
\]

\[\det\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} = \,?\]

\[\begin{pmatrix}
-1 & 0 \\
0 & 1 \\
\end{pmatrix}
\]

\[\operatorname{tr}\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} = \,?\]

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

\[
\begin{pmatrix}
-1 & 1/2 \\
1 & 0 \\
-1 & 1/2 \\
\end{pmatrix}
\begin{pmatrix}
xf \\
yf \\
zf \\
\end{pmatrix} = \begin{pmatrix}
xf \\
yf \\
zf \\
\end{pmatrix}
\]
Description of isometries: 3D

Coordinate system: \( \{ O, \mathbf{a}, \mathbf{b}, \mathbf{c} \} \)

Isometry:

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

\[
\tilde{x} = W x + w.
\]

\[
\tilde{x} = (W, w) x \quad \text{or} \quad \tilde{x} = \{W \mid w\} x
\]

matrix-column pair

Seitz symbol
Short-hand notation for the description of isometries

**Isometry:**

\[ X \to \tilde{X} \]

\[
\begin{align*}
\tilde{x} &= W_{11} x + W_{12} y + W_{13} z + w_1 \\
\tilde{y} &= W_{21} x + W_{22} y + W_{23} z + w_2 \\
\tilde{z} &= W_{31} x + W_{32} y + W_{33} z + w_3.
\end{align*}
\]

**Notation rules:**
- Left-hand side: omitted
- Coefficients 0, +1, -1
- Different rows in one line

**Examples:**

\[
\begin{array}{ccc}
-1 & 1/2 \\
1 & 0 & 1/2 \\
-1 & 1/2
\end{array}
\]

\[ \{ -x+1/2, y, -z+1/2 \} \to \{ \overline{x}+1/2, y, \overline{z}+1/2 \} \]
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. \((x,-y+1/2,z+1/2)\)
Space group \textit{Cmm2} (No. 35)

Diagram of symmetry elements

Diagram of general position points

How are the symmetry operations represented in ITA?

Symmetry operations

For \((0,0,0)\) set

1. \(1\)
2. \(2 \quad 0,0,z\)
3. \(m \quad x,0,z\)
4. \(m \quad 0,y,z\)

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

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

General Position

Coordinates

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

8 \( f \quad 1\)

1. \(x,y,z\)
2. \(\bar{x},\bar{y},z\)
3. \(x,\bar{y},z\)
4. \(\bar{x},y,z\)
(i) coordinate triplets of an image point $\tilde{X}$ of the original point $X = \begin{bmatrix} x \\ y \\ z \end{bmatrix}$ 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 $G$

$(W,w) = (I,t_n)(W,w_0), 0 \leq w_{i0} < 1$
### Space Groups: Infinite Order

#### Coset Decomposition $G:T_G$

<table>
<thead>
<tr>
<th>$(I,0)$</th>
<th>$(W_2, w_2)$</th>
<th>...</th>
<th>$(W_m, w_m)$</th>
<th>...</th>
<th>$(W_i, w_i)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(I,t_1)$</td>
<td>$(W_2, w_2 + t_1)$</td>
<td>...</td>
<td>$(W_m, w_m + t_1)$</td>
<td>...</td>
<td>$(W_i, w_i + t_1)$</td>
</tr>
<tr>
<td>$(I,t_2)$</td>
<td>$(W_2, w_2 + t_2)$</td>
<td>...</td>
<td>$(W_m, w_m + t_2)$</td>
<td>...</td>
<td>$(W_i, w_i + t_2)$</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>$(I,t_j)$</td>
<td>$(W_2, w_2 + t_j)$</td>
<td>...</td>
<td>$(W_m, w_m + t_j)$</td>
<td>...</td>
<td>$(W_i, w_i + t_j)$</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
</tbody>
</table>

#### 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: P1 2/m 1

Coset decomposition $G:T_G$

Point group $P_G = \{1, 2, \bar{1}, m\}$

General position

<table>
<thead>
<tr>
<th>$T_G$</th>
<th>$T_G \ 2$</th>
<th>$T_G \ \bar{1}$</th>
<th>$T_G \ m$</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1,0)</td>
<td>(2,0)</td>
<td>(1,0)</td>
<td>(m,0)</td>
</tr>
<tr>
<td>(1,t_1)</td>
<td>(2,t_1)</td>
<td>(1, t_1)</td>
<td>(m, t_1)</td>
</tr>
<tr>
<td>(1,t_2)</td>
<td>(2,t_2)</td>
<td>(1, t_2)</td>
<td>(m,t_2)</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>(1,t_j)</td>
<td>(2,t_j)</td>
<td>(1, t_j)</td>
<td>(m, t_j)</td>
</tr>
</tbody>
</table>

... ... ... ...

inversion centres $(\bar{1}, t)$:

... ... ... ...

$-I$ ... $-I$ ...

$-I$ $n_1$ $n_2$ $n_3$

$\bar{1}$ at $\bar{1}$

... $n_1/2$ ...

... $n_2/2$ ...

... $n_3/2$ ...
Coset decomposition $P12_1/c1:T$

**Point group?**

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

---

**EXAMPLE**

<table>
<thead>
<tr>
<th>$I,0$</th>
<th>$(2,0 \frac{1}{2} \frac{1}{2})$</th>
<th>$\bar{I},0$</th>
<th>$(m,0 \frac{1}{2} \frac{1}{2})$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$I,t_1$</td>
<td>$(2,0 \frac{1}{2} \frac{1}{2}+t_1)$</td>
<td>$\bar{I},t_1$</td>
<td>$(m,0 \frac{1}{2} \frac{1}{2}+t_1)$</td>
</tr>
<tr>
<td>$I,t_2$</td>
<td>$(2,0 \frac{1}{2} \frac{1}{2}+t_2)$</td>
<td>$\bar{I},t_2$</td>
<td>$(m,0 \frac{1}{2} \frac{1}{2}+t_2)$</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>$I,t_j$</td>
<td>$(2,0 \frac{1}{2} \frac{1}{2}+t_j)$</td>
<td>$\bar{I},t_j$</td>
<td>$(m,0 \frac{1}{2} \frac{1}{2}+t_j)$</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
</tbody>
</table>

**inversion centers**

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

**2\_screw axes**

$(2,u \frac{1}{2}+v \frac{1}{2}+w)$

$(2,u \frac{1}{2} \frac{1}{2}+w)$
**Space group \( P2_1/c \) (No. 14)**

**Matrix-column presentation**

**Position**
- Multiplicity: \( 4 \)
- Wyckoff letter: \( e \)
- Site symmetry: \( 1 \)

**Generators selected**
- \( (1); r(1, 0, 0); r(0, 1, 0); r(0, 0, 1); (2); (3) \)

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

**Symmetry operations**
- \( (1) 1 \)
- \( (2) 2(0, \frac{1}{2}, 0) \)
- \( (3) \bar{1} 0, 0, 0 \)
- \( (4) c x, \frac{1}{3}, z \)
Example: Space group $P2_1/c$ (14)

Space-group symmetry operations

short-hand notation

matrix-column presentation

Geometric interpretation

Seitz symbols

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

<table>
<thead>
<tr>
<th>No.</th>
<th>(x,y,z) form</th>
<th>Matrix form</th>
<th>Symmetry operation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>x,y,z</td>
<td>(1 0 0 0 , 0 1 0 0 , 0 0 1 0)</td>
<td>1 { 1</td>
</tr>
<tr>
<td>2</td>
<td>-x,y+1/2,-z+1/2</td>
<td>( -1 0 0 0 , 0 0 1 0 , 0 -1 0 1/2 )</td>
<td>2 (0,1/2,0) 0,y,1/4 { 2010</td>
</tr>
<tr>
<td>3</td>
<td>-x,-y,-z</td>
<td>( -1 0 0 0 , 0 -1 0 0 , 0 0 -1 0 )</td>
<td>-1 0,0,0 { -1</td>
</tr>
<tr>
<td>4</td>
<td>x,-y+1/2,z+1/2</td>
<td>( 1 0 0 0 , 0 -1 0 0 , 0 0 1 0 )</td>
<td>c x,1/4,z { m010</td>
</tr>
</tbody>
</table>

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(0,1/2,0) 0,y,1/4
(3) $\bar{I}$ 0,0,0
(4) $c$ x,1/4,z
Seitz symbols \( \{ R \mid t \} \)

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

- 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.

\[
\begin{align*}
1 \text{ and } \overline{1} & \quad \text{identity and inversion} \\
\text{m} & \quad \text{reflections} \\
2, 3, 4 \text{ and } 6 & \quad \text{rotations} \\
\overline{3}, \overline{4} \text{ and } \overline{6} & \quad \text{rotoinversions}
\end{align*}
\]

translation part t

translation parts of the coordinate triplets of the General position blocks
Seitz symbols for symmetry operations of hexagonal and trigonal crystal systems

<table>
<thead>
<tr>
<th>ITA description</th>
<th>coord. triplet</th>
<th>type</th>
<th>orientation</th>
<th>Seitz symbol</th>
</tr>
</thead>
<tbody>
<tr>
<td>No.</td>
<td>coord. triplet</td>
<td>type</td>
<td>orientation</td>
<td>Seitz symbol</td>
</tr>
<tr>
<td>1)</td>
<td>$x, y, z$</td>
<td>1</td>
<td>0, 0, z</td>
<td>1</td>
</tr>
<tr>
<td>2)</td>
<td>$\bar{y}, x-y, z$</td>
<td>$3^+$</td>
<td>0, 0, z</td>
<td>$3^+_{001}$</td>
</tr>
<tr>
<td>3)</td>
<td>$\bar{x} + y, \bar{x}, z$</td>
<td>$3^-$</td>
<td>0, 0, z</td>
<td>$3^-_{001}$</td>
</tr>
<tr>
<td>4)</td>
<td>$\bar{x}, \bar{y}, z$</td>
<td>2</td>
<td>0, 0, z</td>
<td>$2_{001}$</td>
</tr>
<tr>
<td>5)</td>
<td>$y, \bar{x} + y, z$</td>
<td>$6^-$</td>
<td>0, 0, z</td>
<td>$6^-_{001}$</td>
</tr>
<tr>
<td>6)</td>
<td>$x-y, x, z$</td>
<td>$6^+$</td>
<td>0, 0, z</td>
<td>$6^+_{001}$</td>
</tr>
<tr>
<td>7)</td>
<td>$y, x, \bar{z}$</td>
<td>2</td>
<td>x, x, 0</td>
<td>$2_{110}$</td>
</tr>
<tr>
<td>8)</td>
<td>$x-y, y, \bar{z}$</td>
<td>2</td>
<td>x, 0, 0</td>
<td>$2_{100}$</td>
</tr>
<tr>
<td>9)</td>
<td>$\bar{x}, \bar{x} + y, \bar{z}$</td>
<td>2</td>
<td>0, y, 0</td>
<td>$2_{010}$</td>
</tr>
<tr>
<td>10)</td>
<td>$\bar{y}, \bar{x}, \bar{z}$</td>
<td>2</td>
<td>x, x, 0</td>
<td>$2_{1\bar{1}0}$</td>
</tr>
<tr>
<td>11)</td>
<td>$\bar{x} + y, y, \bar{z}$</td>
<td>2</td>
<td>x, 2x, 0</td>
<td>$2_{120}$</td>
</tr>
<tr>
<td>12)</td>
<td>$x, x-y, \bar{z}$</td>
<td>2</td>
<td>2x, x, 0</td>
<td>$2_{210}$</td>
</tr>
<tr>
<td>13)</td>
<td>$\bar{x}, \bar{y}, \bar{z}$</td>
<td>$\bar{1}$</td>
<td>0, 0, z</td>
<td>$\bar{1}$</td>
</tr>
<tr>
<td>14)</td>
<td>$y, \bar{x} + y, \bar{z}$</td>
<td>$\bar{3}^+$</td>
<td>0, 0, z</td>
<td>$\bar{3}^+_{001}$</td>
</tr>
<tr>
<td>15)</td>
<td>$x-y, x, \bar{z}$</td>
<td>$\bar{3}^-$</td>
<td>0, 0, z</td>
<td>$\bar{3}^-_{001}$</td>
</tr>
<tr>
<td>16)</td>
<td>$x, y, \bar{z}$</td>
<td>m</td>
<td>x, y, 0</td>
<td>$m_{001}$</td>
</tr>
<tr>
<td>17)</td>
<td>$\bar{y}, x-y, \bar{z}$</td>
<td>$\bar{6}^-$</td>
<td>0, 0, z</td>
<td>$\bar{6}^-_{001}$</td>
</tr>
<tr>
<td>18)</td>
<td>$\bar{x} + y, \bar{x}, \bar{z}$</td>
<td>$\bar{6}^+$</td>
<td>0, 0, z</td>
<td>$\bar{6}^+_{001}$</td>
</tr>
<tr>
<td>19)</td>
<td>$\bar{y}, \bar{x}, z$</td>
<td>m</td>
<td>x, x, z</td>
<td>$m_{110}$</td>
</tr>
<tr>
<td>20)</td>
<td>$\bar{x} + y, y, z$</td>
<td>m</td>
<td>x, 2x, z</td>
<td>$m_{100}$</td>
</tr>
<tr>
<td>21)</td>
<td>$x, x-y, z$</td>
<td>m</td>
<td>2x, x, z</td>
<td>$m_{010}$</td>
</tr>
<tr>
<td>22)</td>
<td>$y, x, z$</td>
<td>m</td>
<td>x, x, z</td>
<td>$m_{1\bar{1}0}$</td>
</tr>
<tr>
<td>23)</td>
<td>$x-y, \bar{y}, z$</td>
<td>m</td>
<td>x, 0, z</td>
<td>$m_{120}$</td>
</tr>
<tr>
<td>24)</td>
<td>$\bar{x}, \bar{x} + y, z$</td>
<td>m</td>
<td>0, y, z</td>
<td>$m_{210}$</td>
</tr>
</tbody>
</table>

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

$C_{2h}$

No. 14

$P12_1/c\overline{1}$

**UNIQUE AXIS b, CELL CHOICE 1**

Generators selected

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

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>(1) $x,y,z$</td>
</tr>
<tr>
<td></td>
<td>(2) $\bar{x},y+\frac{1}{2}, \bar{z}+\frac{1}{2}$</td>
</tr>
<tr>
<td></td>
<td>(3) $\bar{x},\bar{y},\bar{z}$</td>
</tr>
<tr>
<td></td>
<td>(4) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$</td>
</tr>
</tbody>
</table>

**Matrix-column presentation**

**Symmetry operations**

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

**Geometric interpretation**

**Seitz symbols**

(1) $\{1|0\}$
(2) $\{2_{o10}|01/21/2\}$
(3) $\overline{1}|0\}$
(4) $\{m_{010}|01/21/2\}$

**NOT in ITA**
SPACE-GROUPS
DIAGRAMS
Diagrams of symmetry elements

three different settings

permutations of $a, b, c$

Diagram of general position points
<table>
<thead>
<tr>
<th>printed symbol</th>
<th>symmetry axis</th>
<th>graphic symbol</th>
<th>nature of the screw translation</th>
<th>printed symbol</th>
<th>symmetry axis</th>
<th>graphic symbol</th>
<th>nature of the screw translation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Identity</td>
<td>none</td>
<td>none</td>
<td>4</td>
<td>Rotation tetrad</td>
<td>⋆</td>
<td>none</td>
</tr>
<tr>
<td>1</td>
<td>Inversion</td>
<td>○</td>
<td>none</td>
<td>4₁</td>
<td></td>
<td></td>
<td>c/4</td>
</tr>
<tr>
<td>2</td>
<td>Rotation diad or twofold rotation axis</td>
<td></td>
<td>none</td>
<td>4₂</td>
<td>Screw tetrads</td>
<td>⋆</td>
<td>2c/4</td>
</tr>
<tr>
<td>2₁</td>
<td>Screw diad or twofold screw axis</td>
<td></td>
<td>c/2</td>
<td>4₃</td>
<td></td>
<td></td>
<td>3c/4</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>4</td>
<td>Inverse tetrad</td>
<td>⬇</td>
<td>none</td>
</tr>
<tr>
<td>2₁</td>
<td></td>
<td></td>
<td></td>
<td>6</td>
<td>Rotation hexad</td>
<td>⬇</td>
<td>none</td>
</tr>
<tr>
<td>3</td>
<td>Rotation triad</td>
<td></td>
<td>none</td>
<td>6₁</td>
<td></td>
<td>⬇</td>
<td>c/6</td>
</tr>
<tr>
<td>3₁</td>
<td>Screw triad</td>
<td></td>
<td>c/3</td>
<td>6₂</td>
<td></td>
<td>⬇</td>
<td>2c/6</td>
</tr>
<tr>
<td>3₂</td>
<td></td>
<td></td>
<td>2c/3</td>
<td>6₃</td>
<td>Screw hexads</td>
<td>⬇</td>
<td>3c/6</td>
</tr>
<tr>
<td>3</td>
<td>Inverse triad</td>
<td></td>
<td>none</td>
<td>6₄</td>
<td></td>
<td>⬇</td>
<td>4c/6</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>6₅</td>
<td></td>
<td></td>
<td>5c/6</td>
</tr>
<tr>
<td>3</td>
<td></td>
<td></td>
<td></td>
<td>6</td>
<td>Inverse hexad</td>
<td>⬇</td>
<td>none</td>
</tr>
<tr>
<td>printed symbol</td>
<td>symmetry plane</td>
<td>graphical symbol</td>
<td>nature of glide translation</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>---------------</td>
<td>----------------</td>
<td>-----------------</td>
<td>----------------------------</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$m$</td>
<td>reflection plane (mirror)</td>
<td>__________</td>
<td>none</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$a, b$</td>
<td>axial glide plane</td>
<td>__________</td>
<td>$a/2$ or $b/2$</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$c$</td>
<td>..................</td>
<td>none</td>
<td>$c/2$</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$n$</td>
<td>diagonal glide plane (net)</td>
<td>__________</td>
<td>$(a+b)/2, (b+c)/2$ or $(c+a)/2$; OR $(a+b+c)/2$ for $t$ and $c$ systems</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$d$</td>
<td>“diamond” glide plane</td>
<td>__________</td>
<td>$(a\pm b)/4, (b\pm c)/4$ or $(c\pm a)/4$; OR $(a\pm b\pm c)/4$ for $t$ and $c$ systems</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
 EXAMPLE

Space group $Cmm2$ (No. 35)

### 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. $b \ \frac{1}{4},y,z$

### Geometric interpretation

- Glide plane, $t=1/2a$
  - at $y=1/4$, $\perp b$
- Glide plane, $t=1/2b$
  - at $x=1/4$, $\perp a$

### General Position

Coordinates

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

1. $x,y,z$
2. $\bar{x},\bar{y},z$
3. $x,\bar{y},z$
4. $\bar{x},y,z$

- $x+1/2,-y+1/2,z$
- $-x+1/2,y+1/2,z$

### Matrix-column presentation of symmetry operations

8 f 1

- $x, y, z$
- $\bar{x}, \bar{y}, z$
- $x, \bar{y}, z$
- $\bar{x}, y, z$
Example: P4mm

Diagram of symmetry elements

Diagram of general position points

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. $m \ x,x,z$

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. $y,x,z$
Symmetry elements

- Geometric element
- Fixed points

Symmetry operations that share the same geometric element

Examples

Rotation axis

- Geometric element: line
- Fixed points: 1st, ..., (n-1)th powers + all coaxial equivalents

All rotations and screw rotations with the same axis, the same angle and sense of rotation and the same screw vector (zero for rotation) up to a lattice translation vector.

Glide plane

- Geometric element: plane
- Fixed points: defining operation + all coplanar equivalents

All glide reflections with the same reflection plane, with glide of d.o. (taken to be zero for reflections) by a lattice translation vector.
# Symmetry operations and symmetry elements

## Geometric elements and Element sets

<table>
<thead>
<tr>
<th>Name of symmetry element</th>
<th>Geometric element</th>
<th>Defining operation (d.o.)</th>
<th>Operations in element set</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mirror plane</td>
<td>Plane A</td>
<td>Reflection in A</td>
<td>D.o. and its coplanar equivalents*</td>
</tr>
<tr>
<td>Glide plane</td>
<td>Plane A</td>
<td>Glide reflection in A; 2ν (not ν) a lattice translation</td>
<td>D.o. and its coplanar equivalents*</td>
</tr>
<tr>
<td>Rotation axis</td>
<td>Line b</td>
<td>Rotation around b, angle 2π/n, n = 2, 3, 4 or 6</td>
<td>1st, …, (n – 1)th powers of d.o. and their coaxial equivalents†</td>
</tr>
<tr>
<td>Screw axis</td>
<td>Line b</td>
<td>Screw rotation around b, angle 2π/n, u = j/n times shortest lattice translation along b, right-hand screw, n = 2, 3, 4 or 6, j = 1, …, (n – 1)</td>
<td>1st, …, (n – 1)th powers of d.o. and their coaxial equivalents†</td>
</tr>
<tr>
<td>Rotoinversion axis</td>
<td>Line b and point P on b</td>
<td>Rotoinversion: rotation around b, angle 2π/n, and inversion through P, n = 3, 4 or 6</td>
<td>D.o. and its inverse</td>
</tr>
<tr>
<td>Center</td>
<td>Point P</td>
<td>Inversion through P</td>
<td>D.o. only</td>
</tr>
</tbody>
</table>

Example: P4mm

Element set of (00z) line

Symmetry operations that share (0,0,z) as geometric element

\[
\begin{array}{|c|c|}
\hline
2 & -x,-y,z \\
4+ & -y,x,z \\
4- & y,-x,z \\
2(0,0,1) & -x,-y,z+1 \\
\ldots & \ldots \\
\hline
\end{array}
\]

All rotations and screw rotations with the same axis, the same angle and sense of rotation and the same screw vector (zero for rotation) up to a lattice translation vector.
Symmetry element diagram (left) and General position diagram (right) of the space group \( P2 \), No. 3 (unique axis \( b \), cell choice 1).
Diagrams of general position points

Example: la\overline{3}d (No. 230)

Polyhedron centre at 0, 0, 0

Polyhedron centre at $\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$
Example: $\text{la3d}$ (No. 230)

Polyhedron centre at $0, 0, 0$

Polyhedra (twisted trigonal antiprism) centres at $(0,0,0)$ and its equivalent points, site symmetry $\cdot-3$.

Polyhedron centre at $\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$

Polyhedra (twisted trigonal antiprism) centres at $(1/8,1/8,1/8)$ and its equivalent points, site symmetry $\cdot32$.

General-position diagrams in perspective projection
ORIGINS AND ASYMMETRIC UNITS
Space group \textit{Cmm2} (No. 35): left-hand page ITA

\textbf{Origin statement}

The site symmetry of the origin is stated, if different from the identity. A further symbol indicates all symmetry elements (including glide planes and screw axes) that pass through the origin, if any.

\textbf{Space groups with two origins}

For each of the two origins the location relative to the other origin is also given.
Example: Different origins for $Pnnn$

$Pnnn$ \hspace{1cm} D_{2h}^2 \hspace{1cm} mmm \hspace{1cm} \text{Orthorhombic}

No. 48 

$P 2/n 2/n 2/n$

ORIGIN CHOICE 1

ORIGIN at $222$, at $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ from $\bar{I}$

ORIGIN CHOICE 2

ORIGIN at $\bar{I}$ at $nnn$, at $-\frac{1}{4}, -\frac{1}{4}, -\frac{1}{4}$ from $222$
An asymmetric unit of a space group is a (simply connected) smallest closed part of space from which, by application of all symmetry operations of the space group, the whole of space is filled.
Example: Asymmetric units for the space group P121

Number of vertices: 8
0, 1, 1/2
1, 1, 0
1, 0, 0
0, 0, 1/2
1, 0, 1/2
0, 0, 0
0, 1, 0
1, 1, 1/2

Number of facets: 6
x>=0
x<1
y>=0
y<1
z>=0 [x<=1/2]
z<=1/2 [x<=1/2]

[Guide to notation]

=output cctbx: Ralf Grosse-Kustelve)
GENERAL
AND
SPECIAL WYCKOFF
POSITIONS
SITE-SYMMETRY
A group action of a group $G$ on a set $\Omega = \{\omega \mid \omega \in \Omega\}$ assigns to each pair $(g, \omega)$ an object $\omega' = g(\omega)$ of $\Omega$ such that the following hold:

(i) applying two group elements $g$ and $g'$ consecutively has the same effect as applying the product $g'g$, i.e. $g'(g(\omega)) = (g'g)(\omega)$

(ii) applying the identity element $e$ of $G$ has no effect on $\omega$, i.e. $e(\omega) = \omega$ for all $\omega$ in $\Omega$.

The set $\omega^G := \{g(\omega) \mid g \in G\}$ of all objects in the orbit of $\omega$ is called the orbit of $\omega$ under $G$.

The set $S_G(\omega) := \{g \in G \mid g(\omega) = \omega\}$ of group elements that do not move the object $\omega$ is a subgroup of $G$ called the stabilizer of $\omega$ in $G$.

Via this equivalence relation, the action of $G$ partitions the objects in $\Omega$ into equivalence classes.
General and special Wyckoff positions

**General position** $X_0$

$S=\{(1,o)\} \cong 1$

Multiplicity: $|P|$

**Special position** $X_0$

$S>1=\{(1,o),\ldots,\}$

Multiplicity: $|P|/|S_0|$

**Site-symmetry group** $S_0=\{(W,w)\}$ of a point $X_0$

$(W,w)X_0 = X_0$

**Orbit of a point** $X_0$

under $G$: $G(X_0)=\{(W,w)X_0, (W,w) \in G\}$

Multiplicity

Site-symmetry group $S_0=\{(W,w)\}$ of a point $X_0$

$(W,w)X_0 = X_0$

### Multiplicity: $|P|/|S_0|$
(i) coordinate triplets of an image point $\tilde{X}$ of the original point $X = \begin{bmatrix} x \\ y \\ z \end{bmatrix}$ under $(W,w)$ of $G$

-presentation of infinite image points $\tilde{X}$ under the action of $(W,w)$ of $G$: $0 \leq x_i < 1$

(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**

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

\[
\begin{array}{cccccc}
(I,0)X & (W_2,w_2)X & \ldots & (W_m,w_m)X & \ldots & (W_i,w_i)X \\
(I,t_1)X & (W_2,w_2+t_1)X & \ldots & (W_m,w_m+t_1)X & \ldots & (W_i,w_i+t_1)X \\
(I,t_2)X & (W_2,w_2+t_2)X & \ldots & (W_m,w_m+t_2)X & \ldots & (W_i,w_i+t_2)X \\
& \ldots & \ldots & \ldots & \ldots & \ldots \\
(I,t_j)X & (W_2,w_2+t_j)X & \ldots & (W_m,w_m+t_j)X & \ldots & (W_i,w_i+t_j)X \\
& \ldots & \ldots & \ldots & \ldots & \ldots \\
\end{array}
\]

-presentation of infinite image points $\tilde{X}$ of $X$ under the action of $(W,w)$ of $G$: $0 \leq x_i < 1$
Example: Calculation of the Site-symmetry groups

Group P-1

\[ S = \{(W, w), (W, w)X_0 = X_0\} \]

\[
\begin{pmatrix}
-1 & 0 & 0 \\
-1 & 0 & 0 \\
-1 & 0 & 0 \\
\end{pmatrix}
\begin{pmatrix}
0 \\
0 \\
0 \\
\end{pmatrix} =
\begin{pmatrix}
0 \\
0 \\
0 \\
\end{pmatrix}
\]

\[ S_f = \{(1, 0), (-1, 000)X_f = X_f\} \]

\[ S_f \simeq \{1, -1\} \text{ isomorphic} \]
QUIZ: Calculation of the Site-symmetry groups

Group P-1

Determine the site symmetry group of the point $X_0 = \begin{pmatrix} 0 \\ 1/2 \\ 1/2 \end{pmatrix}$

$S=\{(W,w), (W,w)X_0 = X_0\}$
**QUICK QUIZ**

**Space group P4mm**

**Site symmetry groups of special Wyckoff positions**

<table>
<thead>
<tr>
<th>Symmetry Operations</th>
<th>Wyckoff Positions</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 g 1</td>
<td>8 (1) x, y, z</td>
</tr>
<tr>
<td></td>
<td>(2) ( \bar{x}, \bar{y}, z )</td>
</tr>
<tr>
<td></td>
<td>(3) ( \bar{y}, x, z )</td>
</tr>
<tr>
<td></td>
<td>(4) ( y, \bar{x}, z )</td>
</tr>
<tr>
<td></td>
<td>(5) x, ( \bar{y}, z )</td>
</tr>
<tr>
<td></td>
<td>(6) ( \bar{x}, y, z )</td>
</tr>
<tr>
<td></td>
<td>(7) ( \bar{y}, \bar{x}, z )</td>
</tr>
<tr>
<td></td>
<td>(8) ( y, x, z )</td>
</tr>
</tbody>
</table>

**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. \( m \ x,x,z \)

**Diagram:**

- 8 g 1
- 4 f . m.
- 4 e . m.
- 4 d . . m
- 2 c 2 m m.
- 1 b 4 m m
- 1 a 4 m m

- \( 1/2,0,z \)
COORDINATE TRANSFORMATIONS IN CRYSTALLOGRAPHY
Co-ordinate transformation

3-dimensional space

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

\[ \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix} \]

\[ (a', b', c') = (a, b, c)P \]

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

(ii) origin shift by a shift vector \( p(p_1, p_2, p_3) \):

\[ O' = O + p \]

the origin \( O' \) has coordinates \( (p_1, p_2, p_3) \) in the old coordinate system.
Write “new in terms of old” as column vectors.
Linear parts as before.
Transformation matrix-column pair \((P,p)\)

\[
(P,p) = \begin{pmatrix}
  1/2 & 1/2 & 0 & 1/2 \\
  -1/2 & 1/2 & 0 & 1/4 \\
  0 & 0 & 1 & 0
\end{pmatrix}
\]

\[
(P,p)^{-1} = \begin{pmatrix}
  1 & -1 & 0 & -1/4 \\
  1 & 1 & 0 & -3/4 \\
  0 & 0 & 1 & 0
\end{pmatrix}
\]

\[
a' = \frac{1}{2}a - \frac{1}{2}b
\]
\[
b' = \frac{1}{2}a + \frac{1}{2}b
\]
\[
c' = c
\]

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

\[
a = a' + b'
\]
\[
b = -a' + b'
\]
\[
c = c'
\]
\[
O = O' + \begin{pmatrix}
  -1/4 \\
  -3/4 \\
  0
\end{pmatrix}
\]
Short-hand notation for the description of transformation matrices

Transformation matrix:

\[(a,b,c), \text{ origin } O\]

\[(P,p)=\begin{pmatrix} P_{11} & P_{12} & P_{13} & p_1 \\ P_{21} & P_{22} & P_{23} & p_2 \\ P_{31} & P_{32} & P_{33} & p_3 \end{pmatrix}\]

\[(a',b',c'), \text{ origin } O'\]

- written by columns
- coefficients 0, +1, -1
- different columns in one line
- origin shift

Example:

\[
\begin{pmatrix}
1 & -1 \\
1 & 1 \\
\end{pmatrix}
\begin{pmatrix}
-1/4 \\
-3/4 \\
0 \\
\end{pmatrix}
\rightarrow \{a+b, -a+b, c; -1/4, -3/4, 0\}
Transformation of the coordinates of a point $X(x,y,z)$:

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

special cases

- origin shift ($P=I$): $x' = x - p$
- change of basis ($p=0$): $x' = P^{-1}x$

EXAMPLE

$X' = (P,p)^{-1}X = \begin{pmatrix} 1 & -1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1/4 \\ 1/4 \\ 0 \end{pmatrix} = \begin{pmatrix} 1/4 \\ 1/4 \\ 0 \end{pmatrix}$
Determine the coordinates $X'$ of a point $X = P, p$ with respect to the new basis $(a', b', c') = (a, b, c)P$, with $P = c, a, b$.

Hint

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

QUICK QUIZ

| 0.70 |
| 0.31 |
| 0.95 |
Covariant and contravariant crystallographic quantities

**direct or crystal basis**

\[(a', b', c') = (a, b, c)^P = (a, b, c) \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix}^{-1} \]

**reciprocal or dual basis**

\[
\begin{pmatrix} a^* \\ b^* \\ c^* \end{pmatrix} = P^{-1} \begin{pmatrix} a^* \\ b^* \\ c^* \end{pmatrix} = \begin{pmatrix} a^* \\ b^* \\ c^* \end{pmatrix} \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix}^{-1} \]

**covariant to crystal basis: Miller indices**

\[(h', k', l') = (h, k, l)^P\]

**contravariant to crystal basis: indices of a direction \([u]\)**

\[
\begin{pmatrix} u' \\ v' \\ w' \end{pmatrix} = \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix}^{-1} \begin{pmatrix} u \\ v \\ w \end{pmatrix}
\]
Transformation of symmetry operations \((W,w)\)

i. \(\tilde{x}' = (W',w')x'\).

ii. \(\tilde{x}' = (P,p)^{-1} \tilde{x} = (P,p)^{-1}(W,w)x = (P,p)^{-1}(W,w)(P,p)x'\).

\[(W',w') = (P,p)^{-1}(W,w)(P,p)\]
The following matrix-column pairs $(W,w)$ are referred with respect to a basis $(a,b,c)$:

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

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

**Hint**

$$(W',w') = (P,p)^{-1}(W,w)(P,p)$$
Problem: SYMMETRY DATA
ITA SETTINGS

530 ITA settings of orthorhombic and monoclinic groups

**Monoclinic descriptions**

<table>
<thead>
<tr>
<th></th>
<th>Transf.</th>
<th>abc</th>
<th>cba</th>
<th>abc</th>
<th>ba̅c</th>
<th>abc</th>
<th>a̅cb</th>
<th>Monoclinic axis b</th>
<th>Monoclinic axis c</th>
<th>Monoclinic axis a</th>
</tr>
</thead>
<tbody>
<tr>
<td>HM</td>
<td>C2/c</td>
<td>C12/c1</td>
<td>A12/a1</td>
<td>A112/a</td>
<td>B112/b</td>
<td>B2/b11</td>
<td>C2/c11</td>
<td>Cell type 1</td>
<td>Cell type 2</td>
<td>Cell type 3</td>
</tr>
<tr>
<td></td>
<td>A12/n1</td>
<td>C12/n1</td>
<td>B112/n</td>
<td>A112/n</td>
<td>C2/n11</td>
<td>B2/n11</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>I12/a1</td>
<td>I12/c1</td>
<td>I112/b</td>
<td>I112/a</td>
<td>I2/c11</td>
<td>I2/b11</td>
<td></td>
<td></td>
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</tr>
</tbody>
</table>

**Orthorhombic descriptions**

<table>
<thead>
<tr>
<th>No.</th>
<th>HM</th>
<th>abc</th>
<th>ba̅c</th>
<th>cab</th>
<th>ċba</th>
<th>bca</th>
<th>a̅cb</th>
</tr>
</thead>
<tbody>
<tr>
<td>33</td>
<td>Pna21</td>
<td>Pna21</td>
<td>Pbn21</td>
<td>P21nb</td>
<td>P21cn</td>
<td>Pc21n</td>
<td>Pn21a</td>
</tr>
</tbody>
</table>
METRIC TENSOR
3D-unit cell and lattice parameters

lattice basis: \{a, b, c\}

unit cell: the parallelepiped defined by the basis vectors

primitive P and centred unit cells: A, B, C, F, I, R

number of lattice points per unit cell

Lattice parameters:

- lengths of the unit translations:
  - \(a\)
  - \(b\)
  - \(c\)

- angles between them:
  - \(\alpha = (\hat{b}, \hat{c})\)
  - \(\beta = (\hat{c}, \hat{a})\)
  - \(\gamma = (\hat{a}, \hat{b})\)
Lattice parameters (3D)

An alternative way to define the metric properties of a lattice \( L \)

Given a lattice \( L \) of \( \mathbb{V}^3 \) with a lattice basis: \( \{a_1, a_2, a_3\} \)

**Definition (D 1.5.3)** The quantities

\[
\begin{align*}
a_1 &= |a_1| = +\sqrt{(a_1 \cdot a_1)}, \\
a_2 &= |a_2| = +\sqrt{(a_2 \cdot a_2)}, \\
a_3 &= |a_3| = +\sqrt{(a_3 \cdot a_3)}, \\
\alpha_1 &= \arccos(|a_2|^{-1}|a_3|^{-1}(a_2, a_3)), \\
\alpha_2 &= \arccos(|a_3|^{-1}|a_1|^{-1}(a_3, a_1)), \\
\text{and } \alpha_3 &= \arccos(|a_1|^{-1}|a_2|^{-1}(a_1, a_2))
\end{align*}
\]

are called the lattice parameters of the lattice.

Remark: the lengths of basis vectors are measured in

\( nm \) (1 nm = 10^{-9} m) \quad \text{Å} \) (1 Å = 10^{-10} m) \quad \text{pm} \) (1 pm = 10^{-12} m)

**Metric tensor \( G \) in terms of lattice parameters**

\[
G = \begin{pmatrix} a \cdot a & a \cdot b & a \cdot c \\
b \cdot a & b \cdot b & b \cdot c \\
c \cdot a & c \cdot b & c \cdot c \end{pmatrix}, \quad G = \begin{pmatrix} a^2 & ab \cos \gamma & ac \cos \beta \\
ab \cos \gamma & b^2 & bc \cos \alpha \\
ac \cos \beta & bc \cos \alpha & c^2 \end{pmatrix}
\]
<table>
<thead>
<tr>
<th>Crystal family</th>
<th>Symbol*</th>
<th>Crystal system</th>
<th>Crystallographic point groups†</th>
<th>No. of space groups</th>
<th>Conventional coordinate system</th>
<th>Parameters to be determined</th>
<th>Bravais lattices*</th>
</tr>
</thead>
<tbody>
<tr>
<td>Triclinic (anorthic)</td>
<td>$a$</td>
<td>Triclinic</td>
<td>1, [1]</td>
<td>2</td>
<td>None</td>
<td>$a, b, c,$ $\alpha, \beta, \gamma$</td>
<td>$aP$</td>
</tr>
<tr>
<td>Monoclinic</td>
<td>$m$</td>
<td>Monoclinic</td>
<td>2, $m$, [2/$m$]</td>
<td>13</td>
<td>$b$-unique setting $\alpha = \gamma = 90^\circ$</td>
<td>$a, b, c$</td>
<td>$\beta$</td>
</tr>
<tr>
<td>Orthorhombic</td>
<td>$o$</td>
<td>Orthorhombic</td>
<td>222, mm2, [mmm]</td>
<td>59</td>
<td>$\alpha = \beta = \gamma = 90^\circ$</td>
<td>$a, b, c$</td>
<td></td>
</tr>
<tr>
<td>Tetragonal</td>
<td>$t$</td>
<td>Tetragonal</td>
<td>4, 4, [4/$m$] 422, 4mm, 42m, [4/mm]</td>
<td>68</td>
<td>$a = b$ $\alpha = \beta = \gamma = 90^\circ$</td>
<td>$a, c$</td>
<td></td>
</tr>
<tr>
<td>Hexagonal</td>
<td>$h$</td>
<td>Trigonal</td>
<td>3, [3] 32, 3$m$, [3$m$]</td>
<td>18</td>
<td>$a = b$ $\alpha = \beta = 90^\circ, \gamma = 120^\circ$</td>
<td>$a, c$</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Hexagonal</td>
<td>$h$</td>
<td>Hexagonal</td>
<td>6, 6, [6/$m$] 622, 6mm, 62m, [6/mm]</td>
<td>27</td>
<td>$a = b$ $\alpha = \beta = 90^\circ, \gamma = 120^\circ$ (hexagonal axes, triple obverse cell)</td>
<td>$a, c$</td>
<td></td>
</tr>
<tr>
<td>Cubic</td>
<td>$c$</td>
<td>Cubic</td>
<td>23, [m3] 432, 43m, [m3m]</td>
<td>36</td>
<td>$a = b = c$ $\alpha = \beta = \gamma = 90^\circ$</td>
<td>$a$</td>
<td></td>
</tr>
</tbody>
</table>
Crystallographic calculations: Volume of the unit cell

Volume of the unit cell:

The volume $V$ of the unit cell of a crystal structure, i.e. the body containing all points with coordinates $0 \leq x_1, x_2, x_3 < 1$, can be calculated by the formula

$$\det(G) = V^2.$$  

Scalar product of arbitrary vectors:

$$(\mathbf{r}, \mathbf{t}) = \mathbf{r}^T \mathbf{G} \mathbf{t}$$

Transformation properties of $\mathbf{G}$ under basis transformation

$$\{\mathbf{a'}_1, \mathbf{a'}_2, \mathbf{a'}_3\} = \{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3\} P$$

$$\mathbf{G'} = P^T \mathbf{G} P$$
Calculate the coefficients of the metric tensor for the body-centred cubic lattice:

(i) for the conventional basis \((a_P, b_P, c_P)\);
(ii) for the primitive basis:
\[
\begin{align*}
a_I &= \frac{1}{2}(-a_P + b_P + c_P), \\
b_I &= \frac{1}{2}(a_P - b_P + c_P), \\
c_I &= \frac{1}{2}(a_P + b_P - c_P)
\end{align*}
\]
(iii) determine the lattice parameters of the primitive cell if \(a_P = 4 \text{ Å}\)

**Hint**

metric tensor transformation \(G' = P^t G P\)