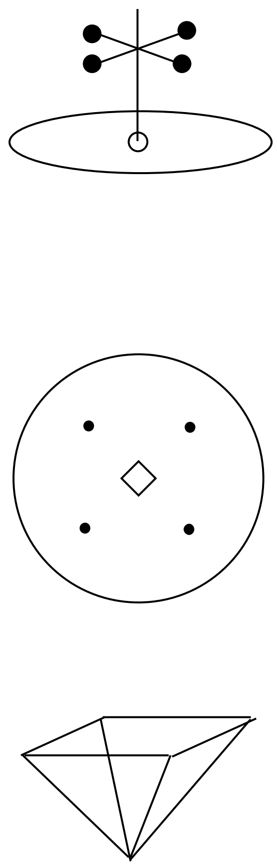
Structural Chemistry Methods Workshop

Crystallography II:

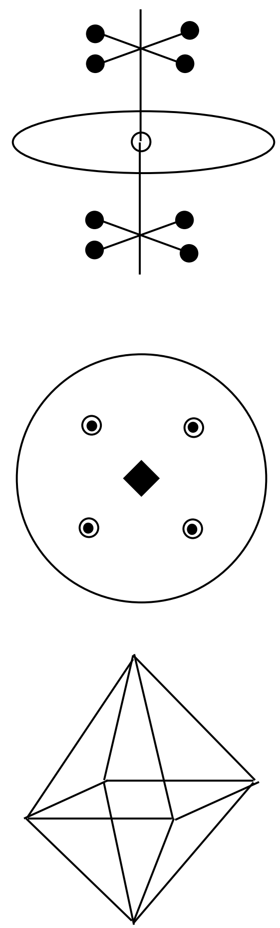
Translational Symmetry Elements,
Coordinate Systems,
and
Symmetry Calculations

Unpolar and polar rotation axes, rota-inversion axes



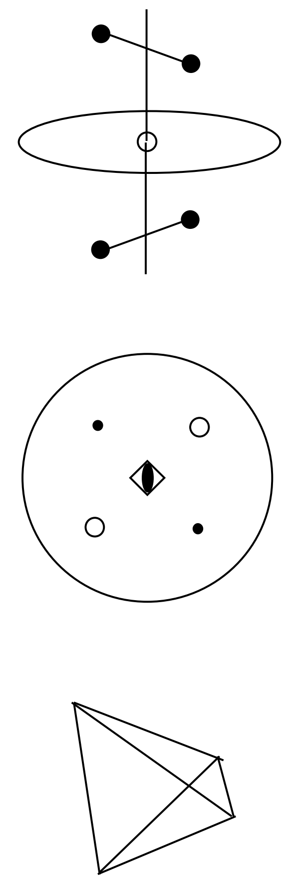
4

polar



4

unpolar



$\bar{4}$

polar

Unpolar and polar rotation axes, rota-inversion axes

Distinction of rotation axes as to polar/unpolar is important, because physical properties of crystals depend on the structural symmetry (Symmetry Principle of Neumann).

E.g., polar directions are a requirement for piezo-electric properties.

Even rota-inversion axes posses no inversion centre!

$\bar{4}$: upper and lower images are crossed over

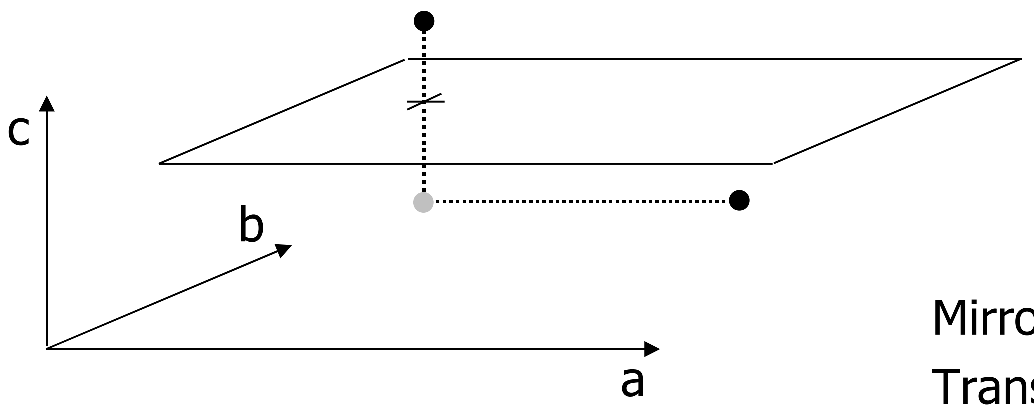
$\bar{2}$, $\bar{6}$: upper and lower images are reflections

Odd rota-inversion axes posses an inversion centre

Addition of translational elements to Rotation and Reflection

The symmetry elements of Rotation and Reflection can be combined with translational elements, resulting in

Glide planes and **screw axes**



Mirror plane m || ab-plane, i.e. ⊥ [001]
Translational component is ½ in $\bar{a}$

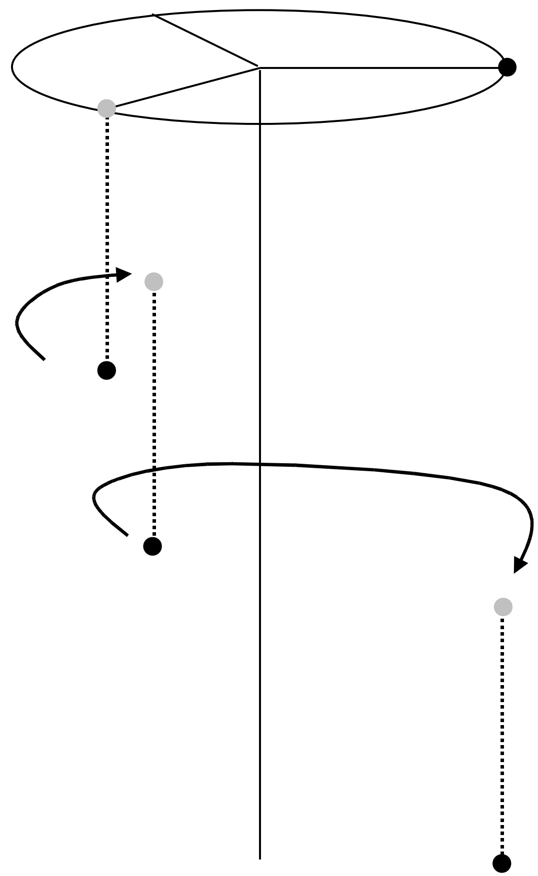
m is a glide plane; new symbol: a

Glide planes

Glide component	Symbol
$\frac{1}{2}\,\bar{a}$	a
$\frac{1}{2}\,\bar{b}$	b
$\frac{1}{2}\,\bar{c}$	c
$\frac{1}{2}(\bar{a}+\bar{b})$, $\frac{1}{2}(\bar{a}+\bar{c})$, $\frac{1}{2}(\bar{b}+\bar{c})$ or $\frac{1}{2}(\bar{a}+\bar{b}+\bar{c})$	n
$\frac{1}{4}(\bar{a}+\bar{b})$, $\frac{1}{4}(\bar{a}+\bar{c})$, $\frac{1}{4}(\bar{b}+\bar{c})$ or $\frac{1}{4}(\bar{a}+\bar{b}+\bar{c})$	d

Screw axes

3_1



For a rotation axis R, the corresponding screw axis R_1 requires subsequently:

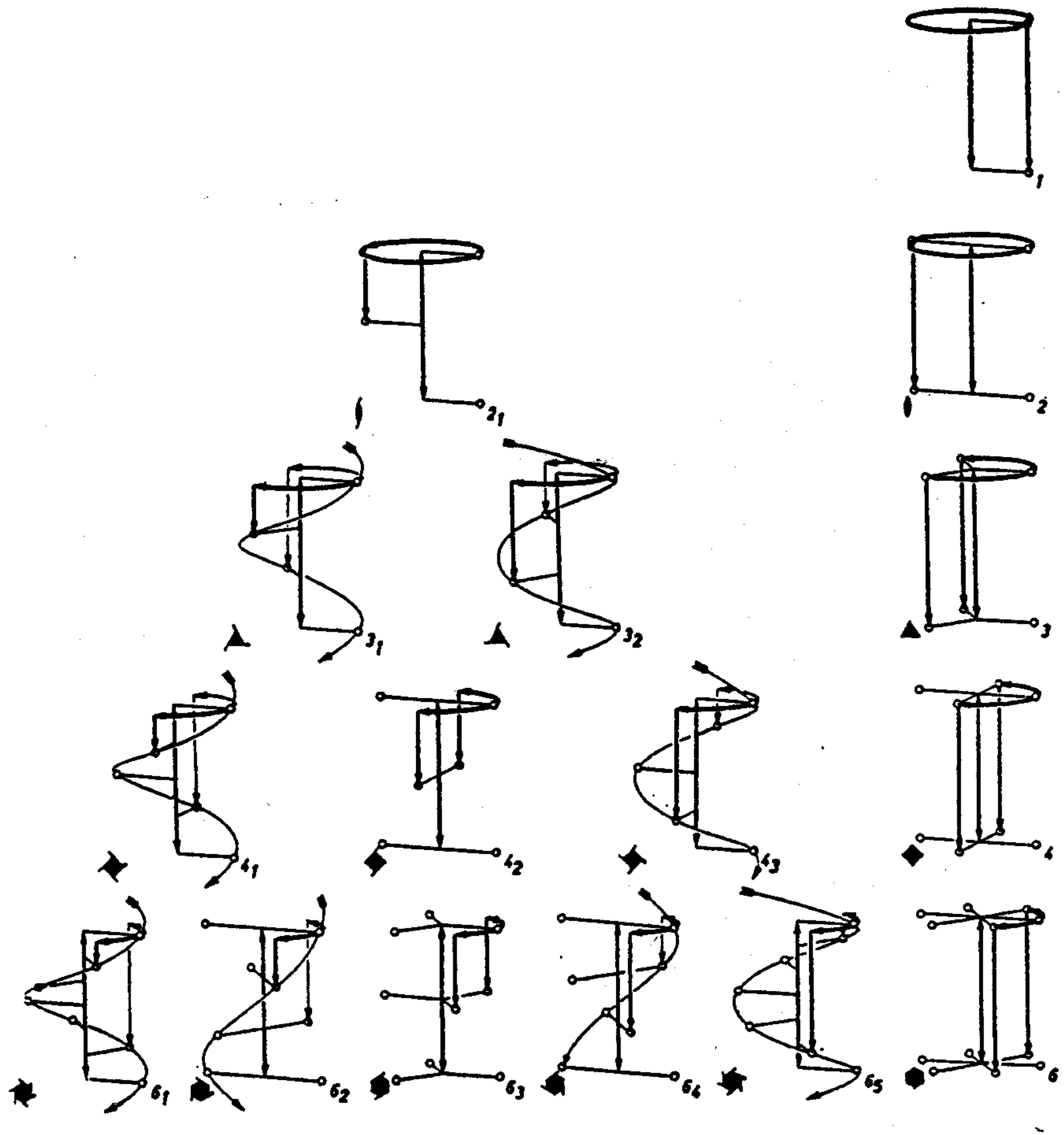
- a clockwise rotation about 360°/R
- a translation of $^1/_R$ parallel to the axis

The counter-clockwise screw operation (enantiomorph) to R_1 is R_{R-1}

Non-enantiomorph: 2_1, 4_2, 6_3

Multiplicity: R-times repetition yields the original position

Screw axes



Special positions

In contrast to symmetry operations without translational elements, glide planes and screw axes produce no special positions.

E.g., a point position on a 2-fold axis, produces no new point after application of the symmetry operator (i.e. reduces the multiplicity).

A point on a 2_1 screw axis, is transported to a new position after the screw operation (i.e. multiplicity is always conserved).

Coordinate Systems

To describe crystal symmetry, one needs exact coordinates of a point in space.

We therefore need an appropriate coordinate system, as well as a calculation procedure for symmetry operations.

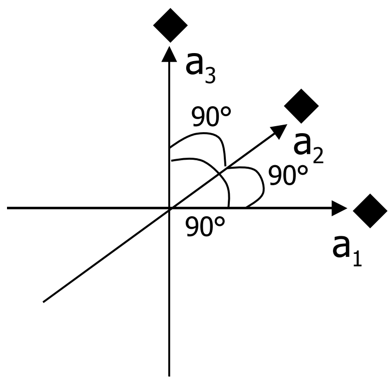
The coordinate system
- consists of three non-coplanar basis vectors
- provides the unit cell

The coordinate system does not have to be cartesian, it can be chosen to fit the particular symmetry.

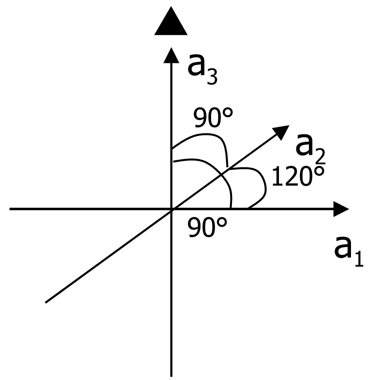
By convention, the axis of highest multiplicity is set as $\bar{c}$-axis of a right-handed coordinate system. $\bar{a}$ and $\bar{b}$ are in the plane, perpendicular to $\bar{c}$. They embrace the angle of the X-fold axis parallel to $\bar{c}$. The angle should be larger than 90°.

Coordinate Systems

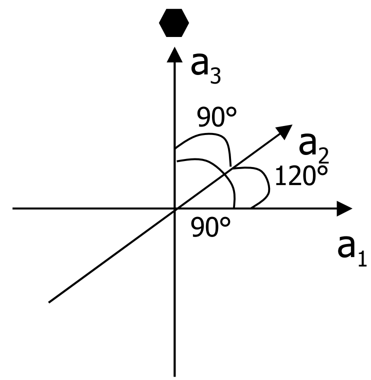
This yields seven different cases



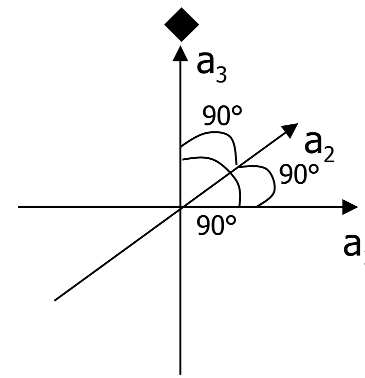
cubic



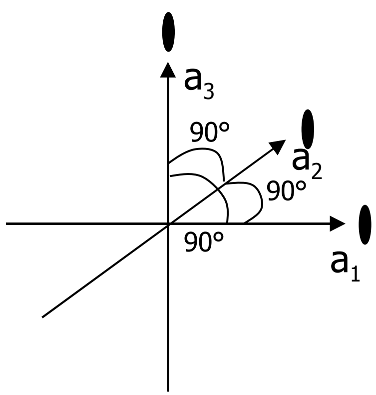
trigonal



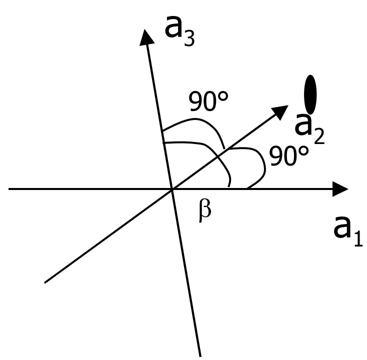
hexagonal



tetragonal

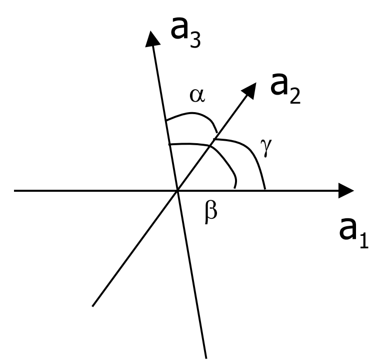


orthorhombic



monoclinic

Note: highest axis is $\bar{b}$!



triclinic

Symmetry Calculations

Any point within a coordinate system can be calculated as a multiple of the three basis vectors of the unit cell:

$$\bar{p} = x\bar{a} + y\bar{b} + z\bar{c} = \Sigma\, x_i \bar{a}_i$$

Crystallographic symmetry operations:

- Keep the ratio of distances (affine transformation)
- Keep lengths and angles

A new point Y (y_1, y_2, y_3) is generated from X (x_1, x_2, x_3) by rotation:

$$y_i = s_{i1}x_1 + s_{i2}x_2 + s_{i3}x_3$$

with i= 1, 2, 3; s_{ij} can equal -1, 0, or 1.

Symmetry Calculations

$$\begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix} = \begin{pmatrix} s_{11} & s_{12} & s_{13} \\ s_{21} & s_{22} & s_{23} \\ s_{31} & s_{32} & s_{33} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$$

$$\bar{Y} = S\,\bar{X}$$

S: Matrix describing the symmetry operator
X: original point
Y: generated point

Note that the notation of the symmetry operator is independent of the coordinate system!

$\bar{Y}$ and $\bar{X}$ are within the same basis (coordinate system).

We can also transform the basis: To obtain the matrix of the new coordinate System (B), the old basis (A) is transformed by the symmetry operator (S).

$$B = AS$$

Impressum

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