Crystallography basics

TABLE 3.4 Space Groups in Standard Orientations[a]

System	Point Group	Space Group					
Triclinic	1	$P1$					
	$\bar{1}$	$P\bar{1}$					
Monoclinic	2	$P2$	$P2_1$	$C2$			
	m	Pm	Pc	Cm	Cc		
	$2/m$	$P2/m$	$P2_1/m$	$C2/m$	$P2/c$	$P2_1/c$	$C2/c$
Orthorhombic	222	$P222$	$P222_1$	$P2_12_12$	$P2_12_12_1$	$C222_1$	$C222$
		$F222$	$I222$	$I2_12_12_1$			
	$mm2$	$Pmm2$	$Pmc2_1$	$Pcc2$	$Pma2$	$Pca2_1$	$Pnc2$
		$Pmn2_1$	$Pba2$	$Pna2_1$	$Pnn2$	$Cmm2$	$Cmc2_1$
		$Ccc2$	$Amm2$	$Abm2$	$Ama2$	$Aba2$	$Fmm2$
		$Fdd2$	$Imm2$	$Iba2$	$Ima2$		
	mmm	$Pmmm$	$Pnnn$	$Pccm$	$Pban$	$Pmma$	$Pnna$
		$Pmna$	$Pcca$	$Pbam$	$Pccn$	$Pbcm$	$Pnnm$
		$Pmmn$	$Pbcn$	$Pbca$	$Pnma$	$Cmcm$	$Cmca$
		$Cmmm$	$Cccm$	$Cmma$	$Ccca$	$Fmmm$	$Fddd$
		$Immm$	$Ibam$	$Ibca$	$Imma$		
Tetragonal	4	$P4$	$P4_1$	$P4_2$	$P4_3$	$I4$	$I4_1$
	$\bar{4}$	$P\bar{4}$	$I\bar{4}$				
	$4/m$	$P4/m$	$P4_2/m$	$P4/n$	$P4_2/n$	$I4/m$	$I4_1/a$
	422	$P422$	$P42_12$	$P4_122$	$P4_12_12$	$P4_222$	$P4_22_12$
		$P4_322$	$P4_32_12$	$I422$	$I4_122$		
	$4mm$	$P4mm$	$P4bm$	$P4_2cm$	$P4_2nm$	$P4cc$	$P4nc$
		$P4_2mc$	$P4_2bc$		$I4cm$	$I4_1md$	$I4_1cd$
	$\bar{4}2m$	$P\bar{4}2m$	$P\bar{4}2c$	$P\bar{4}2_1m$	$P\bar{4}2_1c$	$P\bar{4}m2$	$P\bar{4}c2$
		$P\bar{4}b2$	$P\bar{4}n2$	$I\bar{4}m2$	$I\bar{4}c2$	$I\bar{4}2m$	$I\bar{4}2d$
	$4/mmm$	$P4/mmm$	$P4/mcc$	$P4/nbm$	$P4/nnc$	$P4/mbm$	$P4/mnc$
		$P4/nmm$	$P4/ncc$	$P4/mmc$	$P4_2/mcm$	$P4_2/nbc$	$P4_2/nnm$
		$P4_2/mbc$	$P4_2/mnm$	$P4_2/nmc$	$P4_2/ncm$	$I4/mmm$	$I4/mcm$
		$I4_1/amd$	$I4_1/acd$				
Trigonal/rhombohedral	3	$P3$	$P3_1$	$P3_2$	$R3$		
	$\bar{3}$	$P\bar{3}$	$R\bar{3}$				
	32	$P312$	$P321$	$P3_112$	$P3_121$	$P3_212$	$P3_221$
		$R32$					
	$3m$	$P3m1$	$P31m$	$P3c1$	$P31c$	$R3m$	$R3c$
	$\bar{3}m$	$P\bar{3}1m$	$P\bar{3}1c$	$P\bar{3}m1$	$P\bar{3}c1$	$R\bar{3}m$	$R\bar{3}c$
Hexagonal	6	$P6$	$P6_1$	$P6_5$	$P6_2$	$P6_4$	$P6_3$
	$\bar{6}$	$P\bar{6}$					
	$6/m$	$P6/m$	$P6_3/m$				
	622	$P622$	$P6_122$	$P6_522$	$P6_222$	$P6_422$	$P6_322$
	$6mm$	$P6mm$	$P6cc$	$P6_3cm$	$P6_3mc$		
	$\bar{6}m\bar{2}$	$P\bar{6}m2$	$P\bar{6}c2$	$P\bar{6}2m$	$P\bar{6}2c$		
	$6/mmm$	$P6/mmm$	$P6/mcc$	$P6_3/mcm$	$P6_3/mmc$		
Cubic	23	$P23$	$F23$	$I23$	$P2_13$	$I2_13$	
	$m3$	$Pm3$	$Pn3$	$Fm3$	$Fd3$	$Im3$	$Pa3$
		$Ia3$					
	432	$P432$	$P4_232$	$F432$	$F4_132$	$I432$	$P4_332$
		$P4_132$	$I4_132$				
	$\bar{4}3m$	$P\bar{4}3m$	$F\bar{4}3m$	$I\bar{4}3m$	$P\bar{4}3n$	$F\bar{4}3c$	$I\bar{4}3d$
	$m3m$	$Pm3m$	$Pn3n$	$Pm3n$	$Pn3m$	$Fm3m$	$Fm3c$
		$Fd3m$	$Fd3c$	$Im3m$	$Ia3d$		

[a]The 11 Laue symmetries are separated by horizontal lines.

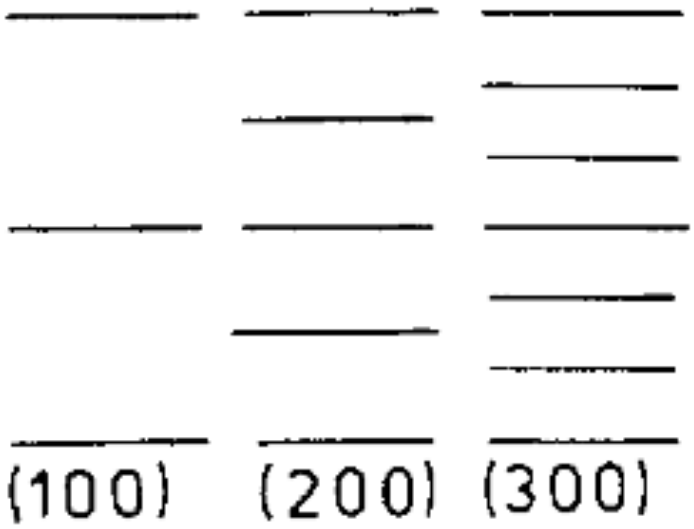
Family of planes

(hkl) - Family of plane: parallel planes and equally spaced. The indices correspond to the plane closer to the origin which intersects the cell at a/h, b/k and c/l.

Miller indices describe the orientation and spacing of a family of planes.

The spacing between adjacent planes of a family is referred to as the "**d-spacing**".

Three different families of planes: The d-spacing of (300) planes is one third of the (100) spacing



Note all (100) planes are members of the (300) family

Planes (and directions) of a form

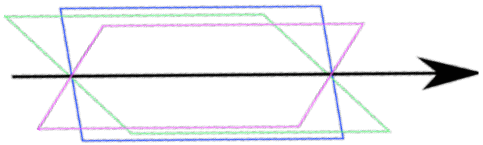
{hkl} - Planes of a form: equivalent lattice planes related by symmetry.

For the cubic system all the planes (100), (010), (001), ($\bar{1}$00), (0$\bar{1}$0) and (00$\bar{1}$) belong to the form {100}.

For a tetragonal material a=b≠c the form {100} would only include (100), (010), ($\bar{1}$00), and (0$\bar{1}$0).

<uvw> - Directions of a form: equivalent lattice directions related by symmetry

Planes of a zone

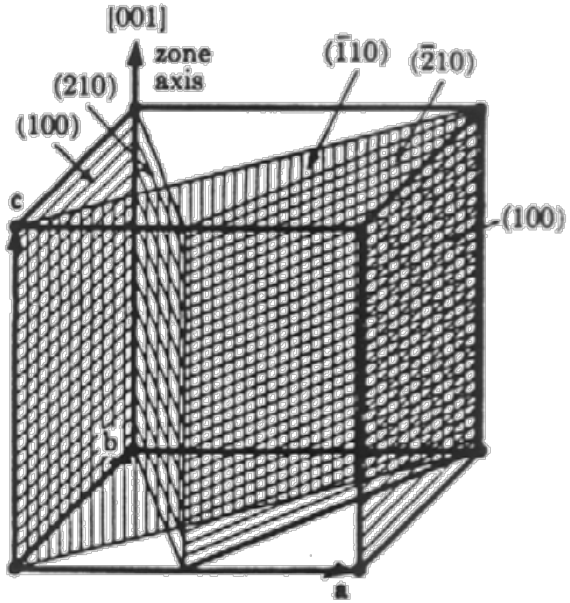


Planes of a zone - The planes of a zone axis **[uvw]** satisfy the Weiss Zone Law:

$$hu + kv + lw = 0$$

This law is valid for all lattices, Cartesian, or not.

In cubic systems [hkl] is normal to the set of planes (hkl) and the Weiss zone law can be expressed as the scalar (dot) product of [uvw] and the plane normal [hkl].



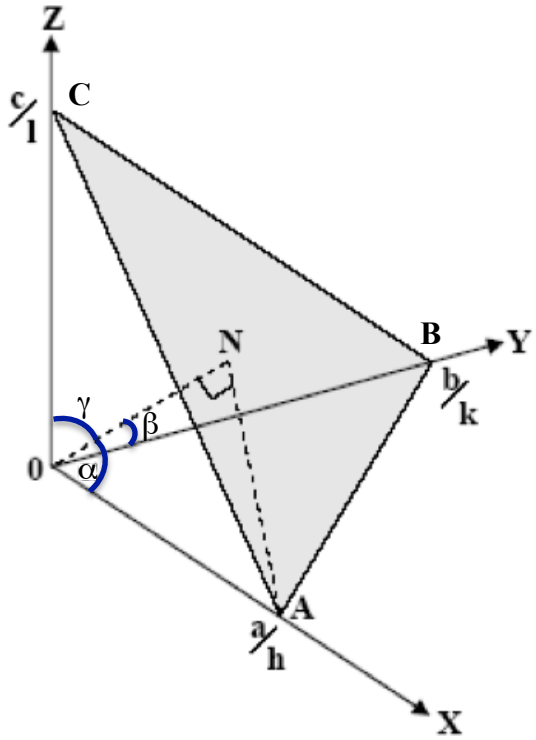
The shaded planes in the cubic lattice are planes of the zone [001].

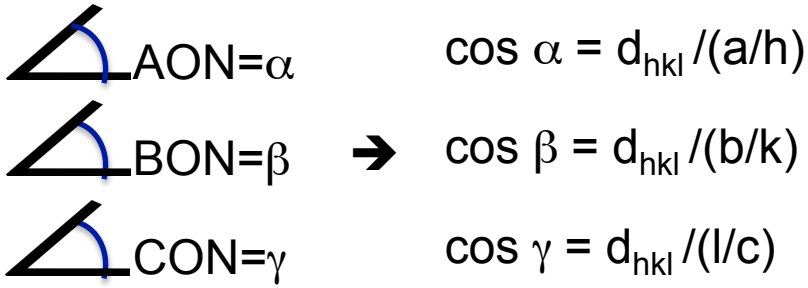
The planes of zone are not all of the same form.

Any direction is a zone axis!

Interplanar distances (d) formulae

In the case of orthogonal systems determination of interplanar distances is simple.





$\cos \alpha = d_{hkl}/(a/h)$

$\cos \beta = d_{hkl}/(b/k)$

$\cos \gamma = d_{hkl}/(l/c)$

For orthogonal axis: $\cos^2\alpha+\cos^2\beta+\cos^2\gamma=1$

Hence: $(h/a)^2.d_{hkl}^2+ (k/b)^2.d_{hkl}^2 + (l/c)^2.d_{hkl}^2 =1$

As a result: $(h/a)^2 + (k/b)^2 + (l/c)^2 = 1/d_{hkl}^2$

Intercepts of a lattice plane (*hkl) on the unit cell vectors a, b, c. As there is another plane of the same family passing through O the interplanar distance is just: ON=*d_{hkl}

Interplanar distances (d) formulae

Cubic:
$$\frac{1}{d^2} = \frac{h^2 + k^2 + l^2}{a^2}$$

Tetragonal:
$$\frac{1}{d^2} = \frac{h^2 + k^2}{a^2} + \frac{l^2}{c^2}$$

Hexagonal:
$$\frac{1}{d^2} = \frac{4}{3}\left(\frac{h^2 + hk + k^2}{a^2}\right) + \frac{l^2}{c^2}$$

Rhombohedral:
$$\frac{1}{d^2} = \frac{(h^2 + k^2 + l^2)\sin^2\alpha + 2(hk + kl + hl)(\cos^2\alpha - \cos\alpha)}{a^2(1 - 3\cos^2\alpha + 2\cos^3\alpha)}$$

Orthorhombic:
$$\frac{1}{d^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}$$

Monoclinic:
$$\frac{1}{d^2} = \frac{1}{\sin^2\beta}\left(\frac{h^2}{a^2} + \frac{k^2\sin^2\beta}{b^2} + \frac{l^2}{c^2} - \frac{2hl\cos\beta}{ac}\right)$$

Triclinic:
$$\frac{1}{d^2} = \frac{1}{V^2}(S_{11}h^2 + S_{22}k^2 + S_{33}l^2 + 2S_{12}hk + 2S_{23}kl + 2S_{13}hl)$$

In the equation for triclinic crystals,

V = volume of unit cell (see below),

$S_{11} = b^2c^2\sin^2\alpha$,

$S_{22} = a^2c^2\sin^2\beta$,

$S_{33} = a^2b^2\sin^2\gamma$,

$S_{12} = abc^2(\cos\alpha\cos\beta - \cos\gamma)$,

$S_{23} = a^2bc(\cos\beta\cos\gamma - \cos\alpha)$,

$S_{13} = ab^2c(\cos\gamma\cos\alpha - \cos\beta)$.

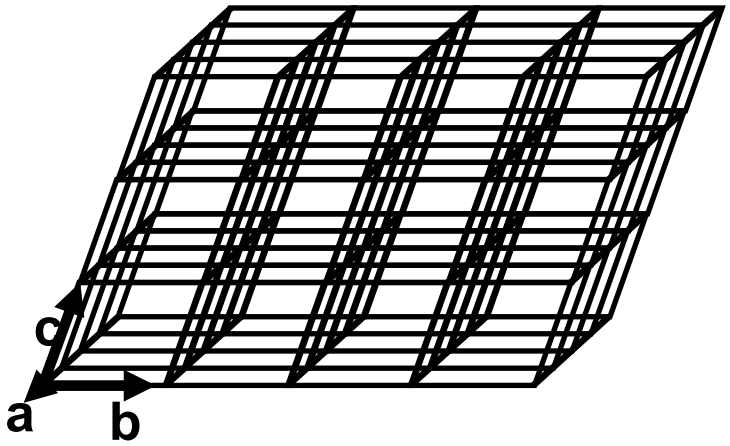
Symmetry operations

- A symmetry element (or operator) when applied to an object leaves that object unchanged

- An object has translational symmetry if it looks the same after a particular translation operation (an example is wallpaper, which has a repeating pattern; if you slide it by the right amount it looks the same as before).

- A point symmetry operation is specified with respect to a point in space which does not move during the operation (eg. inversion, rotation, reflection, improper rotation)

Translational symmetry operations

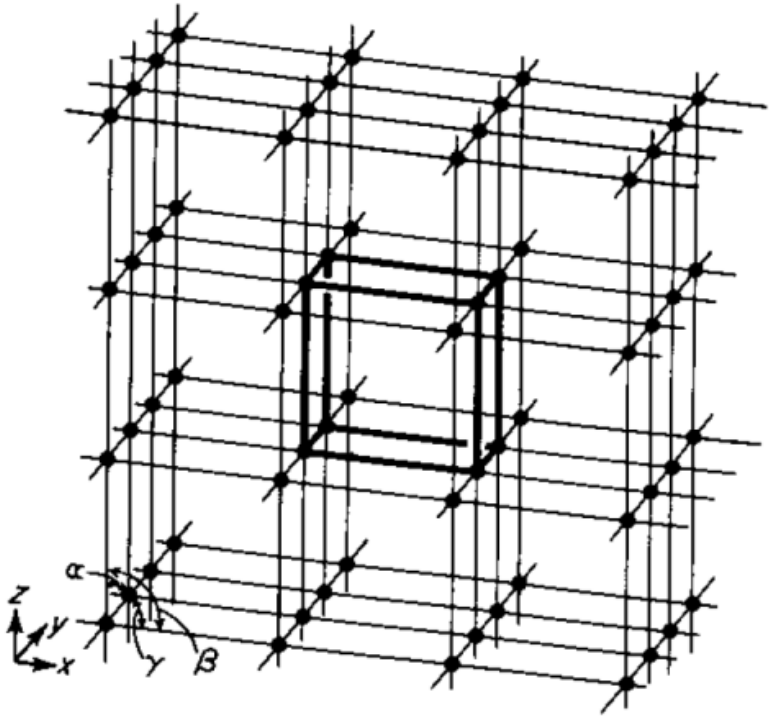


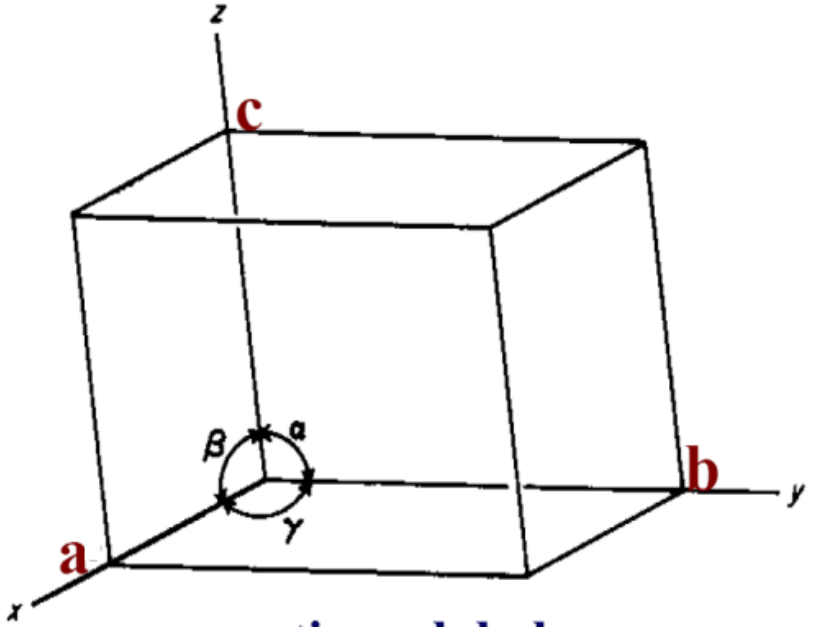
Lattice - Infinite array of points in space, in which each point has identical surroundings.

The simplest way to generate such na array is by using translation invariance (tranlational symmetry operation).

Unit cell

- **The repeat 3d unit in a lattice is called a unit cell**





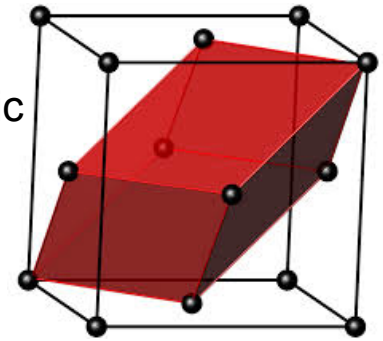
sometimes label a_1, a_2, a_3

- A **unit cell** is defined by six parameters, **a**, **b**, **c**, α, β, and γ
- **a x b • c = c x a • b = b x c • a = volume of the unit cell = V**

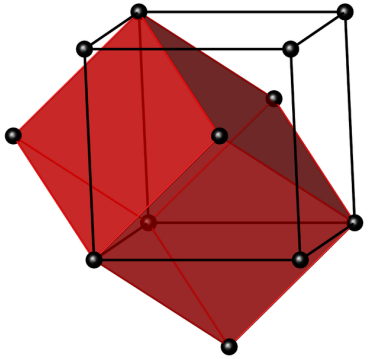
Unit cell choice

- There is always more than one possible choice of unit cell
- By convention the unit cell is usually chosen so that it is as small as possible while reflecting the full symmetry of the lattice
- If the unit cell contains only one lattice point is said to be primitive
- If it contains more than one lattice point it is centered

Face centered cubic
Primitive



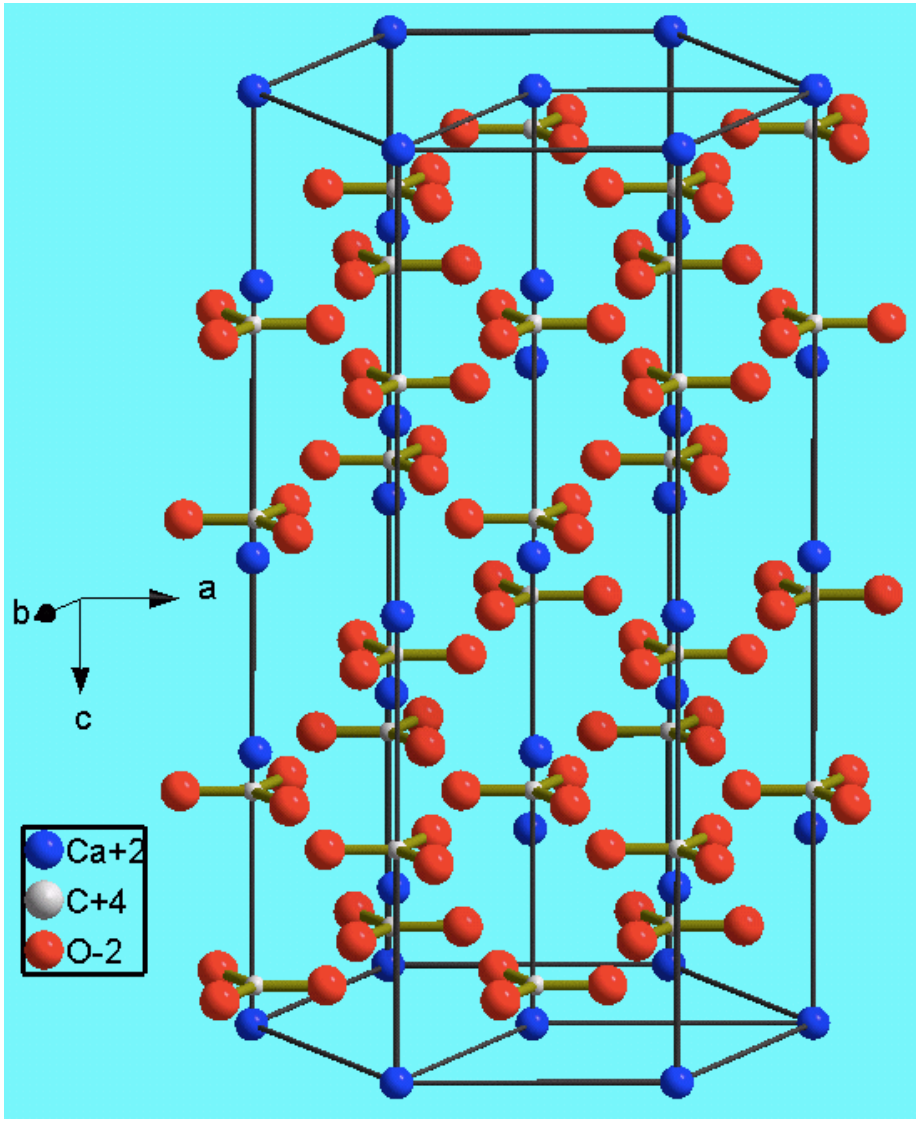
Why?



Body centred cubic
Primitive

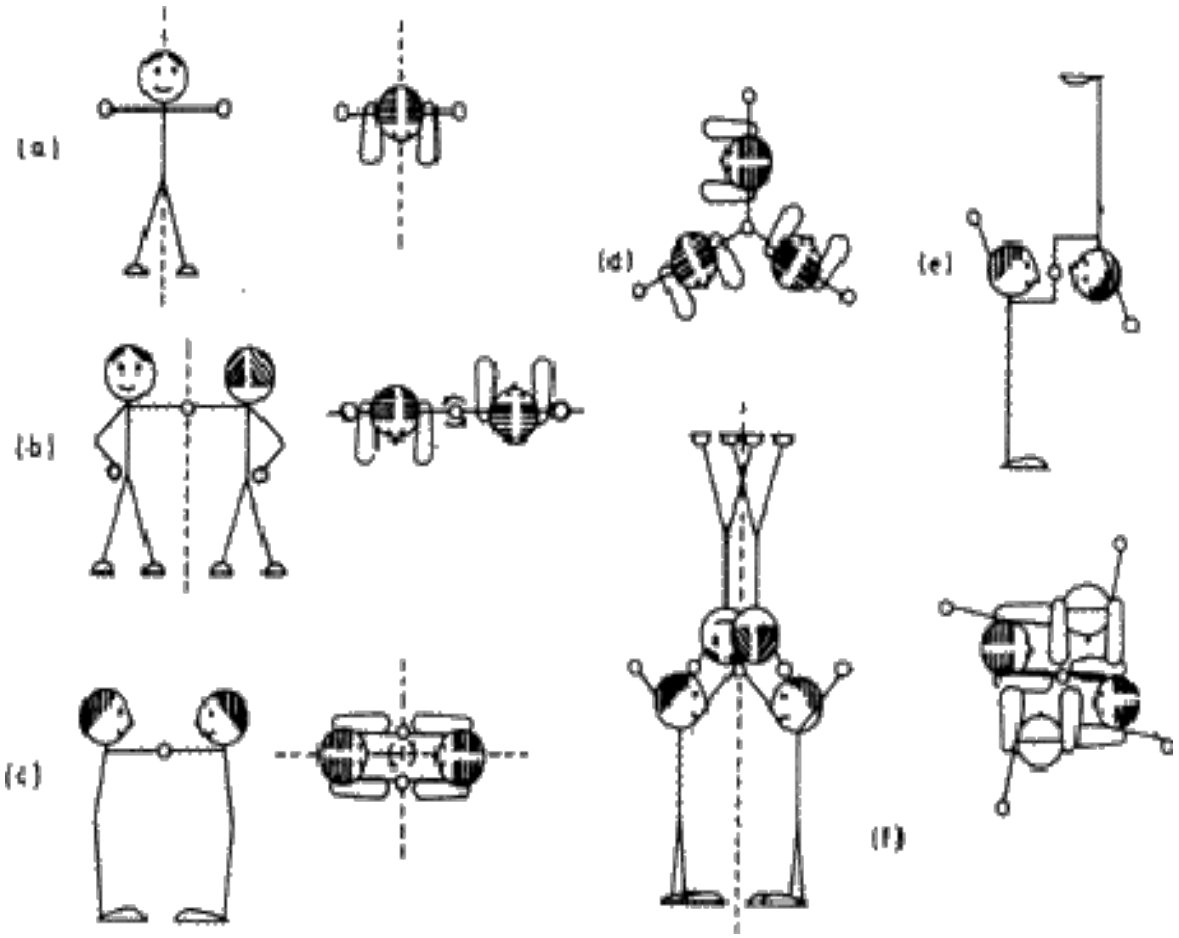
Why does crystallography need symmetry?

Crystal structure of calcite, a form of calcium carbonate



The symmetry of a crystal can be used to reduce the number of unique atom positions we have to specify

Point symmetry operations



Symmetry elements:

(a) Mirror plane, shown as dashed line, in elevation and plan.

(b) Twofold axis, lying along broken line in elevation, passing perpendicularly through clasped hands in plan.

(c) Combination of twofold axis with mirror planes, the position of the symmetry elements given only in plan.

(d) Threefold axis, shown in plan only.

(e) Centre of symmetry (in centre of clasped hands)

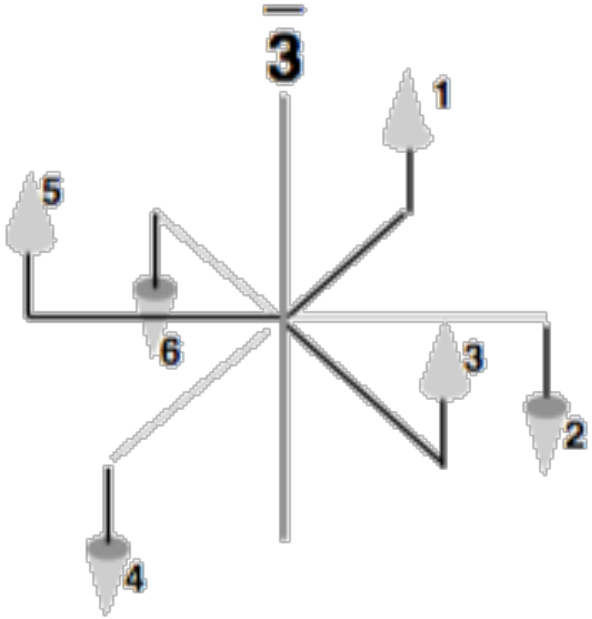
(f) Fourfold inversion axis, in elevation and plan, running along the dashed line and through the centre of the clasped hands **(compound point symmetry operation)**

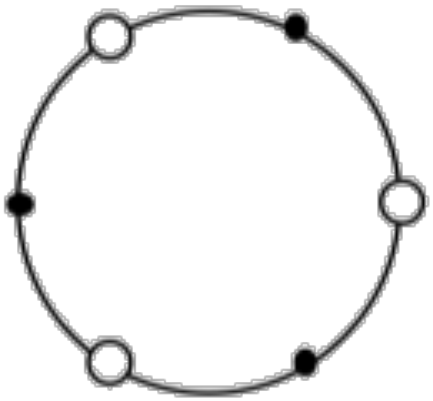
(Compound point symmetry operations)

Compound operations: Combinations of a rotation with a reflection or inversion. Inversion takes a locus on points.

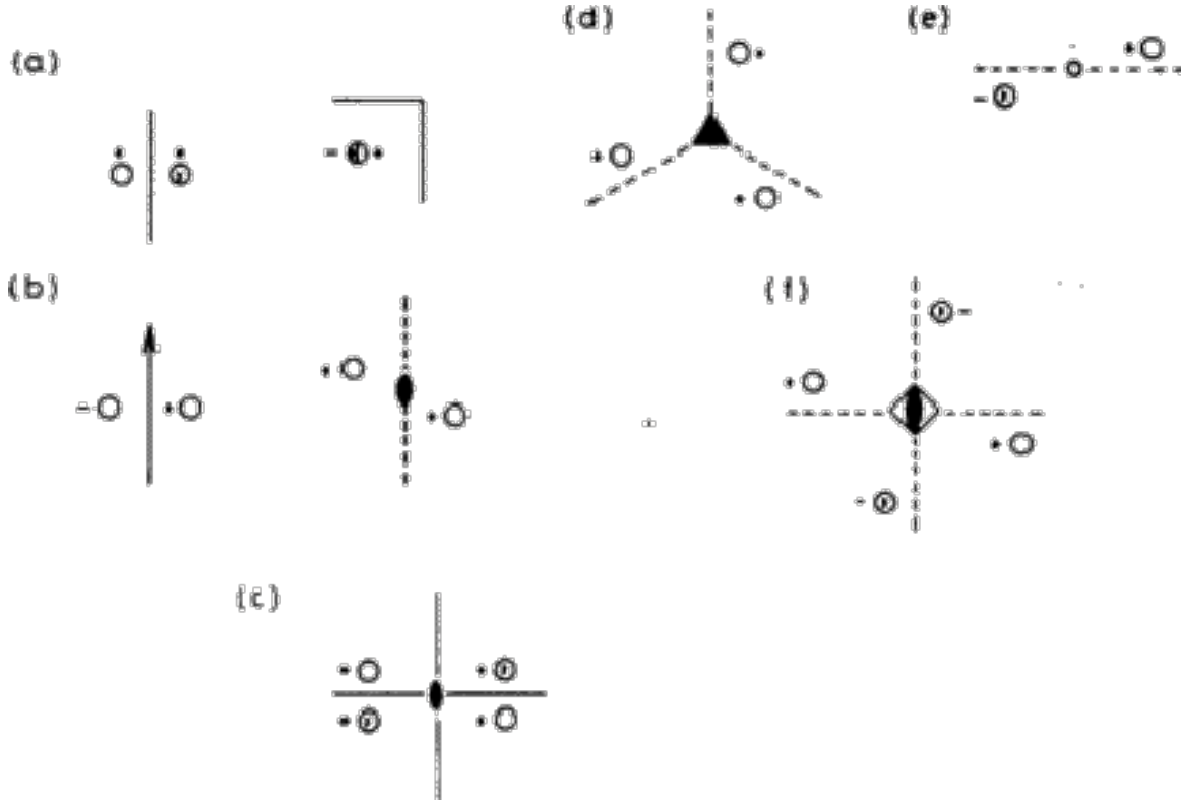
Simple rotations are **proper;** that is, they generate a sequence of objects with the same handedness**. Improper** rotations **(roto-inversions)** produce objects of **alternating handedness.**

Roto-inversions involve rotation and inversion. The overbar is used to designate roto-inversion. The figure below shows the operation of a 3-fold roto-inversion axis.





Point symmetry operations



Symmetry elements using conventional symbols. The right-hand group of (a) is drawn here in a different orientation, and the left-hand groups of (c) and (f) are omitted. Symbols + and - represent equal distances above and below the plane of the paper: open circles represent asymmetric units of one hand, and circles with commas their enantiomorphs. (a) Mirror plane (m), perpendicular to (left) and in the plane of the paper. (b) Twofold axis (2) in the plane of the paper (left) and perpendicular to it (right). (c) Combination of twofold axes and mirror planes. Note that the presence of any two of these elements creates the third. (d) Three fold axis (3). (e) Centre of symmetry (1). (f) Fourfold inversion axis ($\bar{4}$).

In written text mirror planes are given the symbol *m, while axes and the corresponding inversion axes are referred to as* $1, \bar{1}; 2, \bar{2}(\equiv m); 3, \bar{3}; 4, \bar{4}; 6, \bar{6}$. *The symbol 1 (for a onefold axis) means no symmetry at all, while the corresponding inversion axis (* $\bar{1}$ *) is equivalent, as already remarked, to a centre of symmetry.*

Describing symmetry operations with matrices

Rotation axes,
A $2\pi/n$ anti-clockwise rotation about axis *r*.
(If no *r* is given, use the principal (*z*) axis.)

$$\begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

(for $r = z$)

Determinant of matrix

$D = (\cos\theta)^2 + (\sin\theta)^2 = 1.0$

$\theta = 180°$ (two-fold):

(x,y,z) ➔ (-x, -y, z)

$$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Mirror planes
A reflection through a horizontal plane perpendicular to axis *r*.
(x,y,z) ➔ (x, y, -z)

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

(for $r = z$)

D = -1

Inversion centres,
Inversion through the centre point.
(x,y,z) ➔ (-x, -y, -z)

$$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

D = -1

Improper rotations,
A $2\pi/n$ anti-clockwise rotation about axis *r* followed by
a reflection through a horizontal plane perpendicular to *r*.

$$\begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

(for $r = z$)

D = -1

Improper operations (change of hand)

Translation,
Translation along one of the lattice vectors.

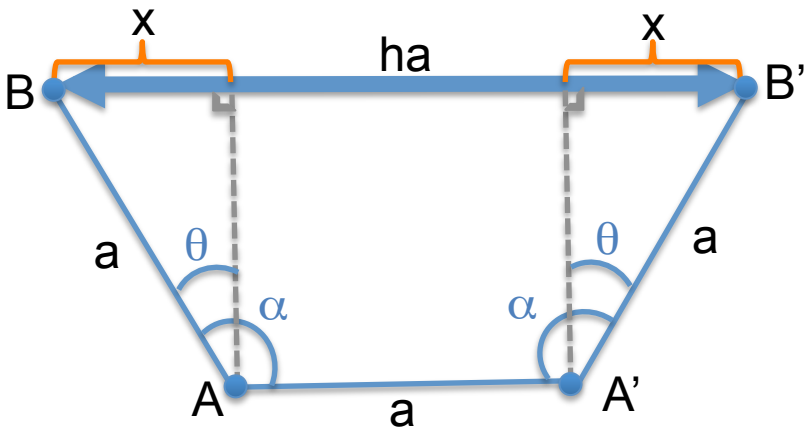
t = 0***x**+0***y**+1***z**

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}$$

(for $r = z$)

Rotations compatible with a lattice

Assume two lattice points, A and B, and that the minimum lattice spacing is **a** (unit translation). B generates a new point A' which is rotated from A by a generic angle α. Applying the same rotational operation R at A' generates a new point B'. If A' and B' are both lattice points then R is a symmetry operation. Due to the (translational) periodicity of the crystal, the new vector **ha,** which connects B and B', must be an integral multiple of a



$$\cos(\theta + \tfrac{\pi}{2}) = -\sin\theta$$

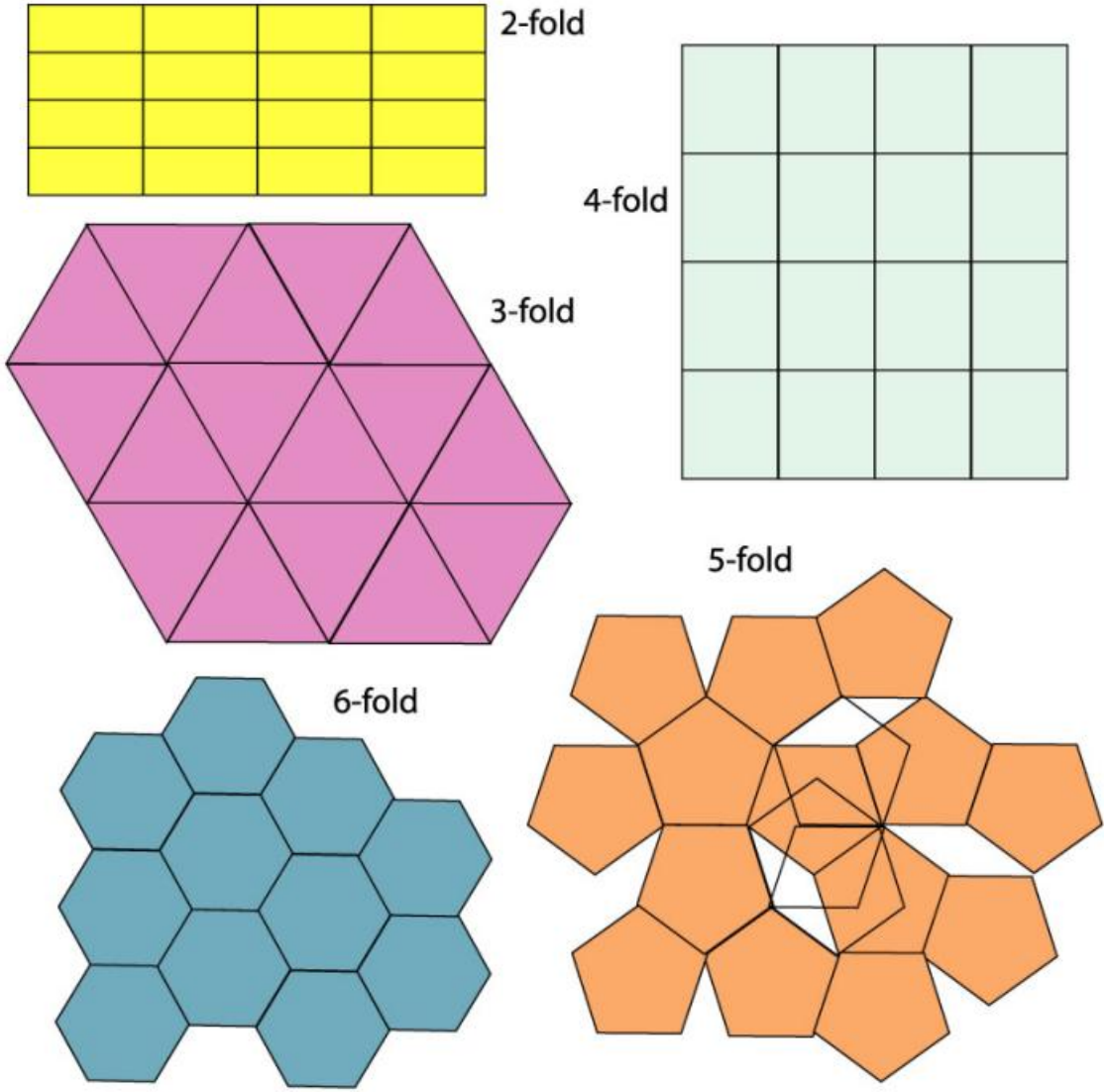
AA' = a
BB' = ha = a + 2x
$x = a.\sin(\theta) = -a.\cos(\theta+\pi/2) = -a.\cos(\alpha)$
$ha = a - 2a.\cos(\alpha)$
$ha - a = -2a.\cos(\alpha)$
$(h-1)/2 = -\cos\alpha$
For h integer: h = -1,0,1,2,3
Hence: $\cos\alpha = 0, \pm\frac{1}{2}, \pm 1$

$\alpha = 0°, 60°, 90°\ 120°, 180°$, or $360°$

Since an n-fold is 360°/n, this constrains a lattice to containing 1-, 2-, 3-, 4-, or 6-fold symmetry (not 5 or 7, etc.)

Rotations compatible with a lattice

Only 2, 3, 4 and 6-fold rotations can produce space filling patterns



Point symmetry operations compatible with a lattice

Rotations

- 1-fold 360° I Identity
- 2-fold 180° 2
- 3-fold 120° 3
- 4-fold 90° 4
- 6-fold 60° 6

Roto-Inversions (Improper Rotations)

- 1-fold 360° $\bar{1}$
- 2-fold 180° $\bar{2}$
- 3-fold 120° $\bar{3}$
- 4-fold 90° $\bar{4}$
- 6-fold 60° $\bar{6}$

Crystal systems

Crystals are axiomatically divided in 7 systems according to their symmetry

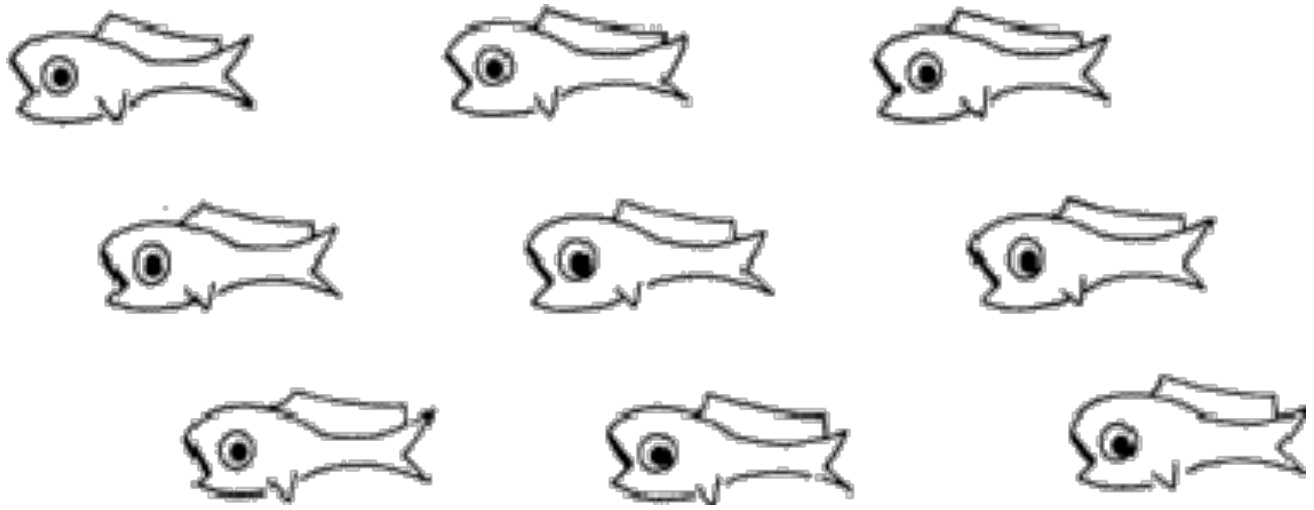
System	Conventional unit cell		Defining symmetry
Triclinic	$\mathbf{a_1} \neq \mathbf{a_2} \neq \mathbf{a_3}$	$\alpha \neq \beta \neq \gamma$	Identity
Monoclinic	$\mathbf{a_1} \neq \mathbf{a_2} \neq \mathbf{a_3}$	$\alpha = \gamma, \quad \beta \geq 90°$	1 * 2-fold
Orthorhombic	$\mathbf{a_1} \neq \mathbf{a_2} \neq \mathbf{a_3}$	$\alpha = \beta = \gamma = 90°$	3 * 2-fold
Tetragonal	$\mathbf{a_1} = \mathbf{a_2} \neq \mathbf{a_3}$	$\alpha = \beta = \gamma = 90°$	1 * 4-fold
Trigonal	$\mathbf{a_1} = \mathbf{a_2} = \mathbf{a_3}$	$\alpha = \beta = \gamma \neq 90°$	1 * 3-fold
Hexagonal	$\mathbf{a_1} = \mathbf{a_2} \neq \mathbf{a_3}$	$\alpha = \beta = 90°, \gamma = 120°$	1 * 6-fold
Cubic	$\mathbf{a_1} = \mathbf{a_2} = \mathbf{a_3}$	$\alpha = \beta = \gamma = 90°$	4 * 3-fold

NB: Axiomatically = self-evident

Symmetry operations compatible with the triclinic system

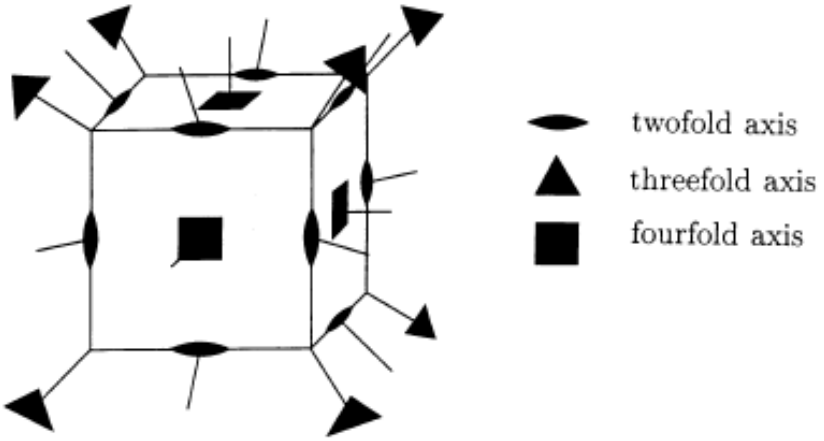
Only translational symmetry, no rotational symmetry other than 1 or $\bar{1}$

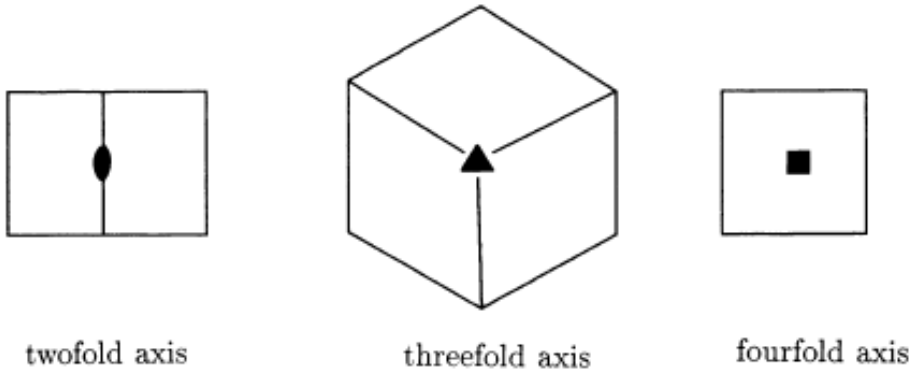
Illustrative 2D example (a planar lattice…)



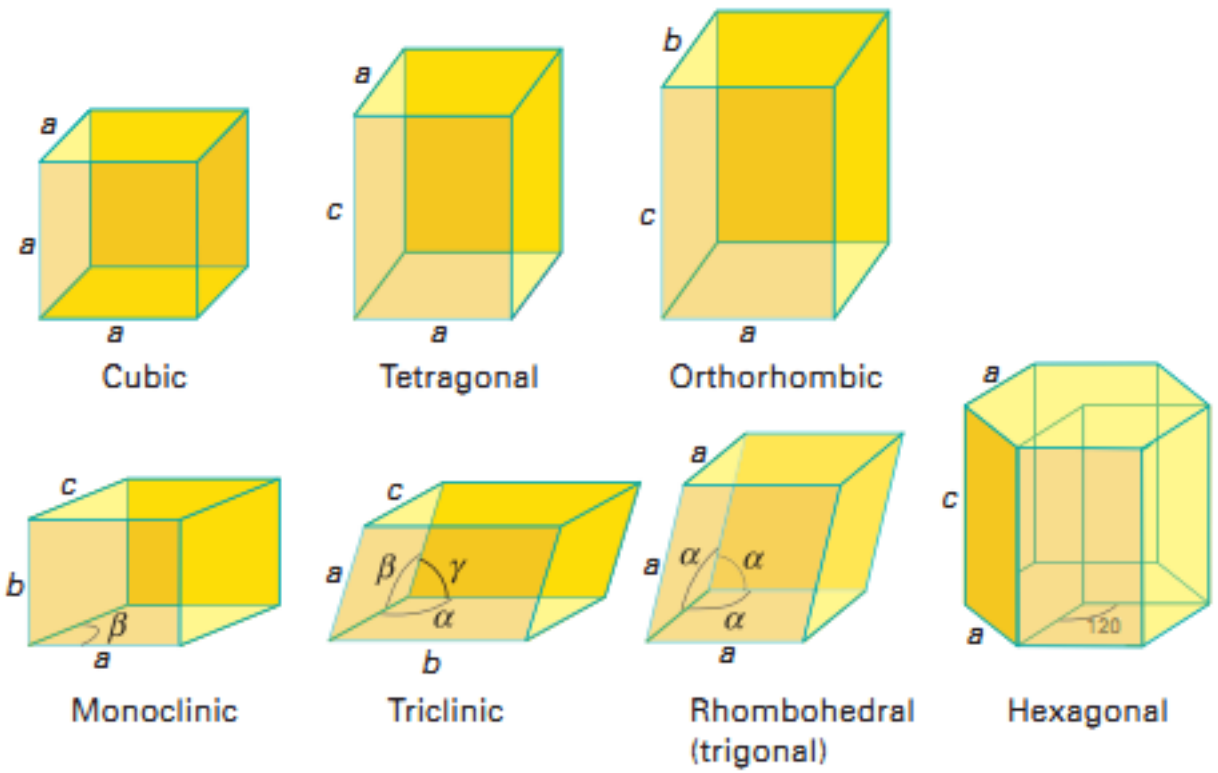
An array of repeating motifs: neither the motif nor the lattice contains any elements of symmetry other than 1 or $\bar{1}$

Symmetry operations compatible with the cubic system





Crystal systems

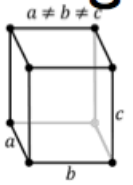


Centering

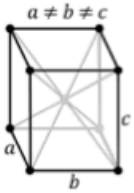
- What happens when other points are added to each of the previous lattices while maintaining the rotation symmetry (added at centered positions, centering involves only translation operations = centering operators)
- In each situation is it still a lattice? Is it a new lattice?

Four possible lattice centerings

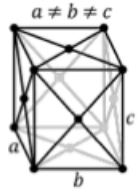
P: Primitive - lattice points on cell corners



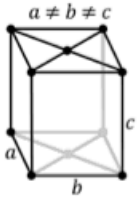
I: Body-centred - additional lattice point at cell centre



F: Face-centred - one additional lattice point at centre of each face



A/B/C: Centred on a single face - one additional lattice point centred on A, B or C face



The location of the additional lattice points within the unit cell is described by a set of **centering operators**:

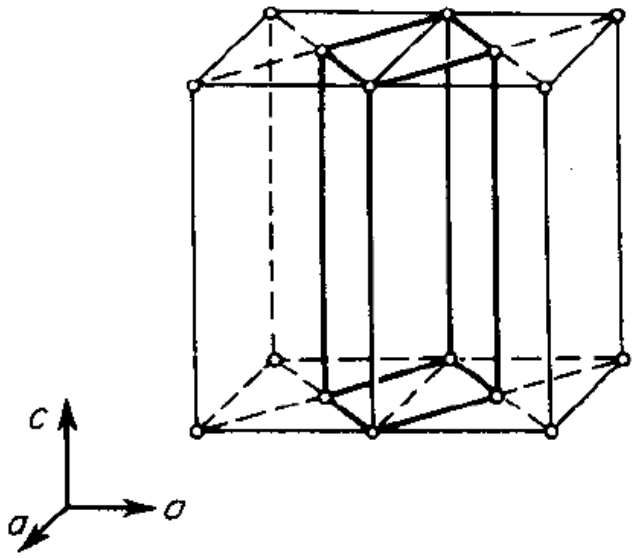
- Body centered (I) has additional lattice point at (1/2,1/2,1/2)
- Face centered (F) has additional lattice points at (0,1/2,1/2), (1/2,0,1/2), and (1/2,1/2,0)
- Side centered (C) has an additional lattice point at (1/2,1/2,0)

Centering

Not all centering possibilities occur for each of the seven crystal systems: Only 14 unique combinations (Bravais lattices):

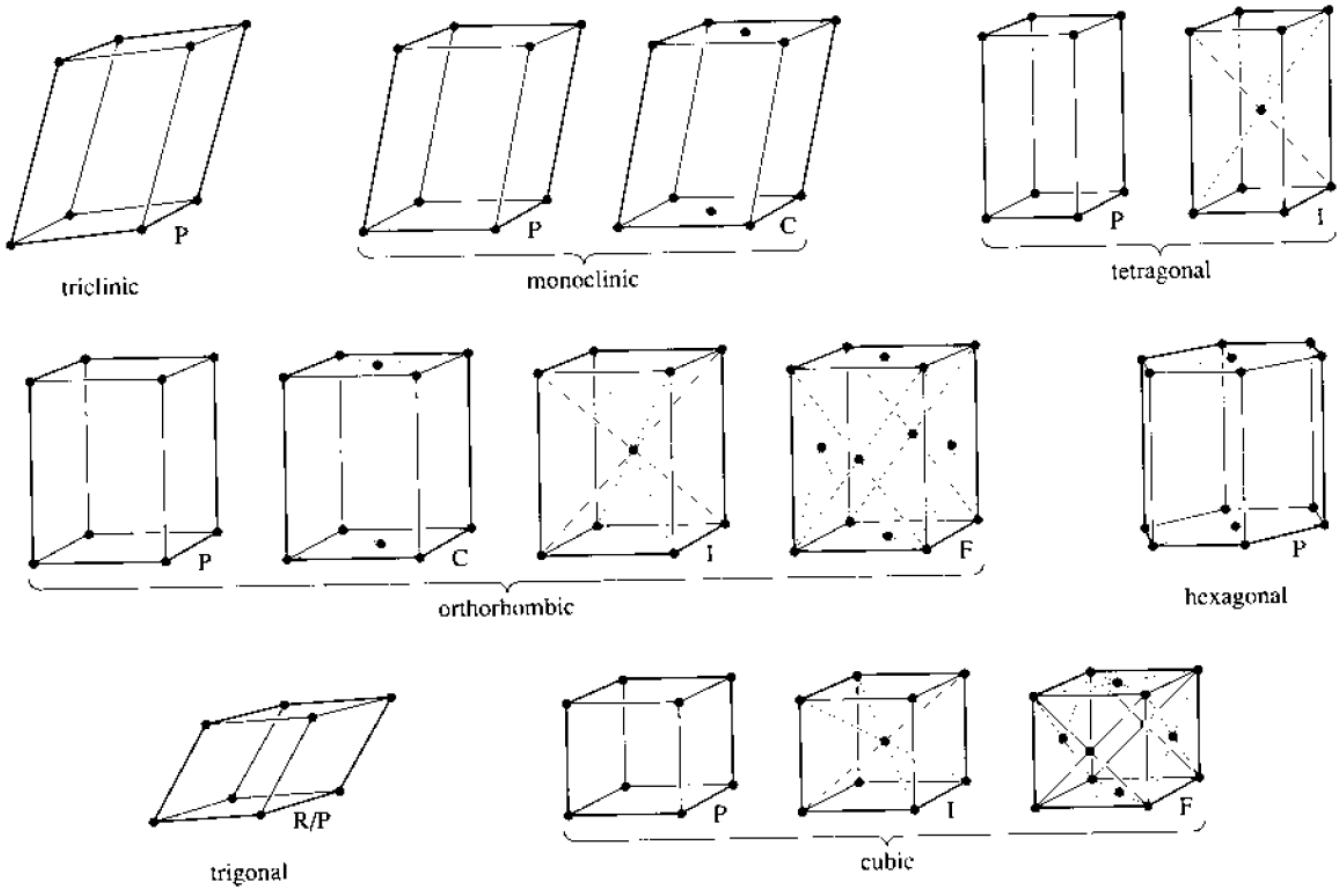
- Some centering types are not allowed because they would lower the symmetry of the unit cell (e.g. side centered cubic is not possible as this would destroy the three-fold symmetry that is an essential component of cubic symmetry)

- Some centering types are redundant (e.g. C-centered tetragonal can always be described using a smaller primitive tetragonal cell, see figure)



Bravais lattices

The combination of crystal system and centering gives 14 Bravais lattices



A Bravais lattice is an infinite array of discrete points with **identical environment**: seven crystal systems + four lattice centering types = 14 Bravais lattices

Point symmetry groups

A set of symmetry operations that leave an object invariant. Generically, there are infinite point symmetry groups. However, not all can be combined with a lattice.

In crystallography we are interested in objects that can be combined with the lattices: there are only 32 point groups compatible with periodicity in 3-D.

Crystallographic point symmetry groups

- A crystallographic point group is a **set of symmetry operations**, like rotations or reflections, that leave a central point fixed while moving other directions and faces of the crystal to the positions of features of the same kind.

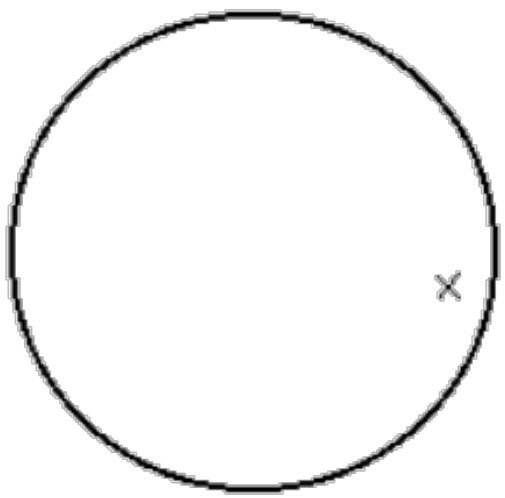
- For a true crystal the group must also be consistent with maintenance of the three-dimensional translational symmetry that defines crystallinity.

- The macroscopic properties of a crystal would look exactly the same before and after any of the operations in its point group. In the classification of crystals, each point group is also known as a crystal class.

- There are infinitely many three-dimensional point groups; However, the crystallographic restriction of the infinite families of general point groups results in there being only **32 crystallographic point groups**.

The 32 point groups in stereographic projection

Triclinic system



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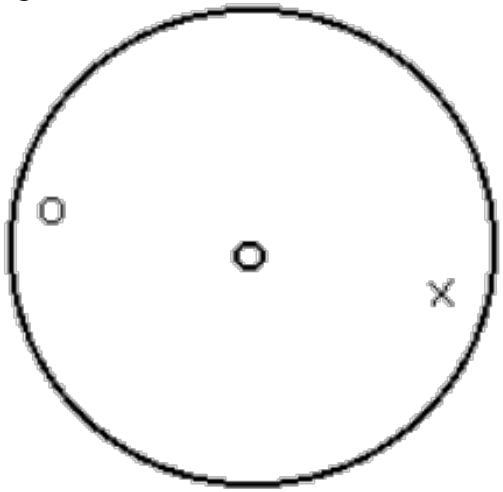
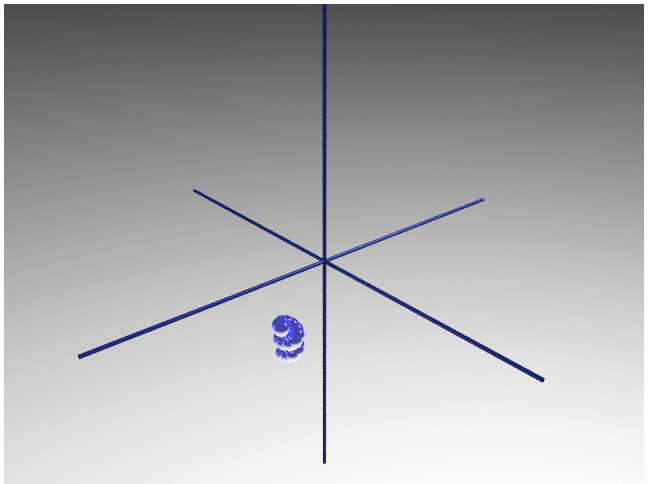
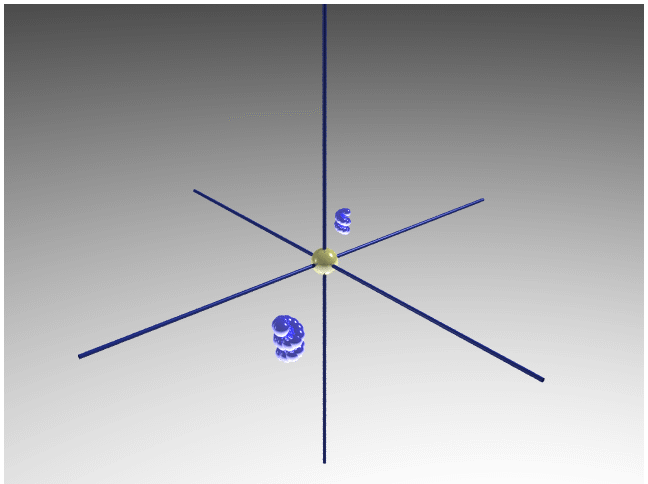


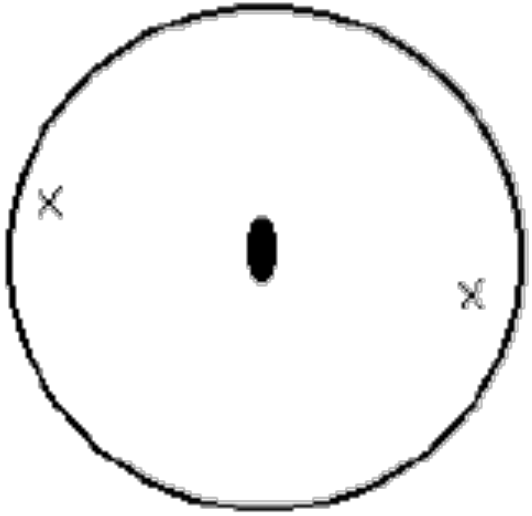
$\bar{1}$





Point Groups in Stereographic projection

Monoclinic System



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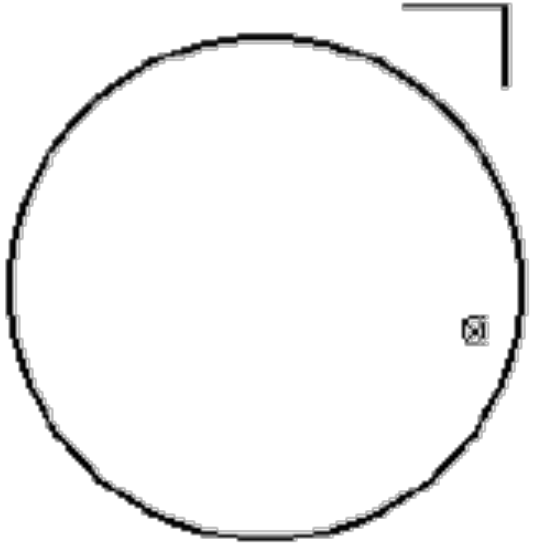
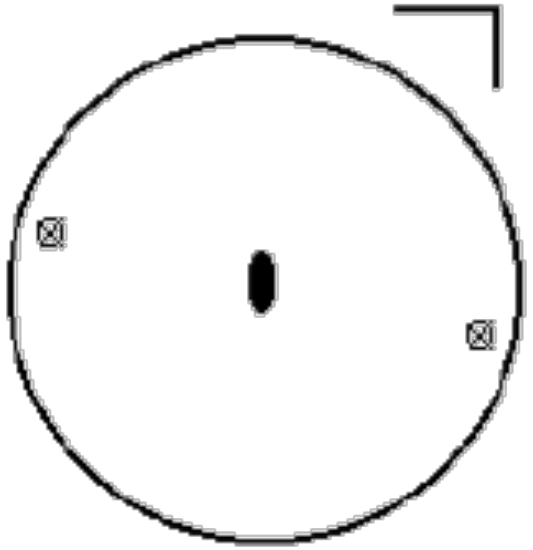
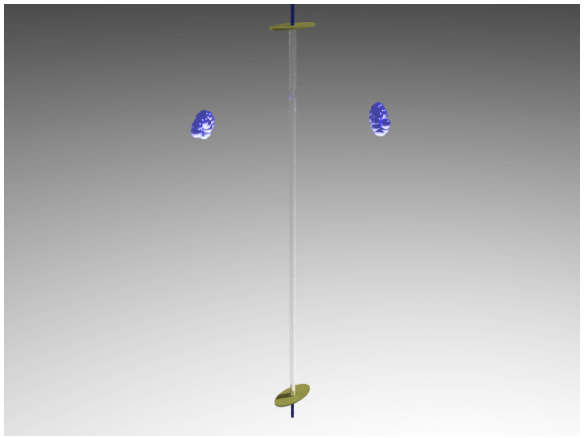
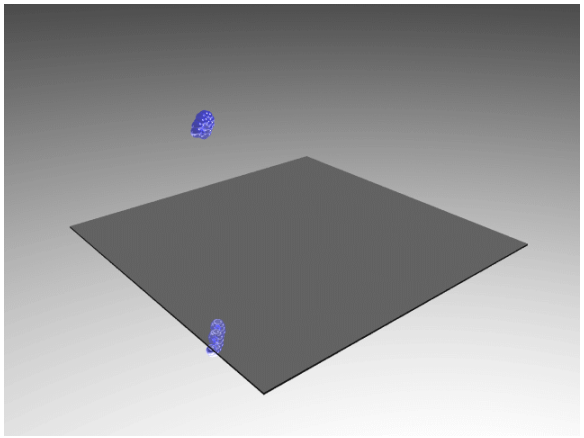


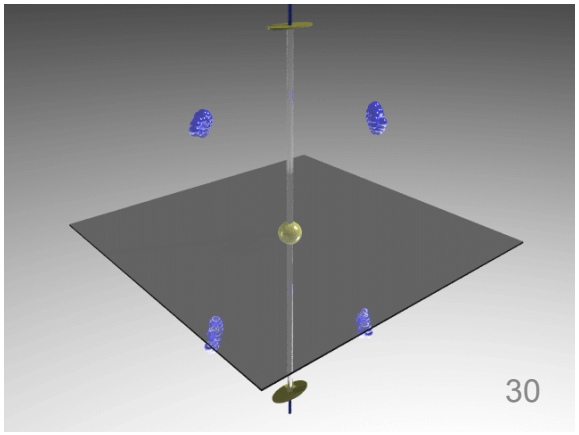
$\bar{2} = m$



$2/m$

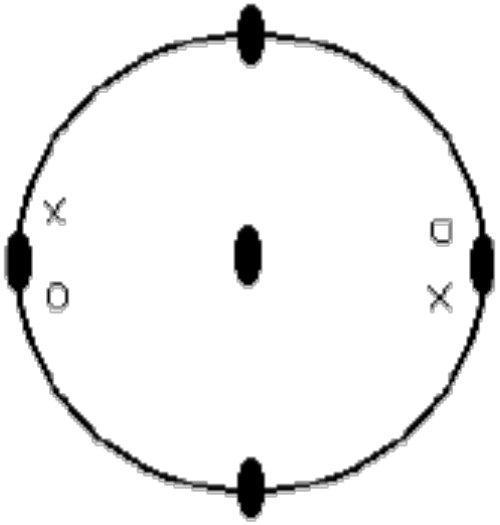






Point Groups in Stereographic projection

Orthorhombic System



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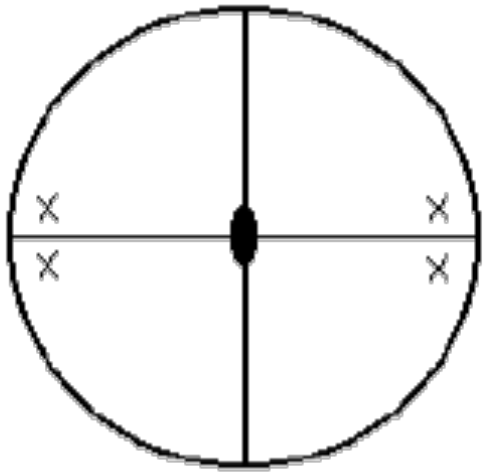
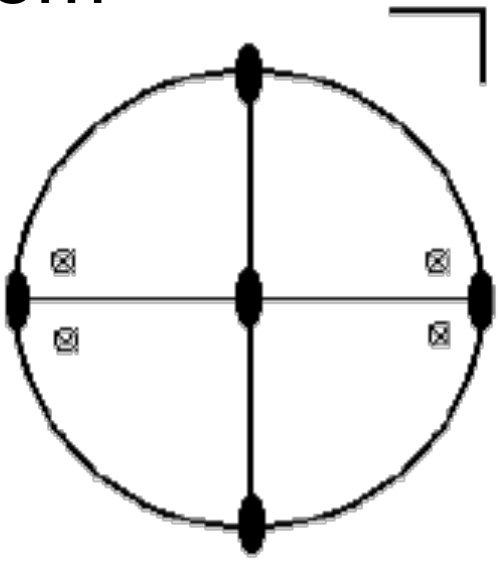
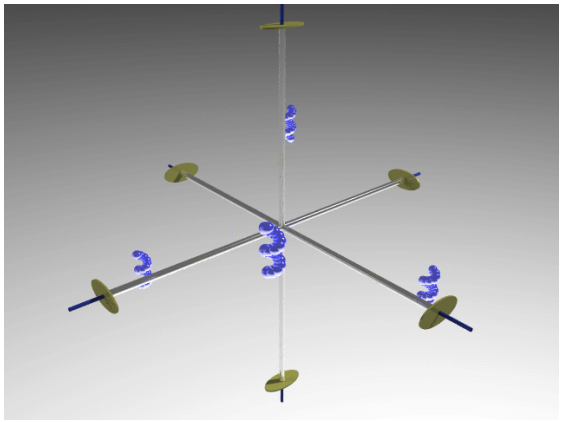
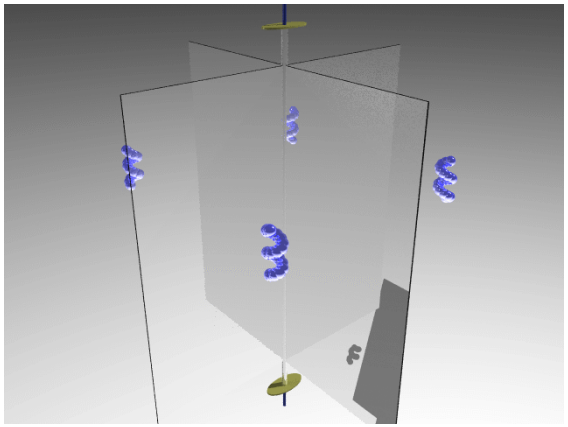


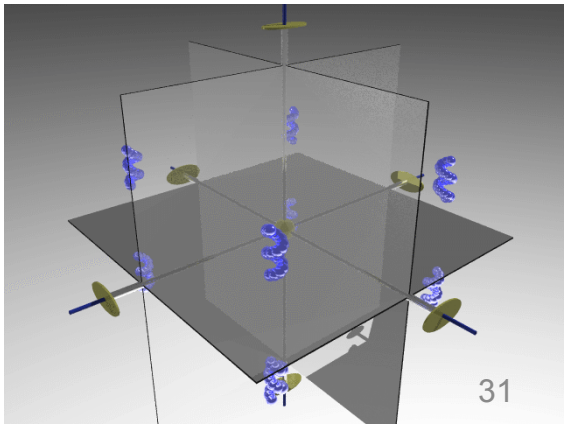
$2mm = mm2$



$2/m2/m2/m = mmm$

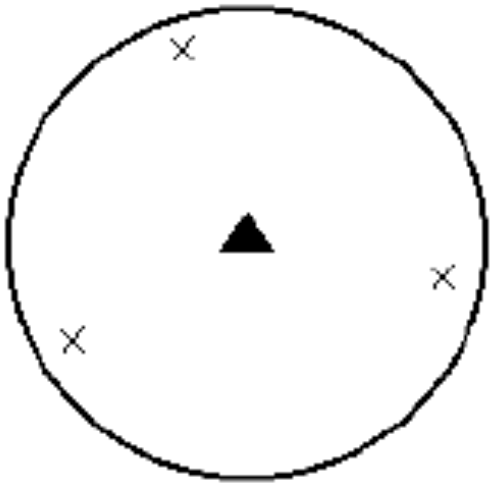






Point Groups in Stereographic projection

Trigonal System



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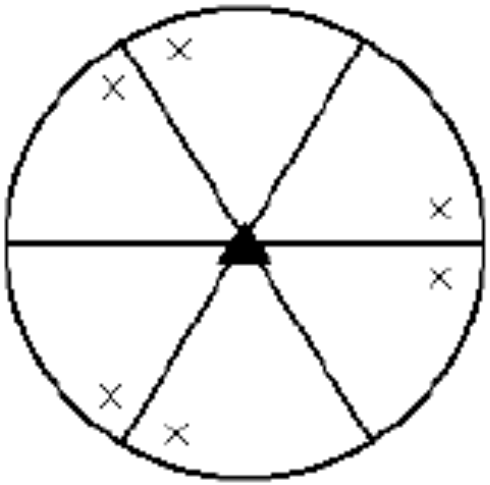
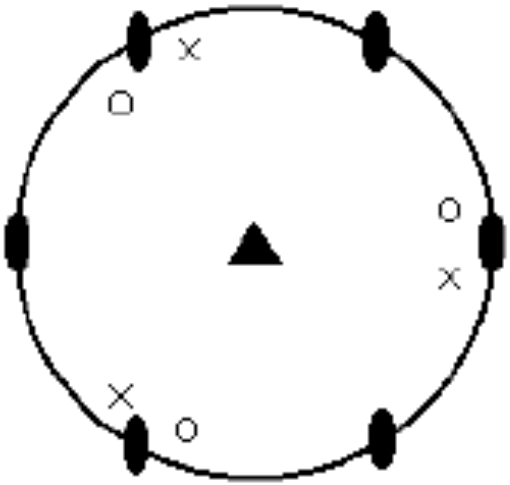
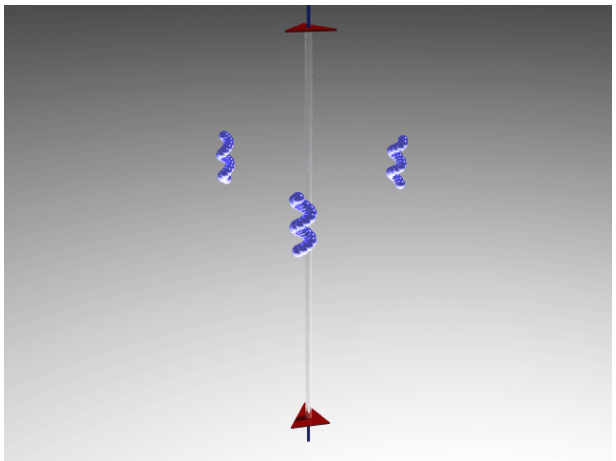
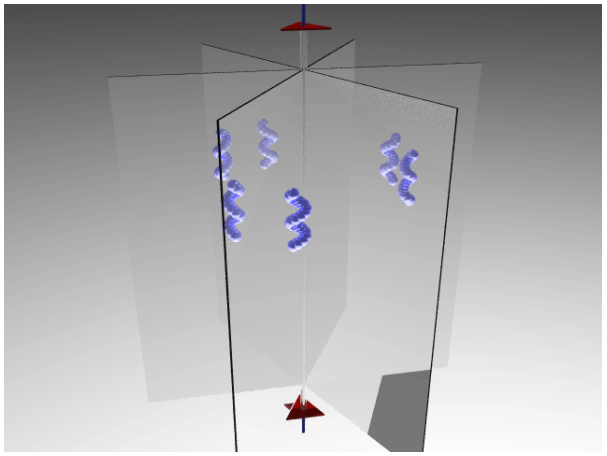


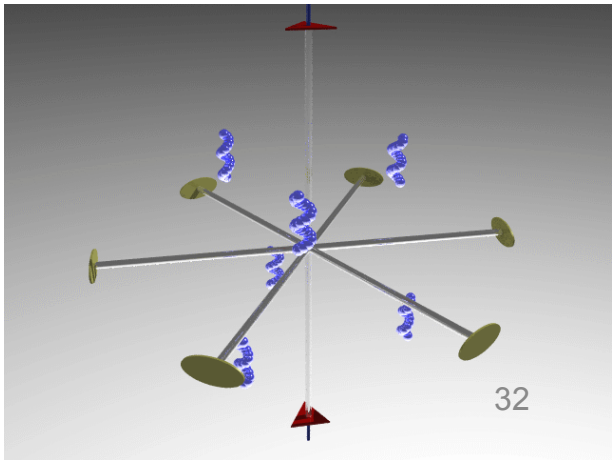
3m



32

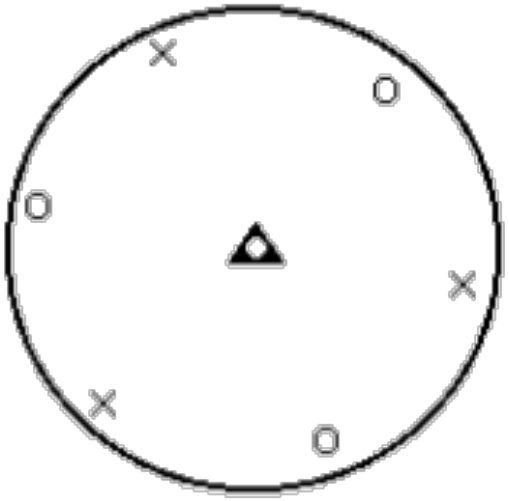




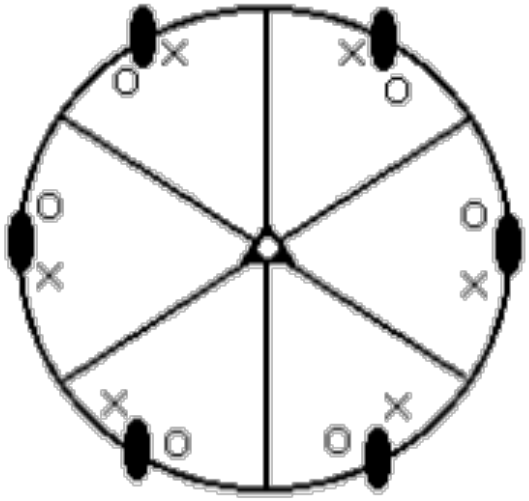


Point Groups in Stereographic projection

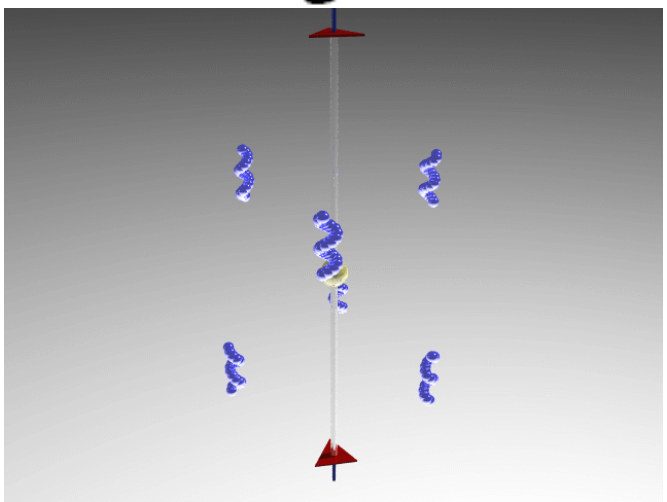
Trigonal System

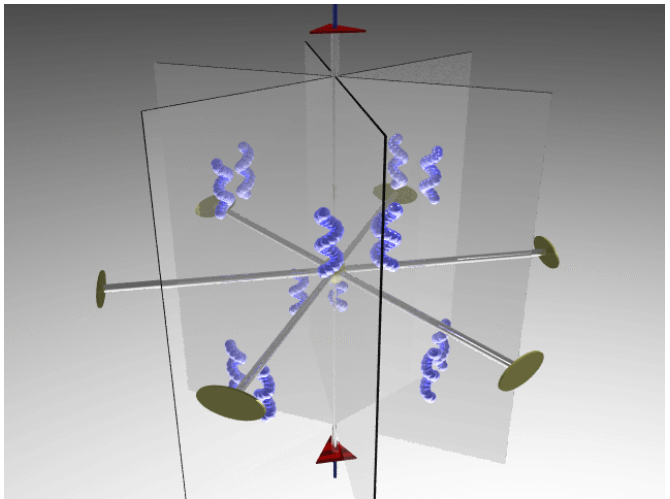


$\bar{3}$

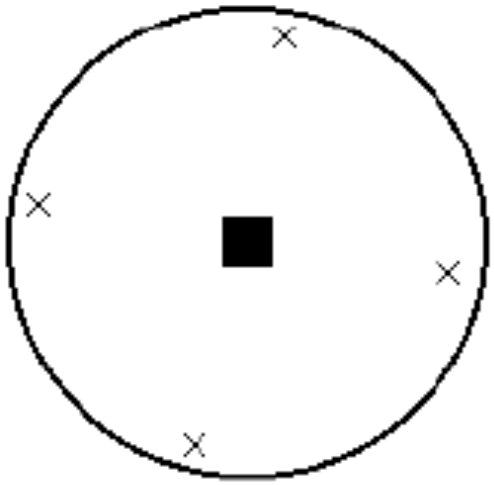


$\bar{3}2/m = \bar{3}m$





Point Groups in Stereographic projection
Tetragonal System



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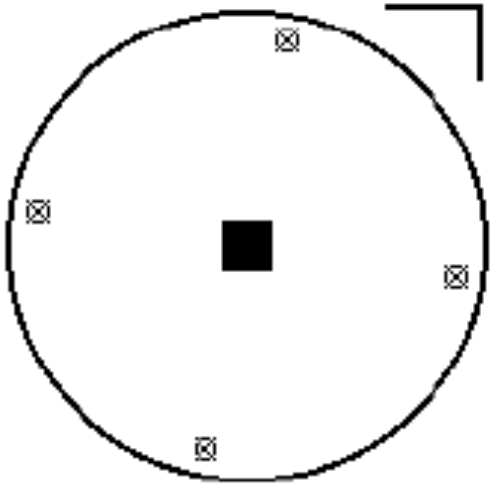
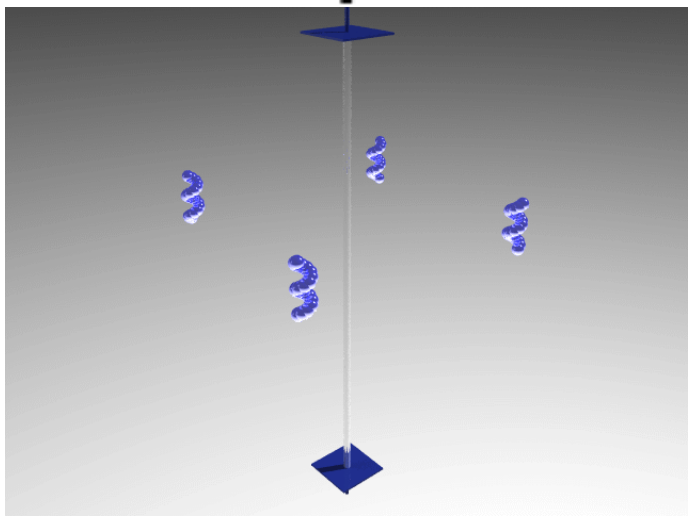
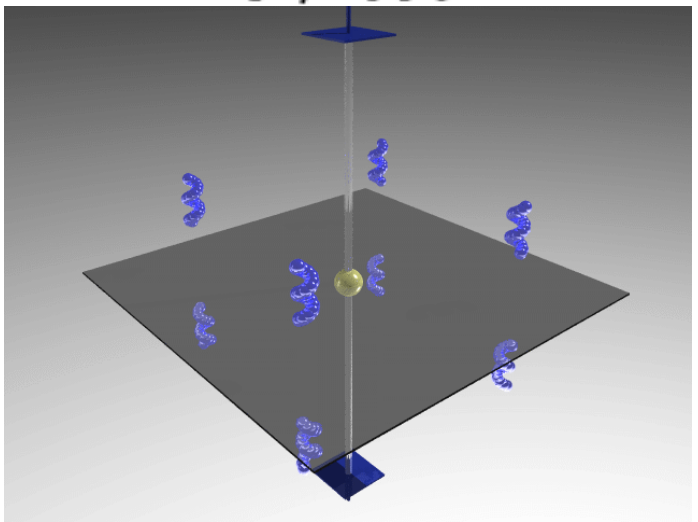


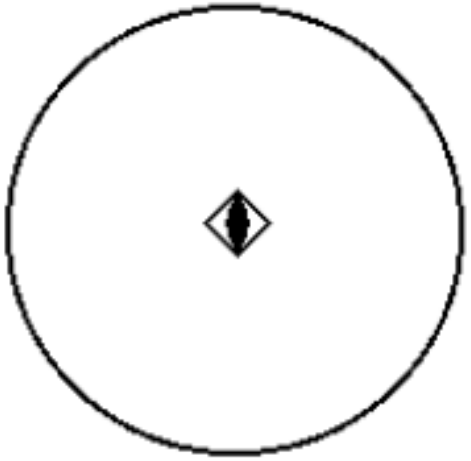
$4/m$



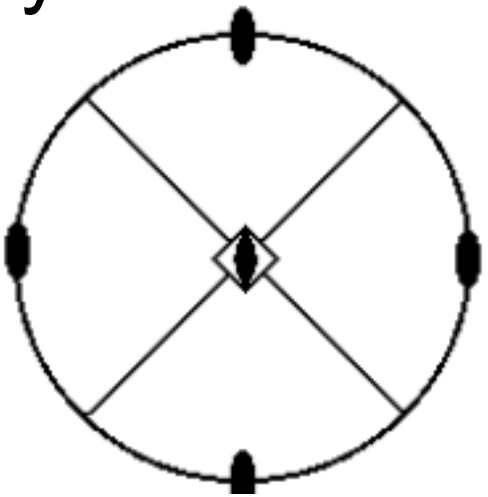


Point Groups in Stereographic projection

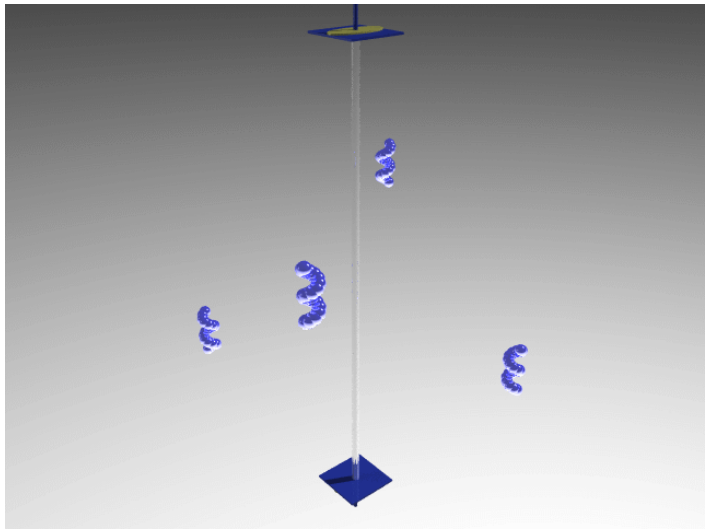
Tetragonal System

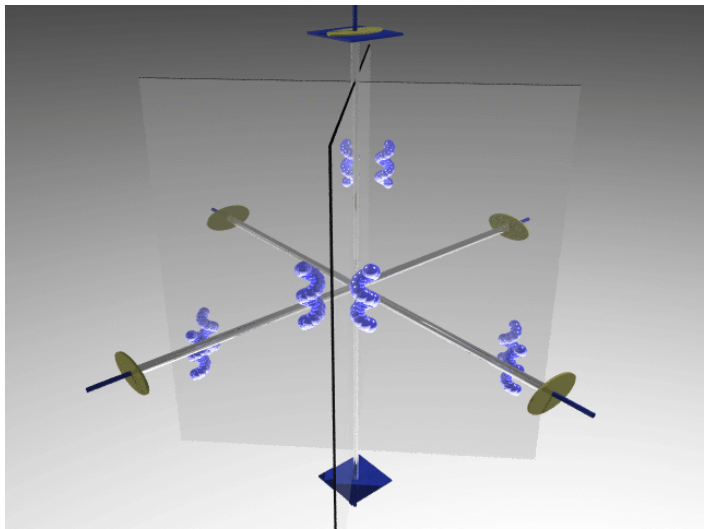


$\bar{4}$

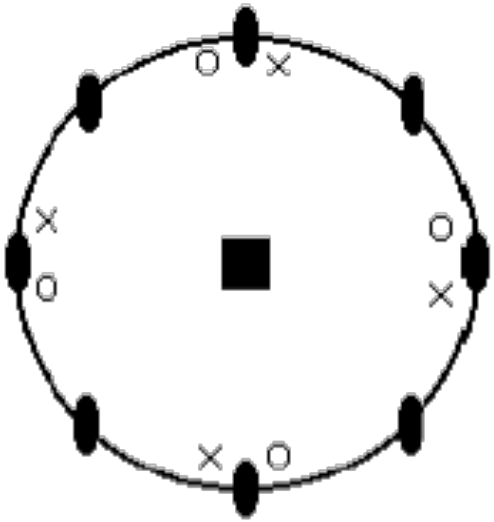


$\bar{4}2m$





Point Groups in Stereographic projection
Tetragonal System



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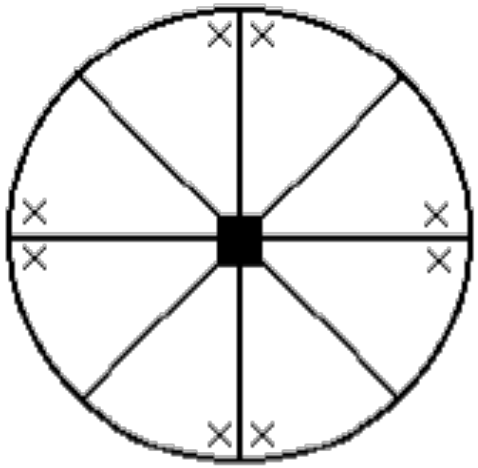
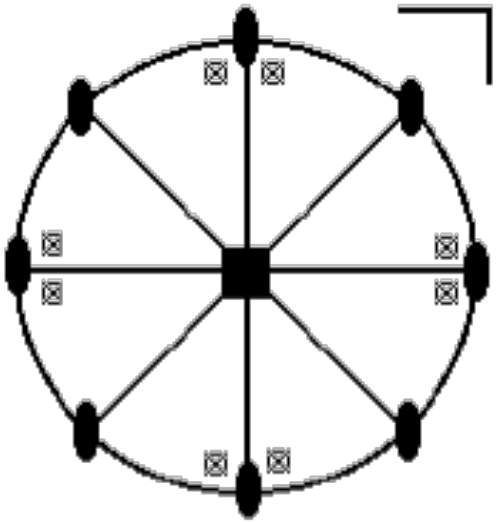
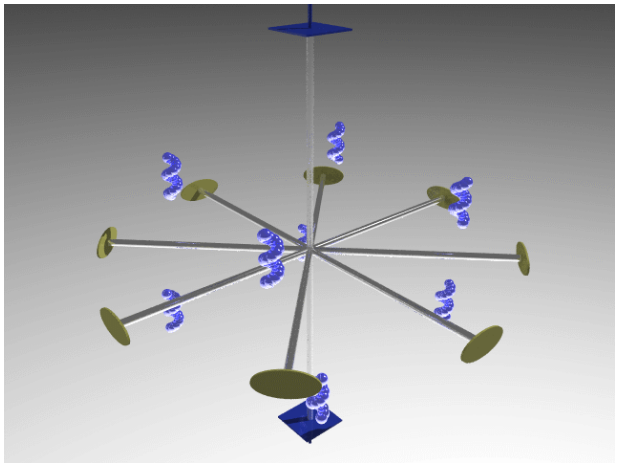
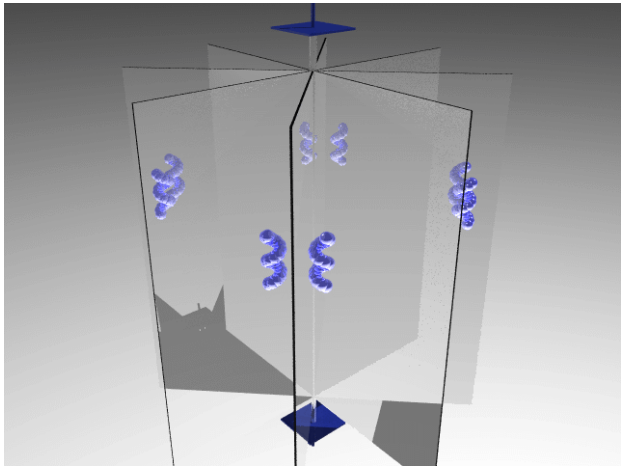


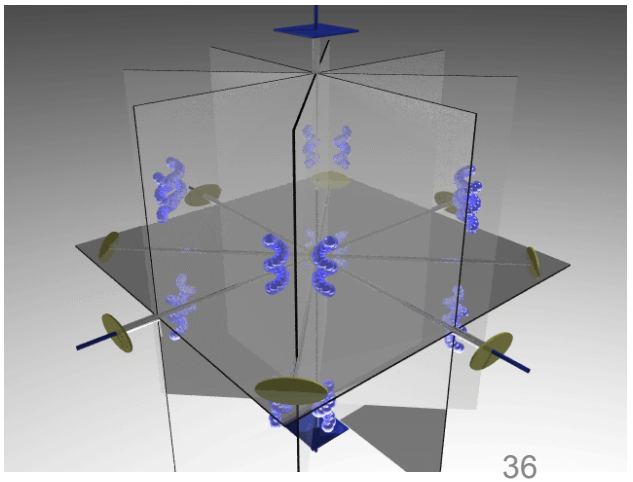
$4mm$



$4/m2/m2/m = 4/mmm$

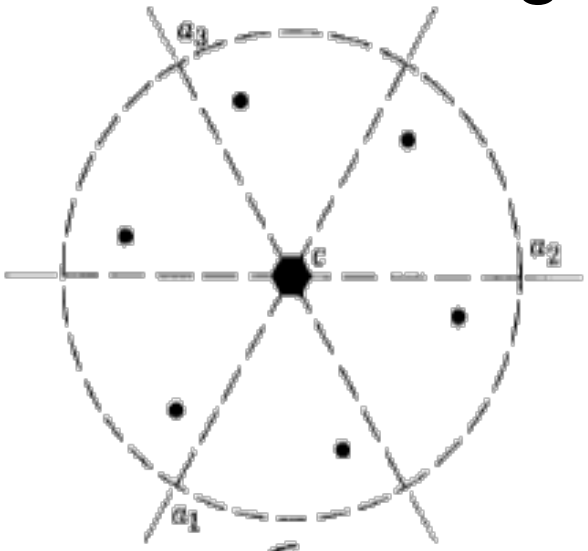




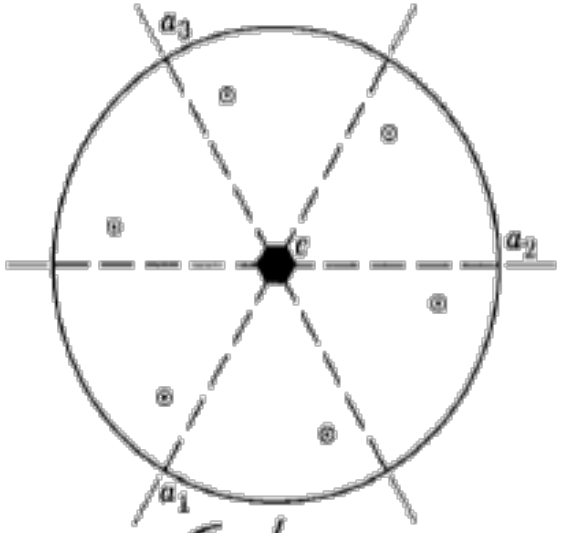


Point Groups in Stereographic projection

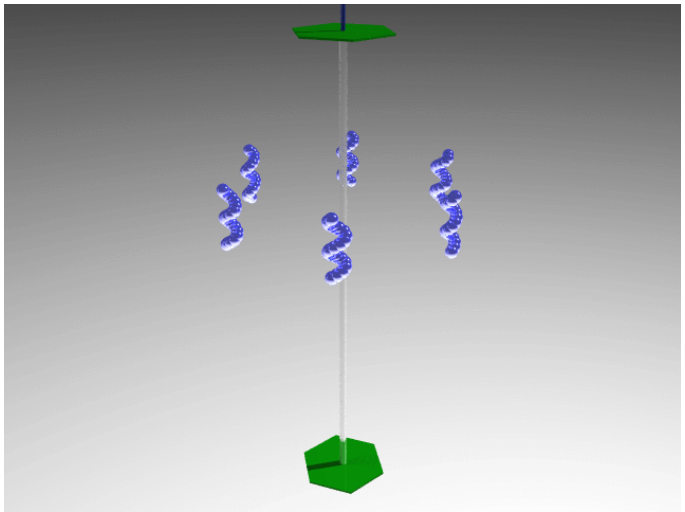
Hexagonal System

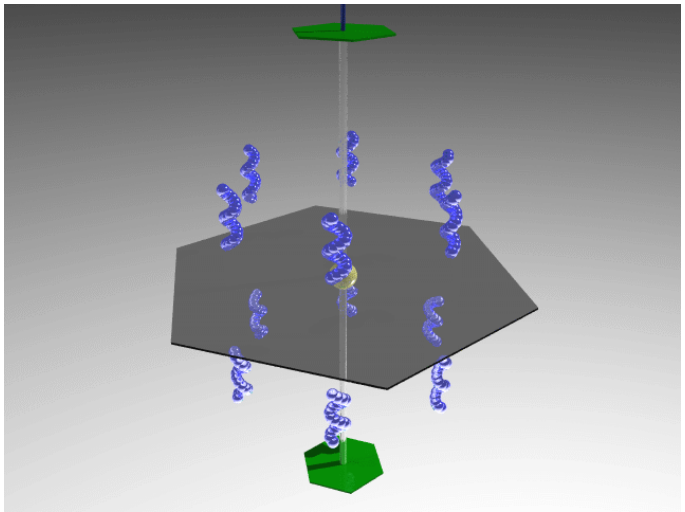


6

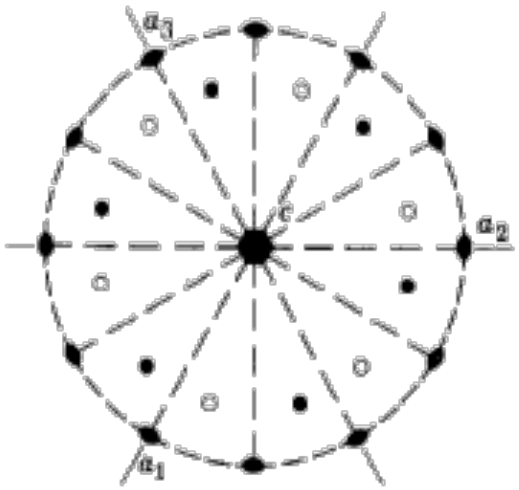


6 / m

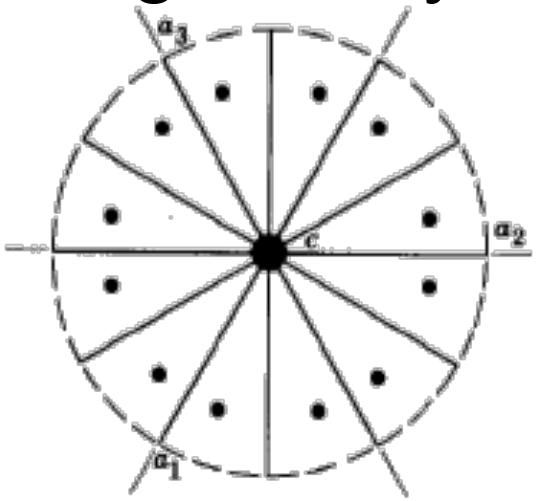




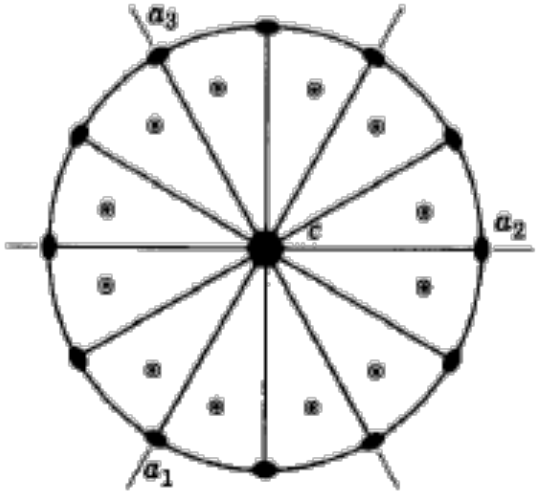
Point Groups in Stereographic projection
Hexagonal System



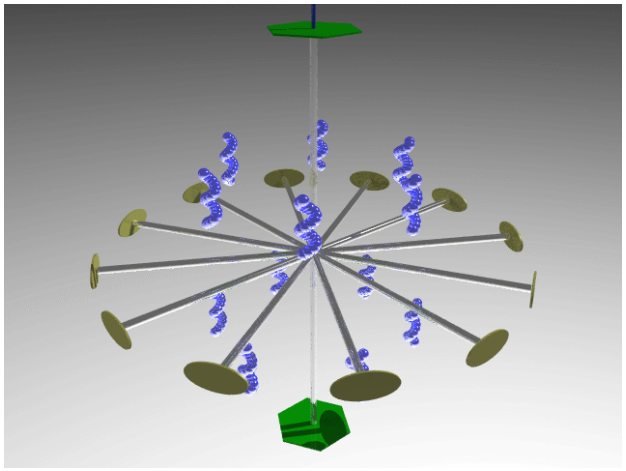
622

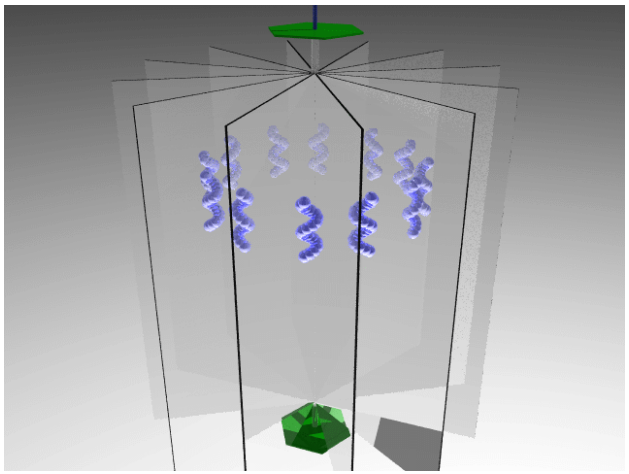


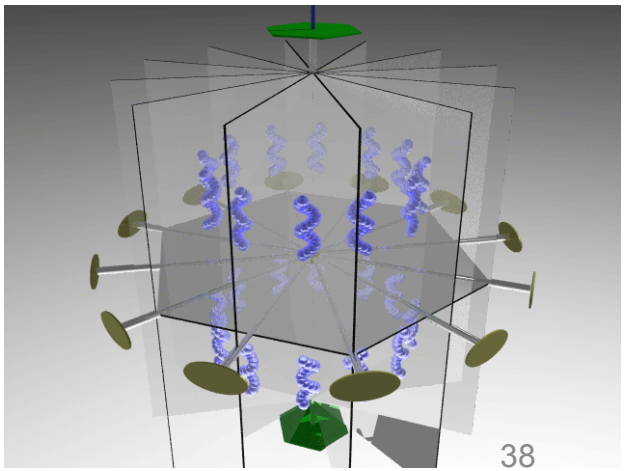
6mm



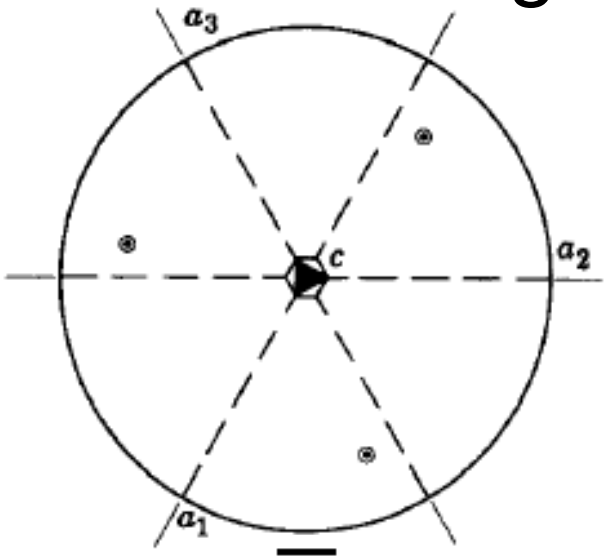
$6/m2/m2/m = 6/mmm$



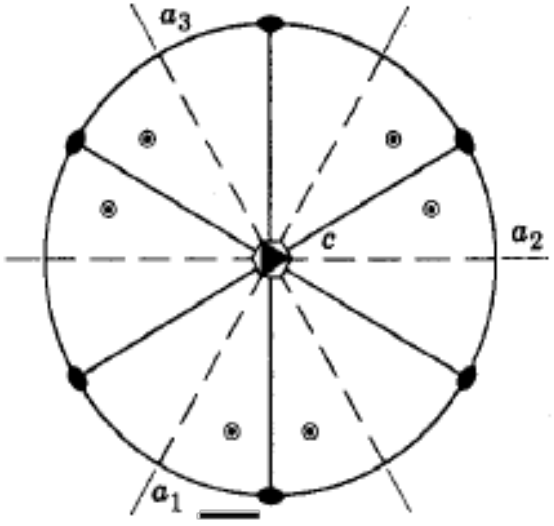




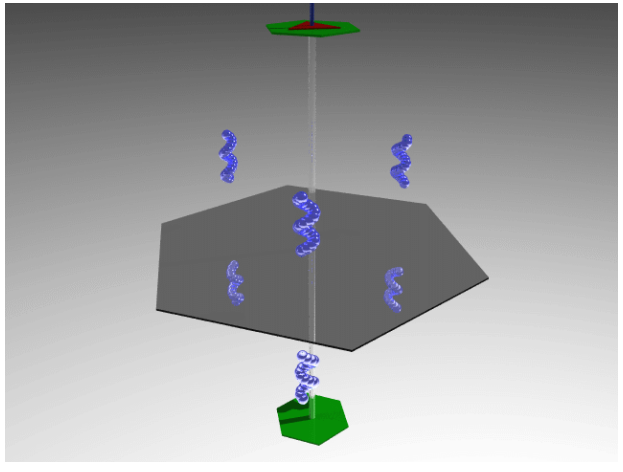
Point Groups in Stereographic projection
Hexagonal System

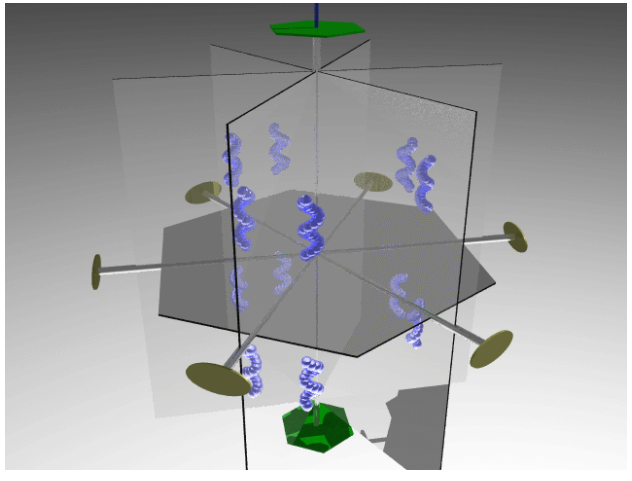


$\bar{6}$



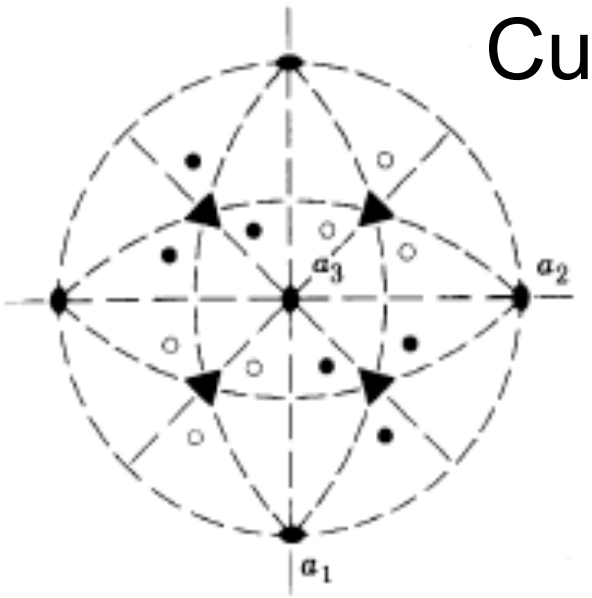
$\bar{6}m2$



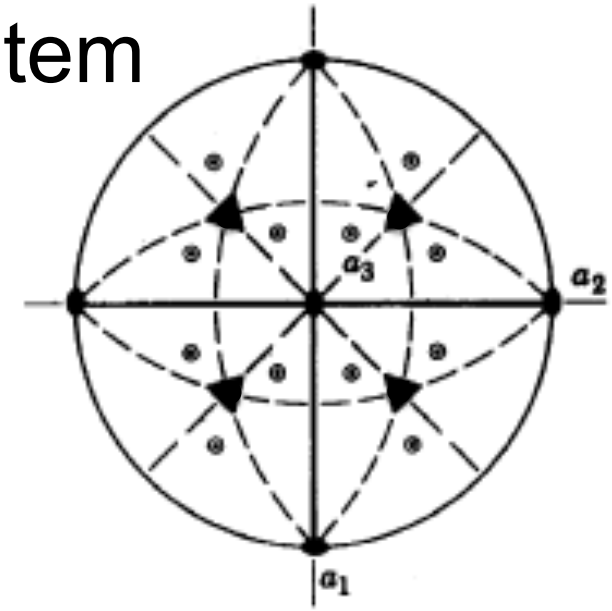


Point Groups in Stereographic projection

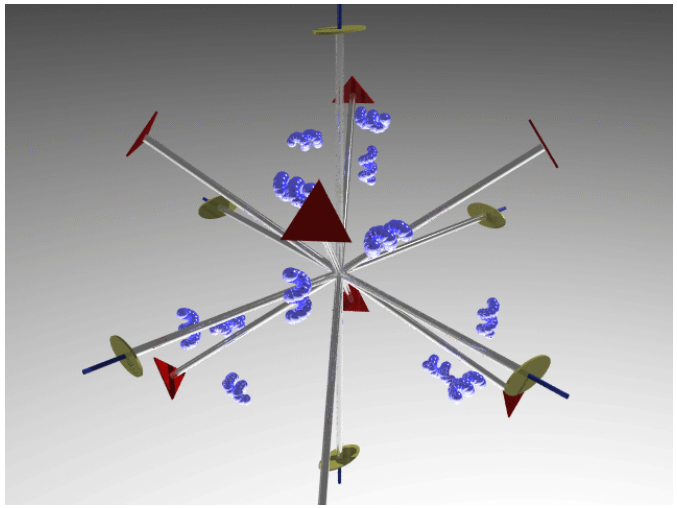
Cubic System

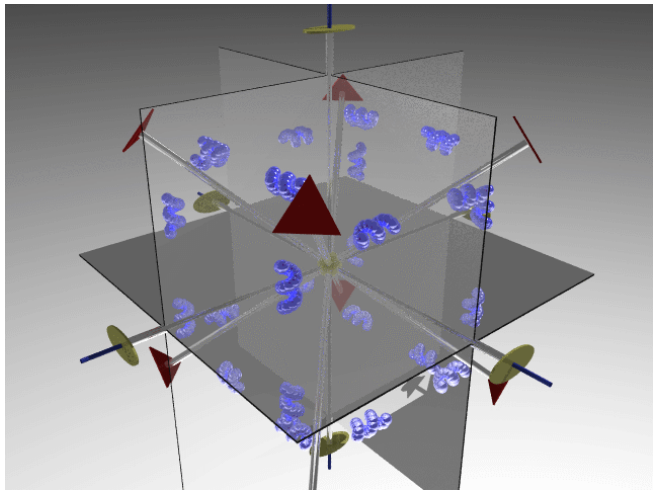


23



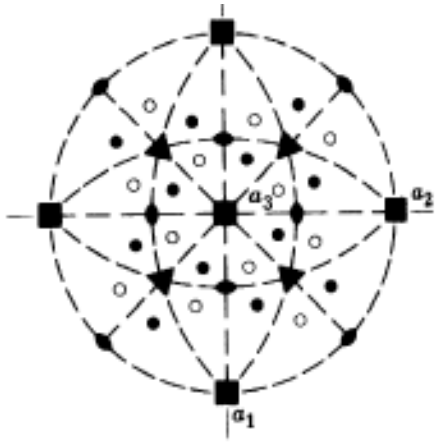
$2/m3 = m3$

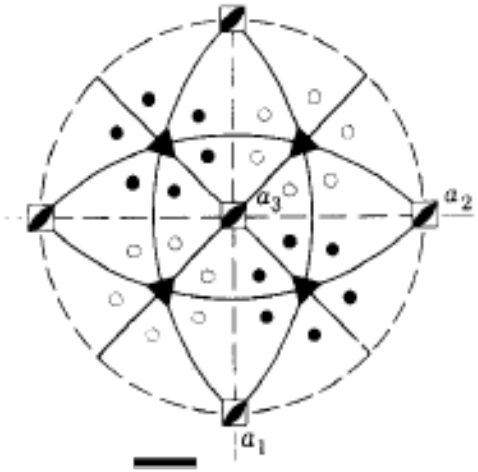


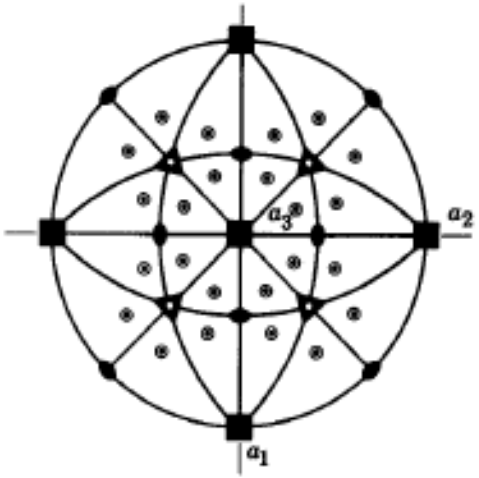


Point Groups in Stereographic projection

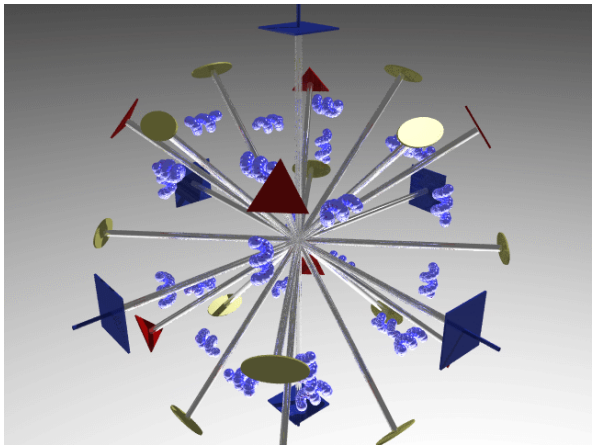
Cubic System

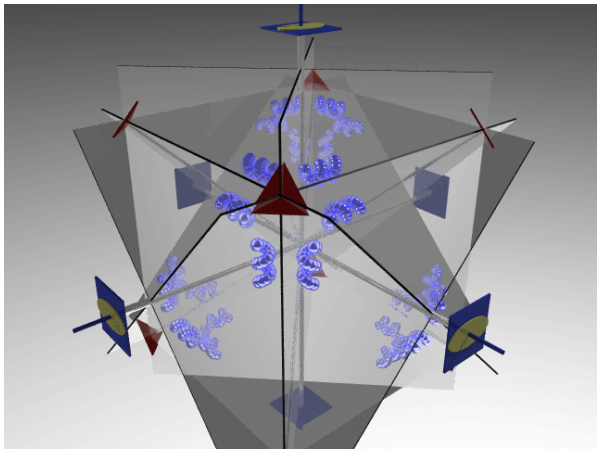


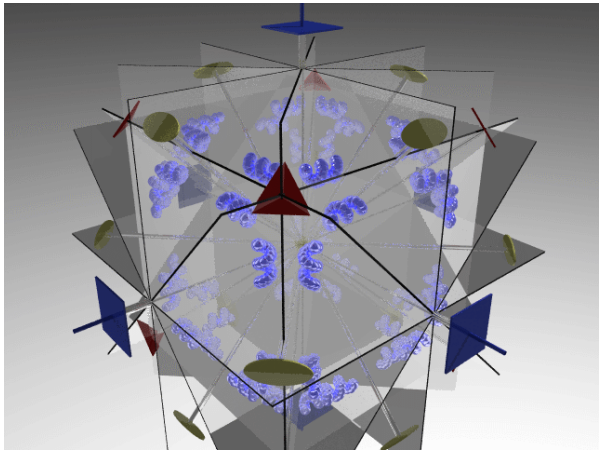




432 $\bar{4}3m$ $4/m32/m = m3m$







In short…

Crystal Class	Point Groups
Triclinic	1, $\bar{1}$
Monoclinic	2, m, 2/m
Orthorhombic	222, mm2, 2/m 2/m 2/m
Trigonal	3, $\bar{3}$, 32, 3m, $\bar{3}$2/m
Hexagonal	6, $\bar{6}$, 6/m, 622, 6mm, $\bar{6}$m2, 6/m 2/m 2/m
Tetragonal	4, $\bar{4}$, 4/m, 422, 4mm, $\bar{4}$2m, 4/m 2/m 2/m
Isometric ??	23, 2/m$\bar{3}$, 432, $\bar{4}$3m, 4/m$\bar{3}$2/m

32 point groups

Space groups

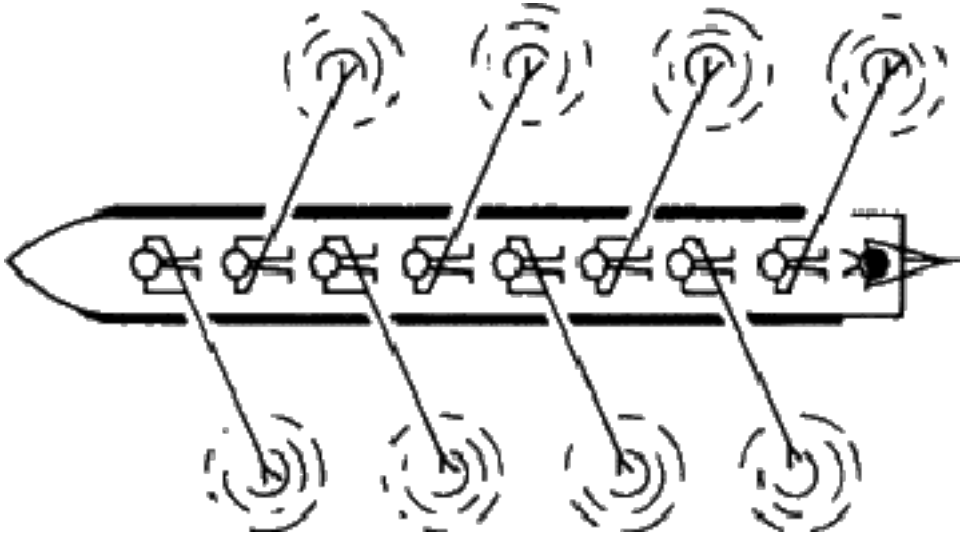
Periodic solids have:

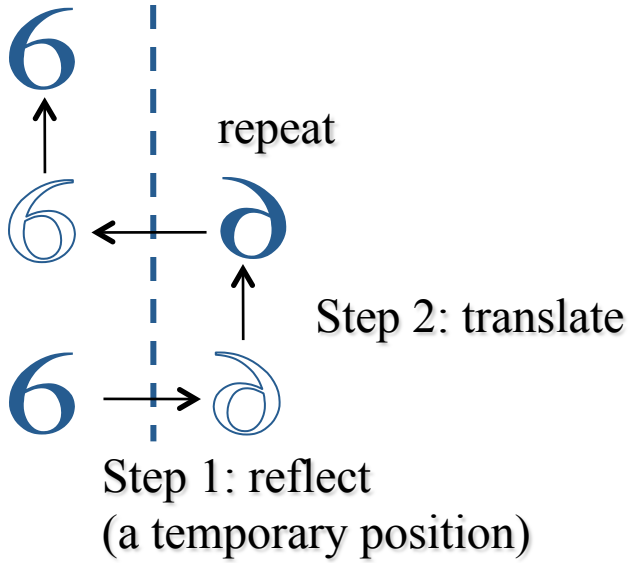
- lattice symmetry (purely translational)
- point symmetry (no translational component)
- possibly glide and/or screw axes (partly translational)

Together all the symmtery operations make up the space group

Glide planes

Combined reflections and translations (the translation is not a pure translational symmetry vector):

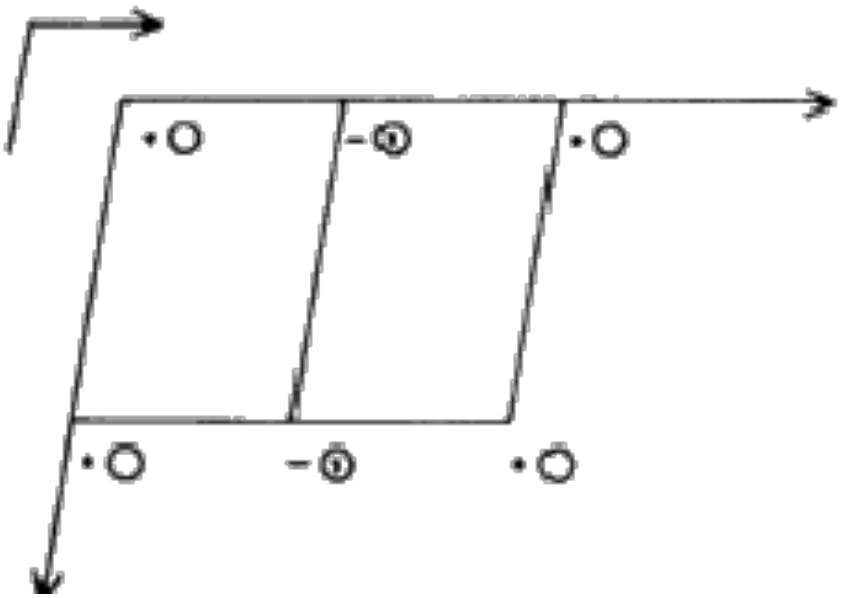




Change of hand…

A stylised aerial view of a well coached 'eight', showing a translational symmetry operation: each rower is related to the next by a combination of translation and reflection.

Glide planes



A glide plane. Translation from left to right across the page is accompanied by reflection through the plane of the paper.

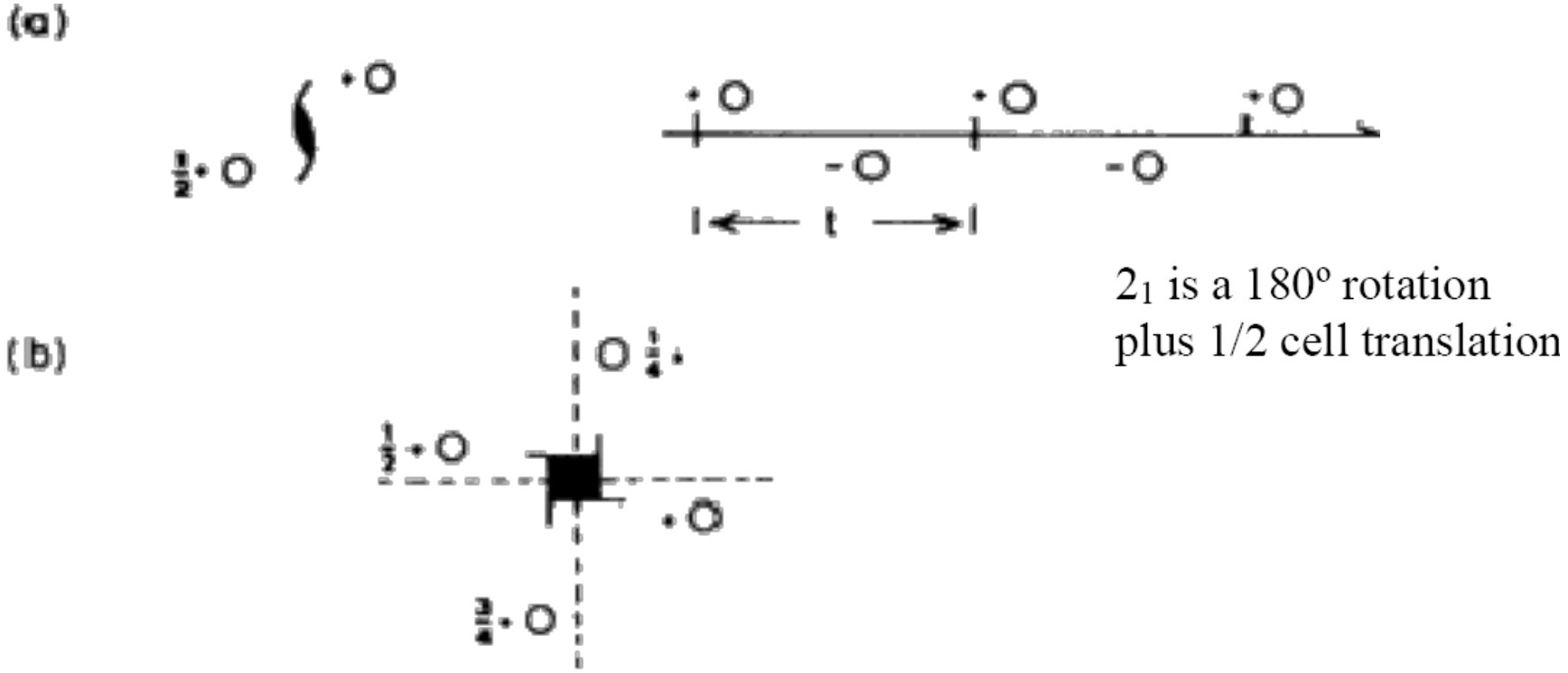
Glide operations

- a-glide
  - Translate by $\frac{1}{2}\mathbf{a}$
- b-glide
  - Translate by $\frac{1}{2}\mathbf{b}$
- c-glide
  - Translate by $\frac{1}{2}\mathbf{c}$
- n-glide ($\perp$ to **a**)
  - Translate by $\frac{1}{2}\mathbf{b}+\frac{1}{2}\mathbf{c}$
- n-glide ($\perp$ to **b**)
  - Translate by $\frac{1}{2}\mathbf{a}+\frac{1}{2}\mathbf{c}$
- n-glide ($\perp$ to **c**)
  - Translate by $\frac{1}{2}\mathbf{a}+\frac{1}{2}\mathbf{b}$
- d-glide
  - Translate by $\frac{1}{4}\mathbf{a}+\frac{1}{4}\mathbf{b}+\frac{1}{4}\mathbf{c}$

The glide translation must always be parallel to the glide plane.

Screw axes

Combined rotations and translations (the translation is not a pure translational symmetry vector). The general symbol for a screw axis is N_n, where N is the order (2, 3, 4 or 6) of the axis, and n/N the translation distance expressed as a fraction of the repeat unit.



(a) A two-fold screw axis, 2_1, shown perpendicular to the plane of the paper (left) and in the plane of the paper (right). Each half revolution is accompanied by a translation through half the repeat distance. (b) A fourfold screw axis, 4_1.

Limitations on combination of symmetry elements

- Not all symmetry elements can be combined in the crystallographic point groups (only 32 point groups are compatible with periodicity in 3-D)

- Furthermore not all of the 32 point groups can be combined will all the lattices. For 3-D lattices there are:
  - 14 Bravais lattices
  - 32 point groups
  - but only **230** space groups

TABLE 3.4 Space Groups in Standard Orientations[a]

System	Point Group	Space Group					
Triclinic	1	$P1$					
	$\bar{1}$	$P\bar{1}$					
Monoclinic	2	$P2$	$P2_1$	$C2$			
	m	Pm	Pc	Cm	Cc		
	$2/m$	$P2/m$	$P2_1/m$	$C2/m$	$P2/c$	$P2_1/c$	$C2/c$
Orthorhombic	222	$P222$	$P222_1$	$P2_12_12$	$P2_12_12_1$	$C222_1$	$C222$
		$F222$	$I222$	$I2_12_12_1$			
	$mm2$	$Pmm2$	$Pmc2_1$	$Pcc2$	$Pma2$	$Pca2_1$	$Pnc2$
		$Pmn2_1$	$Pba2$	$Pna2_1$	$Pnn2$	$Cmm2$	$Cmc2_1$
		$Ccc2$	$Amm2$	$Abm2$	$Ama2$	$Aba2$	$Fmm2$
		$Fdd2$	$Imm2$	$Iba2$	$Ima2$		
	mmm	$Pmmm$	$Pnnn$	$Pccm$	$Pban$	$Pmma$	$Pnna$
		$Pmna$	$Pcca$	$Pbam$	$Pccn$	$Pbcm$	$Pnnm$
		$Pmmn$	$Pbcn$	$Pbca$	$Pnma$	$Cmcm$	$Cmca$
		$Cmmm$	$Cccm$	$Cmma$	$Ccca$	$Fmmm$	$Fddd$
		$Immm$	$Ibam$	$Ibca$	$Imma$		
Tetragonal	4	$P4$	$P4_1$	$P4_2$	$P4_3$	$I4$	$I4_1$
	$\bar{4}$	$P\bar{4}$	$I\bar{4}$				
	$4/m$	$P4/m$	$P4_2/m$	$P4/n$	$P4_2/n$	$I4/m$	$I4_1/a$
	422	$P422$	$P42_12$	$P4_122$	$P4_12_12$	$P4_222$	$P4_22_12$
		$P4_322$	$P4_32_12$	$I422$	$I4_122$		
	$4mm$	$P4mm$	$P4bm$	$P4_2cm$	$P4_2nm$	$P4cc$	$P4nc$
		$P4_2mc$	$P4_2bc$	$I4mm$	$I4cm$	$I4_1md$	$I4_1cd$
	$\bar{4}2m$	$P\bar{4}2m$	$P\bar{4}2c$	$P\bar{4}2_1m$	$P\bar{4}2_1c$	$P\bar{4}m2$	$P\bar{4}c2$
		$P\bar{4}b2$	$P\bar{4}n2$	$I\bar{4}m2$	$I\bar{4}c2$	$I\bar{4}2m$	$I\bar{4}2d$
	$4/mmm$	$P4/mmm$	$P4/mcc$	$P4/nbm$	$P4/nnc$	$P4/mbm$	$P4/mnc$
		$P4/nmm$	$P4/ncc$	$P4_2/mmc$	$P4_2/mcm$	$P4_2/nbc$	$P4_2/nnm$
		$P4_2/mbc$	$P4_2/mnm$	$P4_2/nmc$	$P4_2/ncm$	$I4/mmm$	$I4/mcm$
		$I4_1/amd$	$I4_1/acd$				
Trigonal/rhombohedral	3	$P3$	$P3_1$	$P3_2$	$R3$		
	$\bar{3}$	$P\bar{3}$	$R\bar{3}$				
	32	$P312$	$P321$	$P3_112$	$P3_121$	$P3_212$	$P3_221$
		$R32$					
	$3m$	$P3m1$	$P31m$	$P3c1$	$P31c$	$R3m$	$R3c$
	$\bar{3}m$	$P\bar{3}1m$	$P\bar{3}1c$	$P\bar{3}m1$	$P\bar{3}c1$	$R\bar{3}m$	$R\bar{3}c$
Hexagonal	6	$P6$	$P6_1$	$P6_5$	$P6_2$	$P6_4$	$P6_3$
	$\bar{6}$	$P\bar{6}$					
	$6/m$	$P6/m$	$P6_3/m$				
	622	$P622$	$P6_122$	$P6_522$	$P6_222$	$P6_422$	$P6_322$
	$6mm$	$P6mm$	$P6cc$	$P6_3cm$	$P6_3mc$		
	$\bar{6}m\bar{2}$	$P\bar{6}m2$	$P\bar{6}c2$	$P\bar{6}2m$	$P\bar{6}2c$		
	$6/mmm$	$P6/mmm$	$P6/mcc$	$P6_3/mcm$	$P6_3/mmc$		
Cubic	23	$P23$	$F23$	$I23$	$P2_13$	$I2_13$	
	$m3$	$Pm3$	$Pn3$	$Fm3$	$Fd3$	$Im3$	$Pa3$
		$Ia3$					
	432	$P432$	$P4_232$	$F432$	$F4_132$	$I432$	$P4_332$
		$P4_132$	$I4_132$				
	$\bar{4}3m$	$P\bar{4}3m$	$F\bar{4}3m$	$I\bar{4}3m$	$P\bar{4}3n$	$F\bar{4}3c$	$I\bar{4}3d$
	$m3m$	$Pm3m$	$Pn3n$	$Pm3n$	$Pn3m$	$Fm3m$	$Fm3c$
		$Fd3m$	$Fd3c$	$Im3m$	$Ia3d$		

[a]The 11 Laue symmetries are separated by horizontal lines.

Interpretation of space group symbols

- All space group symbols start with a letter corresponding to the lattice centering, followed by a collection of symbols for symmetry operations in the three lattice directions.

- There are sometimes short notations for space groups symbols:
  - P*121* is usually written as P*2*
    - primitive cell
    - two-fold rotation along the b axis
  - $P2_12_12_1$ (cannot be abbreviated)
    - primitive cell
    - 2_1 screw along each axis, orthorhombic
  - C*mma* (full symbol: C*2/m2/m2/a*)
    - C-centered cell
    - mirror plane perpendicular to a
    - mirror plane perpendicular to b
    - glide plane perpendicular to c
    - other implied symmetry elements (e.g. 2-fold rotations)
  - P*nma*
    - primitive cell
    - n glide plane perpendicular to a
    - mirror plane perpendicular to b
    - glide plane perpendicular to c
    - other implied elements

Lattice centering

- Primitive (P)
- Base centering (C)
  - x, y, z
  - $x+\frac{1}{2}, y+\frac{1}{2}, z$
- Body centering (I)
  - x, y, z
  - $x+\frac{1}{2}, y+\frac{1}{2}, z+\frac{1}{2}$
- Face centering (F)
  - x, y, z
  - $x+\frac{1}{2}, y+\frac{1}{2}, z$
  - $x+\frac{1}{2}, y, z+\frac{1}{2}$
  - $x, y+\frac{1}{2}, z+\frac{1}{2}$
- Rhombohedral centering (R)
  - x, y, z
  - $x+{}^1/_3, y+{}^2/_3, z+{}^1/_3$
  - $x+{}^2/_3, y+{}^1/_3, z+{}^2/_3$

Interpretation of space group symbols

Point Groups (Crystal Classes)

- Hermann-Mauguin Symbols (three positions)
  - Triclinic & monoclinic systems: one position
  - / means 'perpendicular to' as 2/*m*
  - Orthorhombic: three positions for a, b, c
  - Trigonal, Hexagonal, Tetragonal: 3 positions: c, a, [110]
  - Cubic: 3 positions: [100] (a), [111], [110]

Interpretation of space group symbols

TABLE 3.3 Symbols for Symmetry Elements

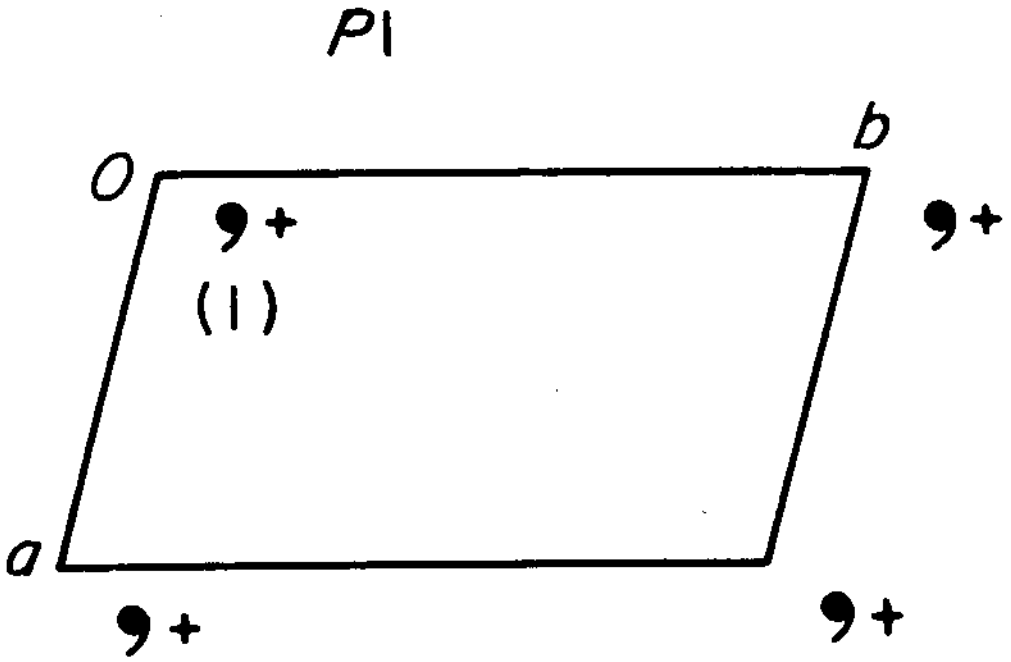
Symmetry	Symbol	Designation If Parallel to Plane of Projection	Designation If Perpendicular to Plane of Projection
Center	$\bar{1}$		
2-Fold axis	2		
3-Fold axis	3		
4-Fold axis	4		
6-Fold axis	6		
2-Fold screw axis	2_1		
3-Fold screw axis	3_1		
3-Fold screw axis	3_2		
4-Fold screw axis	4_1		
4-Fold screw axis	4_2		
4-Fold screw axis	4_3		
6-Fold screw axis	6_1		
6-Fold screw axis	6_2		
6-Fold screw axis	6_3		
6-Fold screw axis	6_4		
6-Fold screw axis	6_5		
Mirror	*m*		
a Glide plane	*a*		
b Glide plane	*b*		
c Glide plane	*c*		
n Glide plane	*n*		
d Glide plane	*d*		

Interpretation of space group symbols

TABLE 3.2 Some Symmetry Elements and Their Equivalent Positions

			Equivalent Positions	
Axis	2	Parallel to a	x, y, z	$x, \bar{y}, \bar{z}$
	2	b	x, y, z	$\bar{x}, y, \bar{z}$
	2	c	x, y, z	$\bar{x}, \bar{y}, z$
	2_1	a	x, y, z	$x+\frac{1}{2}, \bar{y}, \bar{z}$
	2_1	b	x, y, z	$\bar{x}, y+\frac{1}{2}, \bar{z}$
	2_1	c	x, y, z	$\bar{x}, \bar{y}, z+\frac{1}{2}$
Plane	m	Perpendicular to a	x, y, z	$\bar{x}, y, z$
	m	b	x, y, z	$x, \bar{y}, z$
	m	c	x, y, z	$x, y, \bar{z}$
	a	b	x, y, z	$x+\frac{1}{2}, \bar{y}, z$
	a	c	x, y, z	$x+\frac{1}{2}, y, \bar{z}$
	b	a	x, y, z	$\bar{x}, y+\frac{1}{2}, z$
	b	c	x, y, z	$x, y+\frac{1}{2}, \bar{z}$
	c	a	x, y, z	$\bar{x}, y, z+\frac{1}{2}$
	c	b	x, y, z	$x, \bar{y}, z+\frac{1}{2}$
	n	a	x, y, z	$\bar{x}, y+\frac{1}{2}, z+\frac{1}{2}$
	n	b	x, y, z	$x+\frac{1}{2}, \bar{y}, z+\frac{1}{2}$
	n	c	x, y, z	$x+\frac{1}{2}, y+\frac{1}{2}, \bar{z}$
	d	a	x, y, z	$\bar{x}, y+\frac{1}{4}, z+\frac{1}{4}$
	d	b	x, y, z	$x+\frac{1}{4}, \bar{y}, z+\frac{1}{4}$
	d	c	x, y, z	$x+\frac{1}{4}, y+\frac{1}{4}, \bar{z}$

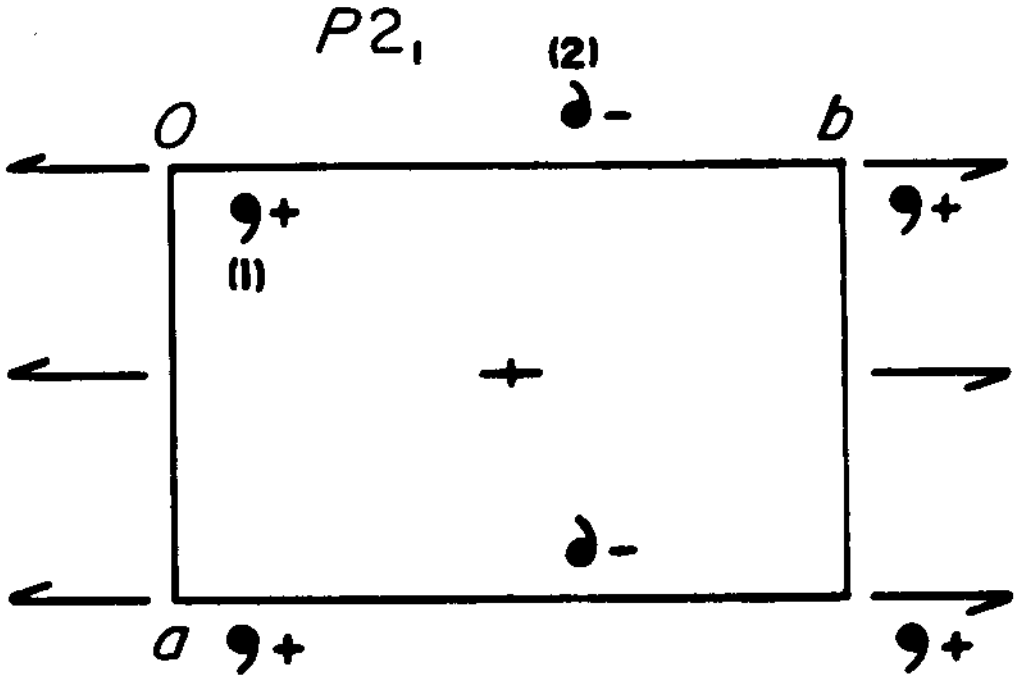
Interpretation of space group symbols



P1, equivalent positions: (1) *x, y, z*

x,y,z are fractions of the length along each unit cell edge (values ranging from 0.0 to 1.0)

Interpretation of space group symbols



$P2_1$, equivalent positions: (1) *x, y, z*; (2) *-x, y+1/2, -z*

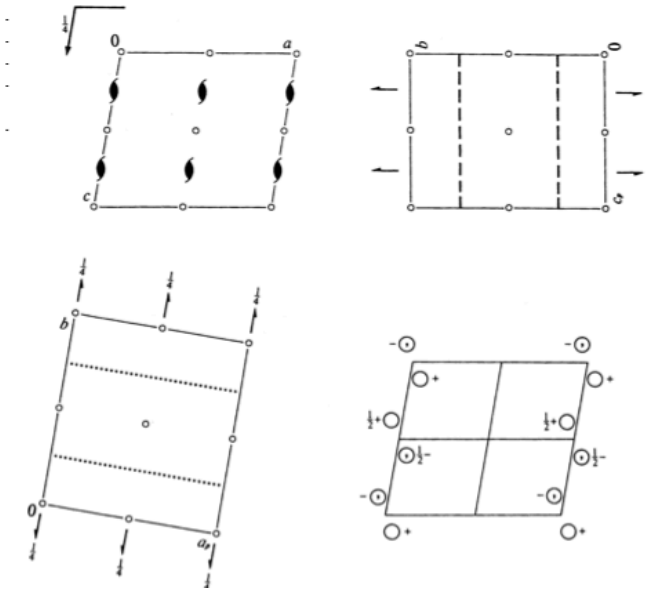
International Tables for Crystallography – Volume A
Entry for Space Group $P2_1/c$ (#14)

Page 1

$P2_1/c$ C_{2h}^5 $2/m$ Monoclinic

No. 14 $P12_1/c1$ Patterson symmetry $P12/m1$

UNIQUE AXIS b, CELL CHOICE 1



Origin at $\bar{1}$

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le \frac{1}{4};\quad 0 \le z \le 1$

Symmetry operations

(1) 1 (2) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{4}$ (3) $\bar{1}$ $0,0,0$ (4) c $x,\frac{1}{4},z$

Page 2

CONTINUED No. 14 $P2_1/c$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	e	1	(1) x,y,z	(2) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	$h0l$: $l=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
2	d	$\bar{1}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			hkl : $k+l=2n$
2	c	$\bar{1}$	$0,0,\frac{1}{2}$	$0,\frac{1}{2},0$			hkl : $k+l=2n$
2	b	$\bar{1}$	$\frac{1}{2},0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $k+l=2n$
2	a	$\bar{1}$	$0,0,0$	$0,\frac{1}{2},\frac{1}{2}$			hkl : $k+l=2n$

Symmetry of special projections

Along [001] $p2gm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p2gg$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [010] $p2$
$\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $P1c1$ (Pc, 7) 1; 4
[2] $P12_1/1$ ($P2_1/c$, 4) 1; 2
[2] $P\bar{1}$ (2) 1; 3

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [2] $P12_1/c1$ ($\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{a}' = 2\mathbf{a}, \mathbf{c}' = 2\mathbf{a}+\mathbf{c}$) ($P2_1/c$, 14); [3] $P12_1/c1$ ($\mathbf{b}' = 3\mathbf{b}$) ($P2_1/c$, 14)

Minimal non-isomorphic supergroups

I [2] $Pnna$ (52); [2] $Pmna$ (53); [2] $Pcca$ (54); [2] $Pbam$ (55); [2] $Pccn$ (56); [2] $Pbcm$ (57); [2] $Pnnm$ (58); [2] $Pbcn$ (60); [2] $Pbca$ (61); [2] $Pnma$ (62); [2] $Cmce$ (64)

II [2] $A12/m1$ ($C2/m$, 12); [2] $C12/c1$ ($C2/c$, 15); [2] $I12/c1$ ($C2/c$, 15); [2] $P12_1/m1$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) ($P2_1/m$, 11); [2] $P12/c1$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) ($P2/c$, 13)

Schoenflies Space Group

$P\,2_1/c$

No. 14

C_{2h}^5

$P\,12_1/c\,1$

UNIQUE AXIS b, CELL CHOICE 1

$2/m$

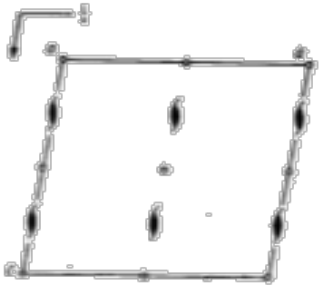
Crystal System

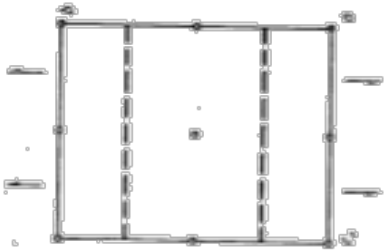
Monoclinic

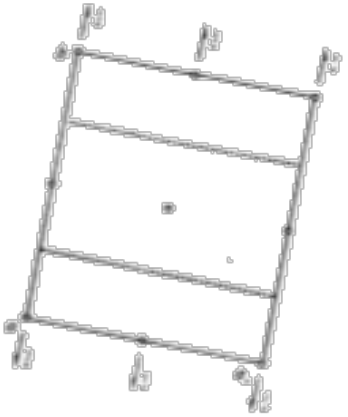
Patterson symmetry $P\,12/m\,1$

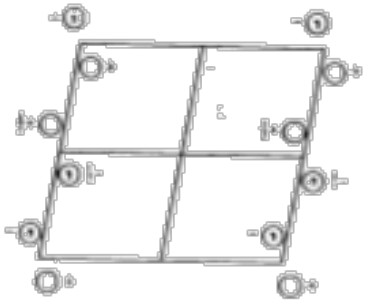
Herman-Mauguin Space Group Symbols (Short & Long)

Point Group









Origin at $\bar{1}$

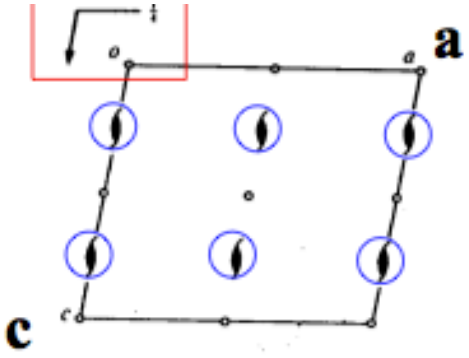
Asymmetric unit $0\le x\le 1;\ 0\le y\le 1;\ 0\le z\le 1$

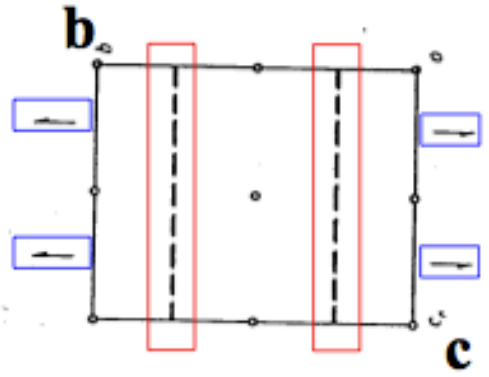
Symmetry operations

(1) 1 (2) $2(0,1,0)\ 0,y,\frac{1}{2}$ (3) $\bar{1}$ 0,0,0 (4) c $x,\frac{1}{4},z$

P 1 2_1/c 1

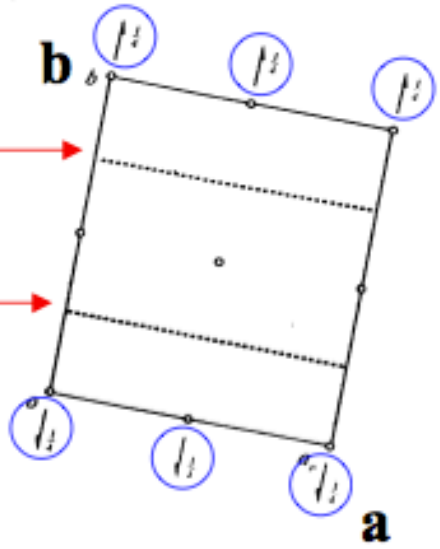
Axes parallel to or planes perpendicular to the b-axis

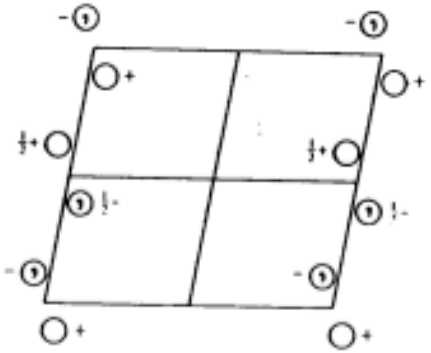




Glide translation in the plane of the projection

Glide translation perpendicular to the plane of the projection





Origin at $\bar{1}$

Asymmetric unit $0 \le x \le 1;\ 0 \le y \le \frac{1}{4};\ 0 \le z \le 1$

Symmetry operations

(1) 1 | (2) $2(0,\frac{1}{4},0)$ $0,y,\frac{1}{4}$ | (3) $\bar{1}$ 0,0,0 | (4) c $x,\frac{1}{4},z$

Inversion Center

c-glide plane

2_1 Screw Axis

Wyckoff positions

- A useful piece of information contained in the International Tables are the Wyckoff positions that tell us where the atoms in a crystal can be found.
- The **letter** is simply a label and has no physical meaning. They are assigned alphabetically from the bottom up.
- The **multiplicity** tells us how many atoms are generated by symmetry if we place a single atom at that position.
- The **symmetry** tells us what symmetry elements the atom resides upon. The **uppermost** Wyckoff position, corresponding to an atom at an arbitrary **position never resides upon any symmetry elements**. This Wyckoff position is called the general position. The coordinates column tells us the coordinates of all of the symmetry related atoms
- All of the remaining Wyckoff positions are called **special positions**. They correspond to atoms which lie upon one of more symmetry elements, because of this they always have a smaller multiplicity than the general position. Furthermore, one or more of their fractional coordinates must be fixed otherwise the atom would no longer lie on the symmetry element.

Asymmetric Unit

- **Definition**: smallest part of the unit cell which will generate the whole cell if all symmetry operators of the space groups are applied to it.

- Knowing the asymmetric unit and the symmetry of the structure allows generating the unit cell.

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
4	*e*	1	(1) x,y,z	(2) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$

General position

2	*d*	$\bar{1}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$
2	*c*	$\bar{1}$	$0,0,\frac{1}{2}$	$0,\frac{1}{2},0$
2	*b*	$\bar{1}$	$\frac{1}{2},0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$
2	*a*	$\bar{1}$	$0,0,0$	$0,\frac{1}{2},\frac{1}{2}$

Wyckoff Sites

Reflection Conditions/ Systematic Absences

Reflection conditions

General:

$h0l$: $l=2n$
$0k0$: $k=2n$
$00l$: $l=2n$

Special: as above, plus

hkl : $k+l=2n$

hkl : $k+l=2n$

hkl : $k+l=2n$

hkl : $k+l=2n$

Symmetry of special projections

Along [001] $p\,2g\,m$
$\boldsymbol{a}'=\boldsymbol{a}_p$ $\boldsymbol{b}'=\boldsymbol{b}$
Origin at $0,0,z$

Along [100] $p\,2g\,g$
$\boldsymbol{a}'=\boldsymbol{b}$ $\boldsymbol{b}'=\boldsymbol{c}_p$
Origin at $x,0,0$

Along [010] $p\,2$
$\boldsymbol{a}'=\frac{1}{2}\boldsymbol{c}$ $\boldsymbol{b}'=\boldsymbol{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I	[2]$P\,1\,2_1\,1\,(P\,2_1)$	1; 2
	[2]$P\,\bar{1}$	1; 3
	[2]$P\,1\,c\,1\,(P\,c)$	1; 4
IIa	none	
IIb	none	

Subgroups = Space group symmetry if certain symmetry operations are eliminated

Supergroups = Space group symmetry if certain symmetry operations are added

Maximal isomorphic subgroups of lowest index

IIc [3]$P\,1\,2_1/c\,1\,(\boldsymbol{b}'=3\boldsymbol{b})(P\,2_1/c)$; [2]$P\,1\,2_1/c\,1\,(\boldsymbol{a}'=2\boldsymbol{a}$ or $\boldsymbol{a}'=2\boldsymbol{a},\boldsymbol{c}'=2\boldsymbol{a}+\boldsymbol{c})(P\,2_1/c)$

Minimal non-isomorphic supergroups

I [2]$P\,n\,n\,a$; [2]$P\,m\,n\,a$; [2]$P\,c\,c\,a$; [2]$P\,b\,a\,m$; [2]$P\,c\,c\,n$; [2]$P\,b\,c\,m$; [2]$P\,n\,n\,m$; [2]$P\,b\,c\,n$; [2]$P\,b\,c\,a$; [2]$P\,n\,m\,a$; [2]$C\,m\,c\,a$

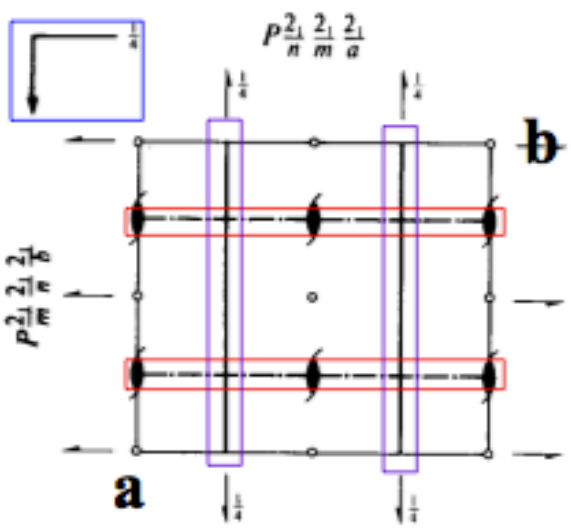
II [2]$C\,1\,2/c\,1\,(C\,2/c)$; [2]$A\,1\,2/m\,1\,(C\,2/m)$; [2]$I\,1\,2/c\,1\,(C\,2/c)$; [2]$P\,1\,2_1/m\,1\,(2\boldsymbol{c}'=\boldsymbol{c})(P\,2_1/m)$; [2]$P\,1\,2/c\,1\,(2\boldsymbol{b}'=\boldsymbol{b})(P\,2/c)$

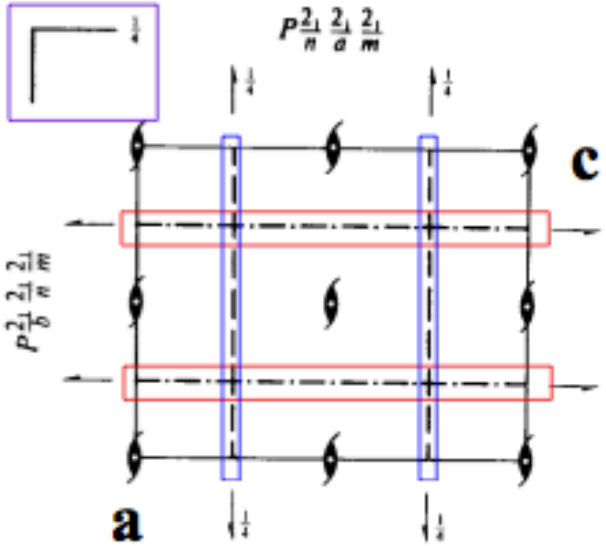
Orthorhombic

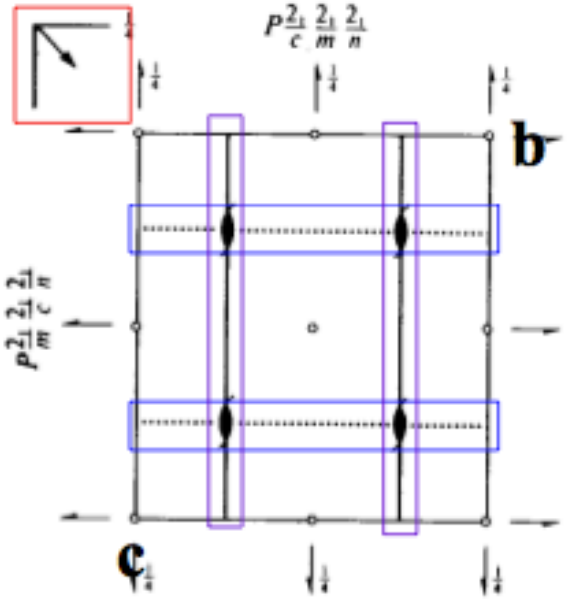
$P\,n\,m\,a$ $\quad D_{2h}^{16}$

No. 62

$P\,2_1/n\,2_1/m\,2_1/a$







P $2_1/n$ $2_1/m$ $2_1/a$

2_1 screw axis || to the a-axis + n-glide plane ⊥ to the a-axis

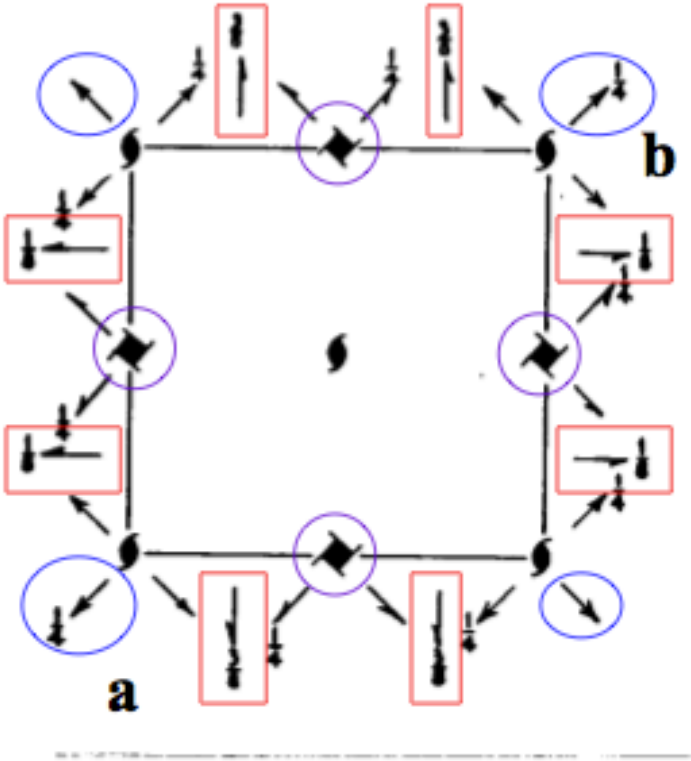
2_1 screw axis || to the b-axis + mirror plane ⊥ to the b-axis

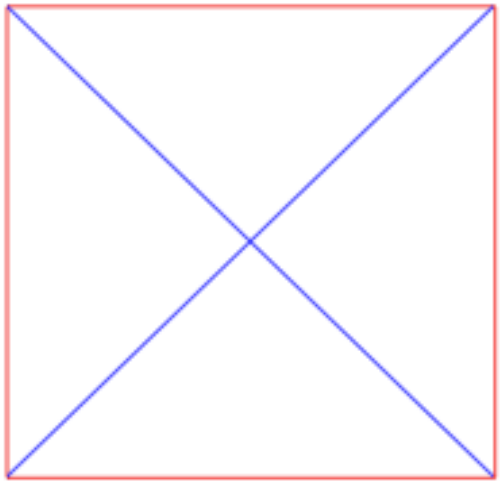
2_1 screw axis || to the c-axis + a-glide plane ⊥ to the c-axis

Tetragonal

$P\,4_1\,2_1\,2$ $\quad D_4^4$

No. 92 $\quad P\,4_1\,2_1\,2$





P 4_1 — 4_1 screw axis || to the c-axis, No glides or mirrors ⊥ to the c-axis

2_1 — 2_1 screw axis || to the a- & b-axes, No glides or mirrors ⊥ to these axes

2 — 2-fold axes || to the face diagonals in the ab plane ([110]), No glides or mirrors ⊥ to these axes

Trigonal

$P\bar{3}m1$ D_{3d}^{3}

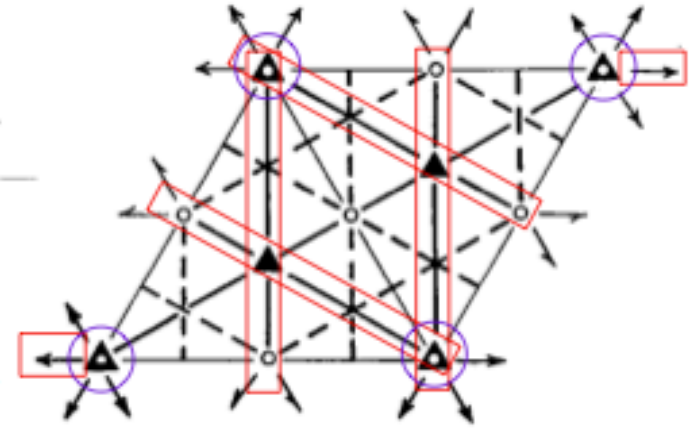
No. 164

$P\bar{3}2/m1$

3-fold rotoinversion axis || to the c-axis,

2-fold axis || to the a- & b-axes, Mirror planes ⊥ to these axes

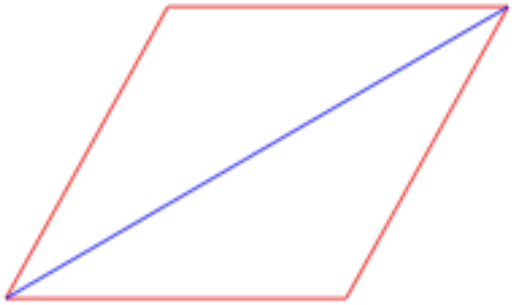
no axes || to the face diagonals in the ab plane ([110]), No glides or mirrors ⊥ to the diagonals

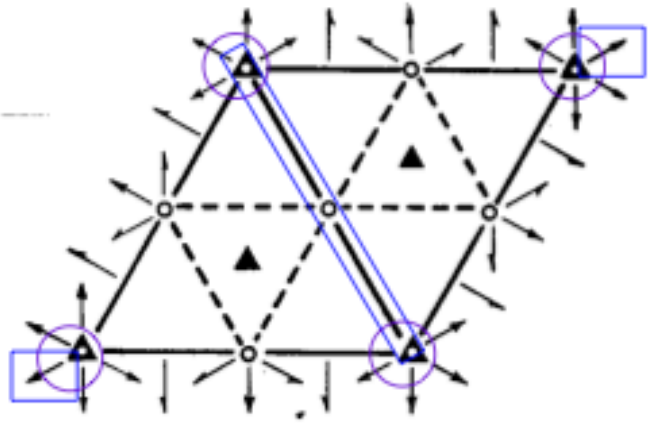


$P\bar{3}1m$ D_{3d}^{1}

No. 162

$P\bar{3}12/m$

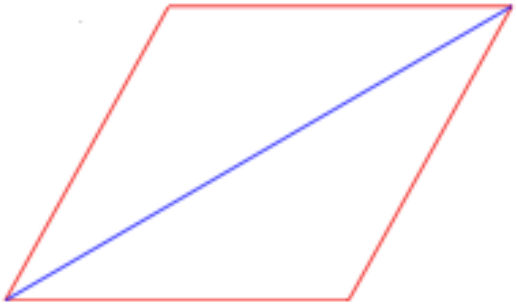


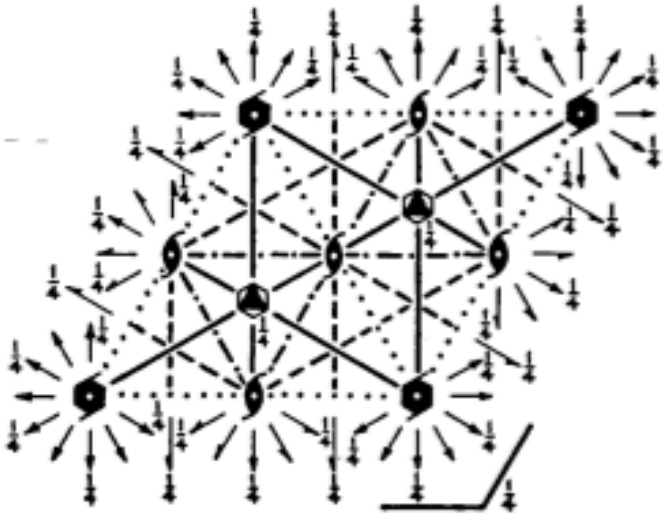


Hexagonal

$P\,6_3/m\,m\,c$ $\quad D^4_{6h}$

No. 194 $\quad P\,6_3/m\,2/m\,2/c$



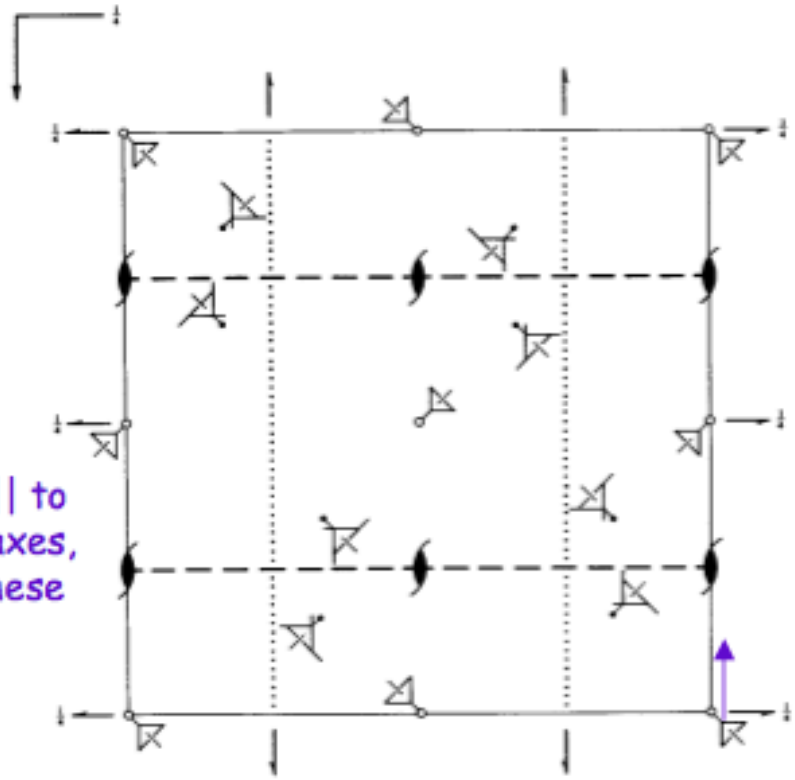


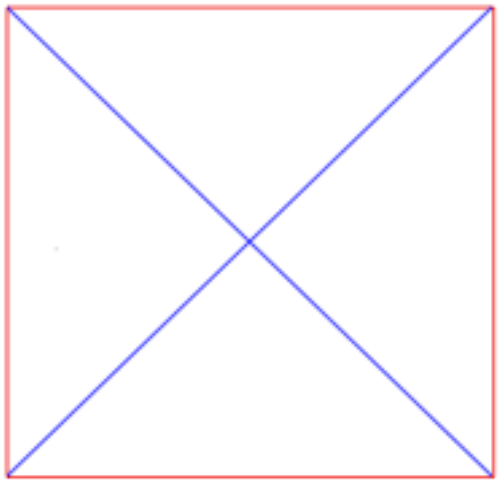
Directions and conventions for naming space group are the same as for trigonal.

Cubic

$P\,a\,\bar{3}$ T_h^6 $m\,\bar{3}$ Cubic

No. 205 $P\,2_1/a\,\bar{3}$ Patterson symmetry $P\,m\,\bar{3}$





2_1 screw axis || to the a-, b- & c-axes, a-glide ⊥ to these axes

P 2_1/a $\bar{3}$ 1

No axes || to the face diagonals. No glides or mirrors ⊥ to these axes

3-fold rotoinversion axes || to the body diagonals

Describing crystals structures

- Full symmetry of a crystal is described by its space group

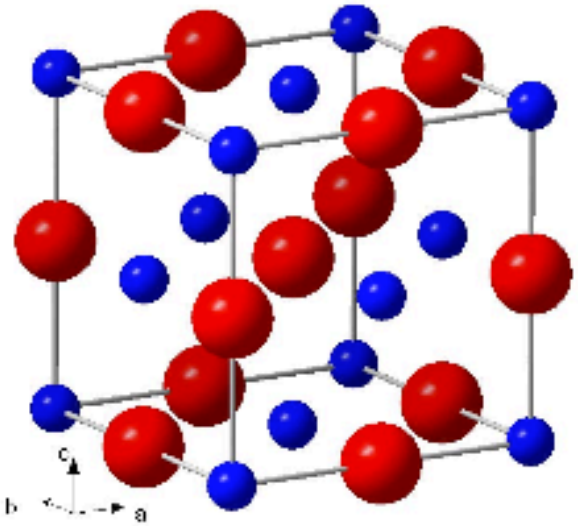
- The location of all atoms in a crystalline solid can be specified by a combination of all the symmetry elements and the fractional coordinates for a unique set of atoms (asymmetric unit)

We specify the atomic coordinates for a small number of atoms. Then we apply all the symmetry elements including the lattice symmetry to build up the full 3D structure.

N.B.: Each lattice point may be associated with many atoms

Examples

NaCl

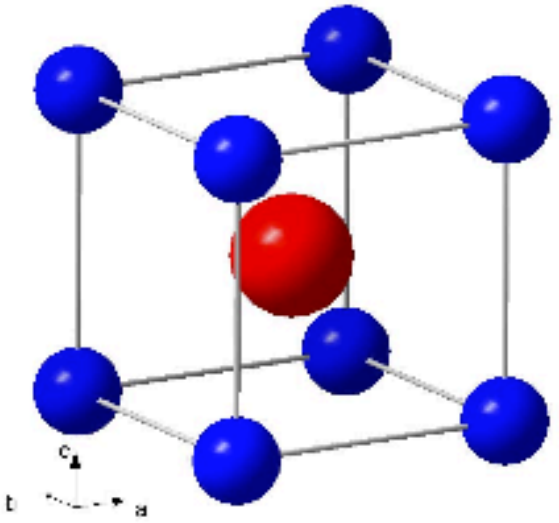


Space Group = $Fm\bar{3}m$ (225)

a = 5.64 Å

Atom	Site	x	y	z
Na	4a	0	0	0
Cl	4b	½	0	0

CsCl



Space Group = $Pm\bar{3}m$ (221)

a = 4.12 Å

Atom	Site	x	y	z
Cs	1a	0	0	0
Cl	1b	½	½	½

Asymmetric units…

Examples

Ta adopts the Ta-type structure with space group Im3m (229) with atoms at 2a (0,0,0) and a=0.33 nm.

Ti adopts the Mg-type structure with space group $p6_3/mmc$ (194) with atoms at 2c (1/3,2/3,1/4) and a=0.295 nm and c=0,4686 nm.

Si adopts the diamond-type structure with space group Fd3m (227) with atoms at (16c) 1/8,1/8,1/8 and a=0.543 nm.

FeO adopts the NaCl-type structure with O in Cl sites (only lattice parameter missing...).