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Commission on Mathematical and Theoretical Crystallography

International School on Fundamental Crystallography
Sixth MaThCryst school in Latin America
Workshop on the Applications of Group Theory in the Study of Phase Transitions

Bogotá, Colombia, 26 November - 1st December 2018
SPACE GROUPS

International Tables for Crystallography, Volume A: Space-group Symmetry

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

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;
1. \( C_{mm2} \)
2. No. 35
3. \( C_{2v} \)
4. \( mm2 \)
5. \text{Ortorhombic}
6. Patterson symmetry \( C_{mmm} \)

4. Origin on \( mm2 \)

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

6. Symmetry operations

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

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

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

Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site symmetry</th>
<th>Coordinates</th>
<th>Reflection conditions</th>
</tr>
</thead>
</table>
| 8 \( f \) 1 \( (1) \ x, y, z \) \( (2) \bar{x}, \bar{y}, z \) \( (3) x, \bar{y}, z \) \( (4) \bar{x}, y, z \) | \( (0,0,0)^+ \) \( \frac{1}{2}, \frac{1}{2}, 0^+ \) | General: \( hkl: h + k = 2n \) \( 0kl: k = 2n \) \( h0l: h = 2n \) \( hk0: h + k = 2n \) \( h00: h = 2n \) \( 0k0: k = 2n \) Special: as above, plus no extra conditions no extra conditions no extra conditions \( hkl: h = 2n \) no extra conditions no extra conditions

Symmetry of special projections

Along [001] 2mm \( a' = a \) \( b' = b \) Origin at 0,0,z
Along [100] p1m1 \( a' = \frac{1}{2}b \) \( b' = c \) Origin at x,0,0
Along [010] p11m \( a' = c \) \( b' = \frac{1}{2}a \) Origin at 0,y,0
Primitive and centred lattice basis in 2D

\{a_1, a_2\}: two translation vectors, linearly independent, form a lattice basis

**Primitive basis:** If all lattice vectors are expressed as integer linear combinations of the basis vectors

**Centred basis:** If some lattice vectors are expressed as linear combinations of the basis vectors with rational, non-integer coefficients

Conventional centred basis (2D): c

Number of lattice points per primitive and centred cells

Fig. 1.5.2 c-centred lattice (net) in the plane with conventional \( \mathbf{a}, \mathbf{b} \) and primitive \( \mathbf{a}', \mathbf{b}' \) bases.
## Crystal families, crystal systems, conventional coordinate system and Bravais lattices in 2D

<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>Bravais lattices*</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Restrictions on cell parameters</td>
<td>Parameters to be determined</td>
</tr>
<tr>
<td>One dimension</td>
<td></td>
<td></td>
<td></td>
<td></td>
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<td></td>
<td></td>
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<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Two dimensions</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Oblique (monoclinic)</td>
<td>m</td>
<td>Oblique</td>
<td>1, [2]</td>
<td>2</td>
<td>None</td>
<td>a, b</td>
</tr>
<tr>
<td>Rectangular (orthorhombic)</td>
<td>o</td>
<td>Rectangular</td>
<td>m, [2mm]</td>
<td>7</td>
<td>$\gamma = 90^\circ$</td>
<td>a, b</td>
</tr>
<tr>
<td>Square (tetragonal)</td>
<td>t</td>
<td>Square</td>
<td>[4], [4mm]</td>
<td>3</td>
<td>$a = b$ $\gamma = 90^\circ$</td>
<td>a</td>
</tr>
<tr>
<td>Hexagonal</td>
<td>h</td>
<td>Hexagonal</td>
<td>3, 6, 3m, [6mm]</td>
<td>5</td>
<td>$a = b$ $\gamma = 120^\circ$</td>
<td>a</td>
</tr>
</tbody>
</table>
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:
\[ \alpha = (\hat{b}, \hat{c}) \]
\[ \beta = (\hat{c}, \hat{a}) \]
\[ \gamma = (\hat{a}, \hat{b}) \]
### Crystal families, crystal systems, lattice systems and Bravais lattices in 3D

<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, α, β, γ</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</td>
<td>a, b, c, β</td>
<td>mP mS (mC, mA, mI)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>α = γ = 90°</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>c-unique setting</td>
<td>a, b, c, γ</td>
<td>mP mS (mA, mB, mI)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>α = β = 90°</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Orthorhombic</td>
<td>o</td>
<td>Orthorhombic</td>
<td>222, mm2, [mmm]</td>
<td>59</td>
<td>α = β = γ = 90°</td>
<td>a, b, c</td>
<td>oP oS (oC, oA, oB)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>oI oF</td>
</tr>
<tr>
<td>Tetragonal</td>
<td>t</td>
<td>Tetragonal</td>
<td>4, 4, [4/m] 422, 4mm, 42m, 4/mmm</td>
<td>68</td>
<td>a = b</td>
<td>a, c</td>
<td>tP tI</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>α = β = γ = 90°</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Hexagonal</td>
<td>h</td>
<td>Trigonal</td>
<td>3, [3] 32, 3m, [3m]</td>
<td>18</td>
<td>a = b</td>
<td>a, c</td>
<td>hP hR</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>α = β = 90°, γ = 120°</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>a = b = c</td>
<td>a, α</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>α = β = γ</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>(rhombohedral axes, primitive cell)</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>a = b</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>α = β = 90°, γ = 120°</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>(hexagonal axes, triple obverse cell)</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/mmm</td>
<td>27</td>
<td>a = b</td>
<td>a, c</td>
<td>hP</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>α = β = 90°, γ = 120°</td>
<td></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</td>
<td>a</td>
<td>cP cI cF</td>
</tr>
</tbody>
</table>
HEADLINE BLOCK
<table>
<thead>
<tr>
<th>Number of space group</th>
<th>Short Hermann-Mauguin symbol</th>
<th>Schoenflies symbol</th>
<th>Full Hermann-Mauguin symbol</th>
<th>Crystal class (point group)</th>
<th>Crystal system</th>
</tr>
</thead>
<tbody>
<tr>
<td>No. 35</td>
<td><em>Cmm2</em></td>
<td><em>C</em>$_{2v}$</td>
<td><em>Cmm2</em></td>
<td><em>mm2</em></td>
<td>Orthorhombic</td>
</tr>
</tbody>
</table>

Patterson symmetry *Cmmm*
HERMANN-MAUGUIN
SYMBOLISM 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>P</strong></td>
<td><strong>I</strong></td>
</tr>
<tr>
<td><strong>F</strong></td>
<td><strong>C</strong></td>
</tr>
<tr>
<td><strong>R</strong></td>
<td></td>
</tr>
<tr>
<td><strong>Triclinic</strong></td>
<td><img src="image" alt="Triclinic" /></td>
</tr>
<tr>
<td><strong>Monoclinic</strong></td>
<td><img src="image" alt="Monoclinic" /></td>
</tr>
<tr>
<td><strong>Orthorhombic</strong></td>
<td><img src="image" alt="Orthorhombic" /></td>
</tr>
<tr>
<td><strong>Tetragonal</strong></td>
<td><img src="image" alt="Tetragonal" /></td>
</tr>
<tr>
<td><strong>Hexagonal</strong></td>
<td><img src="image" alt="Hexagonal" /></td>
</tr>
<tr>
<td><strong>Cubic</strong></td>
<td><img src="image" alt="Cubic" /></td>
</tr>
</tbody>
</table>
Symmetry directions

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></td>
<td>[001] (‘unique axis c’)</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>
</tbody>
</table>
Example:

Orthorhombic

- Bravais lattice
- Screw axis \( 2_1 \parallel \vec{a} \)
- Glide plane \( n \perp \vec{a} \)
- Screw axis \( 2_1 \parallel \vec{b} \)
- Mirror plane \( m \perp \vec{b} \)

Secondary direction

- \( P2_1/n2_1/m2_1/a \)

Tertiary direction

- Screw axis \( 2_1 \parallel \vec{c} \)
- Glide plane \( a \perp \vec{c} \)
PRESENTATION OF SPACE-GROUP SYMMETRY OPERATIONS

IN INTERNATIONAL TABLES FOR CRYSTALLOGRAPHY, VOL. A
Crystallographic symmetry operations

**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

<table>
<thead>
<tr>
<th>Type</th>
<th>Description</th>
<th>Centre Fixed</th>
<th>Axis/Mirror Plane</th>
</tr>
</thead>
<tbody>
<tr>
<td>roto-inversion</td>
<td>centre of roto-inversion fixed</td>
<td>centre of roto-inversion axis</td>
<td></td>
</tr>
<tr>
<td>inversion</td>
<td>centre of inversion fixed</td>
<td></td>
<td></td>
</tr>
<tr>
<td>reflection</td>
<td>plane fixed</td>
<td></td>
<td>reflection/mirror plane</td>
</tr>
<tr>
<td>glide reflection</td>
<td>no fixed point</td>
<td></td>
<td>glide plane</td>
</tr>
</tbody>
</table>

Glide reflection do not preserve handedness.
\[
\begin{pmatrix}
\tilde x \\
\tilde y \\
\tilde z
\end{pmatrix}
= \begin{pmatrix}
W_{11} & W_{12} & W_{13} \\
W_{21} & W_{22} & W_{23} \\
W_{31} & W_{32} & W_{33}
\end{pmatrix}
\begin{pmatrix}
x \\
y \\
z
\end{pmatrix}
+ \begin{pmatrix}
w_1 \\
w_2 \\
w_3
\end{pmatrix}
\]

linear/matrix part

translation column part

\[
\tilde x = W x + w
\]

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

matrix-column pair

Seitz symbol
Space group $Cmm2$ (No. 35)

Diagram of symmetry elements

Diagram of general position points

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

General Position

Coordinates

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

8  $f$  1  

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

$(W, w) = (I, t_n)(W, w_0), 0 \leq w_{i0} < 1$
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: P12/m1

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

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

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

\[
\begin{array}{c}
\bar{1} \at \text{at} \\
n_1/2 \\
n_2/2 \\
n_3/2 \\
\end{array}
\]
Coset decomposition $\text{P12}_1/c1:T$

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

---

**(l,0)**  **(2,0 ½ ½)**  **(I,0)**  **(m,0 ½ ½)**

**(l,t₁)**  **(2,0 ½ ½ + t₁)**  **(I,t₁)**  **(m,0 ½ ½ + t₁)**
**(l,t₂)**  **(2,0 ½ ½ + t₂)**  **(I,t₂)**  **(m,0 ½ ½ + t₂)**
...  ...  ...  ...
**(l,tᵢ)**  **(2,0 ½ ½ + tᵢ)**  **(I,tᵢ)**  **(m,0 ½ ½ + tᵢ)**
...  ...  ...  ...

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

**2₁ screw axes**  
$(2,u ½ + v ½ + w)$

---

General position
Symmetry Operations Block

TYPE of the symmetry operation

SCREW/GLIDE component

ORIENTATION of the geometric element

LOCATION of the geometric element

GEOMETRIC INTERPRETATION OF THE MATRIX-
COLUMN PRESENTATION OF THE SYMMETRY OPERATIONS
Example: Cmm2

Diagram of symmetry elements

Diagram of general position points

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 (1/2,1/2,0) set
(1) t(1/2,1/2,0)
(2) 2 1/2,1/4,z
(3) a x,1/2,z
(4) b 1/4,y,z

Coordinates
(0,0,0) + (1/2,1/2,0) +

<table>
<thead>
<tr>
<th>8</th>
<th>f</th>
<th>1</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1)</td>
<td>x,y,z</td>
<td>(2)</td>
</tr>
</tbody>
</table>

TG  TG  TG  m_y  m_x
(l,0) (2,0) (m_y,0) (m_x,0)
(l,t_1) (2,t_1) (m_y,t_1) (m_x, t_1)
(l,t_2) (2,t_2) (m_y,t_2) (m_x, t_2)
...(l,t_j) (2,t_j) (m_y,t_j) (m_x, t_j)
Space group $P2_1/c$ (No. 14)

No. 14

$P12_1/c1$

$C_{2h}^5$

2/$m$

1

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

4 e 1

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) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{3}$

(3) $\bar{1}$ 0,0,0

(4) $c$ $x,\frac{1}{3},z$
<table>
<thead>
<tr>
<th>Table: Space-group symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>GENPOS</td>
</tr>
<tr>
<td>WYCKPOS</td>
</tr>
<tr>
<td>HKLCOND</td>
</tr>
<tr>
<td>MAXSUB</td>
</tr>
<tr>
<td>SERIES</td>
</tr>
<tr>
<td>WYCKSETS</td>
</tr>
<tr>
<td>NORMALIZER</td>
</tr>
<tr>
<td>KVEC</td>
</tr>
<tr>
<td>SYMMETRY OPERATIONS</td>
</tr>
<tr>
<td>IDENTIFY GROUP</td>
</tr>
</tbody>
</table>

- **New Article in Nature**

- **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 double point groups

- **Subperiodic Groups: Layer, Rod and Frieze Groups**
- **Structure Databases**
- **Raman and Hyper-Raman scattering**
- **Point-group symmetry**
- **Plane-group symmetry**
Problem: Matrix-column presentation
Geometrical interpretation

Generators and General Positions

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

Show:

Standard/Default Setting

Generators only
All General Positions

Non Conventional Setting
ITA Settings
**Example GENPOS: Space group \( P2_1/c \) (14)**

**Space-group symmetry operations**

**Short-hand notation**

\[
\begin{pmatrix}
W_{11} & W_{12} & W_{13} \\
W_{21} & W_{22} & W_{23} \\
W_{31} & W_{32} & W_{33}
\end{pmatrix}
\begin{pmatrix}
w_1 \\
w_2 \\
w_3
\end{pmatrix}
\]

**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>
</table>
| 1   | x,y,z        | \[
\begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0
\end{pmatrix}
\] | 1                |
| 2   | -x,y+1/2,-z+1/2 | \[
\begin{pmatrix}
-1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & -1 & 1/2
\end{pmatrix}
\] | 2 0,1/2,0 0,y,1/4 |
| 3   | -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+1/2,z+1/2 | \[
\begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 \\
0 & 0 & 1 & 1/2
\end{pmatrix}
\] | c x,1/4,z         |

**General positions**

\[
\begin{align*}
4 & \quad e & \quad 1 & \quad (1) \ x,y,z \\
   & \quad & \quad & \quad (2) \ x,y+\frac{1}{2},z+\frac{1}{2} \\
   & \quad & \quad & \quad (3) \ x,\bar{y},\bar{z} \\
   & \quad & \quad & \quad (4) \ x,\bar{y}+\frac{1}{2},z+\frac{1}{2}
\end{align*}
\]

**Symmetry operations**

\[
\begin{align*}
(1) & \quad 1 & \quad (2) \ 2(0,\frac{1}{2},0) \ 0,y,\frac{1}{4} \\
(3) & \quad \bar{I} \ 0,0,0 & \quad (4) \ c \ x,\frac{1}{4},z
\end{align*}
\]
Seitz symbols \{ R | t \}

- 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.

<table>
<thead>
<tr>
<th>Seitz symbol</th>
<th>Symmetry Operation</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \bar{1} )</td>
<td>identity and inversion</td>
</tr>
<tr>
<td>( m )</td>
<td>reflections</td>
</tr>
<tr>
<td>2, 3, 4, 6</td>
<td>rotations</td>
</tr>
<tr>
<td>( \bar{3}, \bar{4}, \bar{6} )</td>
<td>rotoinversions</td>
</tr>
</tbody>
</table>

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

### EXAMPLE

<table>
<thead>
<tr>
<th>ITA description</th>
<th>Seitz symbol</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>No.</strong></td>
<td><strong>coord. triplet</strong></td>
</tr>
<tr>
<td>1)</td>
<td>(x, y, z)</td>
</tr>
<tr>
<td>2)</td>
<td>(\bar{y}, x - y, z)</td>
</tr>
<tr>
<td>3)</td>
<td>(x + y, \bar{x}, z)</td>
</tr>
<tr>
<td>4)</td>
<td>(\bar{x}, \bar{y}, z)</td>
</tr>
<tr>
<td>5)</td>
<td>(y, \bar{x} + y, z)</td>
</tr>
<tr>
<td>6)</td>
<td>(x - y, x, z)</td>
</tr>
<tr>
<td>7)</td>
<td>(y, x, \bar{z})</td>
</tr>
<tr>
<td>8)</td>
<td>(x - y, \bar{y}, \bar{z})</td>
</tr>
<tr>
<td>9)</td>
<td>(\bar{x}, \bar{x} + y, \bar{z})</td>
</tr>
<tr>
<td>10)</td>
<td>(\bar{y}, x, \bar{z})</td>
</tr>
<tr>
<td>11)</td>
<td>(\bar{x} + y, y, \bar{z})</td>
</tr>
<tr>
<td>12)</td>
<td>(x, x - y, \bar{z})</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>ITA description</th>
<th>Seitz symbol</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>No.</strong></td>
<td><strong>coord. triplet</strong></td>
</tr>
<tr>
<td>13)</td>
<td>(\bar{x}, \bar{y}, \bar{z})</td>
</tr>
<tr>
<td>14)</td>
<td>(y, \bar{x} + y, \bar{z})</td>
</tr>
<tr>
<td>15)</td>
<td>(x - y, x, \bar{z})</td>
</tr>
<tr>
<td>16)</td>
<td>(x, y, \bar{z})</td>
</tr>
<tr>
<td>17)</td>
<td>(\bar{y}, x - y, \bar{z})</td>
</tr>
<tr>
<td>18)</td>
<td>(\bar{x} + y, \bar{x}, \bar{z})</td>
</tr>
<tr>
<td>19)</td>
<td>(\bar{y}, x, \bar{z})</td>
</tr>
<tr>
<td>20)</td>
<td>(\bar{x} + y, y, z)</td>
</tr>
<tr>
<td>21)</td>
<td>(x, x - y, z)</td>
</tr>
<tr>
<td>22)</td>
<td>(y, x, z)</td>
</tr>
<tr>
<td>23)</td>
<td>(x - y, \bar{y}, z)</td>
</tr>
<tr>
<td>24)</td>
<td>(\bar{x}, \bar{x} + y, z)</td>
</tr>
</tbody>
</table>

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

**Generators selected**

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

**Positions**

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

**Symmetry operations**

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

**Seitz symbols**

(1) \{1l0\}  (2) \{2010l01/21/2\}  (3) \{1l0\}  (4) \{m010l01/21/2\}
EXERCISES

Problem 2.16 (b)

1. Characterize geometrically the matrix-column pairs listed under General position of the space group \textit{P4mm} in ITA.

2. Consider the diagram of the symmetry elements of \textit{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.
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</td>
<td>② (⊥ paper)</td>
<td>none</td>
<td>4₂</td>
<td>Screw tetrads</td>
<td>◆</td>
<td>2c/4</td>
</tr>
<tr>
<td>2</td>
<td>or twofold</td>
<td></td>
<td></td>
<td>4₃</td>
<td></td>
<td>◆</td>
<td>3c/4</td>
</tr>
<tr>
<td>2₁</td>
<td>rotation axis</td>
<td>(∥ paper)</td>
<td></td>
<td>4</td>
<td>Inverse tetrad</td>
<td>◆</td>
<td>none</td>
</tr>
<tr>
<td>2₁</td>
<td>Screw diad</td>
<td>② (⊥ paper)</td>
<td>c/2</td>
<td>6</td>
<td>Rotation hexad</td>
<td>◆</td>
<td>none</td>
</tr>
<tr>
<td>2₁</td>
<td>or twofold</td>
<td>(∥ paper)</td>
<td>a/2 or b/2</td>
<td>6₁</td>
<td></td>
<td>◆</td>
<td>c/6</td>
</tr>
<tr>
<td>3</td>
<td>Rotation triad</td>
<td>② paper</td>
<td>none</td>
<td>6₂</td>
<td></td>
<td>◆</td>
<td>2c/6</td>
</tr>
<tr>
<td>3</td>
<td></td>
<td>△</td>
<td></td>
<td>6₃</td>
<td>Screw hexads</td>
<td>◆</td>
<td>3c/6</td>
</tr>
<tr>
<td>3</td>
<td></td>
<td>△</td>
<td>c/3</td>
<td>6₄</td>
<td></td>
<td>◆</td>
<td>4c/6</td>
</tr>
<tr>
<td>3</td>
<td></td>
<td>△</td>
<td>2c/3</td>
<td>6₅</td>
<td></td>
<td>◆</td>
<td>5c/6</td>
</tr>
<tr>
<td>3</td>
<td>Inverse triad</td>
<td>② paper</td>
<td>none</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>diagonal glide plane (net)</td>
<td></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>
Space group *Cmm2* (No. 35)

**Symmetry operations**

For \((0,0,0)^+\) set

1. \(1\)
   - \((0,0,0,0)^+\)
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. \(b\) \(\frac{1}{4},y,z\)

**General Position**

Coordinates

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

- \(8\) \(f\) \(1\)
- \((1)\) \(x,y,z\)
- \((2)\) \(x,\frac{1}{2},z\)
- \((3)\) \(x,\frac{1}{2},z\)
- \((4)\) \(x,\frac{1}{2},z\)

How many general position points per unit cell are there?

Diagram of symmetry elements

Diagram of general position points
Space group *Cmm2* (No. 35)

**General Position**

Coordinates

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

<table>
<thead>
<tr>
<th>(x, y, z)</th>
<th>(\bar{x}, \bar{y}, z)</th>
<th>(x, \bar{y}, z)</th>
<th>(\bar{x}, y, z)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(x+1/2, -y+1/2, z)</td>
<td>(-x+1/2, y+1/2, z)</td>
<td>(-x+1/2, y+1/2, z)</td>
<td>(x+1/2, -y+1/2, z)</td>
</tr>
</tbody>
</table>

**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. \(b \quad \frac{1}{4}, y, z\)

- Glide plane, \(t = 1/2a\) at \(y = 1/4, \perp b\)
- Glide plane, \(t = 1/2b\) at \(x = 1/4, \perp a\)
Example: P4mm

Diagram of symmetry elements

Diagram of general position points

(1) 1
(5) m x,0,z
(2) 2 0,0,z
(6) m 0,y,z
(3) 4+ 0,0,z
(7) m x,\bar{x},z
(4) 4- 0,0,z
(8) m x,x,z

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

\{ Symmetry operations that share the same geometric element \}

\{ Fixed points \}

\{ Geometric element \}

\{ Symmetry element \}

\{ Element set \}

\{ 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. \}

\{ All glide reflections with the same reflection plane, with glide of d.o. (taken to be zero for reflections) by a lattice translation vector. \}

Examples

**Rotation axis**

\{ line \}

\( 1^{\text{st}}, \ldots, (n-1)^{\text{th}} \) powers + all coaxial equivalents

**Glide plane**

\{ plane \}

defining operation + all coplanar equivalents
### 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 $2\pi/n$, $n = 2, 3, 4$ 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 $2\pi/n$, $u = j/n$ times shortest lattice translation along b, right-hand screw, $n = 2, 3, 4$ or 6, $j = 1, \ldots, (n-1)$</td>
<td>1st, …, $(n-1)$th powers of d.o. and their coaxial equivalents†</td>
</tr>
<tr>
<td>Roto-inversion axis</td>
<td>Line b and point P on b</td>
<td>Roto-inversion: rotation around b, angle $2\pi/n$, 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 \( \{ 1^{\text{st}}, 2^{\text{nd}}, 3^{\text{rd}} \text{ powers} + \text{all coaxial equivalents} \} \)

**Element set of (0,0,z) line**

<table>
<thead>
<tr>
<th>Operation</th>
<th>Transformation</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>(-x, -y, z)</td>
</tr>
<tr>
<td>4+</td>
<td>(-y, x, z)</td>
</tr>
<tr>
<td>4-</td>
<td>(y, -x, z)</td>
</tr>
<tr>
<td>2(0,0,1)</td>
<td>(-x, -y, z+1)</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
</tr>
</tbody>
</table>

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).
Figure 2.5 General position diagrams of the space group $I4_132$, No. 214. Left diagram: polyhedra (twisted trigonal antiprisms) centres at $(\frac{1}{8}, \frac{1}{8}, \frac{1}{8})$ and its equivalent points, site-symmetry group $32$. Right diagram: polyhedra (sphenoids) attached to $(0, 0, 0)$ and its equivalent points, site-symmetry group $3$.
ORIGINS AND ASYMMETRIC UNITS
Space group \(Cmm2\) (No. 35): left-hand page ITA

\[
\begin{align*}
Cmm2 & & C_{2v}^{11} & & mm2 & & \text{Orthorhombic} \\
\text{No. 35} & & Cmm2 & & & & \text{Patterson symmetry } Cmmm
\end{align*}
\]

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.

Origin on \(mm2\)

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**

No. 48

\[ D_{2h}^2 \]

\[ P \ 2/n \ 2/n \ 2/n \]

**mmm**

Orthorhombic

Patterson symmetry *Pmmm*

**ORIGIN CHOICE 1**

Origin at 2 2 2, at \( \frac{1}{4}, \frac{1}{4}, \frac{1}{4} \) from \( \bar{1} \)

**ORIGIN CHOICE 2**

Origin at \( \bar{1} \) at *nnn*, at \( -\frac{1}{4}, -\frac{1}{4}, -\frac{1}{4} \) from 2 2 2
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

<table>
<thead>
<tr>
<th>Number of vertices: 8</th>
</tr>
</thead>
<tbody>
<tr>
<td>0, 1, 1/2</td>
</tr>
<tr>
<td>1, 1, 0</td>
</tr>
<tr>
<td>1, 0, 0</td>
</tr>
<tr>
<td>0, 0, 1/2</td>
</tr>
<tr>
<td>1, 0, 1/2</td>
</tr>
<tr>
<td>0, 0, 0</td>
</tr>
<tr>
<td>0, 1, 0</td>
</tr>
<tr>
<td>1, 1, 1/2</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Number of facets: 6</th>
</tr>
</thead>
<tbody>
<tr>
<td>x&gt;=0</td>
</tr>
<tr>
<td>x&lt;1</td>
</tr>
<tr>
<td>y&gt;=0</td>
</tr>
<tr>
<td>y&lt;1</td>
</tr>
<tr>
<td>z&gt;=0 [x&lt;=1/2]</td>
</tr>
<tr>
<td>z&lt;=1/2 [x&lt;=1/2]</td>
</tr>
</tbody>
</table>

[Guide to notation]
GENERAL AND SPECIAL WYCKOFF POSITIONS SITE-SYMMETRY
**Group Actions**

A *group action* of a group $\mathcal{G}$ 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 $\mathcal{G}$ has no effect on $\omega$, i.e. $e(\omega) = \omega$ for all $\omega$ in $\Omega$.

**Orbit and Stabilizer**

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

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

**Equivalence classes**

Via this equivalence relation, the action of $\mathcal{G}$ partitions the objects in $\Omega$ into *equivalence classes*.
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: $|P|/|S_0|$

General and special Wyckoff positions

Site-symmetry groups: oriented symbols

General position $X_0$

$S=\{(1,0)\}\approx 1$

Multiplicity: $|P|$

Special position $X_0$

$S>1=\{(1,0),...,\}$

Multiplicity: $|P|/|S_0|$
(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 $G$: $0 \leq x_i < 1$

(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 $X = x \choose y \choose z$ under $(W,w)$ of $G$

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

-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

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

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

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

\[ S_f \cong \{1, -1\} \quad \text{isomorphic} \]
**Example**

**Space group P4mm**

![Diagram](image)

**Generators selected**

(1); \(t(1,0,0); t(0,1,0); t(0,0,1); (2); (3); (5)

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>(g)</td>
<td>(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)</td>
</tr>
<tr>
<td>4</td>
<td>(f)</td>
<td>(x,\frac{1}{2},z) (\bar{x},\frac{1}{2},z) (\frac{1}{2},x,z) (\frac{1}{2},\bar{x},z)</td>
</tr>
<tr>
<td>4</td>
<td>(e)</td>
<td>(x,0,z) (\bar{x},0,z) (0,x,z) (0,\bar{x},z)</td>
</tr>
<tr>
<td>4</td>
<td>(d)</td>
<td>(x,x,z) (\bar{x},\bar{x},z) (\bar{x},x,z) (x,\bar{x},z)</td>
</tr>
<tr>
<td>2</td>
<td>(c)</td>
<td>(\frac{1}{2},0,z) (0,\frac{1}{2},z)</td>
</tr>
<tr>
<td>1</td>
<td>(b)</td>
<td>(\frac{1}{2},\frac{1}{2},z)</td>
</tr>
<tr>
<td>1</td>
<td>(a)</td>
<td>(0,0,z)</td>
</tr>
</tbody>
</table>
Space group P4mm

General and special Wyckoff positions of P4mm

<table>
<thead>
<tr>
<th>Number</th>
<th>Symbol</th>
<th>Position</th>
<th>Equivalent Positions</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>g</td>
<td>1</td>
<td>(1) $x, y, z$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(2) $x, y, z$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(3) $y, x, z$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(4) $y, x, z$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(5) $x, y, z$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(6) $x, y, z$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(7) $y, x, z$</td>
</tr>
<tr>
<td></td>
<td></td>
<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,x,z
(8) m x,x,z
Problem:

- Wyckoff positions
- Site-symmetry groups
- Coordinate transformations

**Wyckoff Positions**

How to select the group

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

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


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

58

**ITA-Settings for the Space Group 58**

*P* must be read by columns. 

\[(a, b, c)_n = (a, b, c)_P\]

<table>
<thead>
<tr>
<th>ITA number</th>
<th>Setting</th>
<th>P</th>
<th>P⁻¹</th>
</tr>
</thead>
<tbody>
<tr>
<td>58</td>
<td>C   c   e</td>
<td>a,b,c</td>
<td>a,b,c</td>
</tr>
<tr>
<td>58</td>
<td>A   e   a</td>
<td>c,a,b</td>
<td>b,c,a</td>
</tr>
<tr>
<td>58</td>
<td>B   b   e</td>
<td>b,c,a</td>
<td>c,a,b</td>
</tr>
<tr>
<td>58</td>
<td>C   c   e</td>
<td>a,b,c</td>
<td>a,b,c</td>
</tr>
<tr>
<td>58</td>
<td>A   e   a</td>
<td>c,a,b</td>
<td>b,c,a</td>
</tr>
</tbody>
</table>
### Wyckoff Positions of Group 68 (Ccce) [origin choice 2]

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

### Site Symmetry Group 222

- **x,y,z**
  - 

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

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

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

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

**Bilbao Crystallographic Server**
Example WYCKPOS: Wyckoff Positions Ccce (68)

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 = \( \frac{1}{2} \)
y = \( \frac{1}{4} \)
z = \( \frac{1}{4} \)

Space Group: 68 (Ccce) [origin choice 2]
Point: \( \frac{1}{2}, \frac{1}{4}, \frac{1}{4} \)
Wyckoff Position: 4b

Site Symmetry Group 222

<table>
<thead>
<tr>
<th>( x, y, z )</th>
<th>( \begin{pmatrix} 1 &amp; 0 &amp; 0 &amp; 0 \ 0 &amp; 1 &amp; 0 &amp; 0 \ 0 &amp; 0 &amp; 1 &amp; 0 \end{pmatrix} )</th>
<th>1</th>
</tr>
</thead>
<tbody>
<tr>
<td>(-x+1, y, -z+1/2)</td>
<td>( \begin{pmatrix} -1 &amp; 0 &amp; 0 &amp; 1 \ 0 &amp; 1 &amp; 0 &amp; 0 \ 0 &amp; 0 &amp; -1 &amp; 1/2 \end{pmatrix} )</td>
<td>( 2 \frac{1}{2}, y, 1/4 )</td>
</tr>
<tr>
<td>(-x+1, -y+1/2, z)</td>
<td>( \begin{pmatrix} -1 &amp; 0 &amp; 0 &amp; 1 \ 0 &amp; -1 &amp; 0 &amp; 0 \ 0 &amp; 0 &amp; 1 &amp; 0 \end{pmatrix} )</td>
<td>( 2 \frac{1}{2}, 1/4, z )</td>
</tr>
<tr>
<td>(x, -y+1/2, -z+1/2)</td>
<td>( \begin{pmatrix} 1 &amp; 0 &amp; 0 &amp; 0 \ 0 &amp; -1 &amp; 0 &amp; 1/2 \ 0 &amp; 0 &amp; -1 &amp; 1/2 \end{pmatrix} )</td>
<td>( 2 x, 1/4, 1/4 )</td>
</tr>
</tbody>
</table>
Consider the special Wyckoff positions of 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.
Consider the Wyckoff-positions data of the space group \( \text{I}4_1/\text{amd} \) (No. 141), origin choice 2.

Determine the site-symmetry groups of Wyckoff positions 4a, 4c, 8d and 8e. Compare the results with the listed ITA data.

Compare your results with the results of the program WYCKPOS.

Characterize geometrically the isometries (3), (7), (12), (13) and (16) as listed under General Position. Compare the results with the corresponding geometric descriptions listed under Symmetry operations block in ITA. Comment on the differences between the corresponding symmetry operations listed under the sub-blocks (0, 0, 0) and (1/2, 1/2, 1/2).

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

How do the above results change if origin choice 1 setting of \( \text{I}4_1/\text{amd} \) is considered?
COORDINATE TRANSFORMATIONS IN CRYSTALLOGRAPHY
Co-ordinate transformation

3-dimensional space

(a, b, c), origin O: point X(x, y, z)

(P, p)

(a', b', c'), origin O': point X(x', y', z')

Transformation matrix-column pair (P, p)

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

(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.
Example

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

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

\[X = (3/4, 1/4, 0)\]

\[X' = (\text{?})\]

Write “new in terms of old” as column vectors.
EXAMPLE

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

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

\[ X = \left( \frac{3}{4}, \frac{1}{4}, 0 \right) \]

\[ X' = \left( \frac{1}{2}, 1, 0 \right) \]
Linear parts as before.
Linear parts as before.
Transformation matrix-column pair \((P,p)\)

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

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

\[
\begin{align*}
a' &= \frac{1}{2}a - \frac{1}{2}b \\
b' &= \frac{1}{2}a + \frac{1}{2}b \\
c' &= c
\end{align*}
\]

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

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

Transformation matrix: 

(a, b, c), origin O

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

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

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

Example:

\[
\begin{pmatrix} 1 & -1 & \frac{-1}{4} \\ 1 & 1 & \frac{-3}{4} \\ 1 & 0 & 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

$$X' = (P,p)^{-1}X = \begin{pmatrix} 1 & -1 & 0 & -1/4 & 3/4 & 1/4 \\ 1 & 1 & 0 & -3/4 & 1/4 & 1/4 \\ 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 1/4 \\ 1/4 \\ 0 \end{pmatrix}$$
Covariant and contravariant crystallographic quantities

direct or crystal basis

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

reciprocal or dual basis

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

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 \((W,w)\)

\[
\begin{align*}
\tilde{x}' &= (W', w') x' , \\
\tilde{x}' &= (P, p)^{-1} \tilde{x} = (P, p)^{-1} (W, w) x = (P, p)^{-1} (W, w) (P, p) x'.
\end{align*}
\]

\((W', w') = (P, p)^{-1} (W, w) (P, p)\)
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 ($p=o$):  
  $$x' = P^{-1}x$$

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


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

**metric tensor $G$:**  
$$G' = P^t G P$$
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) \(x,-y+1/2,z+1/2\)

(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 \(X=\begin{bmatrix} 0.70 \\ 0.31 \\ 0.95 \end{bmatrix}\) with respect to the new basis \((a',b',c')\).

\[
\begin{align*}
(W',w') &= (P,p)^{-1}(W,w)(P,p) \\
(X') &= (P,p)^{-1}(X)
\end{align*}
\]
530 ITA settings of **orthorhombic** and **monoclinic** groups

4. **SYNOPTIC TABLES OF SPACE-GROUP SYMBOLS**

**Table 4.3.1 (cont.)**

**MONOCLINIC SYSTEM**

<table>
<thead>
<tr>
<th>No. of space group</th>
<th>Schoenflies symbol</th>
<th>Standard short Hermann–Mauguin symbol</th>
<th>Extended Hermann–Mauguin symbols for various settings and cell choices</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>abc</td>
<td>eha</td>
</tr>
<tr>
<td>3</td>
<td>C(_1)</td>
<td>P2</td>
<td>P1 2(_1)</td>
</tr>
<tr>
<td>4</td>
<td>C(_2)</td>
<td>P(_2), P(_2), C2</td>
<td>P1 2(_1)</td>
</tr>
<tr>
<td>5</td>
<td>C(_3)</td>
<td>C2</td>
<td>2(_1)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>B1 2(_1)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>I1 2(_1)</td>
</tr>
<tr>
<td>6</td>
<td>C(_4)</td>
<td>Pm</td>
<td>P1 m1</td>
</tr>
<tr>
<td>7</td>
<td>C(_5)</td>
<td>P(_c)</td>
<td>P1 c1</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>P1 c1</td>
</tr>
<tr>
<td>8</td>
<td>C(_6)</td>
<td>C(_m)</td>
<td>C1 m1</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>C1 m1</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>C1 m1</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>I1 m1</td>
</tr>
<tr>
<td>9</td>
<td>C(_7)</td>
<td>C(_e)</td>
<td>C1 e1</td>
</tr>
<tr>
<td></td>
<td></td>
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<td>C1 e1</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>C1 e1</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>I1 e1</td>
</tr>
<tr>
<td>10</td>
<td>C(_8)</td>
<td>P2/m</td>
<td>P1 2/m</td>
</tr>
<tr>
<td>11</td>
<td>C(_9)</td>
<td>P2/m</td>
<td>P1 2/m</td>
</tr>
</tbody>
</table>
### Monoclinic descriptions

<table>
<thead>
<tr>
<th>Transf.</th>
<th>abc</th>
<th>cba</th>
<th>abc</th>
<th>bač</th>
<th>abc</th>
<th>ācb</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></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></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></td>
<td></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>Cell type 2</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>Cell type 3</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### Orthorhombic descriptions

<table>
<thead>
<tr>
<th>No.</th>
<th>HM</th>
<th>abc</th>
<th>bač</th>
<th>cab</th>
<th>āba</th>
<th>bca</th>
<th>ačb</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>
Problem: Coordinate transformations
Generators
General positions

Generators and General Positions

How to select the group

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

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

Show:

Generators only
All General Positions

Conventional Setting
Non Conventional Setting
ITA Settings

Transformation of the basis
ITA-settings
Symmetry data
Example GENPOS:

- Default setting: \( C12/c1 \)
- Final setting: \( A112/a \)

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

### 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.

\[
(a, b, c)_n = (a, b, c)_s P
\]

<table>
<thead>
<tr>
<th>ITA number</th>
<th>Setting</th>
<th>( P )</th>
<th>( P^{-1} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>( C12/c1 )</td>
<td>a, b, c</td>
<td>a, b, c</td>
</tr>
<tr>
<td>15</td>
<td>( A12/n1 )</td>
<td>-a, c, b, a</td>
<td>c, b, -a, c</td>
</tr>
<tr>
<td>15</td>
<td>( I12/a1 )</td>
<td>c, b, -a, c</td>
<td>-a, c, b, a</td>
</tr>
<tr>
<td>15</td>
<td>( A12/a1 )</td>
<td>c, b, a</td>
<td>c, b, a</td>
</tr>
<tr>
<td>15</td>
<td>( C12/n1 )</td>
<td>a, b, -a, c</td>
<td>a, b, a</td>
</tr>
<tr>
<td>15</td>
<td>( I12/c1 )</td>
<td>-a, c, b, c</td>
<td>-a, c, b, c</td>
</tr>
<tr>
<td>15</td>
<td>( A112/a )</td>
<td>c, a, b</td>
<td>b, c, a</td>
</tr>
<tr>
<td>15</td>
<td>( B112/n )</td>
<td>a, -a, c, b</td>
<td>a, c, -a, b</td>
</tr>
<tr>
<td>15</td>
<td>( I112/b )</td>
<td>-a, c, b, c</td>
<td>-a, b, c, b</td>
</tr>
<tr>
<td>15</td>
<td>( B112/b )</td>
<td>a, c, -b</td>
<td>a, c, b</td>
</tr>
<tr>
<td>15</td>
<td>( A112/n )</td>
<td>-a, c, a, b</td>
<td>b, c, -a, b</td>
</tr>
<tr>
<td>15</td>
<td>( I112/a )</td>
<td>c, a, -c, b</td>
<td>-a, b, c, a</td>
</tr>
<tr>
<td>15</td>
<td>( C2/n1 )</td>
<td>b, a, -a, c</td>
<td>b, a, -b, c</td>
</tr>
<tr>
<td>15</td>
<td>( I12/c1 )</td>
<td>b, a, -c, c</td>
<td>-b, c, a, c</td>
</tr>
<tr>
<td>15</td>
<td>( C2/c1 )</td>
<td>-b, a, c</td>
<td>b, -a, c</td>
</tr>
<tr>
<td>15</td>
<td>( B2/n1 )</td>
<td>b, -a, c, a</td>
<td>c, a, -b, c</td>
</tr>
<tr>
<td>15</td>
<td>( B2/b11 )</td>
<td>-b, a, c, c</td>
<td>-b, c, a, c</td>
</tr>
</tbody>
</table>
### Example GENPOS: ITA settings of C2/c(15)

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

<table>
<thead>
<tr>
<th>N</th>
<th>Standard/Default Setting C2/c</th>
<th>ITA-Setting A 1 1 2/a</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(x,y,z) form</td>
<td>matrix form</td>
</tr>
<tr>
<td>1</td>
<td>x, y, z</td>
<td>[\begin{pmatrix} 1 &amp; 0 &amp; 0 &amp; 0 \ 0 &amp; 1 &amp; 0 &amp; 0 \ 0 &amp; 0 &amp; 1 &amp; 0 \end{pmatrix}]</td>
</tr>
<tr>
<td>2</td>
<td>-x, y, -z+1/2</td>
<td>[\begin{pmatrix} -1 &amp; 0 &amp; 0 &amp; 0 \ 0 &amp; 1 &amp; 0 &amp; 0 \ 0 &amp; 0 &amp; -1 &amp; 1/2 \end{pmatrix}]</td>
</tr>
<tr>
<td>3</td>
<td>-x, -y, -z</td>
<td>[\begin{pmatrix} -1 &amp; 0 &amp; 0 &amp; 0 \ 0 &amp; -1 &amp; 0 &amp; 0 \ 0 &amp; 0 &amp; -1 &amp; 0 \end{pmatrix}]</td>
</tr>
<tr>
<td>4</td>
<td>x, -y, z+1/2</td>
<td>[\begin{pmatrix} 1 &amp; 0 &amp; 0 &amp; 0 \ 0 &amp; -1 &amp; 0 &amp; 0 \ 0 &amp; 0 &amp; 1 &amp; 1/2 \end{pmatrix}]</td>
</tr>
<tr>
<td>5</td>
<td>x+1/2, y+1/2, z</td>
<td>[\begin{pmatrix} 1 &amp; 0 &amp; 0 &amp; 1/2 \ 0 &amp; 1 &amp; 0 &amp; 1/2 \ 0 &amp; 0 &amp; 1 &amp; 0 \end{pmatrix}]</td>
</tr>
<tr>
<td>6</td>
<td>-x+1/2, y+1/2, -z+1/2</td>
<td>[\begin{pmatrix} -1 &amp; 0 &amp; 0 &amp; 1/2 \ 0 &amp; 1 &amp; 0 &amp; 1/2 \ 0 &amp; 0 &amp; -1 &amp; 1/2 \end{pmatrix}]</td>
</tr>
<tr>
<td>7</td>
<td>-x+1/2, -y+1/2, -z</td>
<td>[\begin{pmatrix} -1 &amp; 0 &amp; 0 &amp; 1/2 \ 0 &amp; -1 &amp; 0 &amp; 1/2 \ 0 &amp; 0 &amp; -1 &amp; 0 \end{pmatrix}]</td>
</tr>
<tr>
<td>8</td>
<td>x+1/2, -y+1/2, z+1/2</td>
<td>[\begin{pmatrix} 1 &amp; 0 &amp; 0 &amp; 1/2 \ 0 &amp; -1 &amp; 0 &amp; 1/2 \ 0 &amp; 0 &amp; 1 &amp; 1/2 \end{pmatrix}]</td>
</tr>
</tbody>
</table>

**default setting**

**A 1 1 2/a setting**
Problem: Coordinate transformations Wyckoff positions

Wyckoff Positions

How to select the group

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

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


ITA-Settings for the Space Group 68

The settings must be read by columns. P is the transformation.

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

<table>
<thead>
<tr>
<th>ITA number</th>
<th>Setting</th>
<th>P</th>
<th>(P^{-1})</th>
</tr>
</thead>
<tbody>
<tr>
<td>68</td>
<td>C c c e [origin 1]</td>
<td>a,b,c</td>
<td>a,b,c</td>
</tr>
<tr>
<td>68</td>
<td>A e a a [origin 1]</td>
<td>c,a,b</td>
<td>b,c,a</td>
</tr>
<tr>
<td>68</td>
<td>B b e b [origin 1]</td>
<td>b,c,a</td>
<td>c,a,b</td>
</tr>
<tr>
<td>68</td>
<td>C c c e [origin 2]</td>
<td>a,b,c</td>
<td>a,b,c</td>
</tr>
<tr>
<td>68</td>
<td>A e a a [origin 2]</td>
<td>c,a,b</td>
<td>b,c,a</td>
</tr>
<tr>
<td>68</td>
<td>B b e b [origin 2]</td>
<td>b,c,a</td>
<td>c,a,b</td>
</tr>
</tbody>
</table>
Consider the space group \( P2_1/c \) (No. 14). Show that the relation between the General and Special position data of \( P1 \bar{1}2_1/a \) (setting unique axis \( c \)) can be obtained from the data \( P12_1/c1 \) (setting unique axis \( b \)) applying the transformation \((a',b',c')_c = (a,b,c)_b P\), with \( P = c,a,b \).

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 2.24

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 \textit{Im-3m} (No. 229). Using the option \textit{Non-conventional setting} obtain the matrix-column pairs of the symmetry operations with respect to a primitive basis, applying the transformation \((a',b',c') = 1/2(-a+b+c,a-b+c,a+b-c)\)
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:
\[
\begin{align*}
a & \\
b & \\
c & 
\end{align*}
\]

angles between them:
\[
\begin{align*}
\alpha &= (b, c) \\
\beta &= (c, a) \\
\gamma &= (a, b)
\end{align*}
\]
Lattice parameters (3D)

An alternative way to define the metric properties of a lattice $L$

Given a lattice $L$ of $\mathbf{V}^3$ with a lattice basis: $\{a_1, a_2, a_3\}$

**Definition (D 1.5.3)** The quantities

$$a_1 = |a_1| = +\sqrt{(a_1 \cdot a_1)}, \quad a_2 = |a_2| = +\sqrt{(a_2 \cdot a_2)},$$

$$a_3 = |a_3| = +\sqrt{(a_3 \cdot a_3)},$$

$$\alpha_1 = \arccos(|a_2|^{-1}|a_3|^{-1}(a_2 \cdot a_3)), \quad \alpha_2 = \arccos(|a_3|^{-1}|a_1|^{-1}(a_3 \cdot a_1)),$$

and $$\alpha_3 = \arccos(|a_1|^{-1}|a_2|^{-1}(a_1 \cdot a_2))$$

are called the **lattice parameters** of the lattice.

Remark: the lengths of basis vectors are measured in

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

**Metric tensor $G$** in terms of lattice parameters

$$G = \begin{pmatrix} a \cdot a & a \cdot b & a \cdot c \\ b \cdot a & b \cdot b & b \cdot c \\ c \cdot a & c \cdot b & c \cdot c \end{pmatrix}, \quad G = \begin{pmatrix} a^2 & ab \cos \gamma & ac \cos \beta \\ ab \cos \gamma & b^2 & bc \cos \alpha \\ ac \cos \beta & bc \cos \alpha & c^2 \end{pmatrix}$$
Given a lattice $L$ of $V^3$ with a lattice basis: $\{a_1, a_2, a_3\}$

The lattice $L$ inherits the metric properties of the Euclidean space and they are conveniently expressed with respect to a lattice basis (right-handed coordinate system).

**Metric tensor $G$ of $L$**

$G = \{a_1, a_2, a_3\}^T. \{a_1, a_2, a_3\} = \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix}$

$G = \begin{bmatrix} G_{11} & G_{12} & G_{13} \\ G_{21} & G_{22} & G_{23} \\ G_{31} & G_{32} & G_{33} \end{bmatrix}$

**Metric tensor $G$ is symmetric:** $G_{ik} = G_{ki}$

$G_{ik} = (a_i, a_k) = a_i a_k \cos \alpha_j,$

**Scalar product of arbitrary vectors:** $(r, t) = r^T G t$

Transformation properties of $G$ under basis transformation

$\{a'_1, a'_2, a'_3\} = \{a_1, a_2, a_3\} P$

$G' = \{a'_1, a'_2, a'_3\}^T. \{a'_1, a'_2, a'_3\} = P^T \{a_1, a_2, a_3\}^T. \{a_1, a_2, a_3\} P$

$G' = P^T G P$
Crystallographic calculations: 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

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

In the general case one obtains

$$V^2 = \begin{vmatrix} G_{11} & G_{12} & G_{13} \\ G_{21} & G_{22} & G_{23} \\ G_{31} & G_{32} & G_{33} \end{vmatrix} =$$

$$= a^2 b^2 c^2 (1 - \cos^2 \alpha - \cos^2 \beta - \cos^2 \gamma + 2 \cos \alpha \cos \beta \cos \gamma).$$
Volume of the unit cell in terms of lattice parameters (Buerger, 1941)

Basis vectors with respect to Cartesian basis

\[
a = ia_x + ja_y + ka_z, \\
b = ib_x + jb_y + kb_z, \\
c = ic_x + jc_y + kc_z,
\]

\[
V = a \cdot (b \times c) = \begin{vmatrix} a_x & a_y & a_z \\ b_x & b_y & b_z \\ c_x & c_y & c_z \end{vmatrix}
\]

\[
V^2 = \begin{vmatrix} a_x & a_y & a_z \\ b_x & b_y & b_z \\ c_x & c_y & c_z \end{vmatrix} = \begin{vmatrix} a \cdot a & a \cdot b & a \cdot c \\ b \cdot a & b \cdot b & b \cdot c \\ c \cdot a & c \cdot b & c \cdot c \end{vmatrix} = \det \begin{vmatrix} a^2 & ab \cos \gamma & ac \cos \beta \\ ab \cos \gamma & b^2 & bc \cos \alpha \\ ac \cos \beta & bc \cos \alpha & c^2 \end{vmatrix}
\]

\[
V = abc(1 - \cos^2 \alpha - \cos^2 \beta - \cos^2 \gamma + 2 \cos \alpha \cos \beta \cos \gamma)^{1/2}
\]
Write down the metric tensors of the seven crystal systems in parametric form using the general expressions for their lattice parameters. For each of the cases, express the volume of the unit cell as a function of the lattice parameters.

For example:

tetragonal crystal system: \(a=b, c, \alpha=\beta=\gamma=90\)

\[
G = \begin{bmatrix}
a^2 & 0 & 0 \\
0 & a^2 & 0 \\
0 & 0 & c^2
\end{bmatrix}
\]

\(V=\)?
A body-centred cubic lattice (cl) 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 \(\frac{1}{2}\mathbf{a}_P + \frac{1}{2}\mathbf{b}_P + \frac{1}{2}\mathbf{c}_P\) 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:

\[ \mathbf{a}_I = \frac{1}{2}(-\mathbf{a}_P + \mathbf{b}_P + \mathbf{c}_P), \quad \mathbf{b}_I = \frac{1}{2}(\mathbf{a}_P - \mathbf{b}_P + \mathbf{c}_P), \quad \mathbf{c}_I = \frac{1}{2}(\mathbf{a}_P + \mathbf{b}_P - \mathbf{c}_P) \]

(iii) determine the lattice parameters of the primitive cell if \(a_P = 4\ \text{Å}\)

**Hint**

metric tensor transformation \(G' = P^t G P\)
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 \(1/2b_P + 1/2c_P, \ 1/2a_P + 1/2c_P, \ 1/2a_P + 1/2b_P\), 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:

\[
\begin{align*}
    a_F &= 1/2(b_P + c_P), \\
    b_F &= 1/2(a_P + c_P), \\
    c_F &= 1/2(a_P + b_P)
\end{align*}
\]

(iii) determine the lattice parameters of the primitive cell if \(a_P = 4 \text{ Å}\)