Any shape, symbol, unit, or object can be arranged so that it is periodic in space.

This is done by:

- Symmetry
- Translation
  - Rotation
  - Reflection
  - Inversion

Ex. Translation  
Ex. 2-fold  
Ex. Mirror.

Unit Cell: What is the smallest pattern that will contain the point (i.e., \( B \)) and the symmetry:

Ex.  
Ex.  

\[ \begin{array}{c}
\uparrow \\
\\downarrow \\
\  \\
\  \\
\end{array} \]
A repeating pattern has three defining aspects:
1) the shape of the unit cell
2) the symmetry within it.
3) the translation of the unit cell to fill space.

The smallest cell that can be translated must have a shape that is compatible with the symmetry within it.

The symmetry within a cell is defined with respect to specific points and operations. These symmetry operations are called point point groups.

Each point group contains a unique set of such symmetry operations. There is a finite number of point groups.

1. Dimensions 3: 2 point groups,
2. D 6: 10
3. D 3: 32
There is also a finite set of basic unit cells:

1-D: 1 type
2-D: 4 types
3-D: 7 types

Combining symmetry operations with translation (unit cells) there are a total of 230 space groups.

When atoms are added (motif) they are called crystal structures.

Point Groups:

- Rotation
- Reflection
- Inversion

Only 1, 2, 3, 4, 6 fold rotations exist.

The unit being operated on may be an atom or a group of atoms.
Rotation

- motif - in the plane
- rotation symbol

n-fold: $\frac{360}{n}$ e.g. $\frac{360}{3}$

RoToReflection

rotate - reflect - rotate - reflect ... or reflect - rotate - reflect - rotate.

Symbol: $\hat{n}, \hat{1}, \hat{2}, \hat{3}, \hat{4}, \hat{6}$

Ex.

Notation:

- $\circ$ motif in the plane
- $\circ + \circ -$ motif above or below plane
- $\circ$ handedness of motif
  - $\leftarrow$ left empty right
- $\circ +$ two motifs on top of each other
- $\circ \odot$ two motifs on top of each other with different handedness
Roto-inversion: rotate-invert - rotate-invert...

Symbol: \( \overline{n}, \overline{1}, \overline{2}, \overline{3}, \overline{4}, \overline{6} \)

Ex. 4

Mirror plane normal to axis \( \perp \)

Symbol for rotations then mirror

\[ \begin{aligned} &\frac{n}{m} : \frac{2}{m}, \frac{m}{m}, \frac{6}{m} \\ \text{Is this the same as rotoreflection?} & \end{aligned} \]

Mirror plane parallel to axis \( \parallel \)

m
Mirror plane in rotation plane:

Symbol: n mm, 2mm, 4mm, 6mm, 3m

Do mirror operations 1st.

Ex.

3 mirror planes but all are the same.

Point groups by multiple rotation axis.

Ex.

See page 8-16 for more detail.
Plane lattice - two dimensional periodic array of points
Space lattice - three dimensional

Ex.

\[
\begin{array}{ccc}
\uparrow & \uparrow & \uparrow \\
7 & 7 & 7 \\
\end{array}
\]

lattice sites are not, in general, the same as atomic sites

Valid lattice, the same position in each cell must have identical surroundings.

Unit cell: Basic Building unit, contains all crystallographic information about the structure

Unit cell choice is somewhat arbitrary, but by convention the one with smallest area/volume is selected.

Ideal unit cell but others are valid.
Plane Lattice types:

- **Oblique** \(|\vec{a}| \neq |\vec{b}|\)  
  \[\theta \neq 90^\circ\]  
  Point Group  
  \(1, 2\)

- **Rectangular** \(|\vec{a}| \neq |\vec{b}|\)  
  \[\theta = 90^\circ\]  
  Point Group  
  \(m, 2mm\)

- **Hexagonal** \(|\vec{a}| = |\vec{b}|\)  
  \[\theta = 120^\circ\]  
  Point Group  
  \(3, 3m\), \(6, 6mm\)

- **Square** \(|\vec{a}| = |\vec{b}|\)  
  \[\theta = 90^\circ\]  
  Point Group  
  \(4, 4mm\)

- **Centered Rectangular** \(|\vec{a}| = |\vec{b}|\)  
  \[\theta = 90^\circ\]  
  Point Group  
  \(m, 2mm\)
primitive cell - contains only one lattice site but for centered rectangle this misses physical symmetry.

5-fold rotation does not work with lattices

Proof:

\[
\frac{360}{5} = 72^\circ
\]

32 point groups are divided into Crystal Systems. These Systems define unit cells that can characterize all crystal lattices in space.
Seven crystal systems (space groups with minimum symmetry)

- Triclinic: one 1
- Monoclinic: one 2
- Orthorhombic: three 2's
- Tetragonal: one 4
- Trigonal: one 3
- Hexagonal: one 6
- Cubic: four 3's.

When atoms associated with space groups crystal structures,

International Table for Crystallography

europoint - set of symmetry-related positions
number of points or positions in the set is the rank

Ex. corner site in cell

Same atom must appear at all corners due to symmetry.

rank 1 because \( \frac{1}{8} \) of atom at each corner

i.e. 8 europoints \( \times \frac{1}{8} \) atom
• The placement of an atom at a completely general location in a cell results in the highest number of symmetry-related positions, which is the highest rank.

  General position represented by \(x, y, z\) coordinates, no special value i.e., (corner of cells)

• Special positions are located on a site of one or more symmetry elements. Always have lower ranks than general. Described by fixed positions i.e., \(1/2, 1/2, 1/2\)

(see page 30-31)

• Strukturbericht Symbol

  A - elements
  B - phases of composition near \(AB\) stoichiometry
  C - for \(AB_2\) phase
  D, E, \(\frac{1}{2}\) H - complex
  L - intermediate alloy phase, superlattices
Schoenflies:

\( C_n \) - Space group with single axis of rotation

\( D_n \) - two

\( T_n \) - 3

\( O_n \) - 4

Hermann-Mauguin: