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

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

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

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

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

VOLUME A: SPACE-GROUP SYMMETRY

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

- headline with the relevant group symbols;
- diagrams of the symmetry elements and of the general position;
- specification of the origin and the asymmetric unit;
- list of symmetry operations;
- generators;
- general and special positions with multiplicities, site symmetries, coordinates and reflection conditions;
- symmetries of special projections;
- extensive subgroup and supergroup data
1. $C_{mm2}$

2. No. 35

3. Patterson symmetry $C_{mmm}$

4. Origin on $mm2$

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

6. Symmetry operations
   - For $(0,0,0)+$ set:
     - (1) 1
     - (2) $0,0,z$
     - (3) $m,x,0,z$
     - (4) $m,0,y,z$
Left-hand page:

1. **Headline**

2. **Diagrams** for the symmetry elements and the general position (for graphical symbols of symmetry elements see Chapter 1.4)

3. **Origin**

4. **Asymmetric unit**

5. **Symmetry operations**
General Layout: Right-hand page

CONTINUED

No. 35

C \text{mm}2

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

3 Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site symmetry</th>
<th>Coordinates</th>
<th>Reflection conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0,0,0)+ (\frac{1}{2}, \frac{1}{2}, 0)+</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

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

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

4 Symmetry of special projections

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

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

Along [010] \text{p11m}
\( a' = c \quad b' = \frac{1}{2} a \)
Origin at 0,y,0

5 Maximal non-isomorphic subgroups

1 \( [2] C 1 m 1 (Cm, 8) \) (1; 3)+
2 \( [2] C m 1 1 (Cm, 8) \) (1; 4)+
2 \( [2] C 1 1 2 (P2, 3) \) (1; 2)+

IIa \( [2] P ba 2 (32) \) 1; 2; (3; 4) + (\frac{1}{2}, \frac{1}{2}, 0)
2 \( [2] P b m 2 (Pma 2, 28) \) 1; 3; (2; 4) + (\frac{1}{2}, \frac{1}{2}, 0)
Right-hand page:

(6) *Headline* in abbreviated form

(7) *Generators selected*; this information is the basis for the order of the entries under *Symmetry operations* and *Positions*

(8) General and special *Positions*, with the following columns:
   - Multiplicity
   - Wyckoff letter
   - Site symmetry, given by the oriented site-symmetry symbol
   - Coordinates
   - Reflection conditions

*Note*: In a few space groups, two special positions with the same reflection conditions are printed on the same line

(9) *Symmetry of special projections* (not given for plane groups)

(10) *Maximal non-isomorphic subgroups*

(11) *Maximal isomorphic subgroups of lowest index*

(12) *Minimal non-isomorphic supergroups*
Short Hermann-Mauguin symbol: \( \text{Cmm2} \)

Schoenflies symbol: \( C_{2v} \)

Crystal class (point group): \( \text{mm2} \)

Crystal system: Orthorhombic

Number of space group: No. 35

Full Hermann-Mauguin symbol: \( \text{Cmm2} \)

Patterson symmetry: \( Cmnm \)
HERMANN-MAUGUIN
SYMBOLISM FOR SPACE GROUPS
Hermann-Mauguin symbols for space groups

Orthorhombic

- Primary direction
- Secondary direction
- Tertiary direction

Bravais lattice

- Screw axis $2_1 // \tilde{a}$
- Glide plane $n \perp \tilde{a}$
- Screw axis $2_1 // \tilde{c}$
- Glide plane $a \perp \tilde{c}$
- Screw axis $2_1 // \tilde{b}$
- Mirror plane $m \perp \tilde{b}$

$P2_1/n2_1/m2_1/a$
SPACE-GROUP
SYMMETRY OPERATIONS
Crystallographic symmetry operations

characteristics: fixed points of isometries (W,w) ∈ Xf = Xf
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
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

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

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

matrix-column pair

Seitz symbol
Space Groups: infinite order

Coset decomposition $G:T_G$

$(I,0) \quad (W_2, w_2) \quad ... \quad (W_m, w_m) \quad ... \quad (W_i, w_i)$

$(I,t_1) \quad (W_2, w_2 + t_1) \quad ... \quad (W_m, w_m + t_1) \quad ... \quad (W_i, w_i + t_1)$

$(I,t_2) \quad (W_2, w_2 + t_2) \quad ... \quad (W_m, w_m + t_2) \quad ... \quad (W_i, w_i + t_2)$

... \quad ... \quad ... \quad ... \quad ... \quad ...

$(I,t_j) \quad (W_2, w_2 + t_j) \quad ... \quad (W_m, w_m + t_j) \quad ... \quad (W_i, w_i + t_j)$

... \quad ... \quad ... \quad ... \quad ... \quad ...

Factor group $G/T_G$

isomorphic to the point group $P_G$ of $G$

Point group $P_G = \{I, W_1, W_2, ..., W_i\}$
### Coset decomposition $\text{P2}_1/c: T$

<p>| | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$(I,0)$</td>
<td>$(2,0 \ 1/2 \ 1/2)$</td>
<td>$(\bar{I},0)$</td>
<td>$(m,0 \ 1/2 \ 1/2)$</td>
<td></td>
</tr>
<tr>
<td>$(I,t_1)$</td>
<td>$(2,0 \ 1/2 \ 1/2 + t_1)$</td>
<td>$(\bar{I},t_1)$</td>
<td>$(m,0 \ 1/2 \ 1/2 + t_1)$</td>
<td></td>
</tr>
<tr>
<td>$(I,t_2)$</td>
<td>$(2,0 \ 1/2 \ 1/2 + t_2)$</td>
<td>$(\bar{I},t_2)$</td>
<td>$(m,0 \ 1/2 \ 1/2 + t_2)$</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$(I,t_j)$</td>
<td>$(2,0 \ 1/2 \ 1/2 + t_j)$</td>
<td>$(\bar{I},t_j)$</td>
<td>$(m,0 \ 1/2 \ 1/2 + t_j)$</td>
<td></td>
</tr>
<tr>
<td></td>
<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_1 screw axes*

$(2,u \ 1/2+v \ 1/2 +w)$

$(2,u \ 1/2 \ 1/2 +w)$
Space group \( \text{Cmm2} \) (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. \(b \ \frac{1}{4},y,z\)

**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. \(\bar{x},y,z\)

- Glide plane, \(t=\frac{1}{2}a\) at \(y=\frac{1}{4}, \perp b\)
- Glide plane, \(t=\frac{1}{2}b\) at \(x=\frac{1}{4}, \perp a\)

**Matrix-column presentation of symmetry operations**

\(8 f 1\)

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

\(-x+1/2,y+1/2,z\)
Problem 2.21 (a) Space group Cmm2 (No. 35)

General Position

Coordinates

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

\[
\begin{array}{ccc|cccc}
8 & f & 1 & (1) x,y,z & (2) x\bar{y},z & (3) x,\bar{y},z & (4) \bar{x},y,z \\
\end{array}
\]

A) Characterize geometrically the matrix-column pairs listed under General position of the space group Cmm2 in ITA.

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

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 \(\frac{1}{2},\frac{1}{2},z\)

(3) \(a\) \(x,\frac{1}{2},z\)

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

Matrix-column presentation of symmetry operations

Geometric interpretation
## Sections

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

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<td>Generators and General Positions of Space Groups</td>
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<tr>
<td>WYCKPOS</td>
<td>Wyckoff Positions of Space Groups</td>
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<td>HKLCOND</td>
<td>Reflection conditions of Space Groups</td>
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<td>Series of Maximal Isomorphic Subgroups of Space Groups</td>
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<td>WYCKSETS</td>
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<td>NORMALIZER</td>
<td>Normalizer of Space Groups</td>
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<td>KVEC</td>
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<tr>
<td>SYMMETRY OPERATIONS</td>
<td>Interpretation of matrix column representations of symmetry operations</td>
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### Magnetic Space Groups

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<tr>
<th>Tool</th>
<th>Description</th>
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<td>MGENPOS</td>
<td>General Positions of Magnetic Space Groups</td>
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<tr>
<td>WYCKPOS</td>
<td>Wyckoff Positions of Magnetic Space Groups</td>
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<td>EXTINCTION</td>
<td>Extinction Rules of Magnetic Space Groups</td>
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### Group - Subgroup Relations of Space Groups

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<th>Tool</th>
<th>Description</th>
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<td>Lattice of Maximal Subgroups</td>
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<td>HERMANN</td>
<td>Distribution of subgroups in conjugated classes</td>
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<td>COSETS</td>
<td>Coset decomposition for a group-subgroup pair</td>
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<tr>
<td>WYCKSPLIT</td>
<td>The splitting of the Wyckoff Positions</td>
</tr>
<tr>
<td>MINSUP</td>
<td>Minimal Supergroups of Space Groups</td>
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<tr>
<td>SUPERGROUPS</td>
<td>Supergroups of Space Groups</td>
</tr>
<tr>
<td>CELLSUB</td>
<td>List of subgroups for a given k-index.</td>
</tr>
<tr>
<td>CELLSUPER</td>
<td>List of supergroups for a given k-index.</td>
</tr>
<tr>
<td>NONCHAR</td>
<td>Non Characteristic orbits.</td>
</tr>
<tr>
<td>COMMONSUBS</td>
<td>Common Subgroups of Space Groups</td>
</tr>
<tr>
<td>COMMONSUPER</td>
<td>Common Supergroups of Two Space Groups</td>
</tr>
</tbody>
</table>
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 standard/default setting.

space group
Example GENPOS: Space group $Cmm2(35)$

Matrix-column presentation of symmetry operations

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

Geometric interpretation

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. $2$ $\frac{1}{2},\frac{1}{2},z$
3. $a$ $x,\frac{1}{2},z$
4. $b$ $\frac{1}{2},y,z$
Problem: Geometric Interpretation of \((W,w)\) SYMMETRY OPERATION

Geometric Interpretation of Matrix Column Representation of Symmetry Operation

**Symmetry Operation**

This program calculates the geometric interpretation of matrix column representation of symmetry operation for a given crystal system or space group.

Input:

i) The crystal system or the space group number.

ii) The matrix column representation of symmetry operation.

If you want to work on a non conventional setting click on **Non conventional setting**, this will show you a form where you have to introduce the transformation matrix relating the conventional setting of the group you have chosen with the non conventional one you are interested in.

Output:

We obtain the geometric interpretation of the symmetry operation.

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

\[-x+1/2,y+1/2,z\]
1. Characterize geometrically the matrix-column pairs listed under *General position* of the space group *P4mm* in ITA.

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

3. Compare your results with the results of the program SYMMETRY OPERATIONS.
Problem 2.21(b)

SOLUTION

**Geometric interpretation**

**Matrix-column presentation**

---

**Origin on 4mm**

Asymmetric unit: \(0 \leq x \leq \frac{1}{2};\) \(0 \leq y \leq \frac{1}{2};\) \(0 \leq z \leq 1;\) \(x \leq y\)

**Symmetry operations**

\[\begin{array}{cccc}
(1) & 1 & (2) & 2, 0, 0, z \\
(3) & 4^{-} & 0, 0, z & (4) & 4^{-} & 0, 0, z \\
(5) & m, x, 0, z & (6) & m, 0, y, z & (7) & m, x, x, z & (8) & m, x, z, z \\
\end{array}\]

**Generators selected**

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

**Positions**

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 g 1</td>
<td>(1) (x, y, z)</td>
</tr>
<tr>
<td></td>
<td>(5) (x, y, z)</td>
</tr>
</tbody>
</table>
SPACE GROUPS
DIAGRAMS
Diagrams of symmetry elements

three different settings

permutations of $a, b, c$

Diagram of general position points
Space group \textit{Cmm}2 (No. 35)

Diagram of symmetry elements

Conventional setting

Diagram of general position points

How many general position points per unit cell are there?
Example: P4mm

Diagram of symmetry elements

Diagram of general position points
Symmetry elements

Examples

Rotation axis

Glide plane

Symmetry operations that share the same geometric element

Fixed points

Geometric element

Element set

Symmetry elements

1st, ..., (n-1)th powers + all coaxial equivalents

Rotation axis

plane

defining operation + all coplanar 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.

All glide reflections with the same reflection plane, with glide of d.o. (taken to be zero for reflections) by a lattice translation vector.
# 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; $2\nu$ (not $\nu$) 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>Rotoinversion axis</td>
<td>Line $b$ and point $P$ on $b$</td>
<td>Rotoinversion: 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

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></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.
## The various rotation and screw axes and their symbol

<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 tetrads</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></td>
</tr>
<tr>
<td>2</td>
<td>Rotation diad</td>
<td>(⊥ paper)</td>
<td>none</td>
<td>4₂</td>
<td>Screw tetrads</td>
<td>◆</td>
<td>c/4</td>
</tr>
<tr>
<td>or twofold rotation axis</td>
<td>(∥ paper)</td>
<td></td>
<td></td>
<td>4₃</td>
<td></td>
<td>◆</td>
<td></td>
</tr>
<tr>
<td>2₁</td>
<td>Screw diad</td>
<td>(⊥ paper)</td>
<td>c/2</td>
<td>4</td>
<td>Inverse tetrad</td>
<td>◆</td>
<td></td>
</tr>
<tr>
<td>or twofold screw axis</td>
<td>(∥ paper)</td>
<td></td>
<td>a/2 or b/2</td>
<td>6</td>
<td>Rotation hexad</td>
<td>◆</td>
<td></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></td>
</tr>
<tr>
<td>6</td>
<td></td>
<td>▲</td>
<td>none</td>
<td>6₅</td>
<td></td>
<td>◆</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>Inverse hexad</td>
<td>▲</td>
<td>none</td>
<td>6</td>
<td></td>
<td>◆</td>
<td></td>
</tr>
</tbody>
</table>
### The various symmetry planes and their symbol

<table>
<thead>
<tr>
<th>printed symbol</th>
<th>symmetry plane</th>
<th>graphical symbol</th>
<th>nature of glide translation</th>
</tr>
</thead>
<tbody>
<tr>
<td>(m)</td>
<td>reflection plane (mirror)</td>
<td>________</td>
<td>none</td>
</tr>
<tr>
<td>(a, b)</td>
<td>axial glide plane</td>
<td>________</td>
<td>(a/2) or (b/2)</td>
</tr>
<tr>
<td>(c)</td>
<td>glide plane</td>
<td>________</td>
<td>(c/2)</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>
</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>
</tr>
</tbody>
</table>
ORIGINS
AND
ASYMMETRIC UNITS
Space group $Cmm2$ (No. 35): left-hand page ITA

$Cmm2$
No. 35

$C_{2v}^{11}$
$Cmm2$

$mm2$

Orthorhombic
Patterson symmetry $Cmmm$

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 $P_{nnn}$

$P_{nnn}$  
$D_{2h}^2$  
mmm  
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 $\overline{1}$

**ORIGIN CHOICE 2**

Origin at $\overline{1}$ at $n_{nnn}$, 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-Kustelvse)
SITE-SYMMETRY
GENERAL POSITION
SPECIAL WYCKOFF
POSITIONS
General and special Wyckoff positions

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

$(W,w)X_0 = X_0$

\[
\begin{pmatrix}
a & b & c \\
d & e & f \\
g & h & i \\
\end{pmatrix}
\begin{pmatrix}
w_1 \\
w_2 \\
w_3 \\
\end{pmatrix}
\begin{pmatrix}
x_0 \\
y_0 \\
z_0 \\
\end{pmatrix}
= 
\begin{pmatrix}
x_0 \\
y_0 \\
z_0 \\
\end{pmatrix}
\]

General position $X_0$

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

Special position $X_0$

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

Site-symmetry groups: oriented symbols
(i) coordinate triplets of an image point \( \tilde{X} \) of the original point \( X \) under \((W,w)\) of \( G \)

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

-presentation of infinite symmetry operations of \( G \)
\[
(W,w) = (I,t_n)(W,w_0), 0 \leq w_{i0} < 1
\]
## General Position of Space groups

### Coset decomposition $G: T_G$

<p>| | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$(I,0)$</td>
<td>$(W_2,w_2)$</td>
<td>...</td>
<td>$(W_m,w_m)$</td>
<td>...</td>
</tr>
<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>
</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>
</tr>
<tr>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<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>
</tr>
<tr>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
</tbody>
</table>

### Factor group $G/T_G$

is isomorphic to the point group $P_G$ of $G$

Point group $P_G = \{I, W_1, W_2, ..., W_i\}$
Example: Calculation of the Site-symmetry groups

**Group P-1**

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

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

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

\[ S_f \cong \{1, -1\} \quad \text{isomorphic} \]
Problem: Wyckoff positions
Site-symmetry groups

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:

### 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) (-x+1/2,-y,z) (-x,y-z+1/2) (x+1/2,-y,z+1/2) (-x,y,z) (x+1/2,y,z) (x,y,z+1/2) (-x+1/2,y,z+1/2)</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>

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

#### Site Symmetry Group 222

<table>
<thead>
<tr>
<th>Site</th>
<th>Symmetry</th>
<th>Matrix</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>x,y,z</td>
<td></td>
<td><img src="image" alt="Matrix" /></td>
<td>1</td>
</tr>
<tr>
<td>-x,y,-z+1/2</td>
<td></td>
<td><img src="image" alt="Matrix" /></td>
<td>2.0,y,1/4</td>
</tr>
<tr>
<td>-x,-y+1/2,z</td>
<td></td>
<td><img src="image" alt="Matrix" /></td>
<td>2.0,1/4,z</td>
</tr>
<tr>
<td>x,-y+1/2,-z+1/2</td>
<td></td>
<td><img src="image" alt="Matrix" /></td>
<td>2*x,1/4,1/4</td>
</tr>
</tbody>
</table>
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

\[ x = \frac{1}{2}, \quad y = \frac{1}{4}, \quad z = \frac{1}{4} \]

```
Space Group : 68 (Ccce) [origin choice 2]
Point : \((1/2,1/4,1/4)\)
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 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; 1/2 \ 0 &amp; 0 &amp; 1 &amp; 0 \end{pmatrix}</td>
<td>2 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.
Problem 2.22

Space group P4mm

### Generators selected

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

### Positions

<table>
<thead>
<tr>
<th>Multiplicity, Wyckoff letter, Site symmetry</th>
<th>Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>8  g 1</td>
<td>(1) $x,y,z$</td>
</tr>
<tr>
<td></td>
<td>(5) $x,\bar{y},z$</td>
</tr>
<tr>
<td>4  f . m.</td>
<td>$x,\frac{1}{2},z$</td>
</tr>
<tr>
<td>4  e . m.</td>
<td>$x,0,z$</td>
</tr>
<tr>
<td>4  d . . m</td>
<td>$x,x,z$</td>
</tr>
<tr>
<td>2  c 2 m m.</td>
<td>$\frac{1}{2},0,z$</td>
</tr>
<tr>
<td>1  b 4 m m</td>
<td>$\frac{1}{2},\frac{1}{2},z$</td>
</tr>
<tr>
<td>1  a 4 m m</td>
<td>0,0,z</td>
</tr>
</tbody>
</table>
Consider the special Wyckoff positions of the space group $P4_2/mbc$ (No. 135).

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

Compare your results with the results of the program WYCKPOS.

**P4$_2$/mbc**  
**D$_{4h}^{13}$**  
**4/mmm**  
Tetragonal  

No. 135  

**Origin** at centre (2/m) at 4$_3$/m 1n  

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

**Symmetry operations**

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

(1); \( t(1,0,0); \ t(0,1,0); \ t(0,0,1); \) (2); (3); (5); (9)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

<table>
<thead>
<tr>
<th></th>
<th>i</th>
<th>1</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td>i</td>
<td>1</td>
</tr>
</tbody>
</table>

Coordinates

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

Reflection conditions

General:

hkl : \( k = 2n \)
hhl : \( l = 2n \)
o0l : \( l = 2n \)
h00 : \( h = 2n \)

Special: as above, plus

no extra conditions

<table>
<thead>
<tr>
<th></th>
<th>x, y, 0</th>
<th>( \bar{x}, \bar{y}, 0 )</th>
<th>( y, x, \frac{1}{2} )</th>
<th>( y, \bar{x}, \frac{1}{2} )</th>
<th>( \bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2} )</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( x + \frac{1}{2}, y + \frac{1}{2}, 0 )</td>
<td>( x + \frac{1}{2}, y + \frac{1}{2}, 0 )</td>
<td>( y + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2} )</td>
<td>( y + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2} )</td>
<td>( \bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2} )</td>
</tr>
</tbody>
</table>

hkl : \( l = 2n \)

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

hkl : \( h + k, l = 2n \)

<table>
<thead>
<tr>
<th></th>
<th>0, ( \frac{1}{2}, z )</th>
<th>( \frac{1}{2}, 0, z + \frac{1}{2} )</th>
<th>( \frac{1}{2}, 0, \bar{z} )</th>
<th>( \frac{1}{2}, z + \frac{1}{2} )</th>
<th>( \frac{1}{2}, z + \frac{1}{2} )</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( \frac{1}{2}, 0, z + \frac{1}{2} )</td>
<td>( \frac{1}{2}, 0, \bar{z} + \frac{1}{2} )</td>
<td>( \frac{1}{2}, \bar{z} + \frac{1}{2} )</td>
<td>( \frac{1}{2}, \bar{z} + \frac{1}{2} )</td>
<td>( \frac{1}{2}, \bar{z} + \frac{1}{2} )</td>
</tr>
</tbody>
</table>

hkl : \( h + k, l = 2n \)

<table>
<thead>
<tr>
<th></th>
<th>0, ( 0, z )</th>
<th>( 0, 0, z + \frac{1}{2} )</th>
<th>( \frac{1}{2}, \frac{1}{2}, \bar{z} )</th>
<th>( \frac{1}{2}, \frac{1}{2}, \bar{z} )</th>
<th>( \frac{1}{2}, \frac{1}{2}, \bar{z} )</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( 0, 0, \bar{z} )</td>
<td>( 0, 0, \bar{z} + \frac{1}{2} )</td>
<td>( \frac{1}{2}, \frac{1}{2}, \frac{1}{2} )</td>
<td>( \frac{1}{2}, \frac{1}{2}, \frac{1}{2} )</td>
<td>( \frac{1}{2}, \frac{1}{2}, \frac{1}{2} )</td>
</tr>
</tbody>
</table>

hkl : \( h + k, l = 2n \)

<table>
<thead>
<tr>
<th></th>
<th>0, ( \frac{1}{2}, \frac{1}{2} )</th>
<th>( \frac{1}{2}, 0, \frac{3}{4} )</th>
<th>( \frac{1}{2}, \frac{3}{4}, \frac{1}{2} )</th>
<th>( \frac{1}{2}, 0, \frac{1}{4} )</th>
<th>( \frac{1}{2}, \frac{1}{4}, \frac{1}{2} )</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( \frac{1}{2}, 0, \frac{3}{4} )</td>
<td>( \frac{1}{2}, 0, \frac{1}{4} )</td>
<td>( \frac{1}{2}, 0, \frac{1}{4} )</td>
<td>( \frac{1}{2}, 0, \frac{1}{4} )</td>
<td>( \frac{1}{2}, 0, \frac{1}{4} )</td>
</tr>
</tbody>
</table>

hkl : \( h + k, l = 2n \)

<table>
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<tr>
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<th>( 0, \frac{1}{4}, \frac{1}{2} )</th>
<th>( \frac{1}{2}, \frac{1}{4}, \frac{1}{2} )</th>
<th>( \frac{1}{2}, \frac{1}{4}, \frac{1}{2} )</th>
<th>( \frac{1}{2}, \frac{1}{4}, \frac{1}{2} )</th>
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<td>( 0, \frac{1}{4}, \frac{1}{2} )</td>
<td>( \frac{1}{2}, \frac{1}{4}, \frac{1}{2} )</td>
<td>( \frac{1}{2}, \frac{1}{4}, \frac{1}{2} )</td>
<td>( \frac{1}{2}, \frac{1}{4}, \frac{1}{2} )</td>
</tr>
</tbody>
</table>

hkl : \( h + k, l = 2n \)

<table>
<thead>
<tr>
<th></th>
<th>0, ( 0, 0 )</th>
<th>( 0, 0, \frac{1}{2} )</th>
<th>( \frac{1}{2}, \frac{1}{2}, 0 )</th>
<th>( \frac{1}{2}, \frac{1}{2}, 0 )</th>
<th>( \frac{1}{2}, \frac{1}{2}, 0 )</th>
</tr>
</thead>
<tbody>
<tr>
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<td>( 0, 0, \frac{1}{2} )</td>
<td>( 0, 0, \frac{1}{2} )</td>
<td>( \frac{1}{2}, \frac{1}{2}, 0 )</td>
<td>( \frac{1}{2}, \frac{1}{2}, 0 )</td>
<td>( \frac{1}{2}, \frac{1}{2}, 0 )</td>
</tr>
</tbody>
</table>

hkl : \( h + k, l = 2n \)
COORDINATE TRANSFORMATIONS IN CRYSTALLOGRAPHY
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 ($p=0$):

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

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

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

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

metric tensor $G$:  

$$G' = P^t G P$$
530 ITA settings of orthorhombic and monoclinic groups
## Monoclinic descriptions

<table>
<thead>
<tr>
<th>Transf.</th>
<th>abc</th>
<th>c̄ba</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>A12/c1</td>
<td>A12/a1</td>
<td>A112/a</td>
<td>B112/b</td>
<td>B2/b11</td>
<td>C2/c11</td>
<td>B2/n11</td>
<td>Cell type 1</td>
</tr>
<tr>
<td></td>
<td>A12/n1</td>
<td>C12/n1</td>
<td>B112/n</td>
<td>A112/n</td>
<td>A112/a</td>
<td>C2/n11</td>
<td>B2/n11</td>
<td>I2/c11</td>
<td>Cell type 2</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>
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<td>Cell type 3</td>
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</tbody>
</table>

## Orthorhombic descriptions

<table>
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<th>No.</th>
<th>HM</th>
<th>abc</th>
<th>ba̅c</th>
<th>cab</th>
<th>ćba</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>
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].

Generators and General Positions

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

choose: 15

Show:

Generators only
All General Positions

Transformations of the basis
ITA-settings
Symmetry data

ITA-settings
Symmetry data
Example GENPOS:

default setting $C_{12}/c_1$

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

final setting $A112/a$
### 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>
<th>symmetry operation</th>
<th>(x,y,z) form</th>
<th>matrix form</th>
<th>symmetry operation</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>x, y, z</td>
<td>1</td>
<td>(1 0 0 0)</td>
<td>0 1 0 0</td>
<td>0 0 1 0</td>
<td>(1 0 0 0)</td>
<td>0 1 0 0</td>
<td>0 0 1 0</td>
</tr>
<tr>
<td>2</td>
<td>-x, y, -z +1/2</td>
<td>-x+1/2, -y, -z</td>
<td>2 0, y, 1/4</td>
<td>(1 0 0 0)</td>
<td>-1 0 0 0</td>
<td>1/2</td>
<td>(1 0 0 0)</td>
<td>-1 0 0 0</td>
<td>1/2</td>
</tr>
<tr>
<td>3</td>
<td>-x, -y, -z</td>
<td>-x, -y, -z</td>
<td>-1 0, 0, 0</td>
<td>(1 0 0 0)</td>
<td>0 -1 0 0</td>
<td>0 0 -1 0</td>
<td>(1 0 0 0)</td>
<td>0 -1 0 0</td>
<td>0 0 -1 0</td>
</tr>
<tr>
<td>4</td>
<td>x, -y, z +1/2</td>
<td>x+1/2, -y, -z</td>
<td>c x, 0, z</td>
<td>(1 0 0 0)</td>
<td>0 -1 0 0</td>
<td>0 0 -1 0</td>
<td>(1 0 0 0)</td>
<td>0 -1 0 0</td>
<td>0 0 -1 0</td>
</tr>
<tr>
<td>5</td>
<td>x+1/2, y+1/2, z</td>
<td>x, y+1/2, z +1/2</td>
<td>t (1/2, 1/2, 0)</td>
<td>(1 0 0 0)</td>
<td>0 1 0 0</td>
<td>1/2</td>
<td>(1 0 0 0)</td>
<td>0 1 0 0</td>
<td>1/2</td>
</tr>
<tr>
<td>6</td>
<td>-x+1/2, y+1/2, -z +1/2</td>
<td>-x+1/2, -y+1/2, z +1/2</td>
<td>2 (0, 1/2, 0) 1/4, y, 1/4</td>
<td>(1 0 0 0)</td>
<td>0 1 0 0</td>
<td>1/2</td>
<td>(1 0 0 0)</td>
<td>0 1 0 0</td>
<td>1/2</td>
</tr>
<tr>
<td>7</td>
<td>-x+1/2, -y+1/2, -z</td>
<td>-x, -y+1/2, -z +1/2</td>
<td>-1 1/4, 1/4, 0</td>
<td>(1 0 0 0)</td>
<td>0 -1 0 0</td>
<td>0 0 -1 0</td>
<td>(1 0 0 0)</td>
<td>0 -1 0 0</td>
<td>0 0 -1 0</td>
</tr>
<tr>
<td>8</td>
<td>x+1/2, -y+1/2, z +1/2</td>
<td>x+1/2, y+1/2, -z +1/2</td>
<td>n (1/2, 0, 1/2) 1/4, x, z</td>
<td>(1 0 0 0)</td>
<td>0 -1 0 0</td>
<td>0 0 -1 0</td>
<td>(1 0 0 0)</td>
<td>0 -1 0 0</td>
<td>0 0 -1 0</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 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:

Standard/Default Setting

Non Conventional Setting

ITA Settings

ITA-Settings for the Space Group 68

These must be read by columns. P is the transformation f

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

<table>
<thead>
<tr>
<th>ITA number</th>
<th>Setting</th>
<th>P</th>
<th>P⁻¹</th>
</tr>
</thead>
<tbody>
<tr>
<td>68</td>
<td>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 [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 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 $P112_1/a$ (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.
Problem 2.25

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}-\textit{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 \((a',b',c') = \frac{1}{2}(-a+b+c,a-b+c,a+b-c)\)