Fundamentals. Crystal patterns and crystal structures. Lattices, their symmetry and related basic concepts

Didactic material for the MaThCryst schools

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Ideal vs. real crystal, perfect vs. imperfect crystal

Ideal crystal:
Perfect periodicity, no static (vacancies, dislocations, chemical heterogeneities, even the surface!) or dynamic (phonons) defects.

Real crystal:
A crystal whose structure differs from that of an ideal crystal for the presence of static or dynamic defects.

Perfect crystal:
A real crystal whose structure contains only equilibrium defects.

Imperfect crystal:
A real crystal whose structure contains also non-equilibrium defects (dislocations, chemical heterogeneities...).

What follows describes the structure of an ideal crystals (something that does not exist!), whereas a real crystal is rarely in thermodynamic equilibrium.
What do you get from a (conventional) diffraction experiment?

Time and space averaged structure!

“Time-averaged” because the time span of a diffraction experiment is much larger that the time of an atomic vibration.

The instantaneous position of an atom is replaced by the envelop (most often an ellipsoid) that describes the volume spanned by the atom during its vibration.

“Space-averaged” because a conventional diffraction experiment gives the average of the atomic position in the whole crystal volume, which corresponds to “the” position of the atom only if perfect periodicity is respected.

Importance of studying the “ideal” crystal

Non-conventional experiments (time-resolved crystallography, nanocrystallography etc.) allow to go beyond the ideal crystal model, but also some information that are often neglected in a conventional experiment (diffuse scattering) can give precious insights on the real structure of the crystal under investigation.
Space and time-averaged structure
Transformations

An affine transformation is a deformation that sends corners to corners, parallel lines to parallel lines, mid-points of edges to mid-point of edges but does not preserves distances or angles.

An isometry is a special case of affine transformation which is not a deformation: the object on which it acts can change its orientation and position in space.

A symmetry operation is a special case of isometry: the object on which it acts can change its orientation and position in space only in such a way that its configuration (position, orientation) after the action cannot be distinguished from its configuration before the action.
Symmetry operations of a crystal pattern

• A crystal pattern is an idealized crystal structure which makes abstraction of the defects (including the surface!) and of the atomic nature of the structure.
• A crystal pattern is therefore infinite and perfect.
• A crystal pattern has both translational symmetry and point symmetry; these are described by its space group.
• We have to define the concepts of group and its declinations in crystallography.
Elements and operations

- **geometric element**: the point, line or plane left invariant by the symmetry operation.
- **symmetry element**: the geometric element defined above together with the set of operations (called **element set**) that leave in invariant.
- **symmetry operation**: an isometry that leave invariant the object to which it is applied.

The operation that share a given geometric element differ by a lattice vector. The one characterized by the shortest vector is called **defining operation**.
Crystal structure/pattern vs. crystal lattice

Crystal pattern (crystal structure)

Molecule or coordination polyhedron

Unit cell

Lattice nodes

Translations
Example of crystal pattern which is not a crystal structure
The minimal unit you need to describe a crystal pattern

Asymmetric unit*

Unit cell

*In mathematics, it is called “fundamental region”
Symmetry operations are classified into **first kind** (keep the handedness) and **second kind** (change the handedness).

If the object on which the operation is applied is non-chiral, the effect of the operation on the handedness is not visible but the **nature of the operation** (first or second kind) is not affected!

The **determinant** of the matrix representation of a symmetry operation is $+1$ (first kind) or $-1$ (second kind).

**Chirality**: property of an object not being superimposable to its mirror image by a first-kind operation.

**Handedness**: one of the two configurations (left or right) of chiral object. Also known as **chirality sense**.
Handedness of the object and nature of the operation
Crystal structure, fractional atomic coordinates, crystallographic orbits, Wyckoff positions

Crystal structure: atomic distribution in space that complies with the order and periodicity of the crystal

**Fractional atomic coordinates**: atomic coordinates $x,y,z$ within a unit cell with respect to the basis vectors $a,b,c$.

- $a,b,c$ (bold): basis vectors
- $a,b,c$ (italics): reference axes and cell parameters
- $x,y,z$ (italics): fractional atomic coordinates

Don’t forget the translations!

**Crystallographic orbit**: the infinite set of atoms obtained by applying all the symmetry operations of the space group to a given atom in the unit cell.

**Wyckoff positions**: classification of the crystallographic orbits on the basis of the symmetry of the atomic positions (site-symmetry group) (N to 1 mapping) *.

*More about this follows.
Global vs. local domain of action

**Φ_{pp}** local operations: act only on a specific substructure

**Φ_{qp}** partial operations: relate only a specific pair of substructures

Global (total) operations: that subset of local and partial operations that actually act on the whole structure
A binary operation $\circ$

An “internal law of composition” $S \circ S \rightarrow S$
*(closure property)*

A set $S$

**We've got a “magma”**

**Note:** An “external law of composition” acts on two disjoint sets $S \circ S' \rightarrow S$
Associativity: \( a \circ (b \circ c) = (a \circ b) \circ c \)

Presence of identity (neutral element):
left identity \( e \circ a = a \)
right identity \( a \circ e = a \)

Presence of singular element:
left singular \( s \circ a = s \)
right singular \( a \circ s = s \)

Presence of the inverse (symmetric) element of each element:
left inverse: \( a^{-1} \circ a = e \)
right inverse: \( a \circ a^{-1} = e \)

Commutativity: \( a \circ b = b \circ a \)

Presence of a second binary operation: \( a \in S \star b \in S = c \in S \)
## Algebraic structures

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<thead>
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<th>Globality</th>
<th>Associativity</th>
<th>Identity</th>
<th>Inverse Element</th>
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A symmetry group \((G, \circ)\) is a set \(G\) whose elements are symmetry operations having the following features:

- the combination \(\circ\) (successive application) of two symmetry operations \(g_i\) and \(g_j\) of the set \(G\) is still a symmetry operation \(g_k\) of the set \(G\) (closure property): \(g_i \in G \circ g_j \in G \rightarrow g_k \in G\) \((g_i g_j = g_k)\)
- the binary operation is associative: \(g_i (g_j g_k) = (g_i g_j) g_k\)
- the set \(G\) includes the identity (left and right identical): \(eg_i = g_i e\)
- for each element of the set \(G\) (each symmetry operation) the inverse element (inverse symmetry operation) is in the set \(G\): \(g_i^{-1} g_i = g_i g_i^{-1} = e\)

In the following we will normally speak of a **group** \(G\): it is a shortened expression for group \((G, \circ)\) where \(\circ\) is the “successive application” of symmetry operations \(g \in G\). Rigorously speaking, \(G\) is not a group but just a set!
A special case of Abelian groups: cyclic groups

A cyclic group is a special Abelian group in which all elements of the group are generated from a single element (the generator).

\[ G = \{ g, g^2, g^3, \ldots, g^n = e \} \]
The notion of “order”

**Order of a group element:** the smallest $n$ such that $g^n = e$.

If $n = 2$, then $g^{-1} = g$ and the element is known as an *involution*.

**Order of a group:** the number of elements of the group (finite or infinite)

If $n = \infty$ the group is infinite.
Let $G$ and $H$ be two sets, and $*$ and $#$ two binary operations acting on $G$ and $H$ respectively.

The mapping $f : G \rightarrow H$ that satisfies the relation $f(u * v) = f(u) # f(v)$ is called a **homomorphism**.

- If $G$ contains the neutral element $1_G$, then $H$ too contains a neutral element $1_H$ and the homomorphism $f$ maps them: $1_G \rightarrow 1_H$
- If $G$ contains the inverse of each element $g$, then $H$ too contains the inverse of each element $h$, and the homomorphism $f$ maps the respective elements: $f(u^{-1}) = u'^{-1} = f(u)^{-1}$.

If $H \subseteq G$, the homomorphism takes the name of **endomorphism**.
The **kernel** of the homomorphism $f: G \rightarrow H$ is the subset of elements of $G$ that is mapped by $f$ on to neutral element of $H$.

$$\text{ker } f = \{ g \in G : f(g) = 1_H \}$$

The **image** of the homomorphism $f: G \rightarrow H$ is the set of elements of $G$ that are mapped by $f$ on $H$. The image may coincide with the codomain or be a subset of it.
A 1:1 mapping \( f : G \to H \) is called an isomorphism. For an isomorphism \( \ker(f) = 1 \).

We are especially interested in isomorphic groups, which have the same structure but differ only for the labelling of the elements.
### Dimensions of the space and periodicity of the pattern

$$G^n_m$$ n-dimensional space, m-dimensional periodicity

- **$m = 0$: point groups**
- **$n = m$: space groups**
- **$0 < m < n$: subperiodic groups**

<table>
<thead>
<tr>
<th>$n$</th>
<th>$m$</th>
<th>No. of types of groups</th>
<th>Name</th>
</tr>
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<tbody>
<tr>
<td>1</td>
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<td>1-dimensional point groups</td>
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<tr>
<td></td>
<td>1</td>
<td>2</td>
<td>Line groups: 1-dimensional space groups</td>
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<tr>
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<td>0</td>
<td>10</td>
<td>2-dimensional point groups</td>
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<td>1</td>
<td>7</td>
<td>Frieze groups</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>17</td>
<td>Plane groups, wallpaper groups: 2-dimensional space groups</td>
</tr>
<tr>
<td>3</td>
<td>0</td>
<td>32</td>
<td>3-dimensional point-groups</td>
</tr>
<tr>
<td></td>
<td>1</td>
<td>75</td>
<td>Rod groups</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>80</td>
<td>Layer groups</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>230</td>
<td>(3-dimensional) Space groups</td>
</tr>
</tbody>
</table>
Symmetry group of the crystal

**Space group**: shows the symmetry of the crystal structure and is obtained as intersection of eigensymmetries that build up the structure.

\[ G = \bigcap_i E_i \]

**Translation group**: the group containing only the translations of the crystal structure. It is a normal subgroup of the space group \( G \).

\[ T \triangleleft G \rightarrow \forall t_j \in T, g_i \in G : g_i t_j g_i^{-1} = t_j \]

**Point group**: shows the morphological symmetry of the crystal as well as the symmetry of its physical properties. It is isomorphic to the factor group of the space group and its translation subgroup.

\[ P \cong G/T \]

Some of the definitions will follow
Bravais lattices

- Bravais lattices are sets of (zero-dimensional) points (nodes).
- The lattice nodes are (quite obviously…) different from atoms. **Warning:** In the literature, this difference is often overlooked!
- The space group of a Bravais lattice is a Bravais group (B).
- The subgroup $T$ of $B$ which contains, apart from the identity, only the translations of $B$, is the translation subgroup.
- The subgroup $H$ of $B$ obtained by removing all the translations from $B$ is isomorphic to the point group $P$ of the lattice.

\[ B = \{(W,w)\}\]  \[ T = \{(I,w)\}\]  \[ H = \{(W,0)\}\]  \[ P = \{W\}\]  

The minimal point group of a Bravais lattice is built on $\{I,-I\}$.

\[ W = n \times n \text{ matrix, } I = n \times n \text{ identity matrix, } w = n \times 1 \text{ matrix, } 0 = n \times 1 \text{ zero matrix} \]
The minimal point group of a Bravais lattice is built on \( \{I, -I\} \).

1-dimensional space: \( x \to \bar{x}: -I = \text{reflection (or inversion)} \)

2-dimensional space: \( xy \to \bar{xy}: -I = \text{rotation} \)

3-dimensional space: \( xyz \to \bar{xyz}: -I = \text{inversion} \)

etc....
-I in $E^n$

$$\begin{bmatrix}
\begin{array}{cccc}
\bar{1} & & & \\
& \bar{1} & & \\
& & \bar{1} & \\
& & & \ldots \\
& \ldots & & \\
& & & \bar{1}
\end{array}
\end{bmatrix}
\begin{bmatrix}
x \\
y \\
z \\
w
\end{bmatrix}
\rightarrow
\begin{bmatrix}
-x \\
-y \\
-z \\
-w
\end{bmatrix}$$

$\det(-I_n) = (-1)^n$

Odd-dimensional space: -1

Even-dimensional space: +1

Second kind operation

First kind operation

The inversion does not exist in even-dimensional spaces
One-dimensional lattices

Symmetry operations

Identity
Translations
Reflections

How many 1D lattices are there? Infinite!

How many types of 1D lattice are there? One

$I = 1, -I = m \Rightarrow$ point group of a Bravais lattice: $m = \{1, m\}$
The world in two dimensions

E² : the two-dimensional Euclidean space
Symmetry operations in $E^2$

Operations that leave invariant all the space (2D): the identity
Operations that leave invariant one direction of the space (1D): reflections
Operations that leave invariant one point of the space (0D): rotations
Operations that do not leave invariant any point of the space: translations

The subspace left invariant (if any) by the symmetry operation has dimensions from 0 to $N$ (= 2 here)

Two independent directions in $E^2$ $\Rightarrow$ two axes ($a$, $b$) and one interaxial angle ($\gamma$)

$I = 1$, $-I = 2$ $\Rightarrow$ Minimal point group of a Bravais lattice: 2 = \{1, 2\}
### Symmetry elements in $E^2$

<table>
<thead>
<tr>
<th>Graphic symbol</th>
<th>Hermann-Mauguin symbol</th>
<th>Meaning</th>
<th>Graphic symbol</th>
<th>Hermann-Mauguin symbol</th>
<th>Meaning</th>
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<tbody>
<tr>
<td>2</td>
<td>2-fold rotation point</td>
<td></td>
<td></td>
<td>$m$</td>
<td>Reflection line (mirror)</td>
</tr>
<tr>
<td>3</td>
<td>3-fold rotation point</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>4-fold rotation point</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>6-fold rotation point</td>
<td></td>
<td></td>
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</tbody>
</table>

*Operations obtained as combination with a translation are introduced later*

The orientation in space of a reflection line is always expressed with respect to the lattice direction to which it is perpendicular.
Lattice node coordinates $uv$, lattice direction indices $[uv]$
Choice of the unit cell

- Red: $t(1,0), t(0,1)$
- Green: $t(1,0), t(0,1), t(\frac{1}{2},\frac{1}{2})$
- Orange: $t(1,0), t(0,1), t(\frac{2}{3},\frac{1}{3}), t(\frac{1}{3},\frac{2}{3})$
- Brown: $t(1,0), t(0,1), t(\frac{3}{4},\frac{1}{4}), t(\frac{1}{2},\frac{1}{2}), t(\frac{1}{4},\frac{3}{4})$
Change of reference

\[
\begin{bmatrix}
1 & 1 \\
0 & 1
\end{bmatrix}
\quad \begin{bmatrix}
1 & 1 \\
0 & 1
\end{bmatrix}
\quad \begin{bmatrix}
1 & \frac{1}{2} \\
\frac{1}{2} & 1
\end{bmatrix}
\quad \begin{bmatrix}
\frac{1}{2} & \frac{1}{2} \\
\frac{1}{2} & \frac{1}{2}
\end{bmatrix}
\]

Determ.: 1

\[
\begin{bmatrix}
2 & 0 \\
\frac{1}{2} & 1
\end{bmatrix}
\quad \begin{bmatrix}
\frac{1}{2} & 0 \\
\frac{1}{2} & 1
\end{bmatrix}
\quad \begin{bmatrix}
\frac{1}{2} & \frac{1}{2} \\
\frac{1}{2} & \frac{1}{2}
\end{bmatrix}
\quad \begin{bmatrix}
\frac{1}{2} & \frac{1}{2} \\
\frac{1}{2} & \frac{1}{2}
\end{bmatrix}
\]

Determ.: 2

\[
\begin{bmatrix}
1 & \frac{1}{2} \\
\frac{1}{2} & \frac{1}{2}
\end{bmatrix}
\quad \begin{bmatrix}
\frac{1}{2} & 0 \\
\frac{1}{2} & 1
\end{bmatrix}
\quad \begin{bmatrix}
\frac{1}{2} & \frac{1}{2} \\
\frac{1}{2} & \frac{1}{2}
\end{bmatrix}
\quad \begin{bmatrix}
\frac{1}{2} & \frac{1}{2} \\
\frac{1}{2} & \frac{1}{2}
\end{bmatrix}
\]

Determ.: 2

\[
\begin{bmatrix}
2 & 0 \\
\frac{1}{2} & 1
\end{bmatrix}
\quad \begin{bmatrix}
\frac{1}{2} & 0 \\
\frac{1}{2} & 1
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\quad \begin{bmatrix}
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\]

Determ.: 2

\[
\begin{bmatrix}
1 & \frac{1}{2} \\
\frac{1}{2} & \frac{1}{2}
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\end{bmatrix}
\quad \begin{bmatrix}
\frac{1}{2} & \frac{1}{2} \\
\frac{1}{2} & \frac{1}{2}
\end{bmatrix}
\]

Determ.: 2
Change of the unit cell (cont.)

t(1,0), t(0,1): **primitive** (*p*) unit cell
t(1,0), t(0,1), t(½,½): **centred** (*c*) unit cell

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Cartesian (orthonormal) cell:
unsuitable (in general)

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**Conventional unit cell**
1. Edges of the cell are parallel to the symmetry directions of the lattice (if any);
2. If more than one unit cell satisfies the above condition, the smallest one is the conventional cell.

---

**Reduced cell** (Lagrange-Gauss reduction)
1. Basis vectors correspond to the shortest lattice translation vectors;
2. \(|a| \leq |b|, |b| \leq |b+qa|, q\) any integer. For \(q = \pm 1\), this condition means that the sides of the unit cell are not longer than its diagonals.
Lattice node coordinates $uv$, lattice direction indices $[uv]$
Exercise:
Find the lattice symmetry and \textit{then} choose a suitable unit cell
Exercise:
Find the lattice symmetry and *then* choose a suitable unit cell
Exercise:
Find the lattice symmetry and *then* choose a suitable unit cell
Exercise:
Find the lattice symmetry and *then* choose a suitable unit cell
Exercise:
Find the lattice symmetry and \textbf{then} choose a suitable unit cell

no symmetry direction for this lattice
point group of the lattice: 2 = \{I, -I\}
no symmetry restriction on the cell parameters: 
a; b; \gamma
Exercise:
Find the lattice symmetry and \textit{then} choose a suitable unit cell
Exercise:
Find the lattice symmetry and \textit{then} choose a suitable unit cell

two symmetry directions for this lattice, that are taken as axes $a$ and $b$

point group of the lattice: $2 \, m \, m$

symmetry restriction on the cell parameters: $a; b; \gamma = 90^\circ$

Conventional unit cell

Primitive unit cell
Exercise:
Find the lattice symmetry and \textit{then} choose a suitable unit cell
Exercise:
Find the lattice symmetry and then choose a suitable unit cell

two symmetry directions for this lattice, that are taken as axes $a$ and $b$

point group of the lattice: $2 \overline{m} m$

[10][01]

symmetry restriction on the cell parameters: $a; b; \gamma = 90^\circ$

Conventional (primitive) unit cell
Exercise:
Find the lattice symmetry and *then* choose a suitable unit cell
Exercise:
Find the lattice symmetry and \textit{then} choose a suitable unit cell

This lattice has four symmetry directions. Those corresponding to the shortest period are taken as axes $a_1$ and $a_2$. 
Exercise:
Find the lattice symmetry and \textit{then} choose a suitable unit cell.

This lattice has four symmetry directions. Those corresponding to the shortest period are taken as axes $a_1$ and $a_2$. 
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Exercise:
Find the lattice symmetry and \textit{then} choose a suitable unit cell.
Exercise:
Find the lattice symmetry and *then* choose a suitable unit cell

Point group of the lattice symmetry: $4 \text{m m}$

$\langle 10 \rangle \langle 1\bar{1} \rangle$
Exercise:
Find the lattice symmetry and \textit{then} choose a suitable unit cell

Point group of the lattice symmetry: \(4 \text{\,}_m \text{\,}_m\)

\(a, a_1\) \(b, a_2\)

\(p\) cell (conventional)

\(\langle 10 \rangle \langle 1\bar{1} \rangle\)
Exercise:
Find the lattice symmetry and \textit{then} choose a suitable unit cell.

Restrictions on cell parameters: \(a = b; \gamma = 90^\circ\)
Exercise:
Find the lattice symmetry and *then* choose a suitable unit cell

This lattice has six symmetry directions. Two among the three corresponding to the shortest period are taken as axes $a_1$ et $a_2$. 
Exercise:
Find the lattice symmetry and *then* choose a suitable unit cell.
Exercise:
Find the lattice symmetry and \textit{then} choose a suitable unit cell

Point group of the lattice:
\[ 6 \ m \ m \]

Restrictions on the cell parameters:
\[ a = b; \ \gamma = 120^\circ \]
Direction indices \([uv]\) in the hexagonal lattice of \(E^2\)
Why not 5, then?
Crystal patterns in 2D
The concept of holohedry

Symmetry of the lattice: $S_L = 4mm$

Symmetry of the object: $S_o = 4mm$

Symmetry of the pattern: $S_p = 4mm$

$Lattice$

« Object » (content of the unit cell)

$Pattern$

$S_p = S_L$: holohedry
The concept of holohedry

Symmetry of the lattice: $S_L = 4mm$

Symmetry of the object: $S_o = 3m$

Symmetry of the pattern: $S_p = m = 4mm \cap 3m$

$S_p < S_L : \text{merohedry}$
The concept of holohedry

Symmetry of the lattice: $S_L = 4mm$

Symmetry of the object: $S_o = 3m$

Symmetry of the pattern: $S_p = 1 = 4mm \cap 3m$

$S_p < S_L$: merohedry
The concept of holohedry

The crystallographic restriction \((n = 1, 2, 3, 4, 6)\) applies to the lattice and to the pattern, but not to the content of the unit cell!

Symmetry of the lattice: \(S_L = 4mm\)

Symmetry of the object: \(S_o = 5m\)

Symmetry of the pattern: \(S_p = m = 4mm \cap 5m\)

\[ S_p < S_L : \text{merohedry} \]
The notion of subgroup
Exercise: find the elements, the operations and the symmetry group of a square in E^2

Geometric elements: one point (centre of the square), four lines ([10], [01], [11], [11])

Symmetry elements: one fourfold rotation point: 4
four reflection lines: \( m_{[10]} \), \( m_{[01]} \), \( m_{[11]} \), \( m_{[1\bar{1}]} \)

Symmetry operations:
Four rotations (\( 4^1, 4^2 = 2, 4^3 = 4^{-1}, 4^4 = 1 \))
Four reflections (\( m_{[10]} \), \( m_{[01]} \), \( m_{[11]} \), \( m_{[1\bar{1}]} \))

Check that these operations do form a group

- Isometries are always associative
- The identity belong to the set (it corresponds to \( 4^4 \) and \( m^2 \))
- The inverse of each operation belongs to the set (\( 1^{-1} = 1; m^{-1} = m; 2^{-1} = 2, 4^{-1} = 4^3 \))
- To check the closure, let us build the multiplication (Cayley) table.
From the group \((G, \circ)\) we select a subset of elements forming a subset \(H\). If the \((H, \circ)\) is a group under the same binary operation \(\circ\) as \((G, \circ)\), then \((H, \circ)\) is a subgroup of \((G, \circ)\).
Order and index of a subgroup

group $G$, order $|G|$

$H \subseteq G$

group $H$, order $|H|$

$|H|$ is a divisor of $|G|$ (Lagrange’s theorem)

The ratio $i_G(H) = |G|/|H|$ is called the index of $H$ in $G$

$i_G(H) = 2$: hemihedry
$i_G(H) = 4$: tetartohedry
$i_G(H) = 8$: ogdohedry (3-dimensional space)
By decomposing \((G, \circ)\) with respect to \((H, \circ)\) we get \(i = |G|/|H|\) cosets. Each coset has the same number of elements \(|H|\) as the subgroup, which is called the length of the coset.
By decomposing \((G, \circ)\) with respect to \((H, \circ)\) we get \(i = |G|/|H|\) cosets. Each coset has the same number of elements \(|H|\) as the subgroup, which is called the length of the coset.
## Desymmetrization of the square

<table>
<thead>
<tr>
<th>Order</th>
<th>Index</th>
<th>(4mm) = {1, 4^1, 2, 4^3, m_{[10]}, m_{[01]}, m_{[11]}, m_{[1\overline{1}]}}</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>1</td>
<td>{1, 4^1, 2, 4^3} = 4 {1, 2, m_{[10]}, m_{[01]}} = 2mm. {1, 2, m_{[11]}, m_{[1\overline{1}]}} = 2.mm</td>
</tr>
<tr>
<td>4</td>
<td>2</td>
<td>{1, 4^1, 2, 4^3} = 4 {1, 2, m_{[10]}, m_{[01]}} = 2mm. {1, 2, m_{[11]}, m_{[1\overline{1}]}} = 2.mm</td>
</tr>
<tr>
<td>2</td>
<td>4</td>
<td>{1, 2} = 2 {1, m_{[10]}} = .m. {m_{[01]}} = .m. {1, m_{[11]}} = ..m {1, m_{[1\overline{1}]}} = ..m</td>
</tr>
<tr>
<td>1</td>
<td>8</td>
<td>{1} = 1</td>
</tr>
</tbody>
</table>
Desymmetrization of the square

<table>
<thead>
<tr>
<th>Order</th>
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<tbody>
<tr>
<td>8</td>
<td>1</td>
</tr>
<tr>
<td>4</td>
<td>2</td>
</tr>
<tr>
<td>2</td>
<td>4</td>
</tr>
<tr>
<td>1</td>
<td>8</td>
</tr>
</tbody>
</table>
Cosets
Conjugacy classes
Conjugate subgroups
Normal or invariant subgroups
Left and right cosets

\[ G = H \cup_{i} C_{i} = H \cup_{i} g_{i} H, \ g_{i} \notin (H,C_{j \neq i}) \]  
Left coset

\[ G = 4mm = \{1, 4^1, 4^2 = 2, 4^3 = 4^{-1}, m_{[10]}, m_{[01]}, m_{[11]}, m_{[1\overline{1}]}\} \]

\[ H = 2mm. \]

\[ 4mm = \{2mm.\} \cup g \notin \{2mm.\} = \{1, 2, m_{[10]}, m_{[01]}\} \cup \{4^1, 4^3, m_{[11]}, m_{[1\overline{1}]}\} \]

\[ H = 2.mm \]

\[ 4mm = \{2.mm\} \cup g \notin \{2.mm\} = \{1, 2, m_{[11]}, m_{[1\overline{1}]}\} \cup \{4^1, 4^3, m_{[10]}, m_{[01]}\} \]

\[ H = 4 \]

\[ 4mm = \{4\} \cup g \notin \{4\} = \{1, 4^1, 2, 4^3\} \cup \{m_{[10]}, m_{[01]}, m_{[11]}, m_{[1\overline{1}]}\} \]

Etc. etc.

\[ G = H \cup_{i} C_{i} = H \cup_{i} Hg_{i}, \ g_{i} \notin (H,C_{j \neq i}) \]  
Right coset

Usually, \( g_{i}H \neq Hg_{i} \)

If \( g_{i}H = Hg_{i}, \ \forall i \), then \( H \) is called a \textbf{normal (invariant) subgroup}. 
Decomposition of $4mm$ with respect to 2 and $m_{[10]}$

$$4mm = \{1,2\} \cup 4^1\{1,2\} \cup m_{[10]}\{1,2\} \cup m_{[11]}\{1,2\} =$$

$$\{1,2\} \cup \{4^1,4^3\} \cup \{m_{[10]},m_{[01]}\} \cup \{m_{[11]},m_{[1\bar{1}]}\}$$

$$4mm = \{1,2\} \cup \{1,2\}4^1 \cup \{1,2\}m_{[10]} \cup \{1,2\}m_{[11]} =$$

$$\{1,2\} \cup \{4^1,4^3\} \cup \{m_{[10]},m_{[01]}\} \cup \{m_{[11]},m_{[1\bar{1}]}\}$$

$$4mm = \{1,m_{[10]}\} \cup 4^1\{1,m_{[10]}\} \cup 4^3\{1,m_{[10]}\} \cup 2\{1,m_{[10]}\} =$$

$$\{1,m_{[10]}\} \cup \{4^1,m_{[11]}\} \cup \{4^3,m_{[1\bar{1}]}\} \cup \{2,m_{[01]}\}$$

$$4mm = \{1,m_{[10]}\} \cup \{1,m_{[10]}\}4^1 \cup \{1,m_{[10]}\}4^3 \cup \{1,m_{[10]}\}2 =$$

$$\{1,m_{[10]}\} \cup \{4^1,m_{[1\bar{1}]}\} \cup \{4^3,m_{[11]}\} \cup \{2,m_{[01]}\}$$
Conjugate and normal subgroups

\( H \subset G \)

\( gh_i g^{-1} = h_j ; \quad h_i \in H, \ \forall g \in G : \text{conjugate elements} \)

Conjugation is a similarity transformation: “do the same thing somewhere else”

\( gh_i = h_j g ; \quad h_i \in H, \ \forall g \in G \)

If \( h_i = h_j, \ \forall g \in G, \ h_i \) is a \textbf{self-conjugate element}

The set of conjugate elements form a class \( \bigcup_i g_i h g_i^{-1} = \text{Cl}(h) \) \textbf{conjugacy class}

\[
\text{Cl}(h) = \{ h' \in G | \ \exists g \in G : h' = ghg^{-1} \}
\]

Next consider not one element \( h \) but the whole subgroup \( H \)

\( \bigcup_i g_i H g_i^{-1} = \{H, H', H'' \cdots \} \) are \textbf{conjugate subgroups} of \( G \)

If \( H' = H'' = \cdots = H \) \( (g_i H = H g_i, \ \forall g \in G) \), \( H \) is a \textbf{normal or invariant subgroup} of \( G \): \( H \triangleleft G \).
Conjugacy classes of $4mm$

$$\bigcup_i g_i h g_i^{-1} = \text{Cl}(h): \text{conjugacy class}$$

$h = 1$ \quad $\bigcup_i g_i 1 g_i^{-1} = \bigcup_i g_i g_i^{-1} = \{1\}$

$h = 2$ \quad $\bigcup_i g_i 2 g_i^{-1} = \{2\}$

$h = 4^1$ \quad $\bigcup_i g_i 4^1 g_i^{-1} = \{4^1, 4^3\}$

$h = m_{[10]}$ \quad $\bigcup_i g_i m_{[10]} g_i^{-1} = \{m_{[10]}, m_{[01]}\}$

$h = m_{[11]}$ \quad $\bigcup_i g_i m_{[11]} g_i^{-1} = \{m_{[11]}, m_{[1\bar{1}]}\}$

$4mm = \{1\}, \{2\}, \{4^1, 4^3\}, \{m_{[10]}, m_{[01]}\}, \{m_{[11]}, m_{[1\bar{1}]}\}$
When we apply an isometry • • •

The object is transformed directly \((O \rightarrow O')\)

The symmetry group of the object is transformed by conjugation

\[ hO = O, \quad h \in H \]
\[ h'O' = O', \quad h' \in H' \]
\[ gO = O', \quad g \notin H, H' \]

\[ H' = gHg^{-1} \]
Effects of the operations in a coset

\[ H = 2mm. = \{1, 2, m_{[10]}, m_{[01]} \} \]

\[ gHg^{-1} = H \implies H = 2mm. \triangleleft G = 4mm \]

Normal subgroup

\[ \{4^1, 4^3, m_{[11]}, m_{[1\bar{1}]} \} \]

\[ gHg^{-1} = 2mm. \]
Effects of the operations in a coset

\[ H = 2.mm = \{1, 2, m_{[11]}, m_{[1\bar{1}]}\} \]

\[ gHg^{-1} = H \implies H = 2.mm \triangleleft G = 4mm \]

Normal subgroup

\[ \{4^1, 4^3, m_{[10]}, m_{[01]}\} \]

\[ gHg^{-1} = 2.mm \]
**Effects of the operations in a coset**

$H = 4 = \{1, 4, 2, 4^3\}$

$gHg^{-1} = H \Rightarrow H = 4 \triangleleft G = 4mm$

Normal subgroup

$\{m_{[10]}, m_{[01]}, m_{[11]}, m_{[1\bar{1}]})\}$

$gHg^{-1} = 4$
Effects of the operations in a coset

\[ H = \{1, m_{[10]}\} \]
\[ gHg^{-1} = \{1, m_{[10]}\} \]
\[ g\{1,m_{[01]}\}g^{-1} = \{1,m_{[10]}\} \]
\[ \Rightarrow \{2, m_{[01]}\} \]

Conjugate subgroups

\[ \{4^1, m_{[1]}\} \]
\[ \{4^3, m_{[1]}\} \]
\[ \{4^1, m_{[1]}\} \]
\[ \{2, m_{[01]}\} \]
\[ gHg^{-1} = \{2, m_{[01]}\} \]
\[ gHg^{-1} = \{1, m_{[01]}\} \]
Desymmetrization of the square

Order | Index
--- | ---
8 | 1
4 | 2
2 | 4
1 | 8

Diagram:

```
Order
8
4
2
1

Index
1
2
4
8

Desymmetrization

4.mm

2.mm

.m_{[10]} m_{[01]}

.m_{[11]} m_{[1\bar{1}]}```

Massimo Nespolo, Université de Lorraine
Extra-simple exercise
Show that a subgroup of index 2 is always normal
Holohedries and merohedries in the two-dimensional space
Holohedry 2 : \{1,2\}  Conjugacy classes {1}, \{2\}

**Subgroup 1 : \{1\}**

Holohedry 2\text{\(\text{mm}\)} : \{1,2,m_{[10]},m_{[01]}\}

Conjugacy classes \{1\}, \{2\}, \{m_{[10]}\}, \{m_{[01]}\}

Subgroups 2 : \{1,2\}, \text{\(m\)} : \{1,m_{[10]}\}, \{1,m_{[01]}\}, 1 : \{1\}

Holohedry 4\text{\(\text{mm}\)} : \{1, 4^1, 4^2 = 2, 4^3 = 4^{-1}, m_{[10]}, m_{[01]}, m_{[11]}, m_{[1\overline{1}]}\}

Conjugacy classes \{1\}, \{2\}, \{4^1, 4^3\}, \{m_{[10]}, m_{[01]}\}, \{m_{[11]}, m_{[1\overline{1}]}\}

Subgroups 4 : \{1, 4^1, 4^2, 4^3\}, 2\text{\(\text{mm}\)} : \{1, 2, m_{[10]}, m_{[01]}\}, \{1, 2, m_{[11]}, m_{[1\overline{1}]}\}, 2 : \{1, 2\}, \text{\(m\)} : \{1,m_{[10]}\}, \{1,m_{[01]}\}, \{1,m_{[11]}\}, \{1,m_{[1\overline{1}]}\}, 1 : \{1\}

Holohedry 6\text{\(\text{mm}\)} : \{1, 6^1, 6^2 = 3, 6^3 = 2, 6^4 = 3^{-1}, 6^5 = 6^{-1}, m_{[10]}, m_{[01]}, m_{[11]}, m_{[1\overline{1}]}\}, m_{[12]}, m_{[21]}\}

Conjugacy classes:
\{1\}, \{2\}, \{3^1, 3^2\}, \{6^1, 6^5\}, \{m_{[10]}, m_{[01]}, m_{[11]}\}, \{m_{[1\overline{1}]}, m_{[12]}, m_{[21]}\}

Subgroups 6 : \{1, 6^1, 6^2, 6^3, 6^4, 6^5\}, 3\text{\(\text{m}\)} : \{1, 3^1, 3^2, m_{[10]}, m_{[01]}, m_{[11]}\}, \{1, 3^1, 3^2, m_{[1\overline{1}]}, m_{[12]}, m_{[21]}\}, 3 : \{1, 3, 3^{-1}\}, 2\text{\(\text{mm}\)} : \{1, 2, m_{[10]}, m_{[12]}\}, \{1, 2, m_{[01]}, m_{[21]}\}, \{1, 2, m_{[11]}, m_{[1\overline{1}]}\}, 2 : \{1,2\}, \text{\(m\)} : \{1,m_{[10]}\}, \{1,m_{[01]}\}, \{1,m_{[11]}\}, \{1,m_{[1\overline{1}]}\}, \{1,m_{[12]}\}, \{1,m_{[21]}\}, 1 : \{1\}
Tree of group-subgroups in $E^2$

Tree of maximal group-subgroups (in bold the holohedries)

- Normal subgroup
- Conjugate subgroups
Crystal families

Point-group types that satisfy the following criteria belong to the same crystal family:
1. they correspond to the same holohedry;
2. they are in group-subgroup relation;
3. the types of Bravais lattice on which they act have the same number of free parameters.

- **Tetragonal family**: 1 free parameter ($a$)
  - 4mm
  - 2mm

- **Hexagonal family**: 1 free parameter ($a$)
  - 6mm

- **Orthorhombic family**: 2 free parameters ($a, b$)
  - 6mm

- **Monoclinic family**: 3 free parameters ($a, b, \gamma$)
  - 2mm

The diagram illustrates the relationships between these families and their respective point-group types.
Conventional cell parameters and symmetry directions in the four crystal families of \( E^2 \)

**Monoclinic**
- point group 2 (minimal point group)
- No restriction on \( a, b, \gamma \)
- No symmetry direction

**Orthorhombic**
- point group 2\( \text{mm} \)
- No restriction on \( a, b \); \( \gamma = 90^\circ \)
- \([10]\) and \([01]\)

**Tetragonal**
- point group 4\( \text{mm} \)
- \( a = b \); \( \gamma = 90^\circ \)
- \( \langle 10 \rangle \) ([10] and [01])
- \( \langle 11 \rangle \) ([11] and [11])

**Hexagonal**
- point group 6\( \text{mm} \)
- \( a = b \); \( \gamma = 120^\circ \)
- \( \langle 10 \rangle \) ([10], [01] and [11])
- \( \langle 1\bar{1} \rangle \) ([21], [12] and [1\bar{1}])

Crystal families: **Monoclinic**, **Orthorhombic**, **Tetragonal**, **Hexagonal**

Type of lattice*: **Primitive**, **Centred**

---

*Lattice whose conventional unit cell is primitive or centred
Point-group types that act on the same types of Bravais lattices belong to the same crystal system.

<table>
<thead>
<tr>
<th>Type of group</th>
<th>$mp$</th>
<th>$op$</th>
<th>$oc$</th>
<th>$tp$</th>
<th>$hp$</th>
<th>Crystal system</th>
</tr>
</thead>
<tbody>
<tr>
<td>$2, 1$</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>monoclinic</td>
</tr>
<tr>
<td>$2mm, m$</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td></td>
<td>orthorhombic</td>
</tr>
<tr>
<td>$4mm, 4$</td>
<td></td>
<td></td>
<td></td>
<td>✓</td>
<td></td>
<td>tetragonal</td>
</tr>
<tr>
<td>$6mm, 6, 3m, 3$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>✓</td>
<td>hexagonal</td>
</tr>
</tbody>
</table>

No. of free parameters

<table>
<thead>
<tr>
<th></th>
<th>3</th>
<th>2</th>
<th>2</th>
<th>1</th>
<th>1</th>
</tr>
</thead>
</table>
Lattice systems

Point-group types that correspond to the same lattice symmetry belong to the same lattice system.

\[ 6mm, \ 6, \ 3m, \ 3 : \text{hexagonal lattice system} \]
\[ 4mm, \ 4 : \text{tetragonal lattice system} \]
\[ 2mm, \ m : \text{orthorhombic lattice system} \]
\[ 2, \ 1 : \text{monoclinic lattice system} \]
The world in three dimensions

\( \mathbb{E}^3 : \text{the three-dimensional Euclidean space} \)
Symmetry operations in $E^3$

Operations that leave invariant all the space ($3D$): the identity
Operations that leave invariant a plane ($2D$): the reflections
Operations that leave invariant one direction of the space ($1D$): the rotations
Operations that leave invariant one point of the space ($0D$): the roto-inversions
Operations that do not leave invariant any point of the space: the translations

The subspace left invariant (if any) by the symmetry operation has dimensions from 0 to $N$ (= 3 here)

Three independent directions in $E^3 \Rightarrow$ three axes ($a, b, c$) and three interaxial angles ($\alpha, \beta, \gamma$)

$I = 1, -I = \bar{1} \Rightarrow$ Minimal point group of a Bravais lattice: $\bar{1} = \{1, \bar{1}\}$
Inversion centre vs. inversion point

Rotoinversion: $\bar{n}$

On a mono-dimensional element (axis) a zero-dimensional element (point) exists:
- if $n$ is odd, the inversion operation exists as an independent operation and the corresponding element is called an inversion centre;
- if $n$ is even, the inversion operation does not exist as an independent operation and the corresponding element is an inversion point.

$\bar{3}$ (order 6)  

$\bar{4}$ (order 4)
Labelling of axes and angles in $\mathbb{E}^3$
### Graphic symbols for symmetry elements

<table>
<thead>
<tr>
<th>n-fold rotation axis</th>
<th>n-fold rotoinversion axis</th>
<th>n-fold rotation axis and mirror plane perpendicular to it</th>
</tr>
</thead>
<tbody>
<tr>
<td>♦ 2 2-fold rotation axis</td>
<td>○ $\overline{1}$ one-fold rotoinversion axis (inversion centre)</td>
<td>♦ 2/m</td>
</tr>
<tr>
<td>▲ 3 3-fold rotation axis</td>
<td>▲ $\overline{3}$ three-fold rotoinversion axis</td>
<td>♦ 4/m</td>
</tr>
<tr>
<td>◆ 4 4-fold rotation axis</td>
<td>◆ $\overline{4}$ four-fold rotoinversion axis</td>
<td>♦ 6/m</td>
</tr>
<tr>
<td>● 6 6-fold rotation axis</td>
<td>◇ $\overline{6}$ (3/m) six-fold rotoinversion axis</td>
<td></td>
</tr>
</tbody>
</table>

Two-fold rotoinversion axis is a mirror plane

First-kind operations

Operations including translations are introduced later

The orientation of a mirror plane is indicated by the vector normal to it

Second-kind operations
The orientation of a mirror plane is indicated by the vector normal to it.
An isometry of the second kind, \( f_{\Pi} \), can always be expressed as \( \overline{1} f_{\text{I}} \)

\[
f_{\Pi} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} \quad f_{\Pi} \left( \overline{1} \overline{1} \right) \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} \quad \text{Associativity} \quad \left( f_{\Pi} \overline{1} \right) \overline{1} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} x' \\ y' \\ z' \end{bmatrix}
\]

\[
f_{\text{I}} \overline{1} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} \quad \overline{1} f_{\text{I}} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} \quad \text{Commutativity} \quad \overline{1} = \begin{bmatrix} \overline{1} \\ \overline{1} \\ \overline{1} \end{bmatrix}
\]

If \( f_{\Pi} \) is a symmetry operation of a given object, and if that object is not centrosymmetric, \( f_{\text{I}} \) is not a symmetry operation of the object.
Equivalence of $\tilde{2}$ and $m$
Combination of 2 and $\bar{1}$ gives $m$

Applies to even-fold rotations as well, because they all “contain” a twofold rotation

$4^2 = 2; \ 6^3 = 2$
Choice of the unit cell

\[ t(1,0,0), t(0,1,0), t(0,0,1) : \textbf{Primitive cell} \ (P) \]
\[ t(1,0,0), t(0,1,0), t(0,0,1), t(\frac{1}{2},\frac{1}{2},0) : \textbf{B} \]
\[ t(1,0,0), t(0,1,0), t(0,0,1), t(\frac{1}{2},\frac{1}{2},0) : \textbf{C} \]
\[ t(1,0,0), t(0,1,0), t(0,0,1), t(\frac{1}{2},0,\frac{1}{2}) : \textbf{A} \]
\[ t(1,0,0), t(0,1,0), t(0,0,1), t(\frac{1}{2},0,\frac{1}{2}) : \textbf{I} \]
\[ t(1,0,0), t(0,1,0), t(0,0,1), t(\frac{1}{2},\frac{1}{2},\frac{1}{2}) : \textbf{F} \]
\[ t(1,0,0), t(0,1,0), t(0,0,1), t(\frac{2}{3},\frac{1}{3},0), t(\frac{1}{3},\frac{2}{3},\frac{1}{3}) : \textbf{H} \]
\[ t(1,0,0), t(0,1,0), t(0,0,1), t(\frac{2}{3},\frac{1}{3},\frac{1}{3}), t(\frac{1}{3},\frac{2}{3},\frac{2}{3}) : \textbf{D} \]
\[ t(1,0,0), t(0,1,0), t(0,0,1), t(\frac{2}{3},\frac{2}{3},\frac{2}{3}) : \textbf{R} \]

**Conventional unit cell**
1. the basis vectors \(a, b, c\) form a right-handed reference;
2. edges of the cell are parallel to the symmetry directions of the lattice (if any);
3. if more than one unit cell satisfies the above condition, the smallest one is the conventional cell.

**Reduced cell**
1. the basis vectors \(a, b, c\) form a right-handed reference;
2. its faces are two-dimensional reduced unit cells and its edges are not longer than its diagonals; concretely:
   a. basis vectors correspond to the shortest lattice translation vectors;
   b. the angles between pairs of basis vectors are either all acute (type I reduced cell) or non-acute (type II reduced cell).
Types of unit cells that bring a letter in \( \mathbb{E}^3 \)

\[ \begin{array}{c}
\text{P} & \text{C} & \text{B} & \text{A} \\
\text{I} & \text{F} & \text{R} & \text{H} & \text{D} \\
\end{array} \]

Seldom used
Crystal families and types of lattices in $E^3$: the triclinic (anorthic) family

+ a third direction inclined on the plane

2D $\rightarrow$ 3D

$2 \otimes \overline{1} = \overline{1}$

triclinic crystal family (anorthic)

- One symmetry element: the inversion centre
- No symmetry direction
- The conventional unit cell is not defined – no reason to choose $a priori$ a centred cell
- Point group of the lattice: $\overline{1}$
- No restriction on $a$, $b$, $c$, $\alpha$, $\beta$, $\gamma$
Crystal families and types of lattices in $\mathbb{E}^3$: the \textit{m}onoclinic family

- One symmetry direction (\textit{usually} taken as the $b$ axis).
- The conventional unit cell has two right angles ($\alpha$ and $\gamma$).
- Point group of the lattice: $2/m$.
- Two independent types of unit cell respect these conditions.
A lattice of type $mP$ is equivalent to $mB$

\[
\begin{align*}
  \mathbf{a}_P &= (\mathbf{a}_B - \mathbf{c}_B)/2 ; \\
  \mathbf{c}_P &= (\mathbf{a}_B + \mathbf{c}_B)/2
\end{align*}
\]
A lattice of type $mP$ is NOT equivalent to $mC$
Lattices of type \( mC, mA, mI \) and \( mF \) are all equivalent.
The symbol of a monoclinic space group will change depending on which setting and what type of unit cell you choose, leading to up to 21 possible symbols for a monoclinic space group (the "monoclinic monster").
Crystal families and types of lattices in $E^3$: the orthorhombic family

- Three symmetry directions (axes $a$, $b$, $c$)
- The conventional unit cell has three right angles ($\alpha$, $\beta$, $\gamma$)
- Point group of the lattice: $2/m\ 2/m\ 2/m$
- Four types of cell respect these conditions
- The unit cell with one pair of faces centred can be equivalently described as $A$, $B$ or $C$ by a permutation of the (collective symbol : $S$)

+ a third direction perpendicular to the plane

 orthorhombic crystal family

2D $\rightarrow$ 3D

$2mm$ $\rightarrow$ $2mm \otimes \bar{1} = 2/m2/m2/m$

- $oP$
- $oI$
- $oS$
- $oF$
Three possible setting for the $oS$ type of lattice in $E^3$
Crystal families and types of lattices in E³: the tetragonal family

- Five symmetry directions (c, a & b, the two diagonals in the a-b plane)
- Point group of the lattice: 4/m 2/m 2/m
- The conventional cell has three right angles and two identical edges
- Two independent types of unit cell respect these conditions: tP (equivalent to tC) and tI (equivalent to tF)

+a third direction perpendicular to the plane

tetragonal crystal family

- 2D → 3D
- 4mm → 4mm ⊗ 1
  = 4/m2/m2/m
Why unit cells of type \( tA \) et \( tB \) cannot exist?

4-fold axis!
Why unit cells of type \( tA \) et \( tB \) cannot exist?

4-fold axis!
Why unit cells of type $tA$ et $tB$ cannot exist?

4-fold axis!
Why unit cells of type \( tA \) et \( tB \) cannot exist?

4-fold axis!
Why unit cells of type $tA$ et $tB$ cannot exist?

4-fold axis!

$\begin{align*}
\text{tF!} & \quad \rightarrow \quad \text{tI!}
\end{align*}$
Crystal families and types of lattices in $\mathbb{E}^3$: the cubic family

+ a third direction perpendicular to the plane AND $c = a = b$

cubic crystal family

$cP$  $cI$  $cF$
Three-fold rotoinversion along the \langle111\rangle direction

- First and fourth plane from the observer
- Second plane from the observer
- Third plane from the observer
Crystal families and types of lattices in $E^3$: the cubic family

- Thirteen symmetry directions (the 3 axes; the 4 body diagonals; the six face diagonals)
- Point group of the lattice: $4/m \bar{3} 2/m$
- The conventional unit cell has three right angles and three identical edges
- Three types of unit cell respect these conditions: $cP$, $cI$ et $cF$
Crystal families and types of lattices in $\mathbb{E}^3$: the \textit{hexagonal} family

+ a third direction perpendicular to the plane

$2D \rightarrow 3D$

$6mm \rightarrow 6mm \otimes \tilde{1} = 6/m2/m2/m$

\textit{hexagonal} crystal family

+ a new type of unit cell!
Peculiarity of the hexagonal crystal family in $E^3$

Symmetry directions

$A_1, A_2, C$ hexagonal axes parallel to the symmetry directions

$a_1, a_2, a_3$ rhombohedral axes NOT parallel to the symmetry directions

Two types of lattice with different symmetry in the hexagonal crystal family
Symmetry difference between \( hP \) and \( hR \) types of lattice

\[
\begin{align*}
6/m2/m2/m & \quad \bar{3}2/m \\
[\bar{1}01]_R & \quad [\bar{1}10]_H \\
[0\bar{1}1]_R & \quad [0\bar{1}0]_H \\
[1\bar{1}0]_R & \quad [1\bar{1}0]_H \\
[010]_H & \quad [010]_H \\
[210]_H & \quad [\bar{1}10]_R \\
[110]_H & \quad [10\bar{1}]_R \\
[10\bar{1}]_R & \quad [210]_H \\
\end{align*}
\]

\( z = 0 \) \quad \( z = 1/3 \) \quad \( z = 2/3 \)
7 holohedries → 7 lattice systems but 6 crystal families

- **Hexagonal crystal family:** 2 free parameters ($a,c$ or $a,\alpha$)

- **Tetragonal**
  - $422$
  - $\overline{4}2m$
  - $4mm$
  - $\frac{2}{m}2\overline{m}m$

- **Cubic**
  - $4\overline{3}2$
  - $\overline{4}3m$
  - $\frac{2}{m}3$

- **Orthorhombic**
  - $222$
  - $m2$
  - $\frac{2}{m}$

- **Monoclinic**
  - $2$
  - $m$
  - $\overline{1}$

- **Triclinic**
  - $1$
Lattice systems: classification based on the symmetry of the lattices

- Triclinic: \( \bar{T} \)
- Monoclinic: \( 2/m \)
- Tetragonal: \( 4/m 2/m 2/m (4/mmm) \)
- Orthorhombic: \( 2/m 2/m 2/m (mmm) \)
- Hexagonal: \( 6/m 2/m 2/m (6/mmm) \)
- Rhombohedral: \( \bar{3} 2/m (\bar{3}m) \)
- Cubic: \( 4/m \bar{3} 2/m (m\bar{3}m) \)
Crystal systems: morphological (macroscopic) and physical symmetry

<table>
<thead>
<tr>
<th>Type of group (in bold the holohedries)</th>
<th>$aP$</th>
<th>$mP$</th>
<th>$mS$</th>
<th>$oP$</th>
<th>$oS$</th>
<th>$oI$</th>
<th>$oF$</th>
<th>$tP$</th>
<th>$tI$</th>
<th>$hR$</th>
<th>$hP$</th>
<th>$cP$</th>
<th>$cI$</th>
<th>$cF$</th>
<th>Crystal system</th>
</tr>
</thead>
<tbody>
<tr>
<td>1, $\bar{1}$</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
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<td>✓</td>
<td>✓</td>
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<tr>
<td>2, $m$, $2/m$</td>
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<td>✓</td>
<td>✓</td>
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<td>✓</td>
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<td>✓</td>
<td>✓</td>
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<tr>
<td>222, $mm2$, $2/m2/m2/m$</td>
<td>✓</td>
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<td>✓</td>
</tr>
<tr>
<td>4, $4$, $422$, $42m$, $4/m$, $4mm$, $4/m2/m2/m$</td>
<td>✓</td>
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<tr>
<td>3, $\bar{3}$, $3m$, $32$, $\bar{3}2/m$</td>
<td>✓</td>
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<tr>
<td>6, $\bar{6}$, $622$, $\bar{6}2m$, $6/m$, $6mm$, $6/m2/m2/m$</td>
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</tr>
<tr>
<td>23, $m\bar{3}$, $432$, $43m$, $4/m\bar{3}2/m$</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
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<tr>
<td>No. of free parameters</td>
<td>6</td>
<td>4</td>
<td>4</td>
<td>3</td>
<td>3</td>
<td>3</td>
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<td>2</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>1</td>
</tr>
</tbody>
</table>
Crystal systems: morphological (macroscopic) and physical symmetry

- Triclinic: $A_1$, 1 or $\overline{1}$
- Monoclinic: $A_2$, 2 or $m$ or $2/m$
- Orthorhombic: $3 \times A_2$, Three twofold elements
- Tetragonal: $A_4$
- Trigonal: $A_3$
- Hexagonal: $A_6$
- Cubic: $4 \times A_3$

$A_n = n$ or $\overline{n}$
### Crystal families, crystal systems, lattice systems and types of Bravais lattices in $E^3$

<table>
<thead>
<tr>
<th>6 crystal families</th>
<th>conventional unit cell</th>
<th>7 crystal systems (morphological symmetry)</th>
<th>7 lattice systems (lattice symmetry)</th>
<th>14 types of Bravais lattices (***)</th>
</tr>
</thead>
</table>
| $a = \text{anortic*}$ (triclinic, asymmetric, tetartoprismac...) | no restriction on $a; b; c, \alpha, \beta, \gamma$ | triclinic | triclinic | $aP$
| $m = \text{monoclinic}$ (clinorhombic, monosymmetric, binary, hemiprismatic, monoclinohedral, ...) | no restriction on $a; b; c; \beta.$ $\alpha = \gamma = 90^\circ$ | monoclinic | monoclinic | $mP$ ($mB$) $mS$ ($mC, mA, mI, mF$) |
| $o = \text{orthorhombic}$ (rhombic, trimetric, terbinary, prismatic, anisometric,...) | no restriction on $a; b; c.$ $\alpha = \beta = \gamma = 90^\circ$ | orthorhombic | orthorhombic | $oP$ $oS$ ($oC, oA, oB$) $oI$ $oF$
| $t = \text{tetragonal}$ (quadratic, dimetric, monodimetric, quaternary...) | $a = b; \alpha = \beta = \gamma = 90^\circ$ no restriction on $c$ | tetragonal | tetragonal | $tP$ ($tC$) $tl$ ($tF$) |
| $h = \text{hexagonal}$ (senaiey, monotrimetric...) | $a = b; \alpha = \beta = 90^\circ, \gamma = 120^\circ$ no restriction on $c$ | trigonal (ternary...) (***) | rhombohedral | $hR$ |
| $c = \text{cubic}$ (isometric, monometric, triquaternary, regular, tesseral, tessural...) | $a = b = c$ $\alpha = \beta = \gamma = 90^\circ$ | cubic | cubic | $cP$ $cl$ $cF$

(*) Synonyms within parentheses.

(**) $S = \text{one pair of faces centred.}$ Within parentheses the types of lattices that are equivalent (axial setting change – see the monoclinic example).

(***) Crystals of the trigonal crystal system may have a rhombohedral or hexagonal lattice.
Symmetry directions of the lattices in the three-dimensional space (directions in the same box are equivalents by symmetry)

<table>
<thead>
<tr>
<th>Lattice system</th>
<th>Symmetry restrictions on the parameters of the conventional cell</th>
<th>First symmetry direction</th>
<th>Second symmetry direction</th>
<th>Third symmetry direction</th>
</tr>
</thead>
<tbody>
<tr>
<td>triclinic</td>
<td>No restriction on any parameter</td>
<td>[010]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>monoclinic (b-unique)</td>
<td>$\alpha = \gamma = 90^\circ$ No restriction on $a; b; c; \beta$</td>
<td>[010]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>orthorhombic</td>
<td>$\alpha = \beta = \gamma = 90^\circ$ No restriction on $a; b; c$</td>
<td>[010]</td>
<td>[001]</td>
<td></td>
</tr>
<tr>
<td>tetragonal</td>
<td>$a = b; \alpha = \beta = \gamma = 90^\circ$ No restriction on $c$</td>
<td>[010]</td>
<td>[100]</td>
<td>[100] [100] ≡ ⟨100⟩</td>
</tr>
<tr>
<td>rhombohedral</td>
<td>$a = b = c$ $\alpha = \beta = \gamma$</td>
<td>[111]</td>
<td>[110]</td>
<td></td>
</tr>
<tr>
<td>rhombohedral</td>
<td>hexagonal axes $a = b; \alpha = \beta = 90^\circ; \gamma = 120^\circ$ No restriction on $c$</td>
<td>[001]</td>
<td>[100] [010] [111] [011]</td>
<td></td>
</tr>
<tr>
<td>hexagonal</td>
<td>$a = b; \alpha = \beta = 90^\circ; \gamma = 120^\circ$ No restriction on $c$</td>
<td>[001]</td>
<td>[100] [100] [110] ≡ ⟨110⟩</td>
<td></td>
</tr>
<tr>
<td>cubic</td>
<td>$a = b = c$ $\alpha = \beta = \gamma = 90^\circ$</td>
<td>[111]</td>
<td>[110]</td>
<td>[110] [110] [120] [110]</td>
</tr>
</tbody>
</table>
Symmetry restrictions on cell parameters (conventional cell)

Restrictions incorrectly given in many textbooks

Triclinic family:
none

Monoclinic family
\(\alpha = \gamma = 90^\circ\)

Orthorhombic family
\(\alpha = \beta = \gamma = 90^\circ\)

Tetragonal family
\(a = b\)
\(\alpha = \beta = \gamma = 90^\circ\)

Hexagonal family
Hexagonal axes: \(a = b; \alpha = \beta = 90^\circ; \gamma = 120^\circ\)
Rhombohedral axes: \(a = b = c; \alpha = \beta = \gamma\)

Cubic family
\(a = b = c\)
\(\alpha = \beta = \gamma = 90^\circ\)

For the crystal structure, too restrictive

For the crystal lattice (geometric concept), insufficient

Restrictions incorrectly given in many textbooks

For the crystal structure, too restrictive

For the crystal lattice (geometric concept), insufficient
Why insufficient for the crystal lattice?

A simple example: \(mp\)

if \(\beta = 90^\circ\) the lattice is \(op\) (obviously)

Let us suppose \(\cos \beta = -a/2c\)

<table>
<thead>
<tr>
<th>Bravais type</th>
<th>Centring mode of the cell (a, b, c)</th>
<th>Conditions</th>
</tr>
</thead>
</table>
| cP           | P                                 | \(a = b = c,\)  
\(\alpha = \beta = \gamma = 90^\circ\) |
| ci           | I                                 | \(a = b = c,\)  
\(\alpha = \beta = \gamma = 90^\circ\) |
| cF           | F                                 | \(a = b = c,\)  
\(\alpha = \beta = \gamma = 90^\circ\) |
| tP           | P                                 | \(a = b \neq c,\)  
\(\alpha = \beta = \gamma = 90^\circ\) |
| tI           | I                                 | \(c/\sqrt{2} \neq a = b \neq c,\)  
\(\alpha = \beta = \gamma = 90^\circ\) |
| oP           | P                                 | \(a < b < c,\)  
\(\alpha = \beta = \gamma = 90^\circ\) |
| oI           | I                                 | \(a < b < c,\)  
\(\alpha = \beta = \gamma = 90^\circ\) |
| oF           | F                                 | \(a < b < c,\)  
\(\alpha = \beta = \gamma = 90^\circ\) |
| oC           | C                                 | \(a < b \neq a\sqrt{3},\)  
\(\alpha = \beta = \gamma = 90^\circ\) |
| hP           | P                                 | \(a = b,\)  
\(\alpha = \beta = 90^\circ, \gamma = 120^\circ\) |
| hR           | P                                 | \(a = b = c,\)  
\(\alpha = \beta = \gamma,\)  
\(\alpha \neq 60^\circ, \alpha \neq 90^\circ, \alpha \neq \omega_3\) |
| mP           | P                                 | \(-2c \cos \beta < a < c,\)  
\(\alpha = \gamma = 90^\circ < \beta\)  
\(-c \cos \beta < a < c,\)  
\(\alpha = \gamma = 90^\circ < \beta,\)  
\(a^2 + b^2 = c^2,\)  
\(a^2 + ac \cos \beta = b^2,\)  
\(c^2 + 3b^2 = 9a^2,\)  
\(c = -3a \cos \beta,\)  
\(a^2 + 3b^2 = 9c^2,\)  
\(a = -3c \cos \beta\) \(\text{(9.3.4.2)}\)  
\(\text{but not } a^2 + b^2 = c^2,\)  
\(a^2 + ac \cos \beta = b^2,\)  
\(c^2 + 3b^2 = 9a^2,\)  
\(c = -3a \cos \beta,\)  
\(a^2 + 3b^2 = 9c^2,\)  
\(a = -3c \cos \beta\) \(\text{(9.3.4.3)}\)  
\(\text{nor } a^2 + b^2 = c^2,\)  
\(b^2 + ac \cos \beta = a^2,\)  
\(c^2 + 3b^2 = 9a^2,\)  
\(c = -3a \cos \beta,\)  
\(a^2 + 3b^2 = 9c^2,\)  
\(a = -3c \cos \beta\) \(\text{(9.3.4.4)}\)  
\(\text{nor } c^2 + 3b^2 = 9a^2,\)  
\(c = -3a \cos \beta,\)  
\(a^2 + 3b^2 = 9c^2,\)  
\(a = -3c \cos \beta\) \(\text{(9.3.4.5)}\)  
\(\text{nor } c^2 + 3b^2 = 9a^2,\)  
\(c = -3a \cos \beta,\)  
\(a^2 + 3b^2 = 9c^2,\)  
\(a = -3c \cos \beta\) \(\text{(9.3.4.6)}\)  
| mI           | I                                 | \(\alpha = \gamma = 90^\circ < \beta,\)  
\(a^2 + b^2 = c^2,\)  
\(a^2 + ac \cos \beta = b^2,\)  
\(c^2 + 3b^2 = 9a^2,\)  
\(c = -3a \cos \beta,\)  
\(a^2 + 3b^2 = 9c^2,\)  
\(a = -3c \cos \beta\) \(\text{(9.3.4.2)}\)  
\(\text{but not } a^2 + b^2 = c^2,\)  
\(a^2 + ac \cos \beta = b^2,\)  
\(c^2 + 3b^2 = 9a^2,\)  
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\(a^2 + 3b^2 = 9c^2,\)  
\(a = -3c \cos \beta\) \(\text{(9.3.4.3)}\)  
\(\text{nor } a^2 + b^2 = c^2,\)  
\(b^2 + ac \cos \beta = a^2,\)  
\(c^2 + 3b^2 = 9a^2,\)  
\(c = -3a \cos \beta,\)  
\(a^2 + 3b^2 = 9c^2,\)  
\(a = -3c \cos \beta\) \(\text{(9.3.4.4)}\)  
\(\text{nor } c^2 + 3b^2 = 9a^2,\)  
\(c = -3a \cos \beta,\)  
\(a^2 + 3b^2 = 9c^2,\)  
\(a = -3c \cos \beta\) \(\text{(9.3.4.5)}\)  
\(\text{nor } a^2 + b^2 = c^2,\)  
\(a^2 + ac \cos \beta = b^2,\)  
\(c^2 + 3b^2 = 9a^2,\)  
\(c = -3a \cos \beta,\)  
\(a^2 + 3b^2 = 9c^2,\)  
\(a = -3c \cos \beta\) \(\text{(9.3.4.6)}\)  

Note: All remaining cases are covered by Bravais type \(aP\).