Condense phases:

- Liquids
- Solid materials
  - Amorphous materials
    - Glass
  - Crystalline materials
    - 1 Dim. phases — CrO_3, carbon nanotubes
    - 2 Dim. phases — V_2O_5, graphite
    - 3 Dim. phases — TiO_2, diamond

Inorganic materials / units

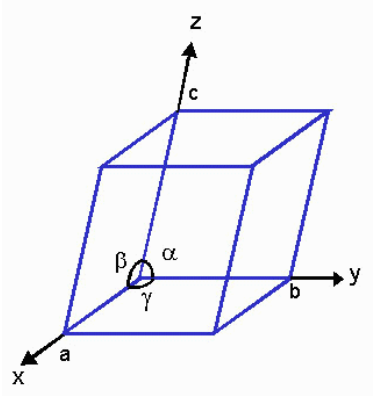
Separate units

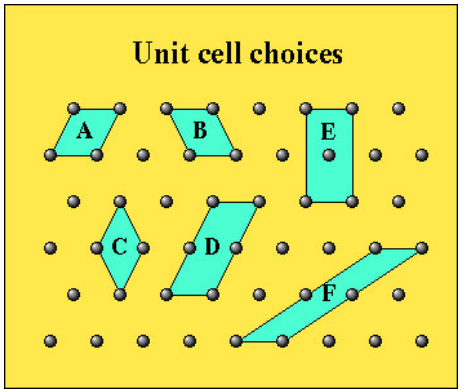
Elements	Molecules	Ions	Complexes
Ar(g)	CO_2(g)	SO_4^{2-}(aq)	$PtCl_4^{2-}$(aq)
	CH_4(g)	CO_3^{2-}(aq)	$Cu(NH_3)_4^{2+}$(aq)
	H_2O(g)(l)		$Ag(NH_3)^{2+}$(aq)
	$XeOF_4$(l)		$Fe(CN)_6^{3-}$(aq)

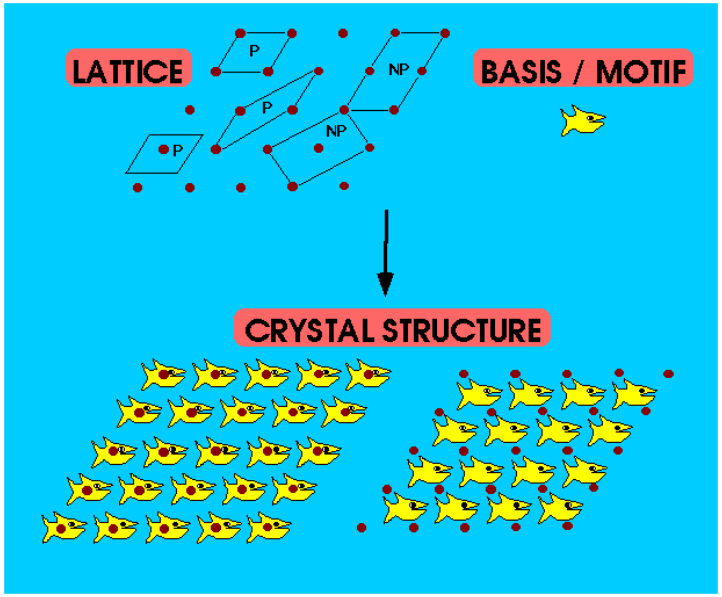
Structur fragments in solid state

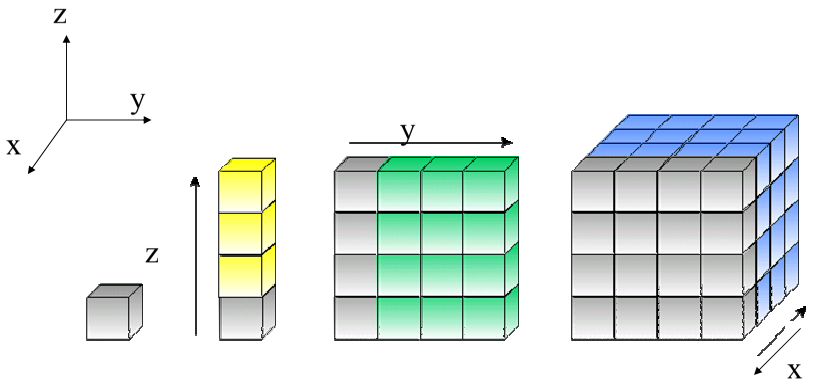
SiO_4^{4-} tetraedral building units in silicates	CN = 4 tetraedral
'CuO_2'-layers in high Tc-materials	CN = 4 planequadratic
'MnO_6'-octahedra in oxides	CN = 6 octahedra

Unit cell



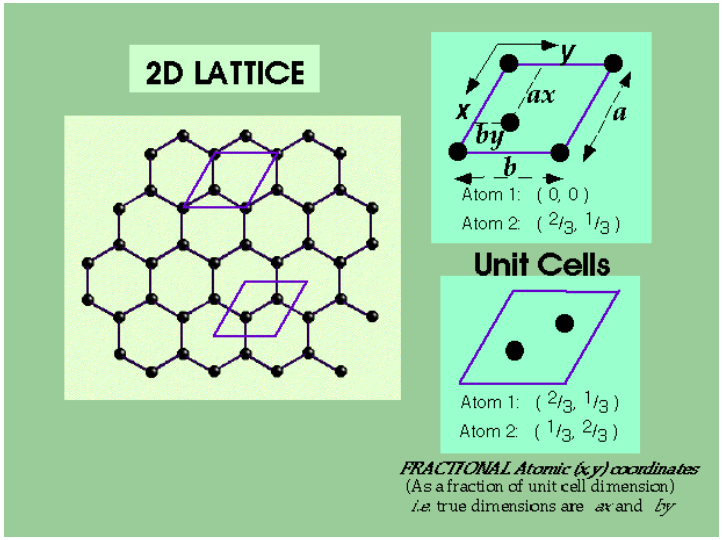


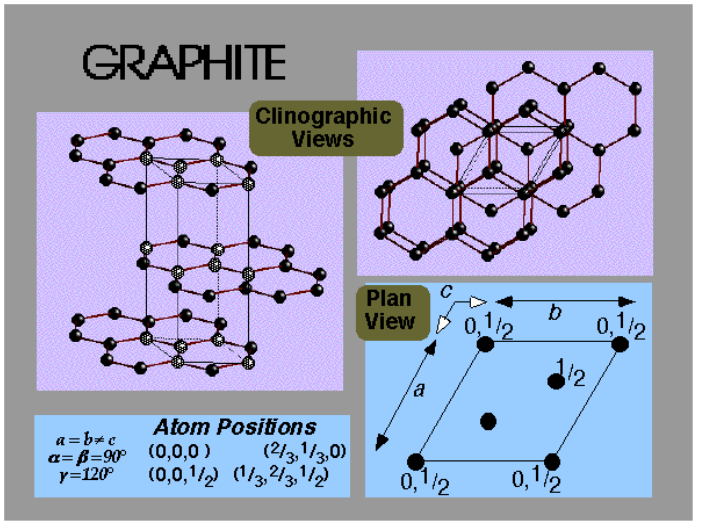


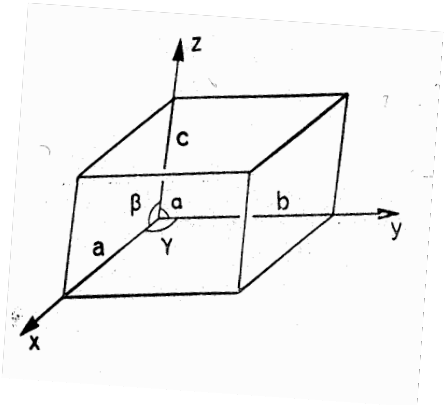


Unitcell

Transtaltion along x, y, z







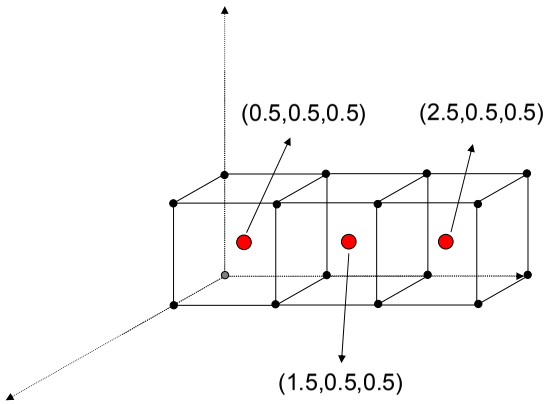
$$V = a \cdot (b \times c)$$

Counting of atoms in 2D

- Atoms in a corner = ¼
- Atoms on an edge = $^1/_2$
- Atoms inside the cell = 1

Counting of atoms in 3D

- A corner-atom is shared between **8** cells ⇒ $^1/_8$ atoms pr. cell
- An edge-atom is shared between mellom **4** cells ⇒ $^1/_4$ atom pr cell
- A surface-atom is shared between **2** cells ⇒ $^1/_2$ atom pr cell
- A atom inside one cell ⇒ **1** atom pr cell



Crystal systems

A collection of point groups that in common give caracteristic symmetry operations

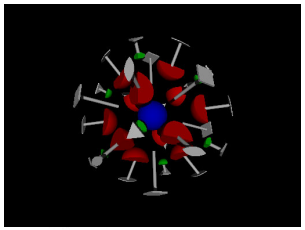


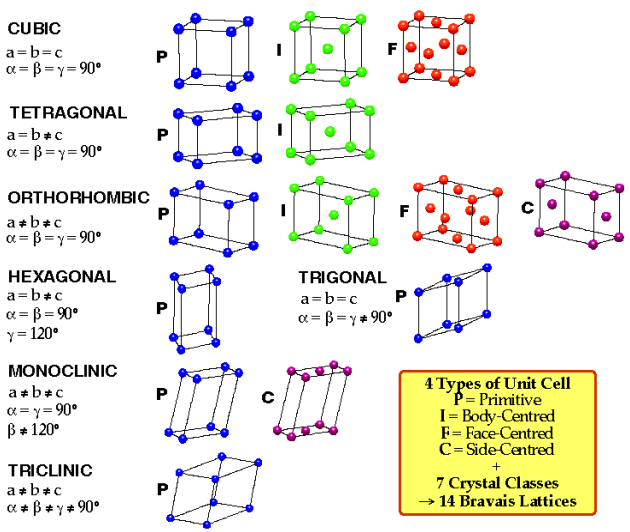
Table 1.1 *The seven crystal systems*

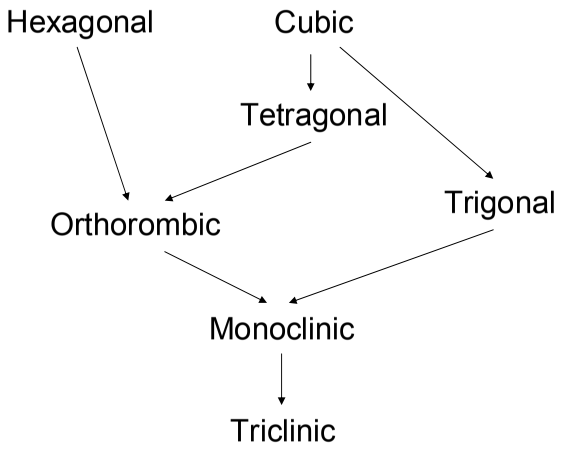
Crystal system	Unit cell shape†	Essential symmetry	Allowed lattices
Cubic	$a = b = c, \alpha = \beta = \gamma = 90°$	Four threefold axes	P, F, I
Tetragonal	$a = b \neq c, \alpha = \beta = \gamma = 90°$	One fourfold axis	P, I
Orthorhombic	$a \neq b \neq c, \alpha = \beta = \gamma = 90°$	Three twofold axes or mirror planes	P, F, I, A (B or C)
Hexagonal	$a = b \neq c, \alpha = \beta = 90°, \gamma = 120°$	One sixfold axis	P
Trigonal (a)	$a = b \neq c, \alpha = \beta = 90°, \gamma = 120°$	One threefold axis	P
(b)	$a = b = c, \alpha = \beta = \gamma \neq 90°$	One threefold axis	R
Monoclinic*	$a \neq b \neq c, \alpha = \gamma = 90°, \beta \neq 90°$	One twofold axis or mirror plane	P, C
Triclinic	$a \neq b \neq c, \alpha \neq \beta \neq \gamma \neq 90°$	None	P

* Two settings of the monoclinic cell are used in the literature, the most commonly used one given here, with b as the unique axis and the other with c defined as the unique axis: $a \neq b \neq c, \alpha = \beta = 90°, \gamma \neq 90°$.
† The symbol ≠ means 'not necessarily equal to'. Sometimes, crystals possess *pseudo-symmetry*. For example, a unit cell may be geometrically cubic but not possess the essential symmetry elements for cubic symmetry; the true symmetry is then lower, perhaps tetragonal.

The unit cell is chosen so that the mention symmetry elements are easily observed.
By describing the symmetry of the unitcell the symmetry of the condensed material is described fully.

Bravais Lattices





Symmety operations

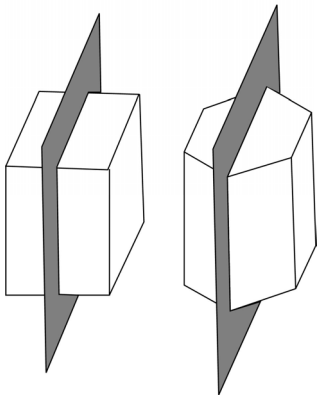
- Mirrorplane *m*
- Rotationaxis *n (2,3,4,6)*
- Invertionaxis $\bar{n}$ ($\bar{1}$,$\bar{2}$…)
- Sentrosymmetry $\bar{1}$

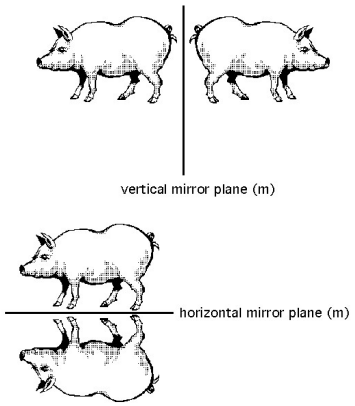
Pointgroup symmetry

- Glidemirrorplane *n, d, a, b, c*
- Screwaxis 2_1, 3_1, ..6_3

Spechial symmetry operations

Mirrorplane *m*

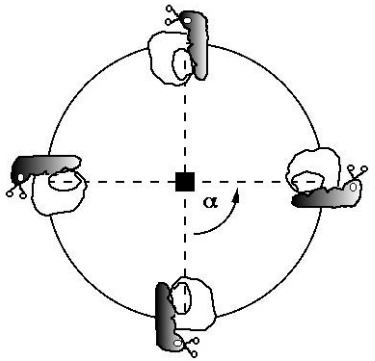


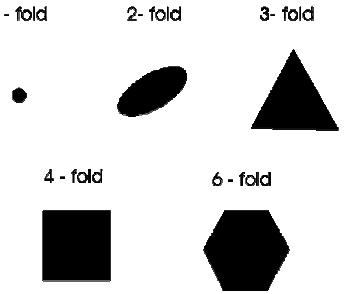


Rotationaxis n

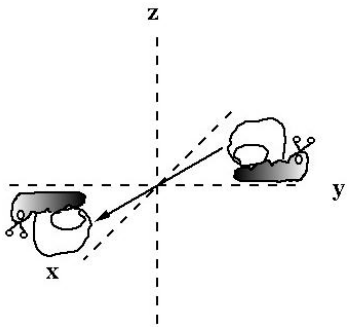
4-fold rotation axis

$\alpha = 360/n$





Inversionaxis $\bar{n}$



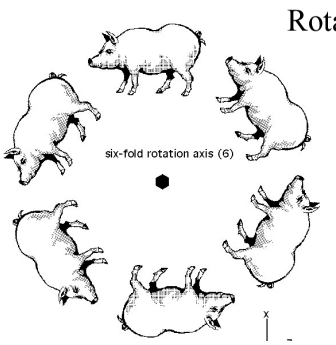
Rotation + inversion

$\alpha = 360^o/n$

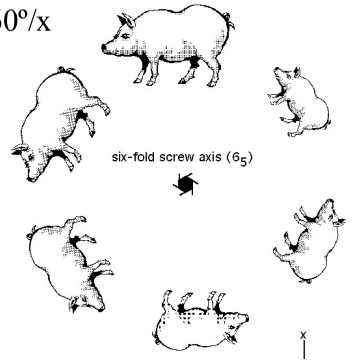
Screw axis, X_y

Translation: y/x

Rotation: 360º/x

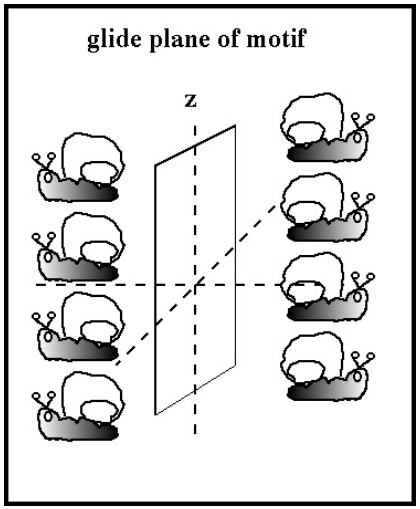


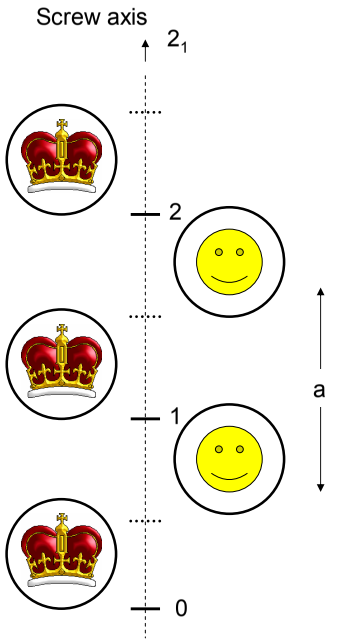
ordinary 6-fold rotation axis

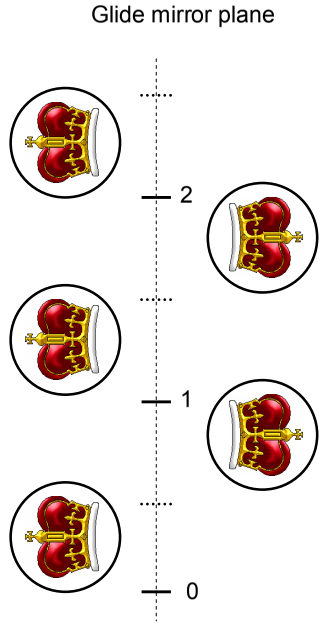


screw rotation axis 6_5

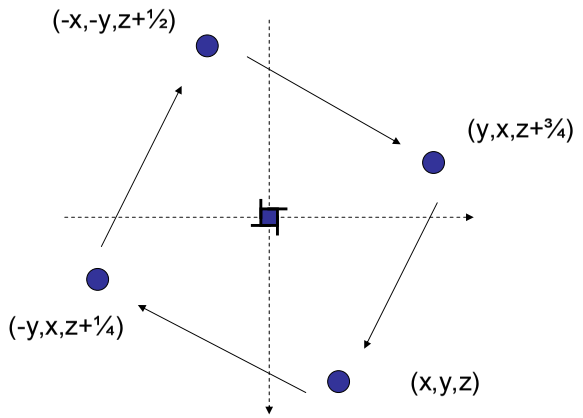
Glide plane







4_1

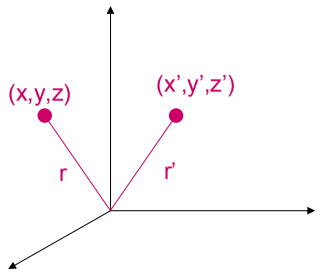


$$\{4 \mid \vec{t}\} = (3\times 3)\mathbf{r} + \vec{t} = \mathbf{R}\mathbf{r} + \mathbf{t}$$

$$\{4 \mid \vec{t}\}^4 = \{1 \mid \vec{t}\}$$

Pointgroups

- A chracteristic collection of symmetry elements
- The symmetry elements has origo as common point
- Symmetry elements and point group symbol:
  Two schemes:
  - Schönflies
  - Hermann Mauguin
- Illustrated in form of stereographic projection



r' = R•r

R is a symmetry operator

$$\begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix}$$

Symmetry operations:

Identity: **I**

$a_{ij} = 0$
$a_{ii} = 1$

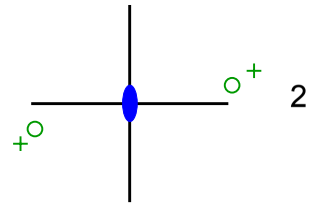
$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

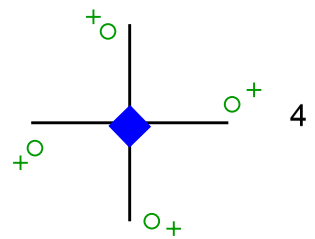
Rotation: n, C_n

+ rotation axis [uvw]
n[uvw] or C_n[uvw]

$$\{2[001]\}(xyz) = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} -x \\ -y \\ z \end{bmatrix}$$

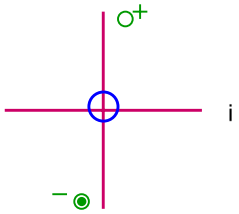
$$\{4[001]\}(xyz) = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} -y \\ x \\ z \end{bmatrix}$$





Inversion / centrosymmetry: $\bar{1}$ i

$$\{\bar{1}(i)\}(x,y,z)=(-x,-y,-z)$$

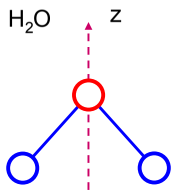
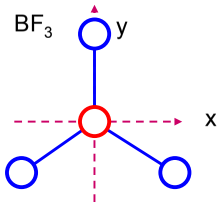


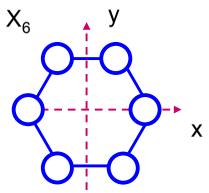
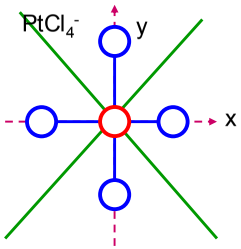
Right hand becomes left hand

Mirrorplane: m

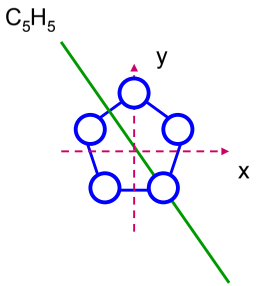
$$\{m[010]\}(x,y,z)=(x,-y,z)$$

m is defined from the normal of the plane

	Rotation axis	Other symmetry elements
	C_2^z 2	Vertical mirrorplane
	C_3^z 3	Horizontal mirrorplane Vertical mirrorplane

	Rotation axis	Other symmetry elements
	C_6^z 6	Two-fold axis Mirror planes Inversion center
	C_4^z 4	C_2 axis Mirror planes Inversion center

Rotation axis **Other symmetry elements**



C_5^z **5**

5 C_2 axis
Mirror planes

Left hand rule for x,y,z
Highest rotation axis || z

Triclin system

1 and $\bar{1}$ does not imply any restrictions for a,b,c or α,β,γ

Point group with elements: **1** **I**
$\bar{1}$ **I,i**

If a 2-fold axis is added, then the system becomes:

Monoclinic system

with the symmetry operations 2 (C_2) or $\bar{2} \equiv$ m (σ_h)

2 **I, C_2**
m **I, σ_h**

Presence of further 2 or m is a criteria for an orthorombic system

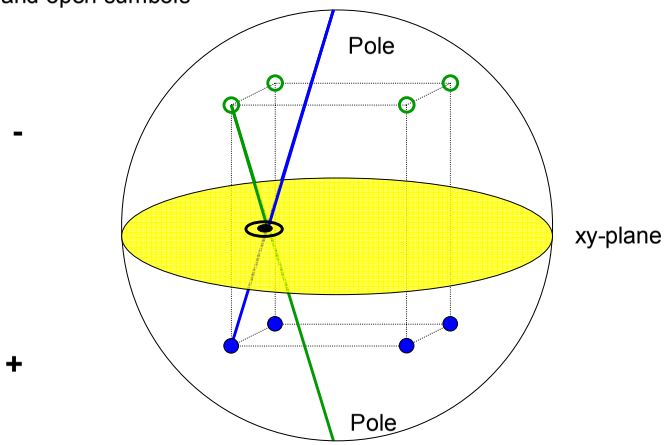
What about m normal to 2?
It does not change the criteria for a,b,c or α,β,γ and is hence possible.

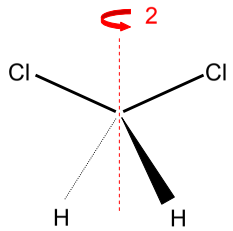
$$\{m[001]\}\{2[001]\} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}\begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} = \{\bar{1}\}$$

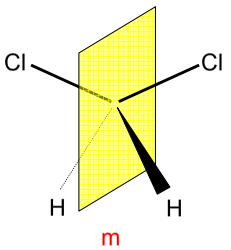
2/m sentrosymmetric, with the operations: I,C_2,σ_h,i

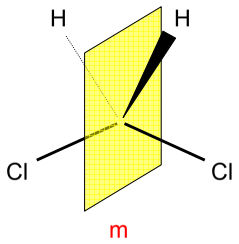
Stereographic projection

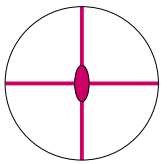
- The crystal is surrounded by a sphere
- We are interested in the projected surface in a xy-plane through the sphere
- The projected point is determined by the intersection of a connection line from the point of interrest to the pole of the opposite side.
- The two halves of the spheres are noted by assigning + and – and to use filled and open sumbols



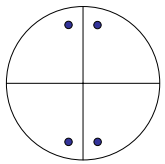




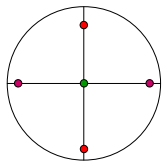




mm2



Generally 4 pos.



Spechially
2 pos.
2 pos.
1 pos.

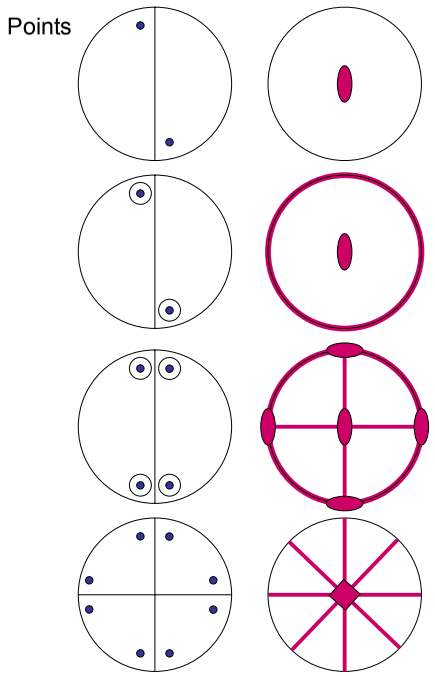
Symmety operations

- Mirrorplane m
- Rotationaxis n (2,3,4,6)
- Invertionaxis $\bar{n}$ ($\bar{1}$,$\bar{2}$…)
- Sentrosymmetry $\bar{1}$

} Pointgroup symmetry

- Glidemirrorplane n, d, a, b, c
- Screwaxis $2_1, 3_1, ..6_3$

} Spechial symmetry operations



Point groups:

A crystallographic pointgroup is a selection of symmetry elements that can operate on a three dimensional lattice.
This is only met by 32 pointgroups.

Crystal system	*Crystallographic point group*
Triklinic	1,-1
Monoklininc	2, m, 2/m
Orthorombic	222, mm2, mmm
Tetragonal	4, -4, 4/m, 422, 4mm, -42m, 4/mmm
Trigonal	3, -3, 32, 3m, -3m
Hexagonal	6, -6, 6/m, 622, 6mm, -6m2, 6/mmm
Cubic	23, m3, 432, -43m, m3m

Of these are 11 centrosymmetric and 21 non-centrosymmetric.