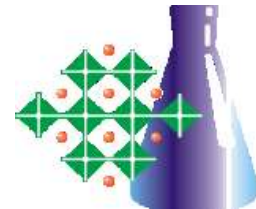


# International school



## Introduction in Rietveld structure refinement



PANalytical



**CRYSTAL  
IMPACT**



**Crystal structure and crystal symmetry (crystal systems, unit cell, reciprocal space, reciprocal lattice, systematic absences, Wyckoff positions)**



**Sofia, Bulgaria,  
28 September - 3 October 2015**



**МИНИСТЕРСТВО  
НА ОБРАЗОВАНИЕТО  
И НАУКАТА**

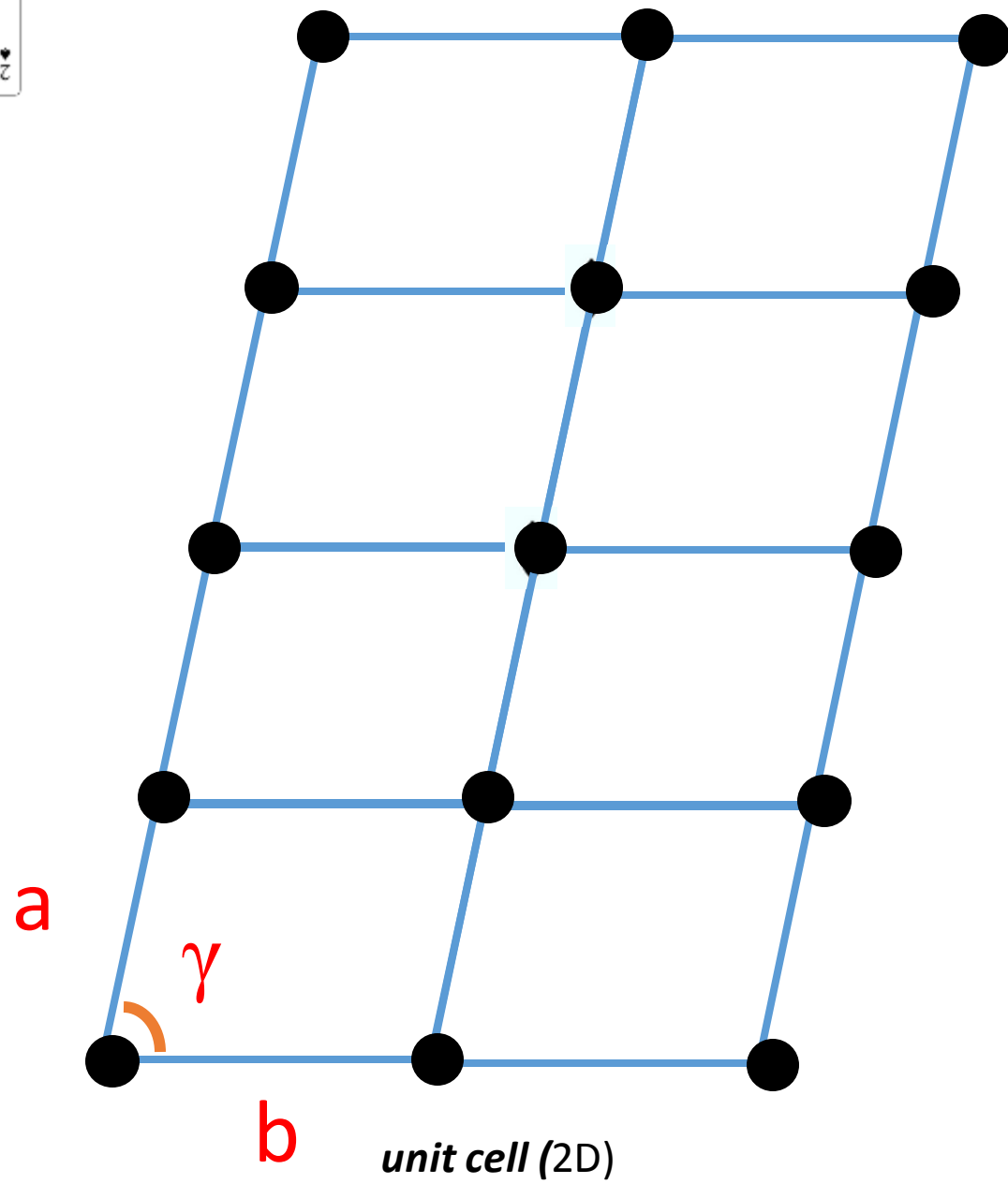
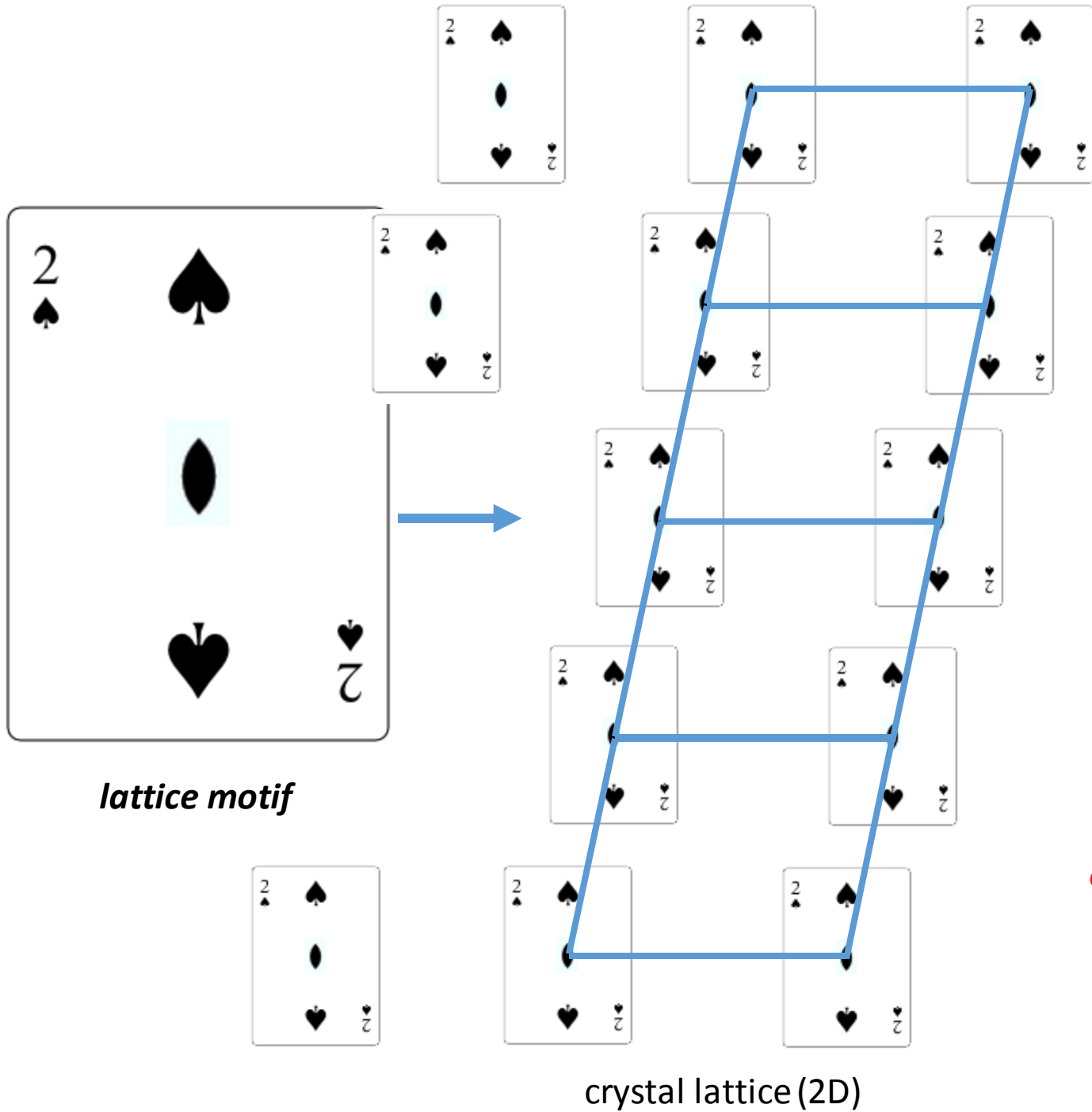
# What is a crystal?

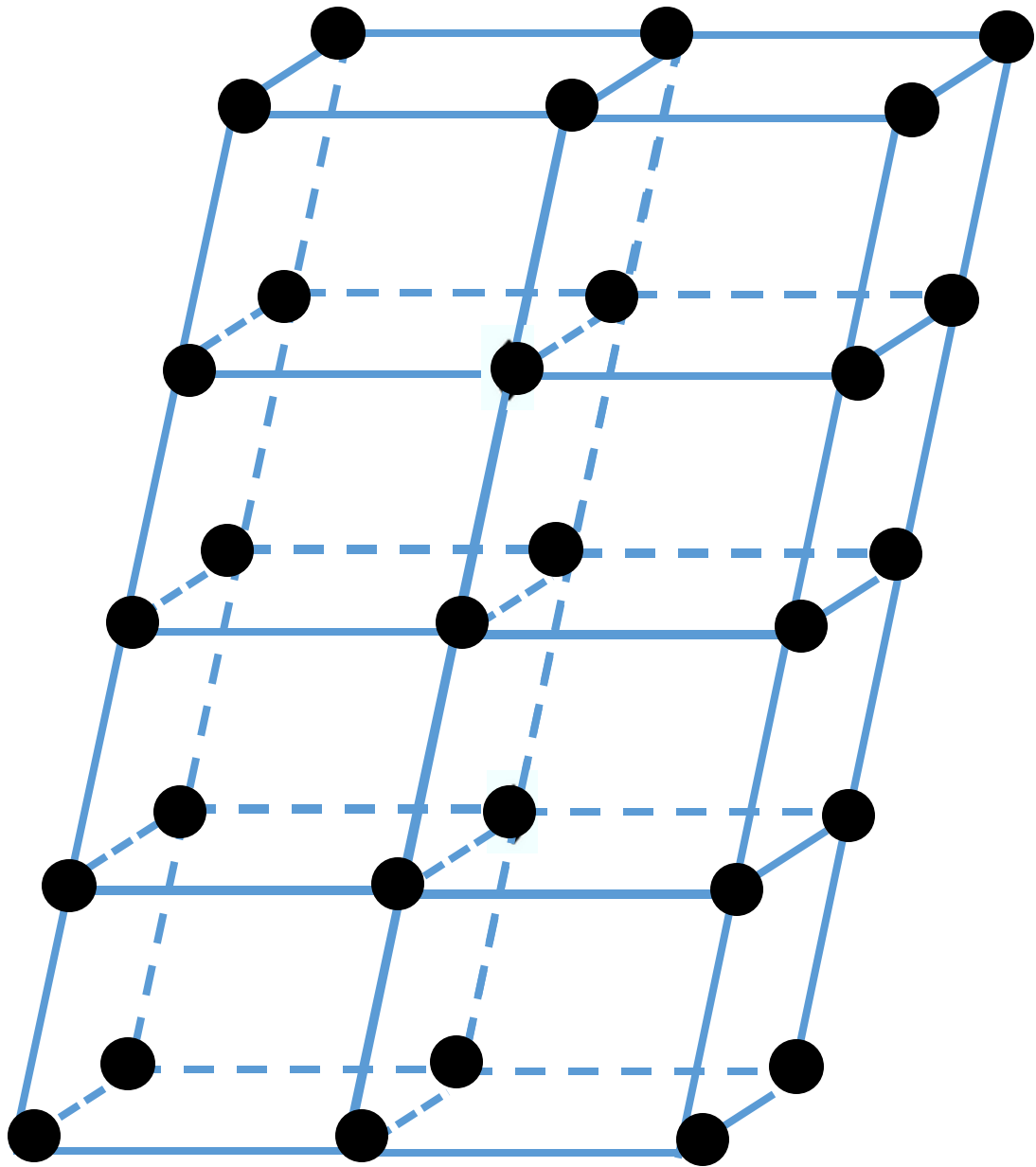
- Solids that are exact repeats of a symmetric motif (the opposite is amorphous/glass)
- In a crystal, the level at which there is no symmetry → ***asymmetric unit***.



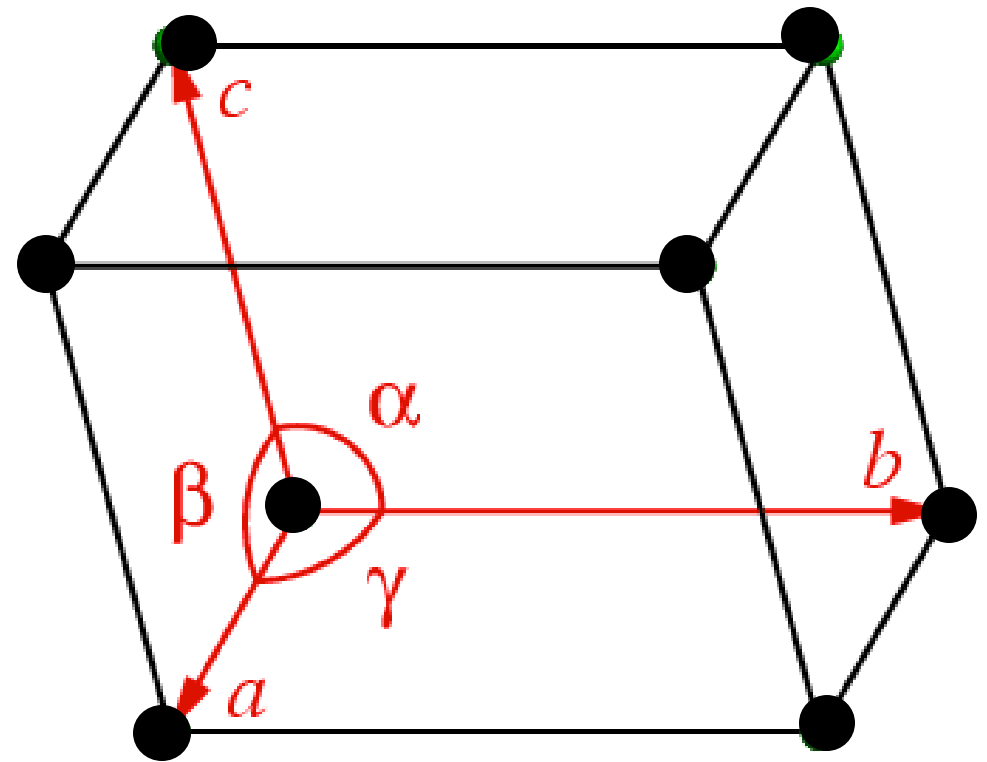
***asymmetric unit***

- Apply an operator (rotational, screw ...) to construct ***lattice motif***.
- Lattice motif is translated in three dimensions to form crystal lattice.
- The lattice points are connected to form the boxes → ***unit cell***.
- The edges define a set of unit vector axes →  $\vec{a}$ ,  $\vec{b}$ ,  $\vec{c}$  unit cell dimensions a, b, c.
- Angles between axes:  $\alpha$  between  $\vec{b}\vec{c}$ ,  $\beta$  between  $\vec{a}\vec{c}$ ,  $\gamma$  between  $\vec{a}\vec{b}$



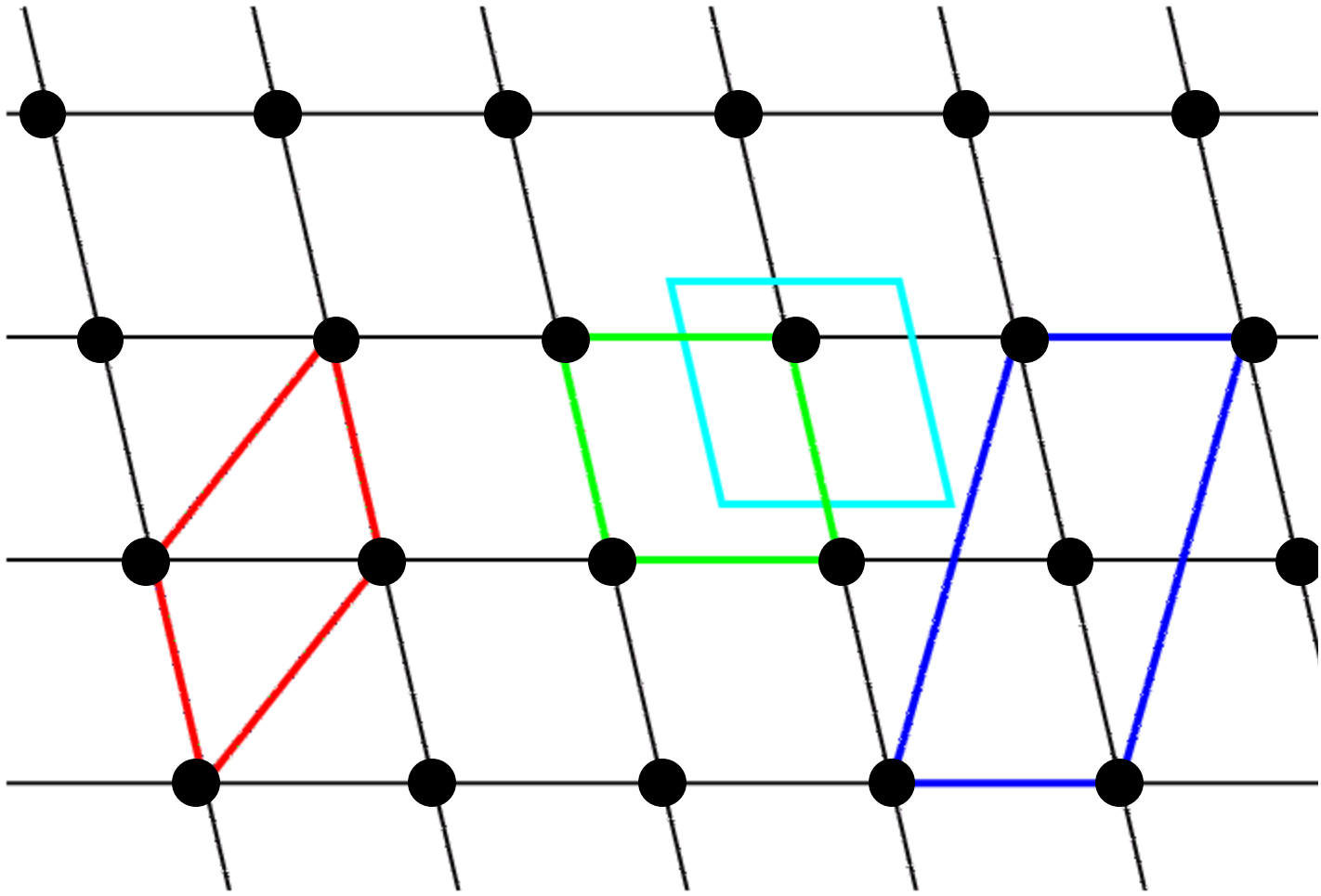


crystal lattice (3D)



*unit cell* (3D)

Sometimes the question arises as to the choice of parallelogram for our three-dimensional or two-dimensional unit cell as shown below .



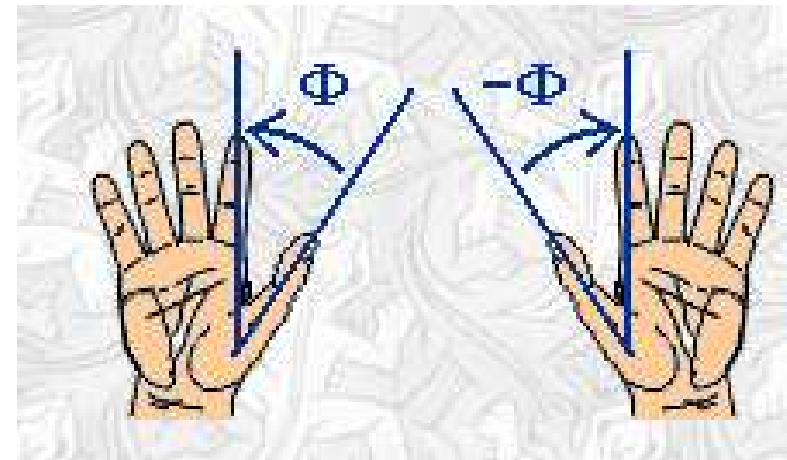
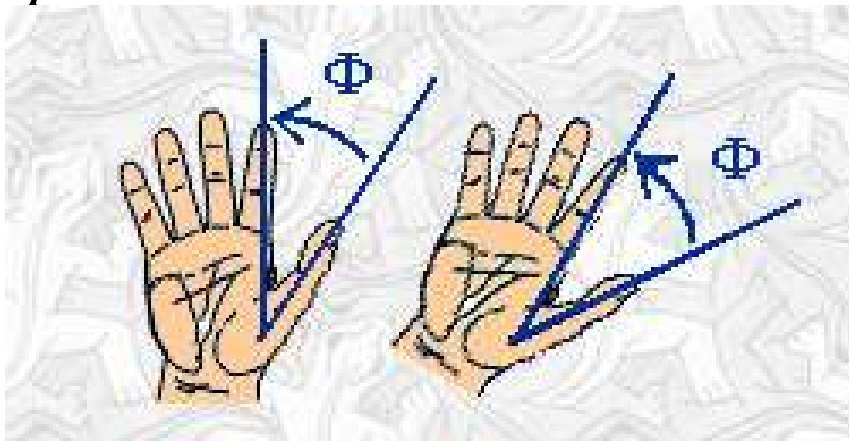
| Centring Type           | Symbol | Multiplicity |
|-------------------------|--------|--------------|
| Primitive - no centring | P      | 1            |
| A-face centred          | A      | 2            |
| B-face centred          | B      | 2            |
| C-face centred          | C      | 2            |
| All-face centred        | F      | 4            |
| Body centred            | I      | 2            |
| Rhombohedrally centred  | R      | 3            |

# Symmetry operations

## Crystallographic symmetry operations

If one object remains unchanged (congruent) after the application of one or more “movements”, we will say that it presents symmetrical properties - referred as isometries, i.e. they are special kind of mappings between an object and its image that leave all distances and angles invariant.

The operations will be called symmetry operations if the object is a crystal pattern, representing a real crystal, its symmetry operations are called *crystallographic symmetry operations*.



congruence may be direct (proper) or opposite (improper, e.g. change of handedness and production of enantiomorphs )

## Two dimensional symmetry

Operations that leave invariant all the space: the identity

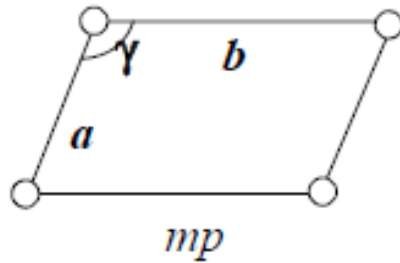
Operations that leave invariant one point of the space: rotations

Operations that leave invariant one direction of the space: reflections

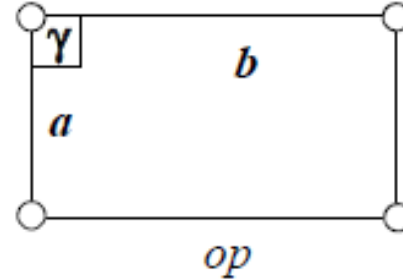
Operations that do not leave invariant any point of the space: translations

## Two dimensional crystal families

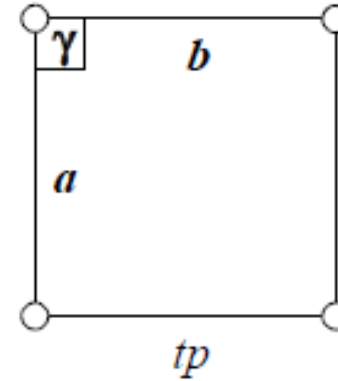
*monoclinic*  
No restriction  
on  $a, b, \gamma$   
No symmetry direction



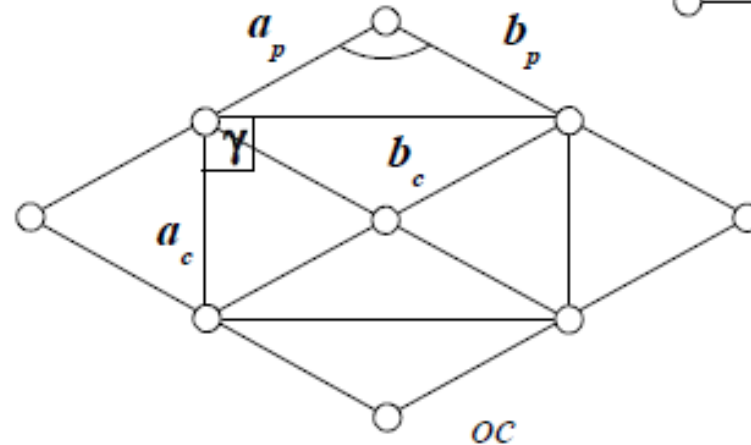
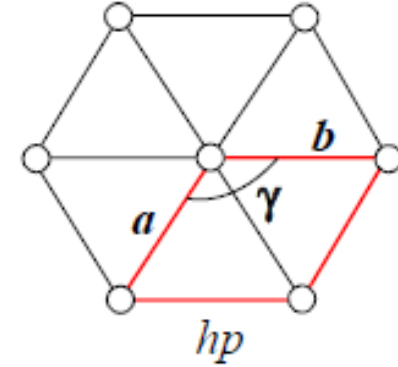
*orthorhombic*  
No restriction  
on  $a, b$  ;  
 $\gamma = 90^\circ$   
[10] et [01]



*tetragonal*  
 $a = b ; \gamma = 90^\circ$   
 $\langle 10 \rangle$  ([10] et [01])  
 $\langle 11 \rangle$  ([11] et  $[1\bar{1}]$ )



*hexagonal*  
 $a = b ; \gamma = 120^\circ$   
 $\langle 10 \rangle$  ([10], [01] et  $[11]$ )  
 $\langle 21 \rangle$  ([21], [12] et  $[1\bar{1}]$ )



Crystal families: *monoclinic*, *orthorhombic*, *tetragonal*, *hexagonal*  
Type of lattice\*: *primitive*, *centred*

In case of direct congruence we can have :

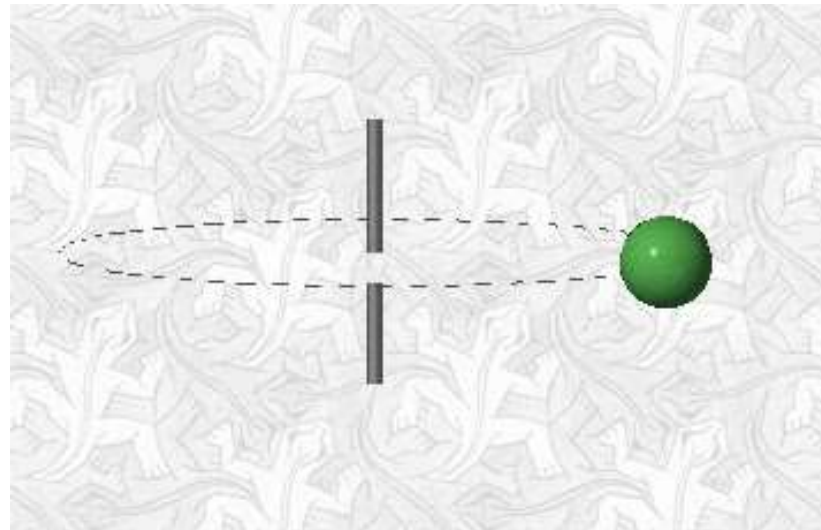
a) **translation**:

when all the points of the object undergo an equal displacement in the same direction;

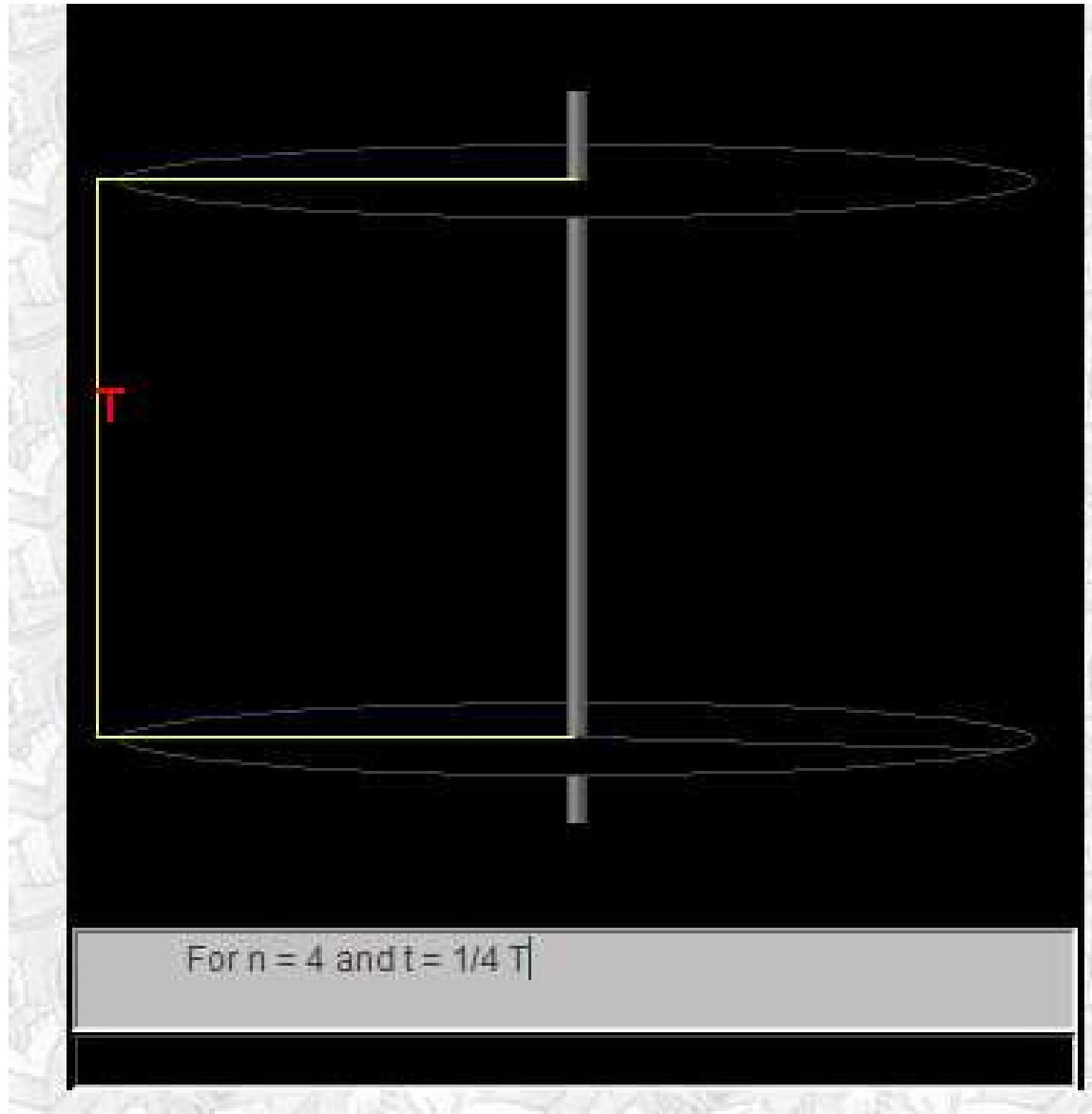
b) **rotation** around an axis (2, 3, 4, 6):

all points on the axis will not change their position;

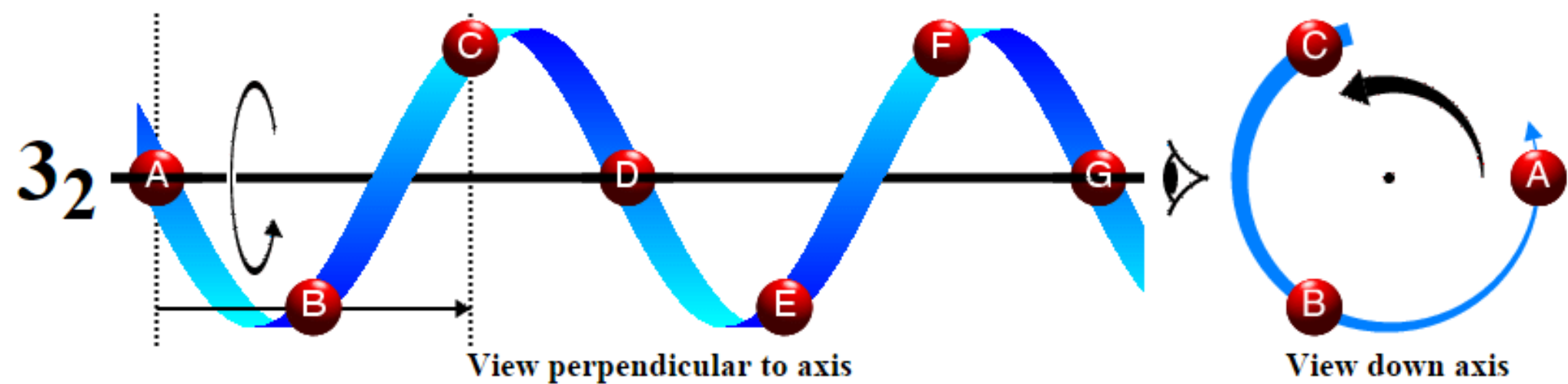
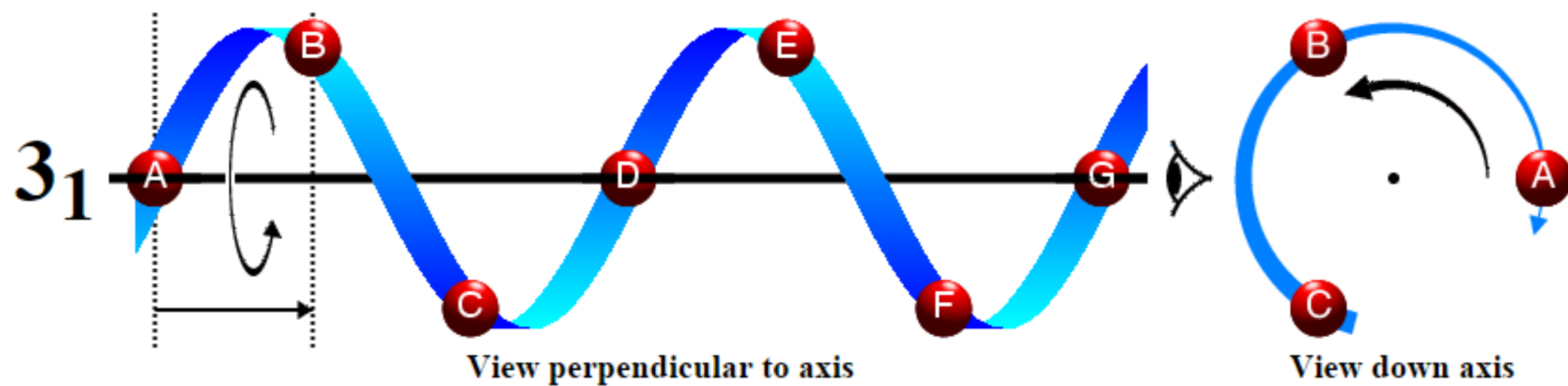
c) **rototranslation** or **screw axis**, which may be considered as the combination of a rotation around the axis and a translation along the axial direction.

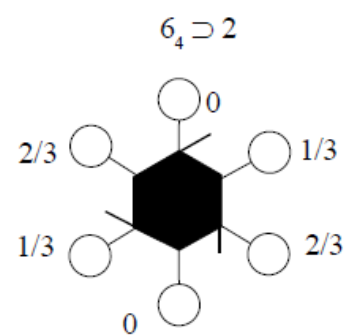
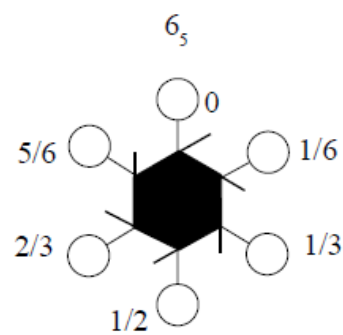
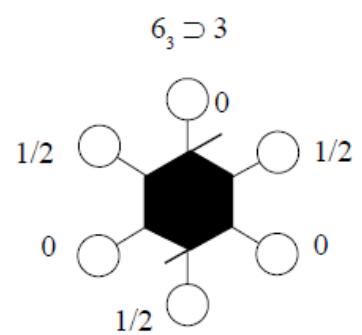
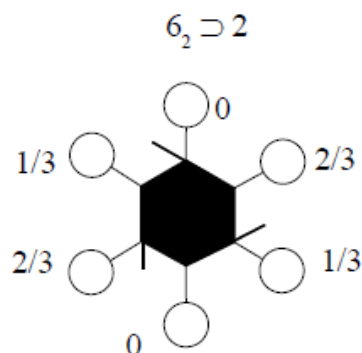
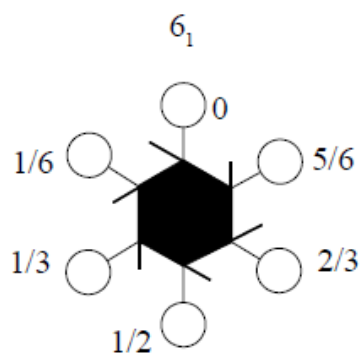
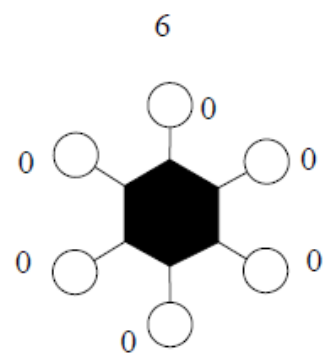
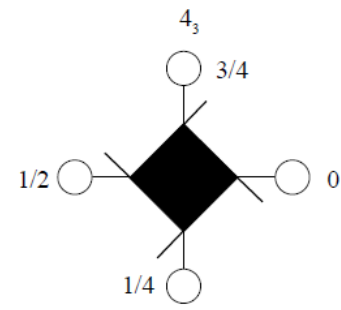
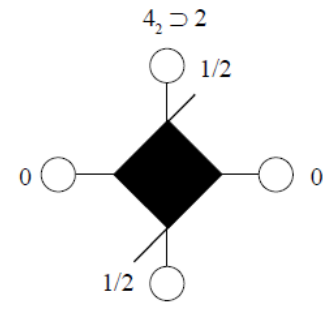
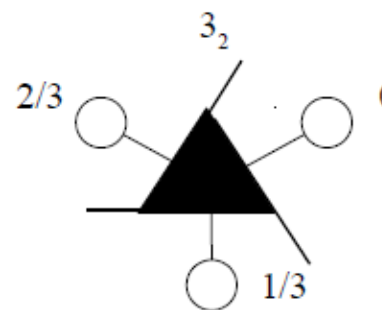
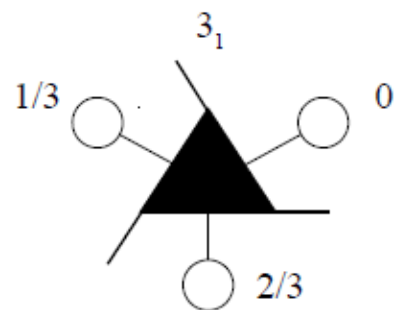
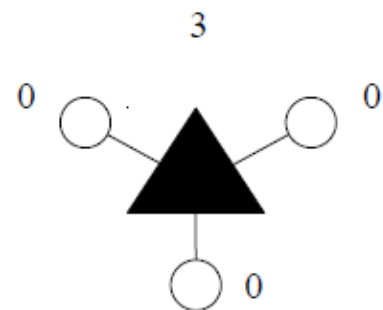
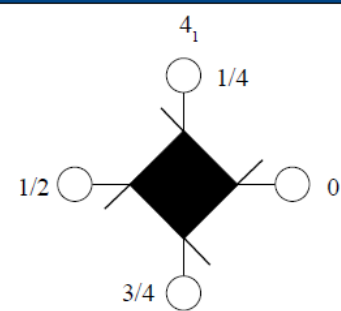
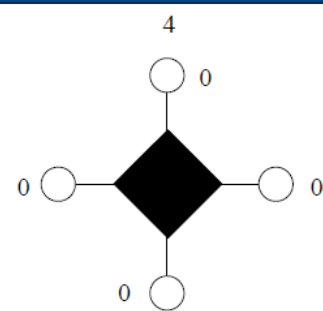
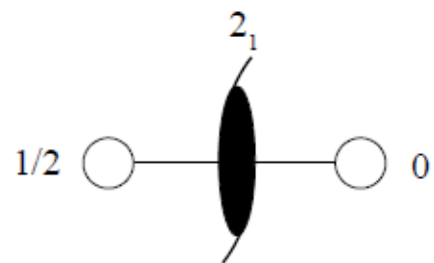
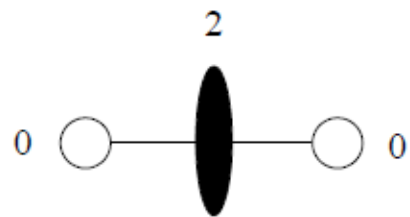


## screw axis



| Order | Screw axes                |
|-------|---------------------------|
| 2     | $2_1$                     |
| 3     | $3_1, 3_2$                |
| 4     | $4_1, 4_2, 4_3$           |
| 6     | $6_1, 6_2, 6_3, 6_4, 6_5$ |

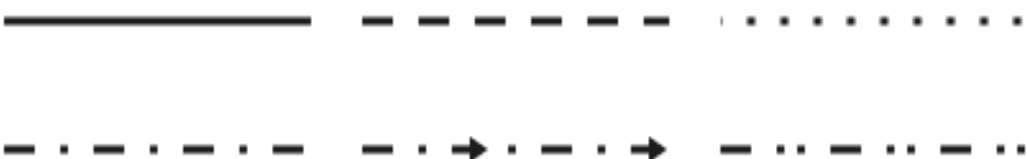




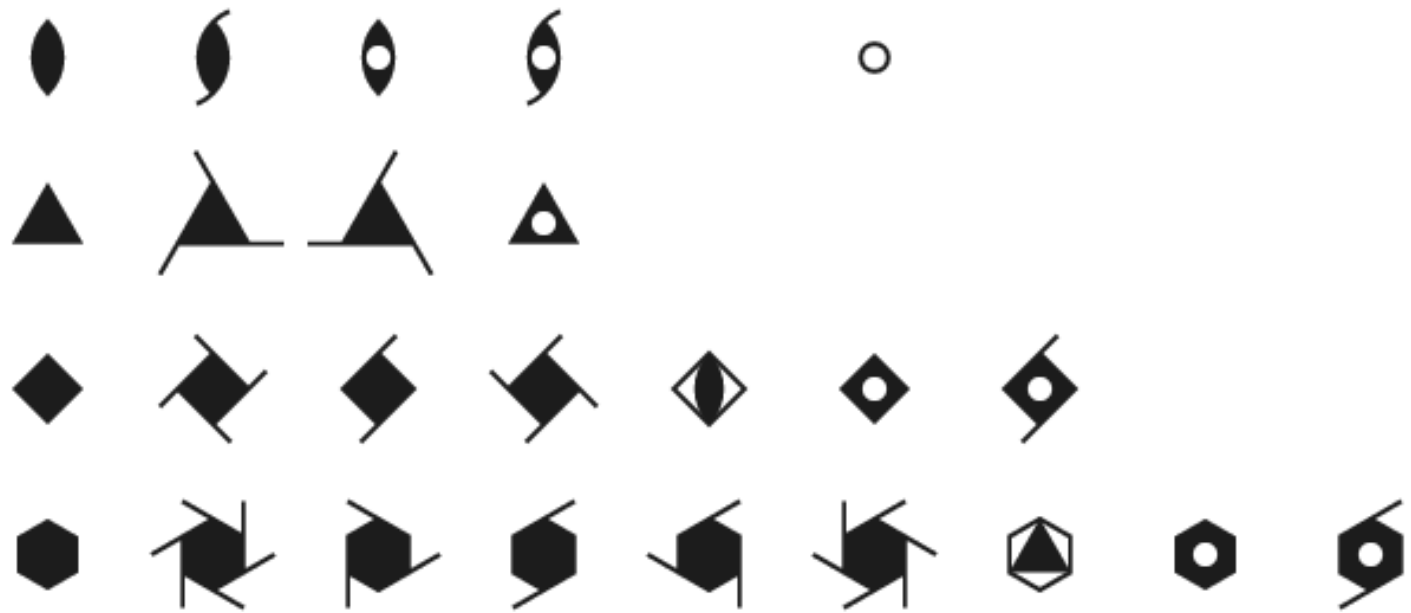
Planes parallel to the plane of the screen



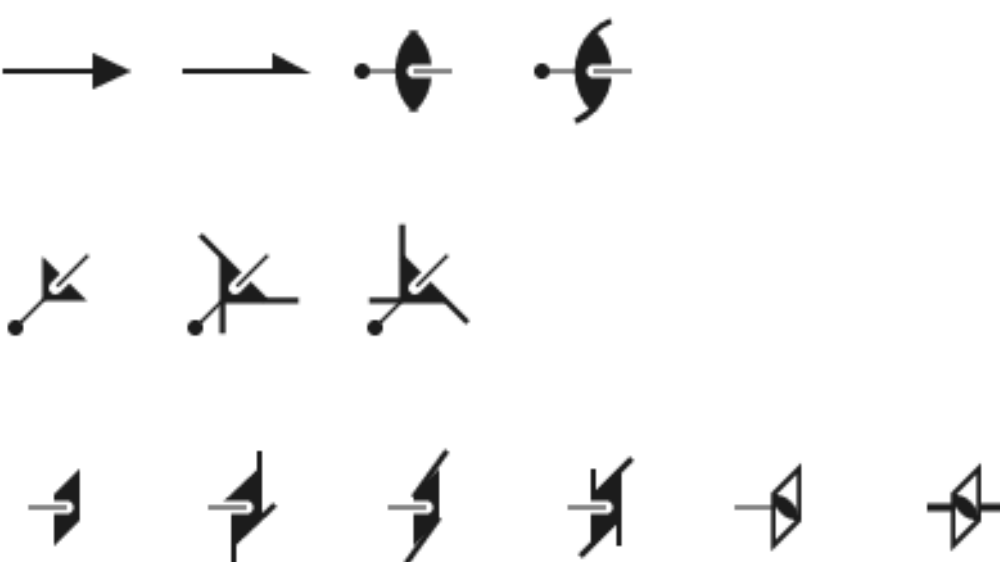
Planes perpendicular to the plane of the screen



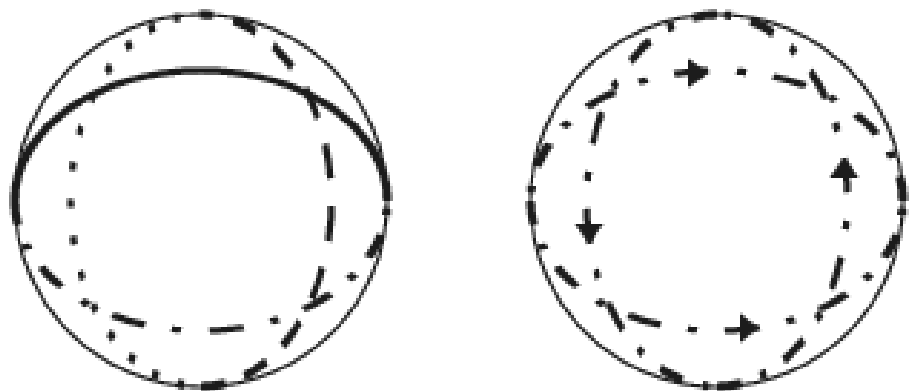
Axes normal to the plane of the screen and centre of inversion



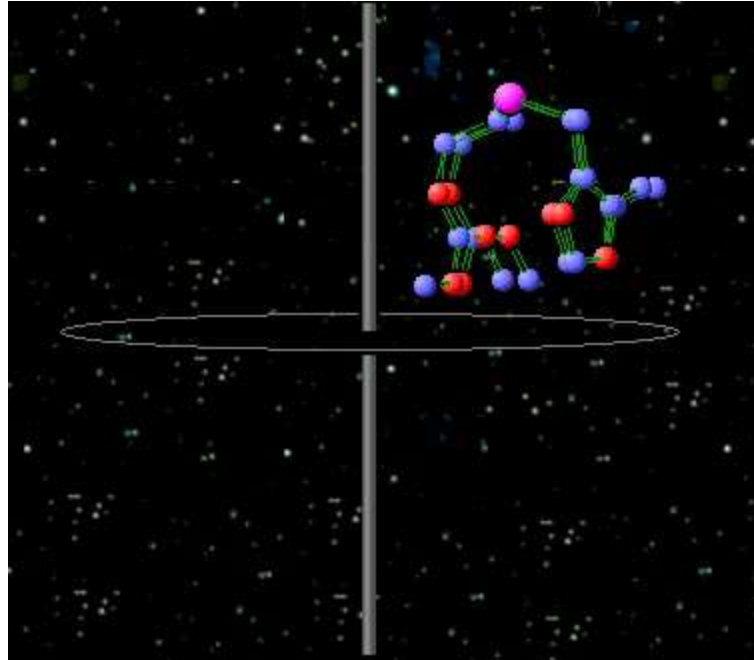
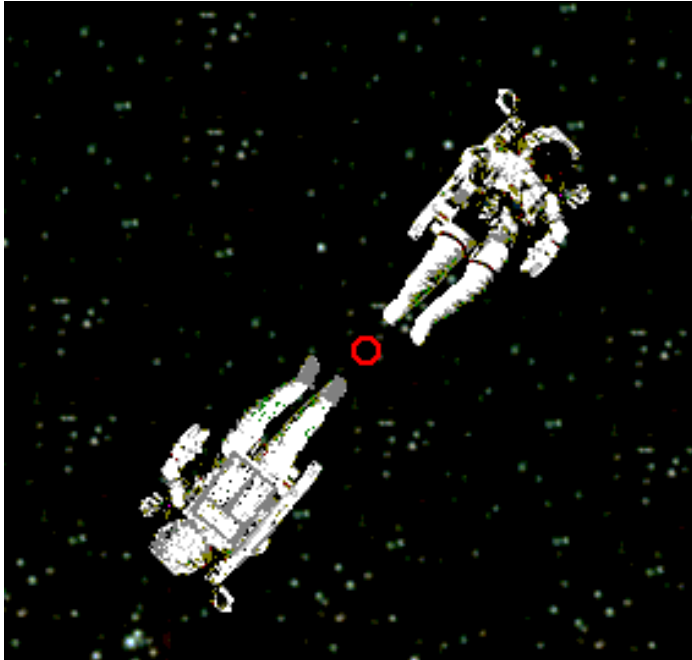
Axes parallel or inclined to the plane of the screen



Planes inclined to the plane of the screen



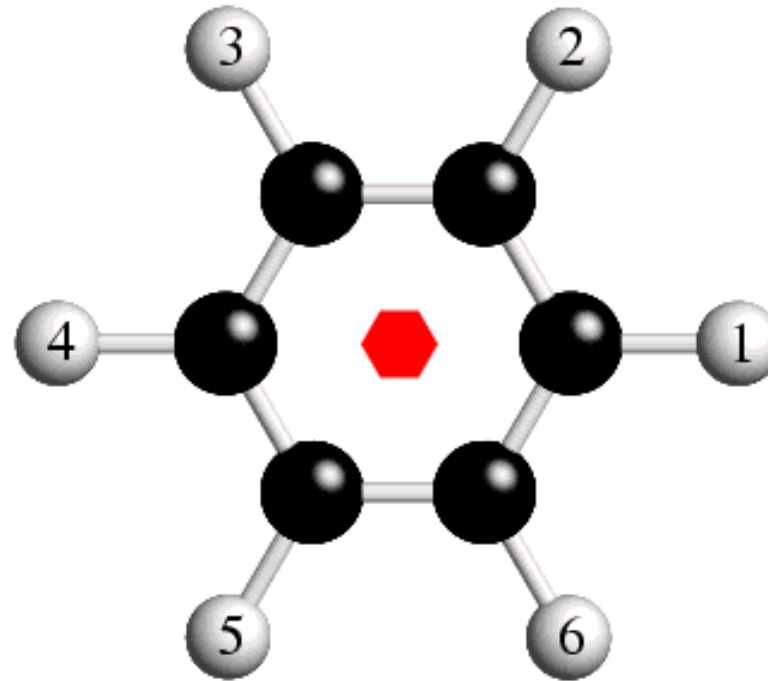
- 1: an [inversion](#), a symmetry operation with respect to a point;
- 2: a [reflection](#), a symmetry operation with respect to a plane (line in 2D);
- 3: a [rotoinversion](#), the product of a rotation around an axis by an inversion with respect to a point on the axis;
- 4: [glide plane](#) operation, the product of a reflection by a translation parallel to the reflection plane;
- 5: a [rotoreflexion](#), the product of a rotation by a reflection with respect to a plane perpendicular to the axis.

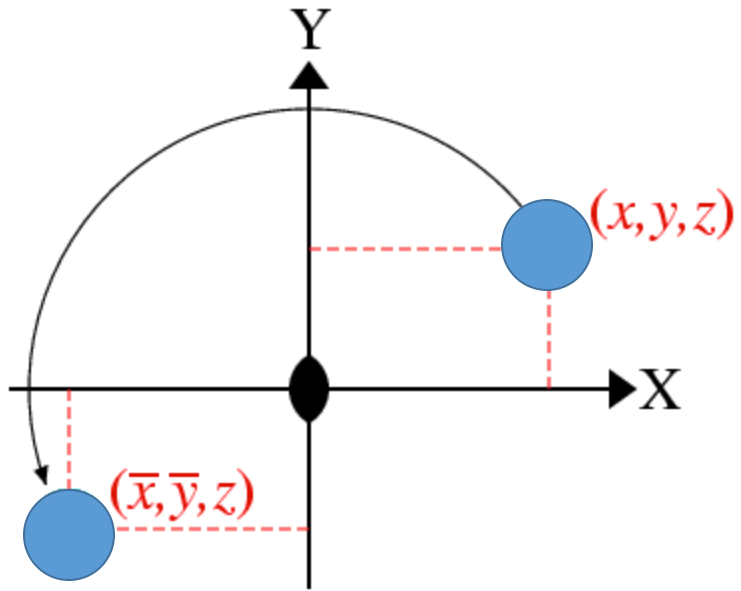


**Symmetry elements** are points, axes or planes with respect to which symmetry operations are performed.

### **Axes of rotation symmetry:**

If all the properties of the object remain unchanged after a rotation of  $2\pi/n$  around an axis, this will be called a symmetry axes of order n for the object; the written symbol is n.

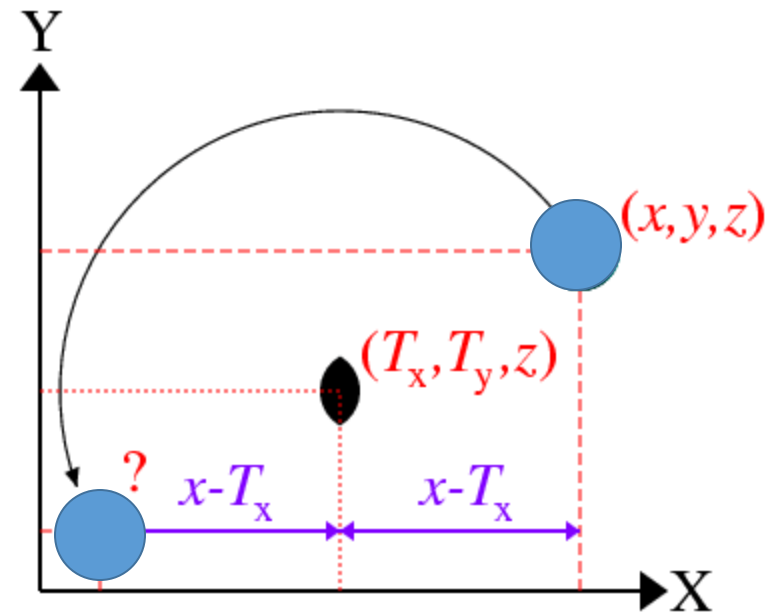




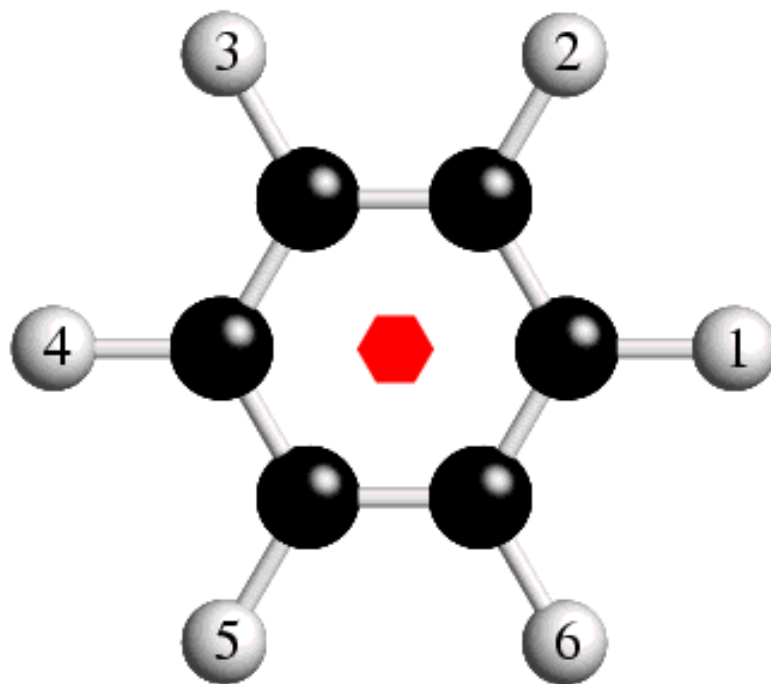
twofold rotation axis parallel to the z-direction  
and passing 0,0,0

### Symmetry Operators

$$(-x, -y, z)$$



twofold rotation axis parallel to the z-direction with x,y coordinates  
 $(T_x, T_y)$



## Symmetry Operators

$6^+$   $3^+$  2  $3^-$   $6^-$  1

Most crystals usually have some type of rotational symmetry combined with the pure translational symmetry of the lattice. **The combination of a lattice with the different orders of rotation symmetry leads to the seven possible crystal systems.**

| Crystal System                      | Characteristic<br>minimal Symmetry |                                      | Unit-Cell Parameters                                                   | Independent<br>Parameters |
|-------------------------------------|------------------------------------|--------------------------------------|------------------------------------------------------------------------|---------------------------|
| Triclinic                           | 1× 1-fold                          | -1                                   | a ; b ; c    α ; β ; γ any                                             | 6                         |
| Monoclinic                          | 1× 2-fold                          | 2/ <i>m</i>                          | a ; b ; c    α = γ = 90°; β                                            | 4                         |
| Orthorhombic                        | 3× 2-fold                          | <i>mmm</i>                           | a ; b ; c    α = β = γ = 90°                                           | 3                         |
| Tetragonal                          | 1× 4-fold                          | 4/ <i>mmm</i>                        | a = b ; c    α = β = γ = 90°                                           | 2                         |
| Rhombohedral<br>( <i>Trigonal</i> ) | 1× 3-fold                          | 6/ <i>mmm</i> (P)<br>-3 <i>m</i> (R) | a = b = c, α = β = γ (old ≠ 90°)<br>a = b ; c    α = β = 90°; γ = 120° | 2                         |
| Hexagonal                           | 1× 6-fold                          | 6/ <i>mmm</i>                        | a = b; c    α = β = 90°; γ = 120°                                      | 2                         |
| Cubic                               | 4× 3-fold                          | <i>m-3m</i>                          | a = b = c; α = β = γ = 90°                                             | 1                         |

Most crystals usually have some type of rotational symmetry combined with the pure translational symmetry of the lattice. **The combination of a lattice with the different orders of rotation symmetry leads to the seven possible crystal systems.**

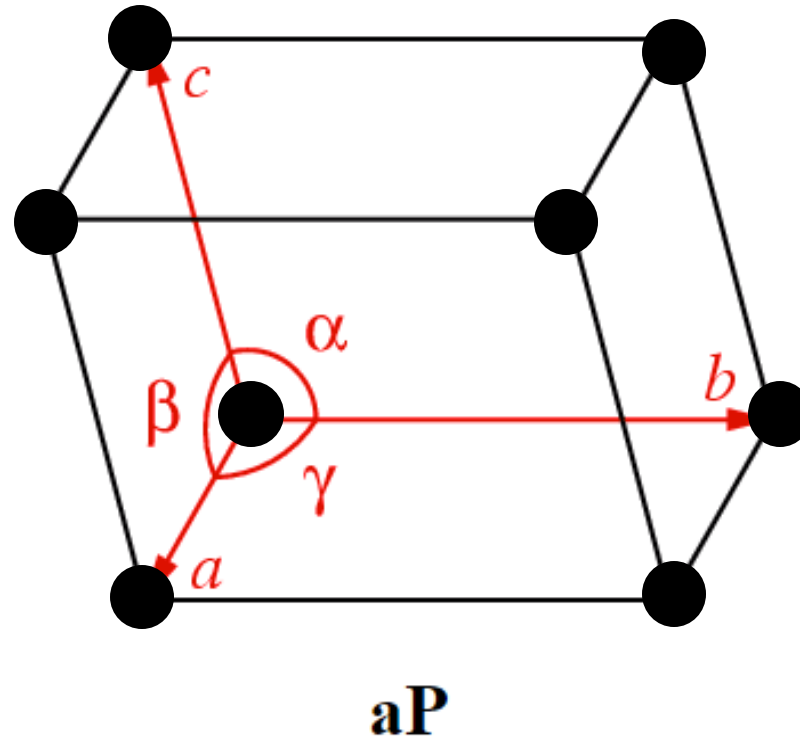
| Lattice system | Parameters                                                                                     |
|----------------|------------------------------------------------------------------------------------------------|
| triclinic      | $a ; b ; c$<br>$\alpha , \beta , \gamma$ any                                                   |
| monoclinic     | $a ; b ; c$<br>$\alpha = \gamma = 90^\circ, \beta$ any                                         |
| orthorhombic   | $a ; b ; c$<br>$\alpha = \beta = \gamma = 90^\circ$                                            |
| tetragonal     | $a = b ; c$<br>$\alpha = \beta = \gamma = 90^\circ$                                            |
| rhombohedral   | <div> rhombohedral<br/>axes </div> $a = b = c$<br>$\alpha = \beta = \gamma$                    |
|                | <div> hexagonal<br/>axes </div> $a = b ; c$<br>$\alpha = \beta = 90^\circ, \gamma = 120^\circ$ |
| hexagonal      | $a = b ; c$<br>$\alpha = \beta = 90^\circ, \gamma = 120^\circ$                                 |
| cubique        | $a = b = c$<br>$\alpha = \beta = \gamma = 90^\circ$                                            |

| Crystal System | Unit-Cell Parameters                                               |
|----------------|--------------------------------------------------------------------|
| Triclinic      | $a \neq b \neq c; \alpha \neq \beta \neq \gamma$                   |
| Monoclinic     | $a \neq b \neq c; \alpha = \gamma = 90^\circ; \beta \neq 90^\circ$ |
| Orthorhombic   | $a \neq b \neq c; \alpha = \beta = \gamma = 90^\circ$              |
| Tetragonal     | $a = b \neq c; \alpha = \beta = \gamma = 90^\circ$                 |
| Trigonal       | $a = b \neq c; \alpha = \beta = 90^\circ; \gamma = 120^\circ$      |
| Hexagonal      | $a = b \neq c; \alpha = \beta = 90^\circ; \gamma = 120^\circ$      |
| Cubic          | $a = b = c; \alpha = \beta = \gamma = 90^\circ$                    |

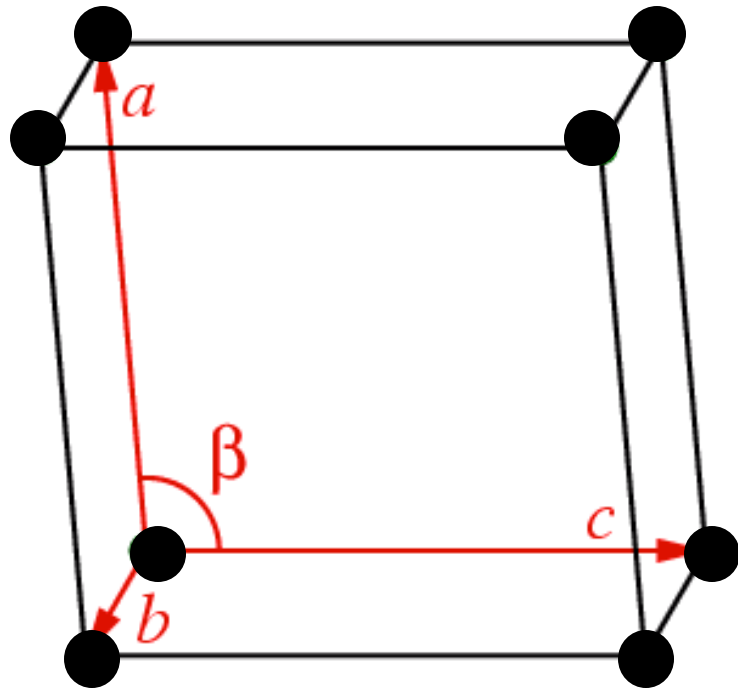
# Bravais Lattices

The combination of the 7 crystal systems with lattice centring ( $P$ ,  $A$ ,  $B$ ,  $C$ ,  $F$ ,  $I$ ,  $R$ ) leads to a maximum of fourteen (14) lattice types which are referred to as the Bravais lattices.

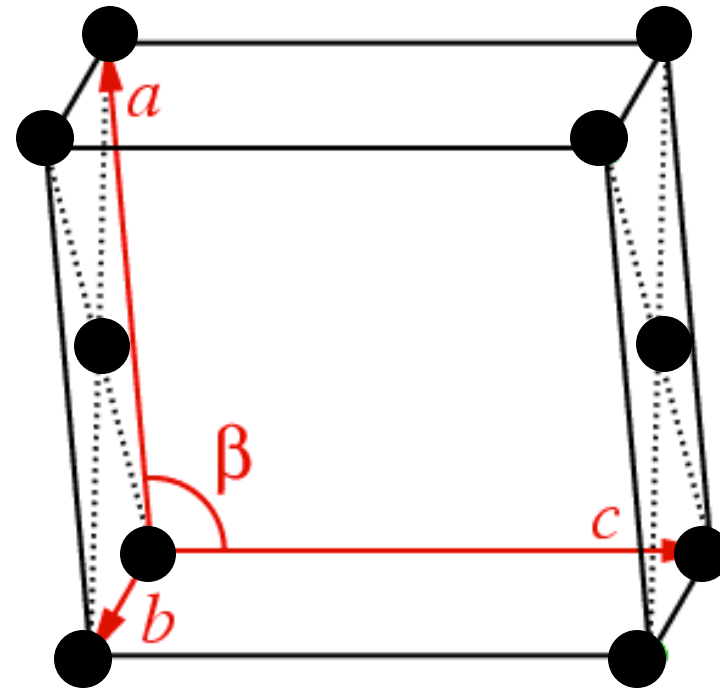
| 6 crystal families                                                                                       | conventional unit cell                                                           | 7 crystal systems<br>(morphological symmetry) | 7 lattice systems<br>(lattice symmetry) | 14 types of Bravais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



The triclinic lattice has no symmetry constraints upon it so that all of the 6 lattice parameters  $a$ ,  $b$ ,  $c$ ,  $\alpha$ ,  $\beta$ ,  $\gamma$ , are independent variables.

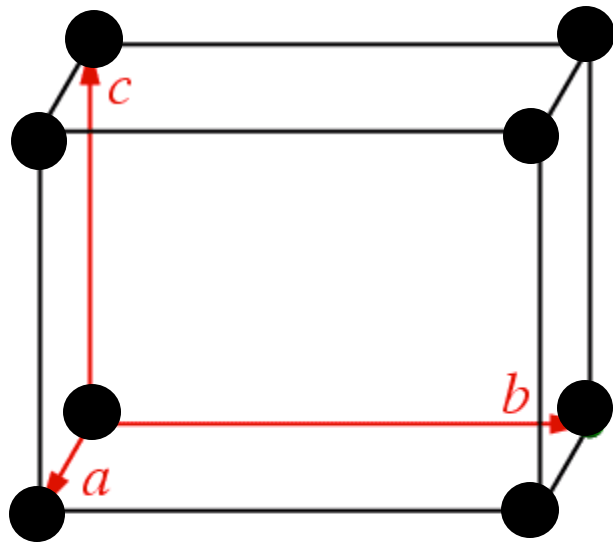


**mP**

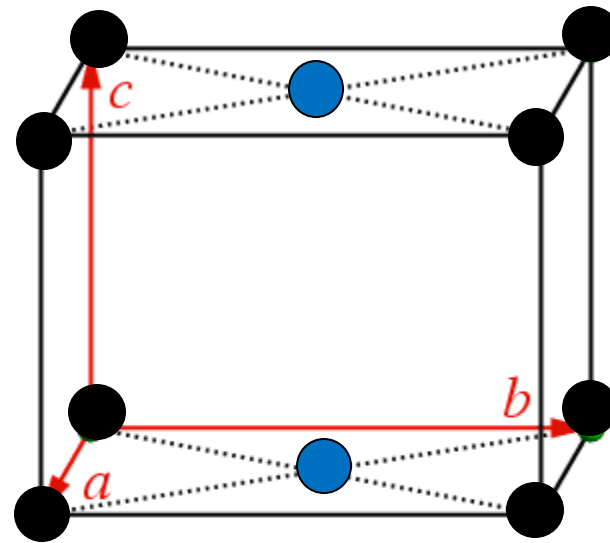


**mC**

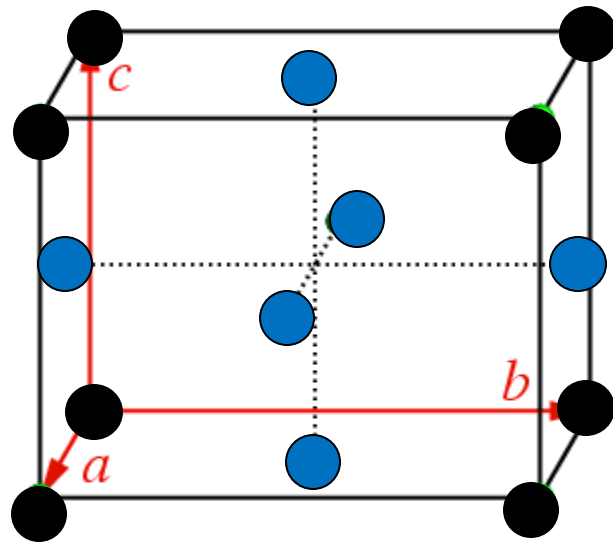
The monoclinic lattice has an axis of order 2 imposed as a symmetry constraint forcing two of the unit cell angles to  $90^\circ$ . The most common convention, is to choose the symmetry axis to be parallel to the ***b*** direction so that  $\alpha = \gamma = 90^\circ$ . The 4 independent lattice parameters are *a*, *b*, *c*, and  $\beta$ .



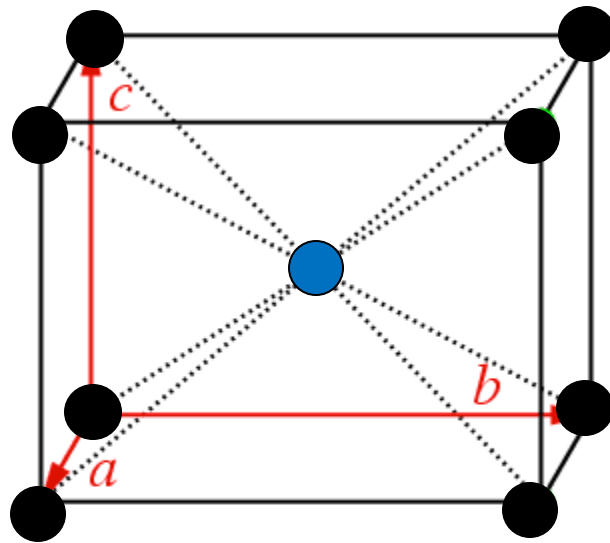
**oP**



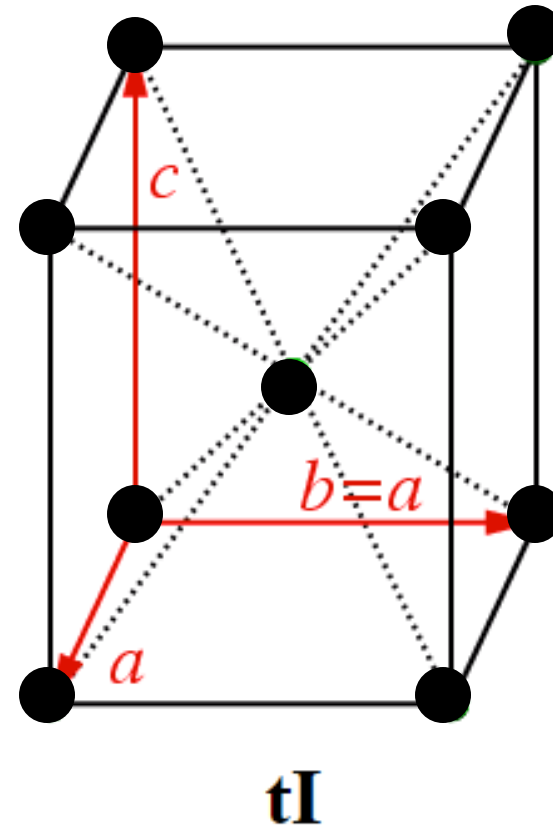
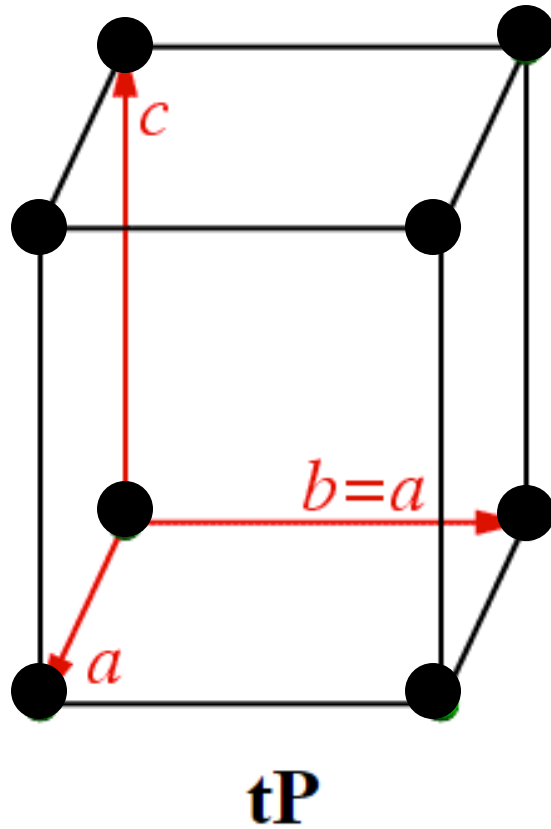
**oC**



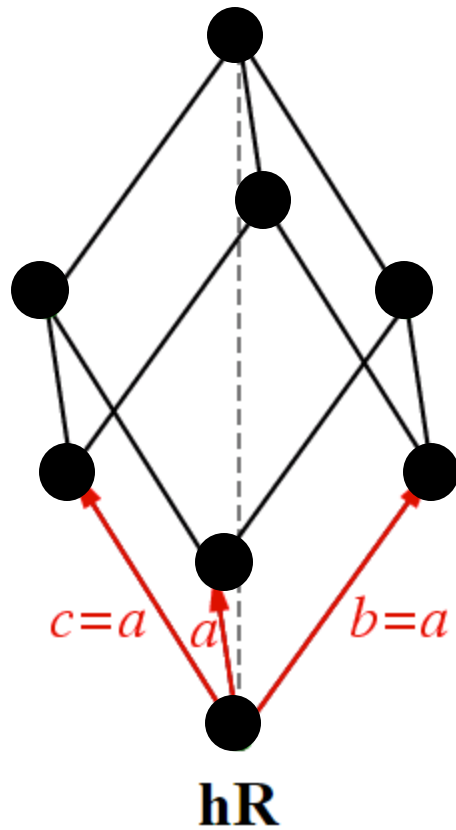
**oF**



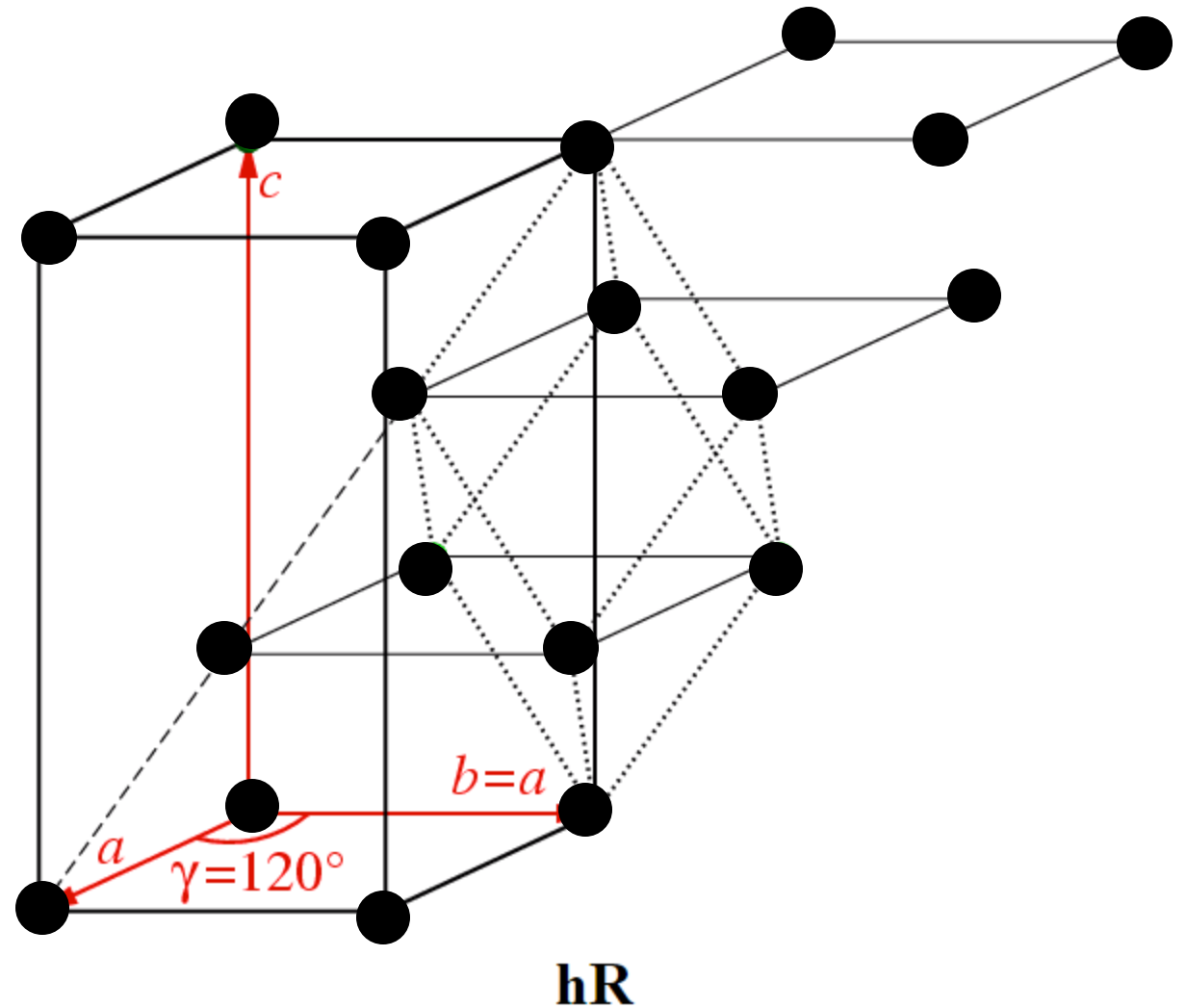
**oI**



The symmetry constraint with tetragonal lattice is an **axis of order 4 along the c-direction** which constrains all of the unit-cell angles to  $90^\circ$  and constrains the unit-cell lengths so that  $a = b$ . Conventional choice of unit cell results in either primitive or body-centred lattices, but these can be enlarged to C-face centred or all-face centred, respectively, by choosing a larger unit cell.

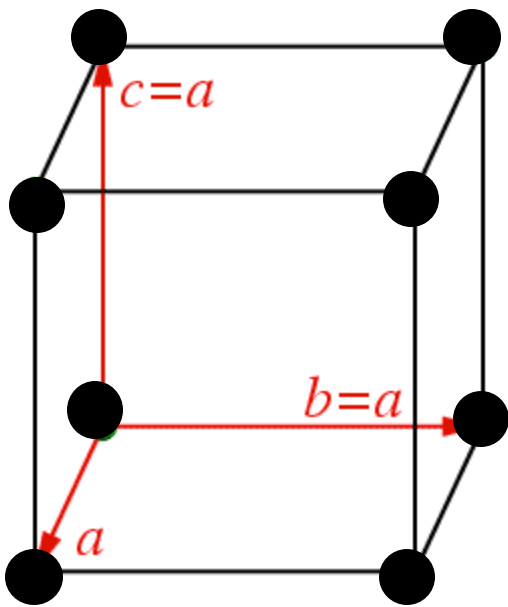


primitive rhombohedral

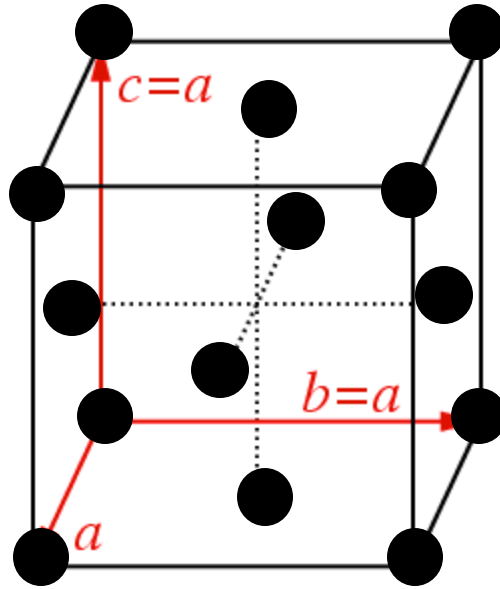


rhombohedrally-centred hexagonal

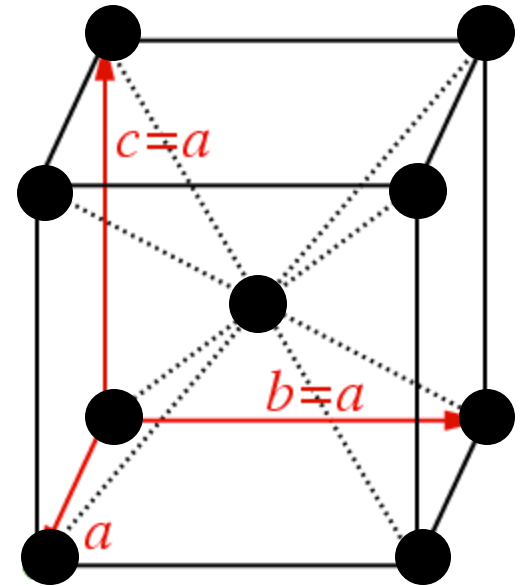
A rotation axis of order 3 along the body-diagonal of the unit cell (shown as a dashed line) constrains all of the sides to be of equal length and all of the angles to be equal, as shown above.



**cP**



**cF**



**cI**

The symmetry constraints on cubic lattices are due to the body-diagonal threefold rotation axis plus axes of order 2 parallel to each of the cell edges. This constrains all of the unit-cell angles to  $90^\circ$  and all of the unit-cell lengths to be equal, i.e.,  $a = b = c$ . Single-faced (A, B, or C) lattice centring is incompatible with the presence of threefold symmetry.

| Lattice system | Parameters                                                                    | First symmetry direction                          | Second symmetry direction                                                                                         | Third symmetry direction                                                                             |
|----------------|-------------------------------------------------------------------------------|---------------------------------------------------|-------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------|
| triclinic      | $a ; b ; c$<br>$\alpha , \beta , \gamma$ any                                  | _____                                             | _____                                                                                                             | _____                                                                                                |
| monoclinic     | $a ; b ; c$<br>$\alpha = \gamma = 90^\circ, \beta$ any                        | [010]                                             | _____                                                                                                             | _____                                                                                                |
| orthorhombic   | $a ; b ; c$<br>$\alpha = \beta = \gamma = 90^\circ$                           | [100]                                             | [010]                                                                                                             | [001]                                                                                                |
| tetragonal     | $a = b ; c$<br>$\alpha = \beta = \gamma = 90^\circ$                           | [001]                                             | [100] [010] $\equiv \langle 100 \rangle$                                                                          | [110] [1 $\bar{1}$ 0] $\equiv \langle 110 \rangle$                                                   |
| rhombohedral   | rhombohedral axes $a = b = c$<br>$\alpha = \beta = \gamma$                    | [111]                                             | [1 $\bar{1}$ 0] [01 $\bar{1}$ ] [ $\bar{1}$ 01]<br>$\equiv \langle 110 \rangle$                                   | _____                                                                                                |
|                | hexagonal axes $a = b ; c$<br>$\alpha = \beta = 90^\circ, \gamma = 120^\circ$ | [001]                                             | [100] [010] [1 $\bar{1}$ 0]<br>$\equiv \langle 100 \rangle$                                                       | _____                                                                                                |
| hexagonal      | $a = b ; c$<br>$\alpha = \beta = 90^\circ, \gamma = 120^\circ$                | [001]                                             | [100] [010] [1 $\bar{1}$ 0]<br>$\equiv \langle 100 \rangle$                                                       | [1 $\bar{1}$ 0] [120] [ $\bar{2}$ 10]<br>$\equiv \langle 110 \rangle$                                |
| cubique        | $a = b = c$<br>$\alpha = \beta = \gamma = 90^\circ$                           | [001] [100] [010]<br>$\equiv \langle 001 \rangle$ | [111] [1 $\bar{1}$ $\bar{1}$ ] [ $\bar{1}$ 1 $\bar{1}$ ] [ $\bar{1}$ $\bar{1}$ 1]<br>$\equiv \langle 111 \rangle$ | [110] [1 $\bar{1}$ 0] [011]<br>[0 $\bar{1}$ 1] [101] [ $\bar{1}$ 01]<br>$\equiv \langle 110 \rangle$ |

## Point groups

A **symmetry group** is a set of symmetry operators that are combined together according to a particular set of rules:

- The resulting action from the combination of two symmetry operators must always be equivalent to the action of a single symmetry operator that belongs to the same group. With reference to the point group 6, the action of a  $60^\circ$  rotation followed by, say, a  $240^\circ$  rotation is equivalent to a rotation of  $300^\circ$ . In symbol form this is written as:  $6^+ * 3^- = 6^-$

Thus the rule is obeyed since the resulting operator ( $6^-$ ) is a member of the point group 6.

- The group must always contain the identity symmetry operator.

Again with reference to the point group 6, this is the rotation axis of order 1 which rotates an object by  $360^\circ$ .

- Each symmetry operator in the group must have an inverse operator belonging to the group.

Thus in the point group 6, the inverse operator for a positive  $60^\circ$  rotation ( $6^+$ ) is a negative rotation ( $6^-$ ) by  $60^\circ$ .

- Beyond the scope of this “reminer” is the associative rule specifying the way in which symmetry operators are combined with each other.

A **point group** may be defined as any group of symmetry operators that leaves one or more *points* in space unmoved. If it is a single point, it is fixed in space by (a) the centre of inversion when the point group possesses rotary-inversion axes (e.g.  $-1, -3, -4, -5, -6, -7, \dots, -\infty$ ), or (b) the intersection of a twofold (2) and one or more axes (e.g. 2, 3, 4, 5, 6, 7, ...,  $\infty$ ) or (c) the intersection of a mirror plane (m) and a rotation axis (e.g. 2, 3, 4, 5, 6, 7, ...,  $\infty$ ) perpendicular to it.

This single fixed point is called the origin. If it involves more than one point unmoved, then the point group is polar.

Although there exists an infinite number of point groups, when crystallographic considerations are taken into account, i.e. rotation and rotary-inversion axes must be of order 1, 2, 3, 4, or 6, then the number of such groups is limited to just 32.

The symmetry operators present in these groups are:

|                       |    |            |    |    |    |
|-----------------------|----|------------|----|----|----|
| Rotation Axes         | 1  | 2          | 3  | 4  | 6  |
| Rotary-Inversion Axes | -1 | $m (= -2)$ | -3 | -4 | -6 |

The 32 point groups consistent with the 7 crystal systems are known as the **3-dimensional crystallographic point groups**.

# Crystal System

# 32 Crystallographic Point Groups

|              |     |                   |             |              |                      |              |
|--------------|-----|-------------------|-------------|--------------|----------------------|--------------|
| Triclinic    | 1   | -1                |             |              |                      |              |
| Monoclinic   | 2   | <i>m</i>          | 2/ <i>m</i> |              |                      |              |
| Orthorhombic | 222 | <b><i>mm2</i></b> | <i>mmm</i>  |              |                      |              |
| Tetragonal   | 4   | -4                | 4/ <i>m</i> | 422          | <b>4<i>mm</i></b>    | -42 <i>m</i> |
| Trigonal     | 3   | -3                | 32          | 3 <i>m</i>   | -3 <i>m</i>          |              |
| Hexagonal    | 6   | -6                | 6/ <i>m</i> | 622          | <b>6<i>mm</i></b>    | -62 <i>m</i> |
| Cubic        | 23  | <i>m</i> -3       | 432         | -43 <i>m</i> | <i>m</i> -3 <i>m</i> |              |

Of the 32 crystallographic point groups, those highlighted in blue possess a centre of inversion and are called centrosymmetric, while those highlighted in red possess only rotation axes and are termed enantiomorphic (the point groups that possess no improper rotations). A third type, highlighted in **bold type**, are referred to as polar.

## Diffraction Symmetry

- Bragg's law provides the condition for a plane wave to be diffracted by a family of lattice planes.
- The observed diffraction pattern is a view of the reciprocal lattice
- The reciprocal lattice is related to the real lattice and  $a^*=1/a$ ,  $a^*.b=0$ ,  $a^*.c=0$  etc.
- By considering the Bragg construction in terms of the reciprocal lattice, we can show that  $\mathbf{K} = \mathbf{G}$  for constructive interference - the Laue condition
- This leads naturally to the imaginary Ewald sphere, which allows us to make calculations from a measured diffraction pattern.
- A diffraction pattern is not a direct representation of the crystal lattice.

$$2 d \sin \theta = n \lambda$$

**BRAGG'S EQUATION**

$$\sin \theta \sim 1/d$$

- Large atomic spacing will produce a small diffraction angle and a small atomic spacing will produce a large diffraction angle.

$$\sin \theta \sim 1/(eV)^{1/2}, \lambda = 1.22 E^{1/2}$$

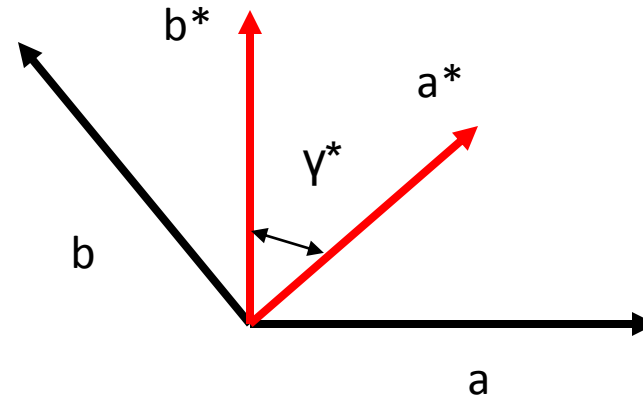
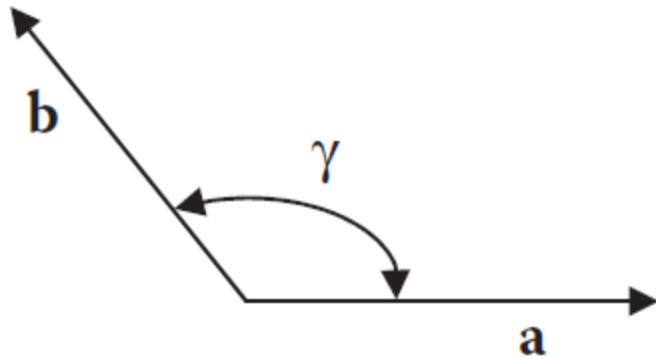
The diffraction angles are invariant under scaling; that is, they depend only on the ratio of the wavelength to the size of the diffracting object.

- Diffraction pattern will vary with incident wave-particle energy. The diffraction angle becomes smaller with increasing incident energy.
- Diffraction has same probability for  $n = 1$  and  $n = -1$ , which implies the diffraction pattern should possess some sort of symmetry.

If the units of **a** are angstroms ( $\text{\AA}$ ), then the units of **a\*** are angstroms  $^{-1}$  ( $\text{\AA}^{-1}$ ).

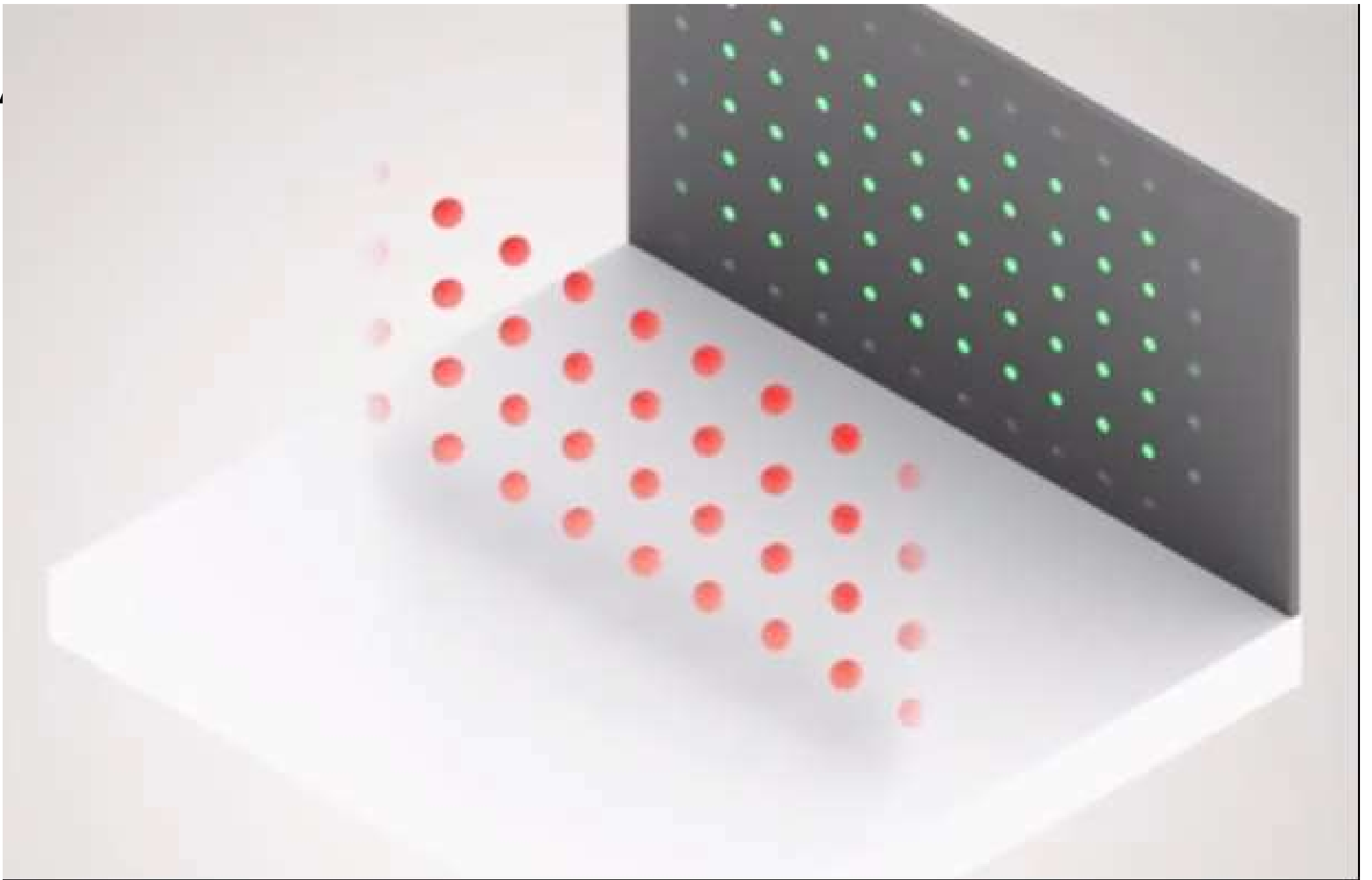
The angle between **a** and **b** is  $\gamma$ ; the angle between **a\*** and **b\*** is  $\gamma^*$ .

Since **a** and **b** are in angstroms and **a\*** and **b\*** are in inverse angstroms, the directions of the vectors are emphasized, not their relative lengths.



Two-dimensional non orthogonal basis vectors **a** and **b**, superimposed reciprocal basis vectors, **a\*** and **b\*** is  $\gamma^*$

$$\sin \theta \sim 1$$



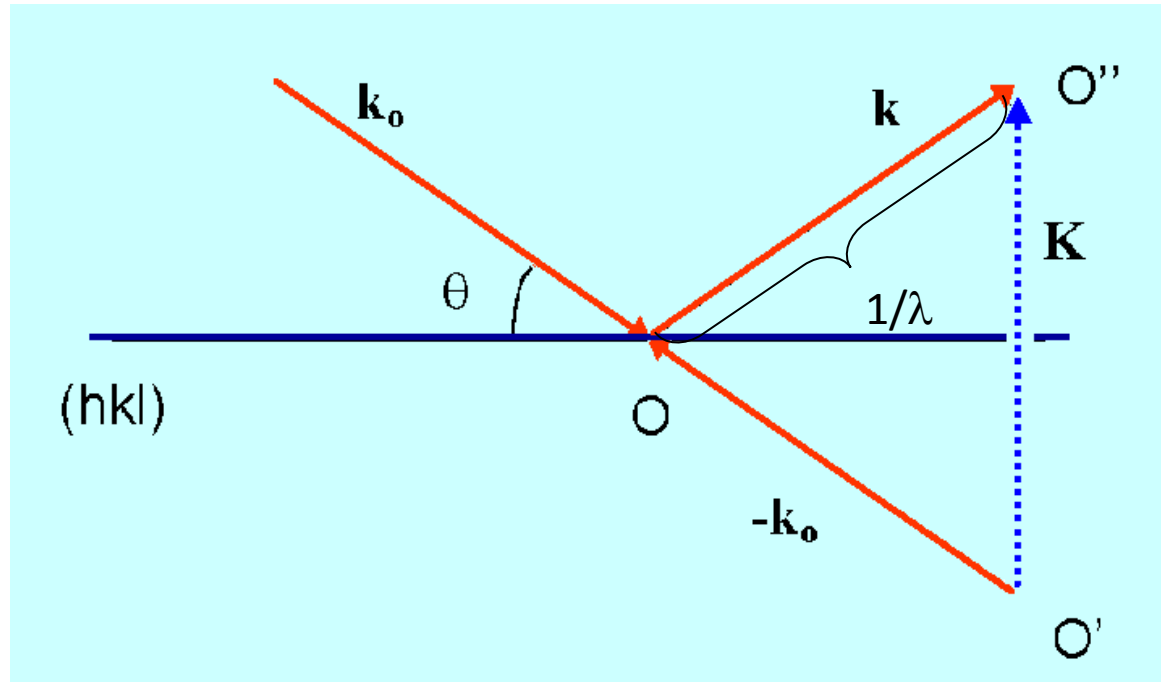
# Diffraction Symmetry

The diffraction experiment measures the spacing of the spots from which the reciprocal lattice is derived. Indeed there are similar constraints that apply equally-well to the reciprocal-space unit-cell parameters.

| Crystal System      | Unit-Cell Parameters                                               | Reciprocal-Space Parameters                                                    |
|---------------------|--------------------------------------------------------------------|--------------------------------------------------------------------------------|
| Triclinic           | $a \neq b \neq c; \alpha \neq \beta \neq \gamma$                   | $a^* \neq b^* \neq c^*; \alpha^* \neq \beta^* \neq \gamma^*$                   |
| Monoclinic          | $a \neq b \neq c; \alpha = \gamma = 90^\circ; \beta \neq 90^\circ$ | $a^* \neq b^* \neq c^*; \alpha^* = \gamma^* = 90^\circ; \beta^* \neq 90^\circ$ |
| Orthorhombic        | $a \neq b \neq c; \alpha = \beta = \gamma = 90^\circ$              | $a^* \neq b^* \neq c^*; \alpha^* = \beta^* = \gamma^* = 90^\circ$              |
| Tetragonal          | $a = b \neq c; \alpha = \beta = \gamma = 90^\circ$                 | $a^* = b^* \neq c^*; \alpha^* = \beta^* = \gamma^* = 90^\circ$                 |
| Trigonal (see note) | $a = b = c; \alpha = \beta = \gamma \neq 90^\circ$                 | $a^* = b^* = c^*; \alpha^* = \beta^* = \gamma^* \neq 90^\circ$                 |
| Hexagonal           | $a = b \neq c; \alpha = \beta = 90^\circ; \gamma = 120^\circ$      | $a^* = b^* \neq c^*; \alpha^* = \beta^* = 90^\circ; \gamma^* = 60^\circ$       |
| Cubic               | $a = b = c; \alpha = \beta = \gamma = 90^\circ$                    | $a^* = b^* = c^*; \alpha^* = \beta^* = \gamma^* = 90^\circ$                    |

# The **K** vector

We define incident and reflected X-rays as  $\mathbf{k}_0$  and  $\mathbf{k}$  respectively, with moduli  $1/\lambda$



Then we define vector  $\mathbf{K} = \mathbf{k} - \mathbf{k}_0$

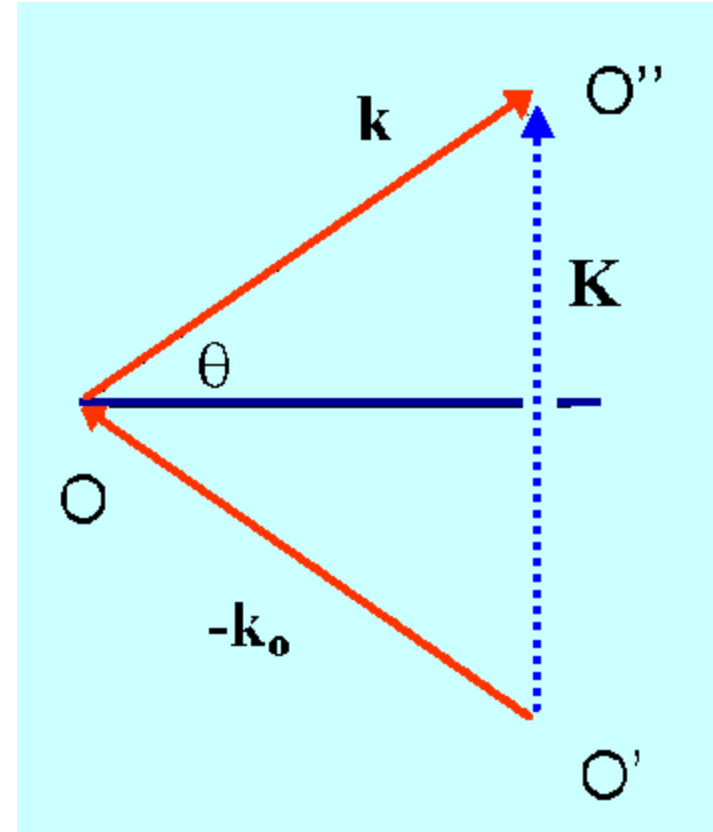
# K vector

As  $\mathbf{k}$  and  $\mathbf{k}_o$  are of equal length,  $1/\lambda$ , the triangle  $O, O', O''$  is isosceles.

The angle between  $\mathbf{k}$  and  $-\mathbf{k}_o$  is  $2\theta_{hkl}$  and the  $hkl$  plane bisects it.

The length of  $\mathbf{K}$  is given by:

$$|\mathbf{K}| = 2|\mathbf{k}|\sin\theta_{hkl} = \frac{2\sin\theta_{hkl}}{\lambda}$$



# The Laue condition

$\mathbf{K}$  is perpendicular to the (hkl) plane, so can be defined as:

$$\mathbf{K} = \left[ \frac{2 \sin \theta_{hkl}}{\lambda} \right] \hat{\mathbf{n}} \quad \text{where } \hat{\mathbf{n}} \text{ is a vector of unit length}$$

$\mathbf{G}$  is also perpendicular to (hkl) so

$$\hat{\mathbf{n}} = \frac{\mathbf{G}_{hkl}}{|\mathbf{G}_{hkl}|}$$

$$\Rightarrow \mathbf{K} = \frac{2}{\lambda |\mathbf{G}_{hkl}|} \sin \theta_{hkl} \mathbf{G}_{hkl} \quad \text{and} \quad |\mathbf{G}_{hkl}| = \frac{1}{d_{hkl}} \quad \text{from previous}$$

$$\Rightarrow \mathbf{K} = \frac{2 d_{hkl} \sin \theta_{hkl}}{\lambda} \mathbf{G}_{hkl}$$

But Bragg:  $2 d \sin \theta = \lambda$

So  $\mathbf{K} = \mathbf{G}_{hkl}$  the Laue condition

Von Laue condition in reciprocal space (orthogonal lattices):

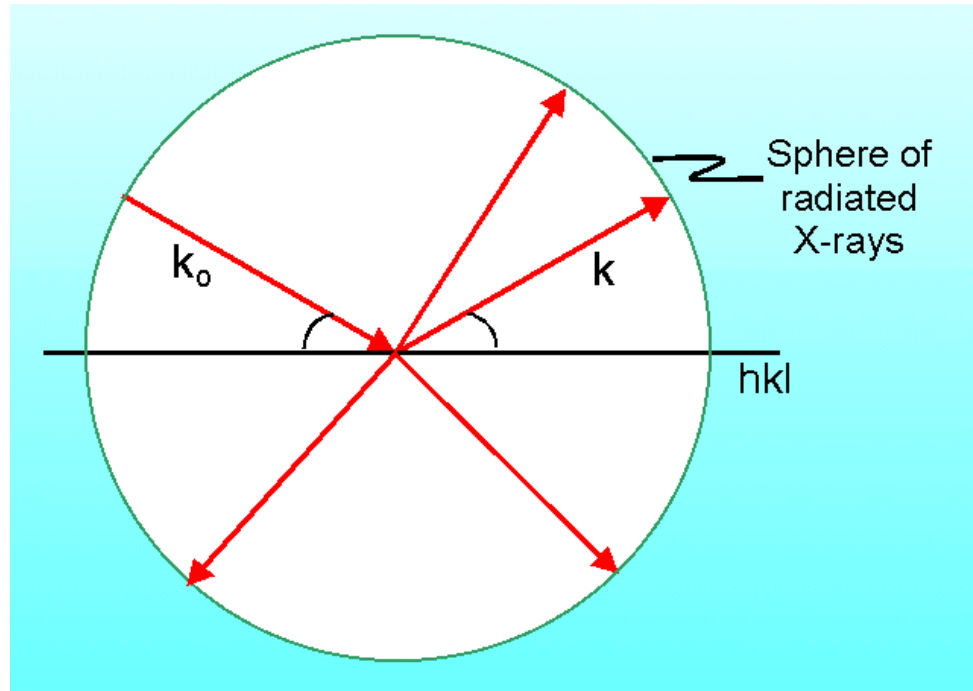
$$\lambda(h^2 a^{*2} + k^2 b^{*2} + l^2 c^{*2})^{1/2} = 2 \sin \theta_{hkl} = \frac{n\lambda}{d_{hkl}}$$

Von Laue condition in reciprocal space for all crystal symmetries:

$$\lambda(h^2 a^{*2} + k^2 b^{*2} + l^2 c^{*2} + 2hka^*c^* \cos \gamma^* + 2hla^*c^* \cos \beta^* + 2klb^*c^* \cos \alpha^*)^{1/2} = 2 \sin \theta_{hkl} = \frac{n\lambda}{d_{hkl}}$$

# What does this mean?!

Laue assumed that each set of atoms could radiate the incident radiation in all directions



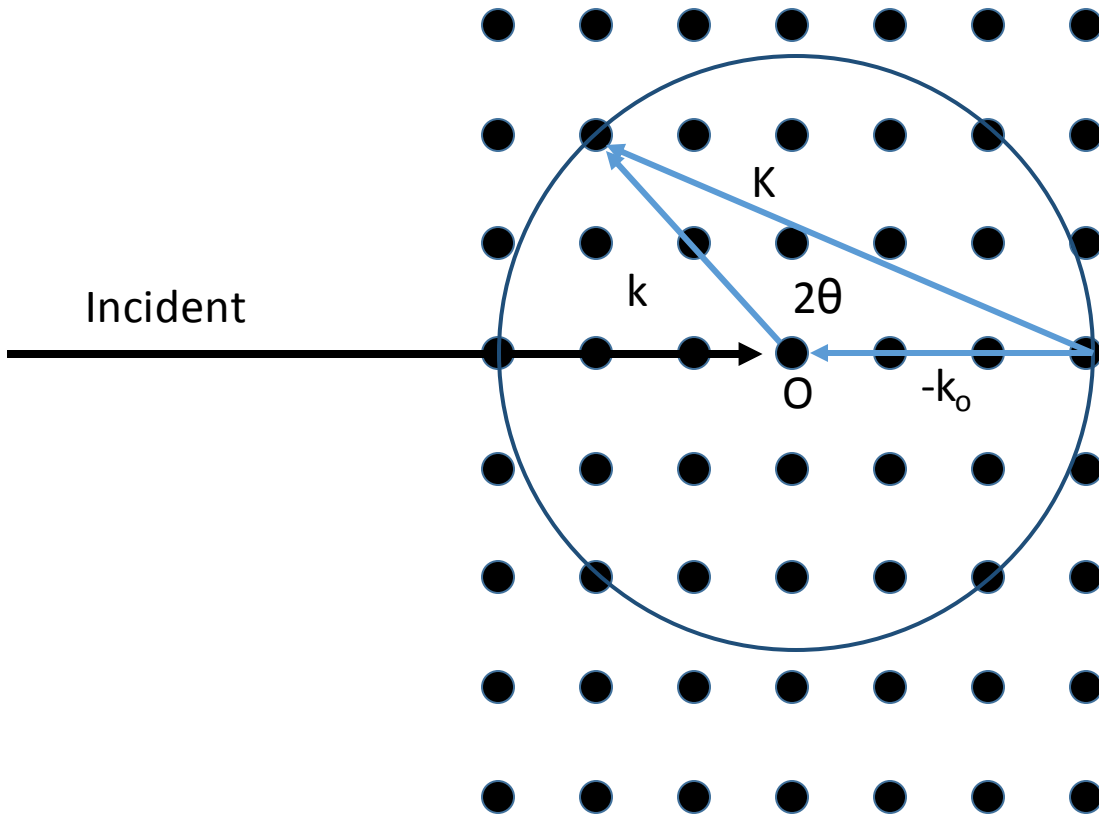
Constructive interference only occurs when the scattering vector,  $\mathbf{K}$ , coincides with a reciprocal lattice vector,  $\mathbf{G}$

This naturally leads to the Ewald Sphere construction

# Ewald Sphere

We superimpose the imaginary “sphere” of radiated radiation upon the reciprocal lattice

For a fixed direction and wavelength of incident radiation, we draw  $-\mathbf{k}_0$  ( $=1/\lambda$ )  
e.g. along  $\mathbf{a}^*$



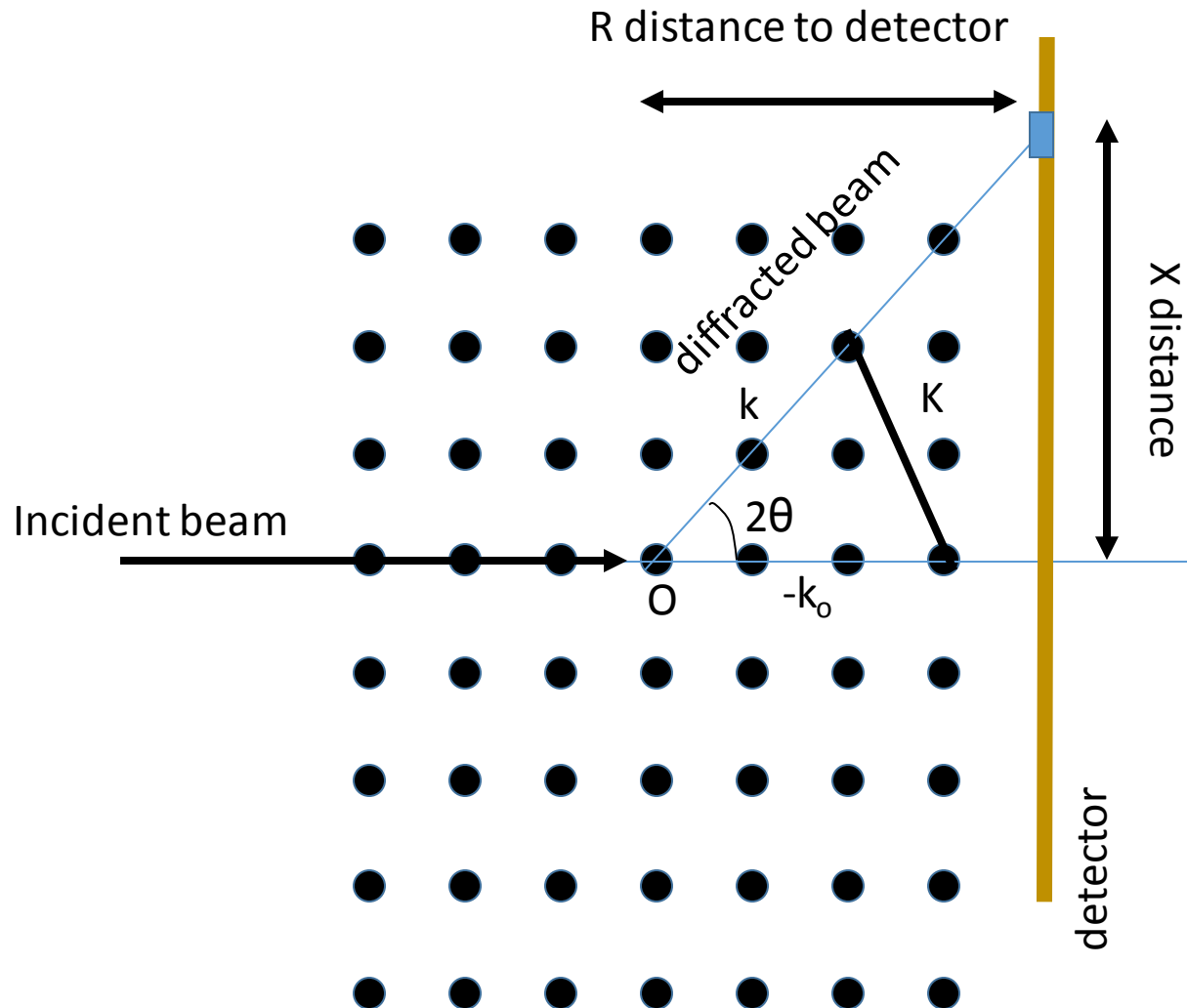
Draw sphere of radius  $1/\lambda$  centred on end of  $\mathbf{k}_0$

Reflection is only observed if sphere intersects a point

i.e. where  **$\mathbf{K}=\mathbf{G}$**

# What does this actually mean?!

Relate to a real diffraction experiment with crystal at O



$K=G$  so scattered beam  
at angle  $2\theta$

Geometry:

$$\tan 2\theta = \frac{x}{R} \Rightarrow 2\theta = \tan^{-1} \frac{x}{R}$$

$$\text{but } |K| = \frac{2 \sin \theta_{hkl}}{\lambda}$$

$$\text{so } |K| = \frac{2}{\lambda} \sin \left( \frac{1}{2} \tan^{-1} \frac{x}{R} \right)$$

In addition, the diffraction experiment measures the intensity of the reciprocal-lattice points, which are proportional to the square of the structure factors,  $\mathbf{F}(hkl)$ . Friedel's law states that, in the absence of anomalous dispersion effects,

$$|\mathbf{F}(hkl)| = |\mathbf{F}(-h-k-l)|.$$

By virtue of this law the reciprocal lattice weighted with  $|\mathbf{F}|$  always contains a [point of inversion](#) in the absence of anomalous dispersion, even when this symmetry element is not present in the crystal structure. Thus the point-group symmetry of the reciprocal lattice is centrosymmetric. Thus determination of this point-group symmetry is the obvious first step in the determination of the crystal symmetry.

# Laue Classes

The eleven centrosymmetric point groups which describe 3-dimensional diffraction symmetry are known as the *Laue classes* (often still referred to as Laue groups).

| Crystal System | Laue Classes |         |
|----------------|--------------|---------|
| Triclinic      | -1           |         |
| Monoclinic     | $2/m$        |         |
| Orthorhombic   | $mmm$        |         |
| Tetragonal     | $4/m$        | $4/mmm$ |
| Trigonal       | -3           | $-3m$   |
| Hexagonal      | $6/m$        | $6/mmm$ |
| Cubic          | $m-3$        | $m-3m$  |

## Reflection Multiplicity

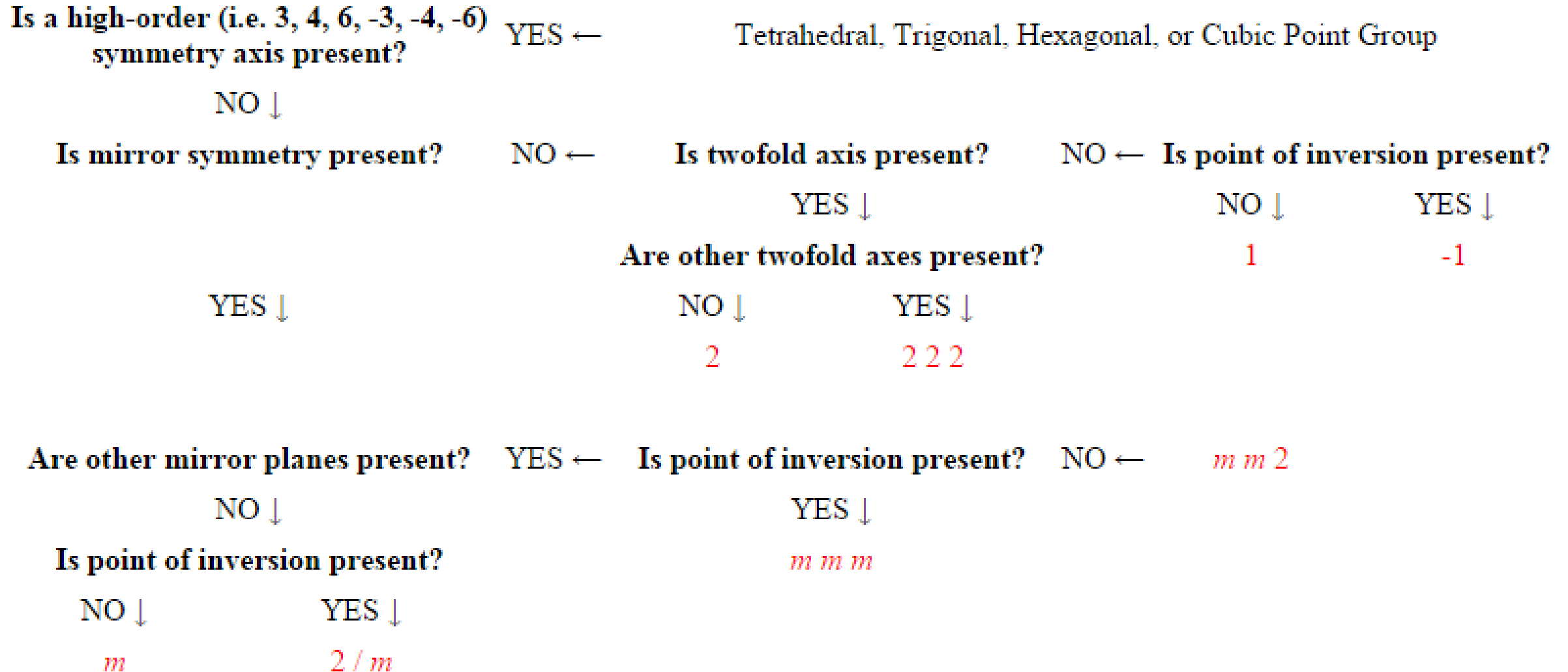
In contrast to single-crystal diffraction in which symmetry-equivalent reflections can be measured individually and checked for equality, the one-dimensional nature of powder diffraction results in the exact superposition of reflections with the same  $d$  spacing.

In calculating the intensity of a peak in a powder diffraction pattern, it is more efficient to calculate the intensity of a single reflection,  $hkl$ , and multiply it by  $j$ , the number of symmetry-equivalent reflections contributing to the single observed peak. This is called the multiplicity of the reflection. Multiplicity only occurs in powder diffraction, and so is not commonly discussed in connection with single-crystal data.

**What determines the multiplicity of a reflection?** There are two factors that need to be considered: firstly, the Laue class of the sample; and secondly, whether the reflection lies on one of the symmetry elements within the particular Laue class.

| Crystal System | Laue Class | Symmetry-Equivalent Reflections                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         | Multiplicity |
|----------------|------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------|
| Triclinic      | -1         | $hkl \equiv -h-k-l$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | 2            |
| Monoclinic     | 2/m        | $hkl \equiv -h\bar{k}-l \equiv -h-k-l \equiv h-kl$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 4            |
| Orthorhombic   | mmm        | $hkl \equiv h-k-l \equiv -h\bar{k}-l \equiv -h-kl \equiv -h-k-l \equiv -hkl \equiv h-kl \equiv h\bar{k}-l$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | 8            |
| Tetragonal     | 4/m        | $hkl \equiv -khl \equiv -h-kl \equiv k-hl \equiv -h-k-l \equiv k-h-l \equiv h\bar{k}-l \equiv -kh-l$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | 8            |
|                | 4/mmm      | $hkl \equiv -khl \equiv -h-kl \equiv k-hl \equiv -h-k-l \equiv k-h-l \equiv h\bar{k}-l \equiv -kh-l \equiv$<br>$khl \equiv -hkl \equiv -k-hl \equiv h-kl \equiv -k-h-l \equiv h-k-l \equiv kh-l \equiv -hk-l$                                                                                                                                                                                                                                                                                                                                                                                                                                           | 16           |
| Cubic          | m-3        | $hkl \equiv -hkl \equiv h-kl \equiv h\bar{k}-l \equiv -h-k-l \equiv h-k-l \equiv -h\bar{k}-l \equiv -h-kl \equiv$<br>$klh \equiv -klh \equiv k-lh \equiv kl-h \equiv -k-l-h \equiv k-l-h \equiv -kl-h \equiv -k-lh \equiv$<br>$lhk \equiv -lhk \equiv l-hk \equiv lh-k \equiv -l-h-k \equiv l-h-k \equiv -lh-k \equiv -l-hk$                                                                                                                                                                                                                                                                                                                            | 24           |
|                | m-3m       | $hkl \equiv -hkl \equiv h-kl \equiv h\bar{k}-l \equiv -h-k-l \equiv h-k-l \equiv -h\bar{k}-l \equiv -h-kl \equiv$<br>$klh \equiv -klh \equiv k-lh \equiv kl-h \equiv -k-l-h \equiv k-l-h \equiv -kl-h \equiv -k-lh \equiv$<br>$lhk \equiv -lhk \equiv l-hk \equiv lh-k \equiv -l-h-k \equiv l-h-k \equiv -lh-k \equiv -l-hk \equiv$<br>$khl \equiv -khl \equiv k-hl \equiv kh-l \equiv -k-h-l \equiv k-h-l \equiv -kh-l \equiv -k-hl \equiv$<br>$lkh \equiv -lkh \equiv l-kh \equiv lk-h \equiv -l-k-h \equiv l-k-h \equiv -lk-h \equiv -l-kh \equiv$<br>$hlk \equiv -hlk \equiv h-lk \equiv hl-k \equiv -h-l-k \equiv h-l-k \equiv -hl-k \equiv -h-lk$ | 48           |

## Point-Group Determination in practice



# Space Groups

The number of permutations of Bravais lattices with rotation and screw axes, mirror and glide planes, plus points of inversion is finite: there are only 230 unique combinations for three-dimensional symmetry, and these combinations are known as the 230 space groups.

The space groups are numbered from 1 to 230 and are classified here according to the 7 crystal systems: triclinic, monoclinic, orthorhombic, tetragonal, trigonal, hexagonal, and cubic.

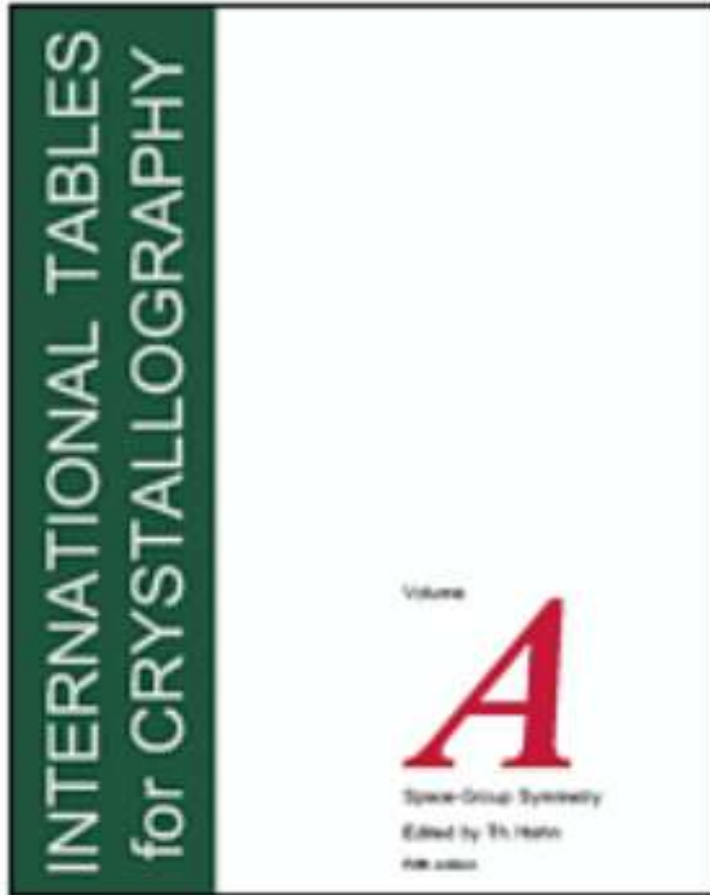
Within each crystal system, the space groups can be ordered by Laue class, crystal class (e.g.  $2 < m < 2/m$ ) and, finally, lattice centering (e.g.  $P < A, B, C < F < I$ ).

Each one of the 230 three-dimensional space groups is unique; however, they are frequently specified by means of space group symbols that are not unique to a particular space group.

# INTERNATIONAL TABLES FOR CRYSTALLOGRAPHY

## VOLUME A: SPACE-GROUP SYMMETRY

Extensive tabulations and illustrations of the 17 plane groups and the 230 space groups



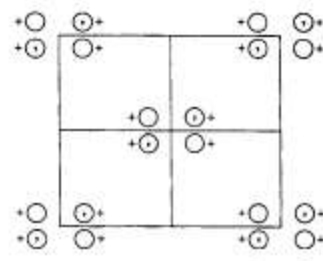
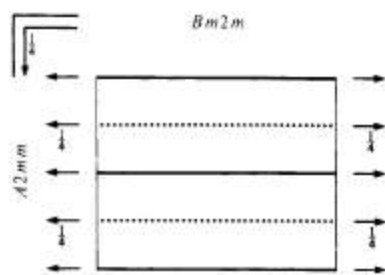
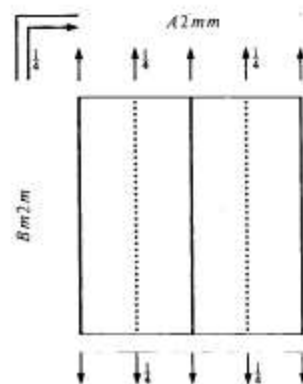
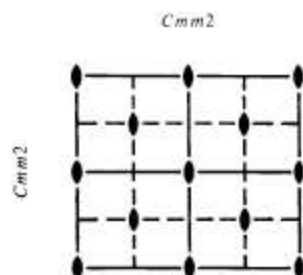
- headline with the relevant group symbols;
- diagrams of the symmetry elements and of the general position;
- specification of the origin and the asymmetric unit;
- list of symmetry operations;
- generators;
- general and special positions with multiplicities, site symmetries, coordinates and reflection conditions;
- symmetries of special projections;
- extensive subgroup and supergroup data

$Cmm2$ 

No. 35

 $C_{2v}^{11}$  $Cmm2$  $mm2$ 

Orthorhombic

Patterson symmetry  $Cmmm$ Origin on  $mm2$ Asymmetric unit  $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq 1$ 

Symmetry operations

For  $(0,0,0)+$  set(1) 1 (2) 2  $0,0,z$  (3)  $m$   $x,0,z$  (4)  $m$   $0,y,z$ For  $(\frac{1}{2},\frac{1}{2},0)+$  set(1)  $t(\frac{1}{2},\frac{1}{2},0)$  (2) 2  $\frac{1}{2},\frac{1}{2},z$  (3)  $a$   $x,\frac{1}{2},z$  (4)  $b$   $\frac{1}{2},y,z$ Generators selected (1);  $t(1,0,0)$ ;  $t(0,1,0)$ ;  $t(0,0,1)$ ;  $t(\frac{1}{2},\frac{1}{2},0)$ ; (2); (3)

Positions

Multiplicity,  
Wyckoff letter,  
Site symmetry

Coordinates

 $(0,0,0)+$   $(\frac{1}{2},\frac{1}{2},0)+$ 8  $f$  1 (1)  $x,y,z$  (2)  $x,y,z$  (3)  $x,y,z$  (4)  $x,y,z$ 

Reflection conditions

General:

 $hkl : h+k=2n$  $0kl : k=2n$  $h0l : h=2n$  $hko : h+k=2n$  $h00 : h=2n$  $0k0 : k=2n$ 

Special: as above, plus

no extra conditions

no extra conditions

 $hkl : h=2n$ 

no extra conditions

no extra conditions

Symmetry of special projections

Along  $[001]$   $c2mm$  $a'=a$   $b'=b$ Origin at  $0,0,z$ Along  $[100]$   $p1m1$  $a'=\frac{1}{2}b$   $b'=c$ Origin at  $x,0,0$ Along  $[010]$   $p1m1$  $a'=c$   $b'=\frac{1}{2}a$ Origin at  $0,y,0$ 

Maximal non-isomorphic subgroups

**I** [2]  $C1m1$  ( $Cm$ , 8) (1; 3)+  
 [2]  $Cm11$  ( $Cm$ , 8) (1; 4)+  
 [2]  $C112$  ( $P2$ , 3) (1; 2)+

**IIa** [2]  $Pba2$  (32) 1; 2; (3; 4) +  $(\frac{1}{2},\frac{1}{2},0)$   
 [2]  $Pbm2$  ( $Pma2$ , 28) 1; 3; (2; 4) +  $(\frac{1}{2},\frac{1}{2},0)$   
 [2]  $Pma2$  (28) 1; 4; (2; 3) +  $(\frac{1}{2},\frac{1}{2},0)$   
 [2]  $Pmm2$  (25) 1; 2; 3; 4

**IIb** [2]  $Ima2$  ( $c'=2c$ ) (46); [2]  $Ibm2$  ( $c'=2c$ ) ( $Ima2$ , 46); [2]  $Iba2$  ( $c'=2c$ ) (45); [2]  $Imm2$  ( $c'=2c$ ) (44); [2]  $Ccc2$  ( $c'=2c$ ) (37);  
 [2]  $Cmc2_1$  ( $c'=2c$ ) (36); [2]  $Ccm2_1$  ( $c'=2c$ ) ( $Cmc2_1$ , 36)

Maximal isomorphic subgroups of lowest index

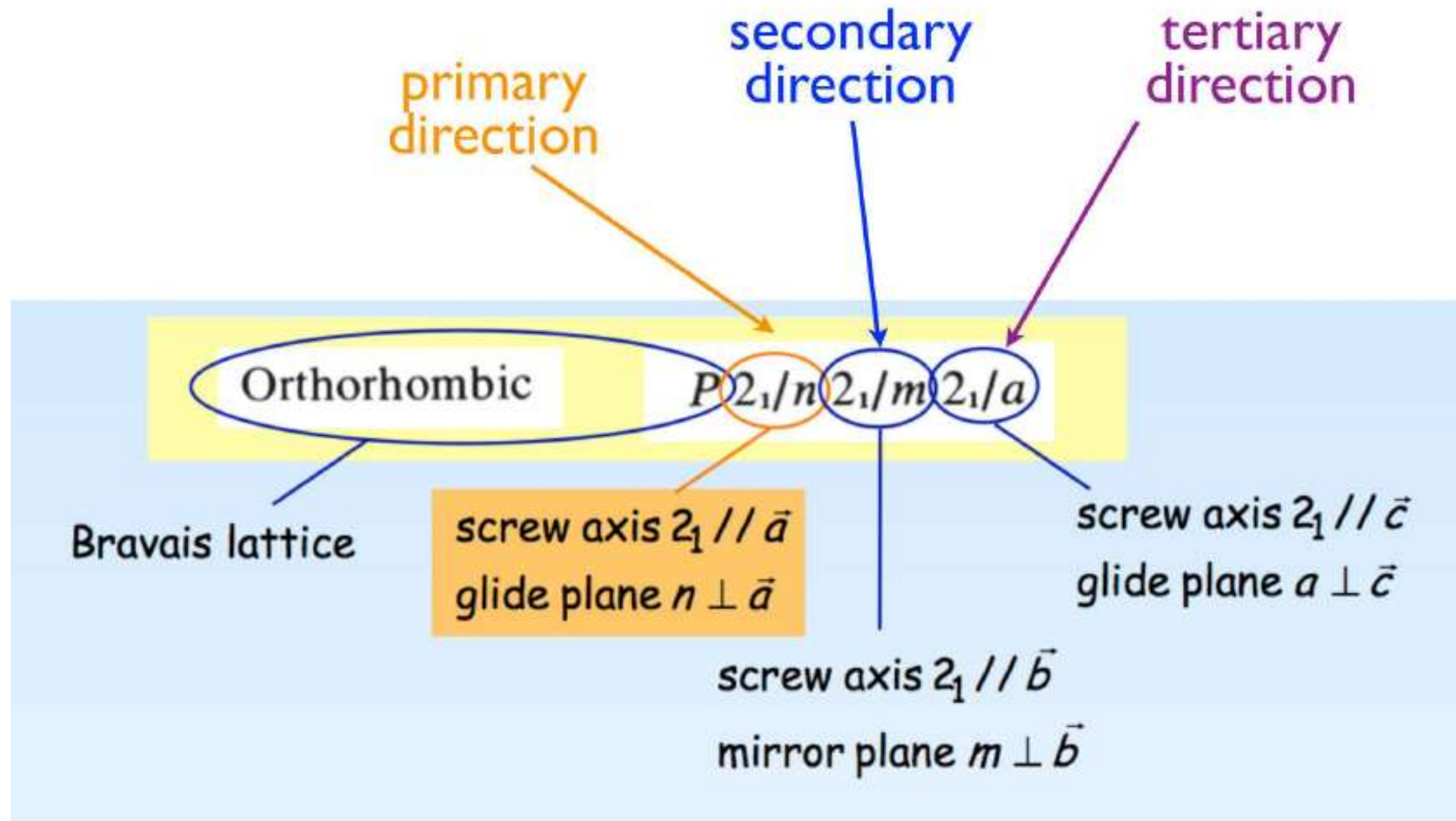
**IIc** [2]  $Cmm2$  ( $c'=2c$ ) (35); [3]  $Cmm2$  ( $a'=3a$  or  $b'=3b$ ) (35)

Minimal non-isomorphic supergroups

**I** [2]  $Cmmm$  (65); [2]  $Cmme$  (67); [2]  $P4mm$  (99); [2]  $P4bm$  (100); [2]  $P4_2cm$  (101); [2]  $P4_2nm$  (102); [2]  $P42m$  (111);  
 [2]  $P42_1m$  (113); [3]  $P6mm$  (183)

**II** [2]  $Fmm2$  (42); [2]  $Pmm2$  ( $a'=\frac{1}{2}a, b'=\frac{1}{2}b$ ) (25)

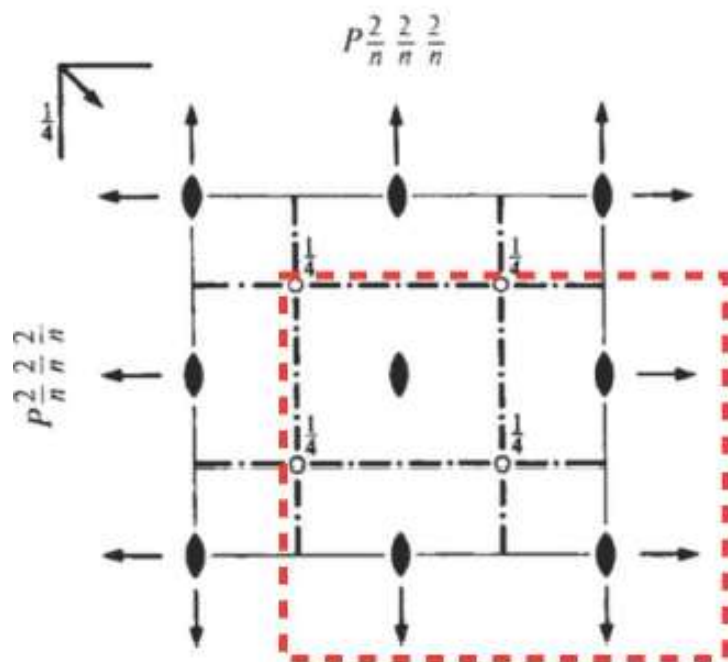
| Short Hermann-Mauguin symbol | Schoenflies symbol          | Crystal class (point group) | Crystal system            |
|------------------------------|-----------------------------|-----------------------------|---------------------------|
| ① $Cmm2$                     | $C_{2v}^{11}$               | $mm2$                       | Orthorhombic              |
| ② No. 35                     | $Cmm2$                      |                             | Patterson symmetry $Cmmm$ |
| Number of space group        | Full Hermann-Mauguin symbol |                             | Patterson symmetry        |



$Pnnn$

No. 48

ORIGIN CHOICE 1



Origin at 222, at  $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$  from  $\bar{1}$

$D_{2h}^2$

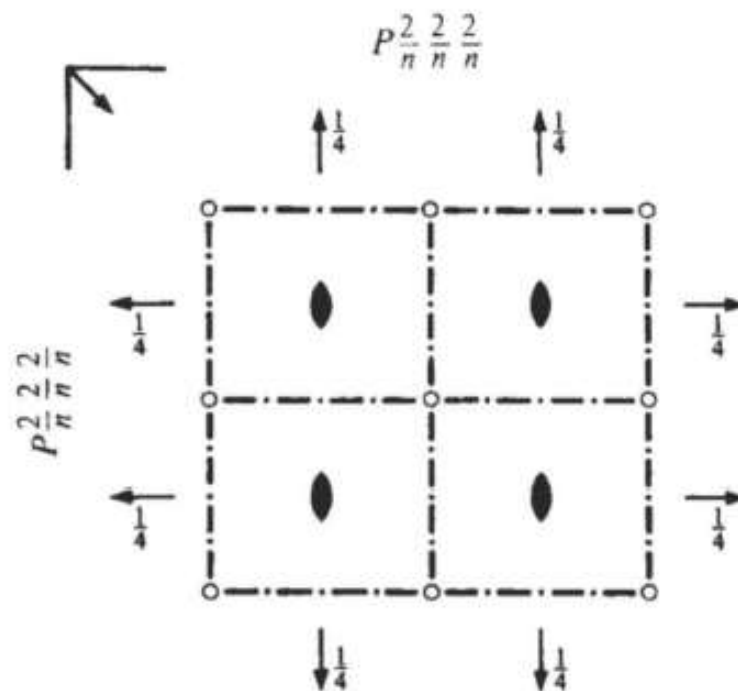
$P \frac{2}{n} \frac{2}{n} \frac{2}{n}$

$mmm$

Orthorhombic

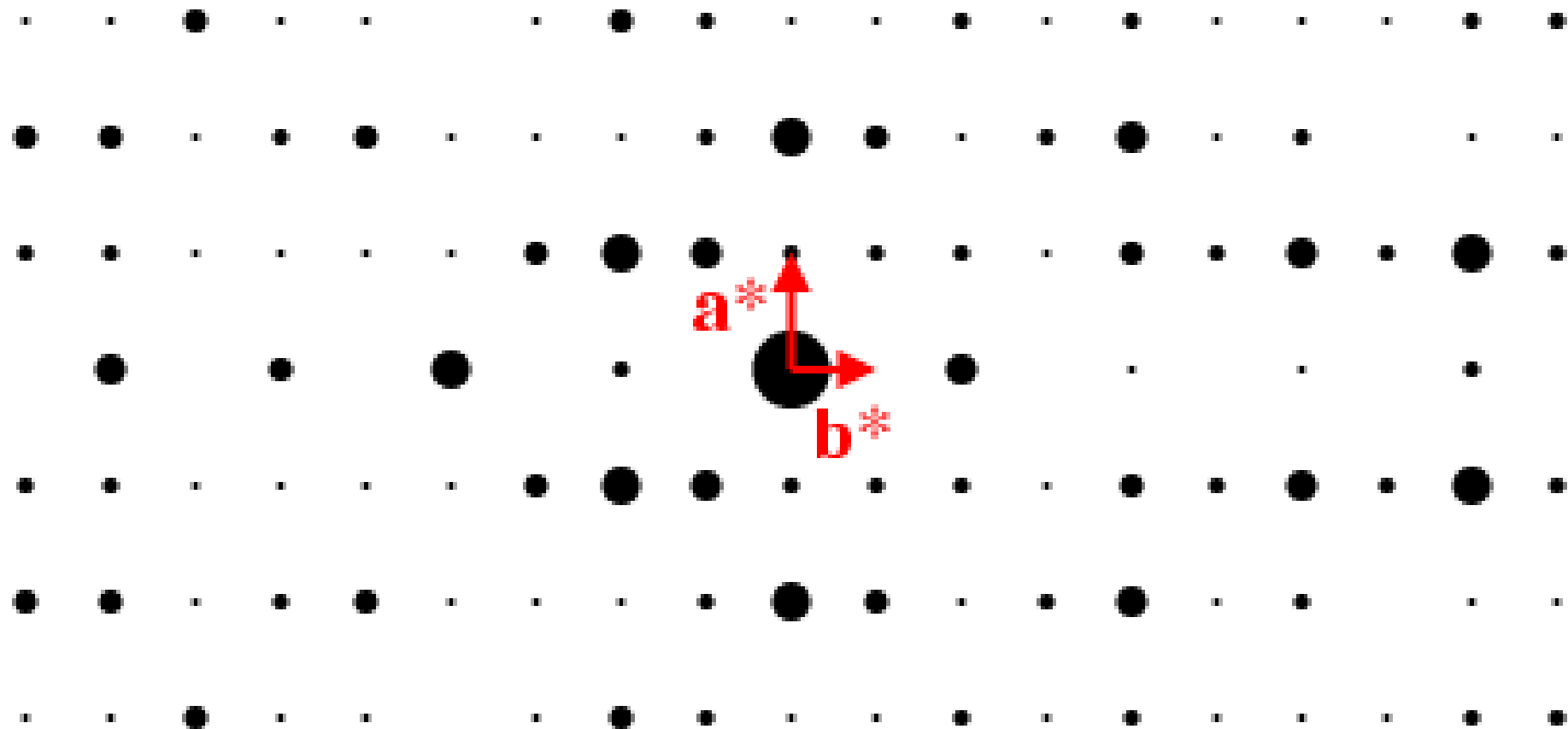
Patterson symmetry  $Pmmm$

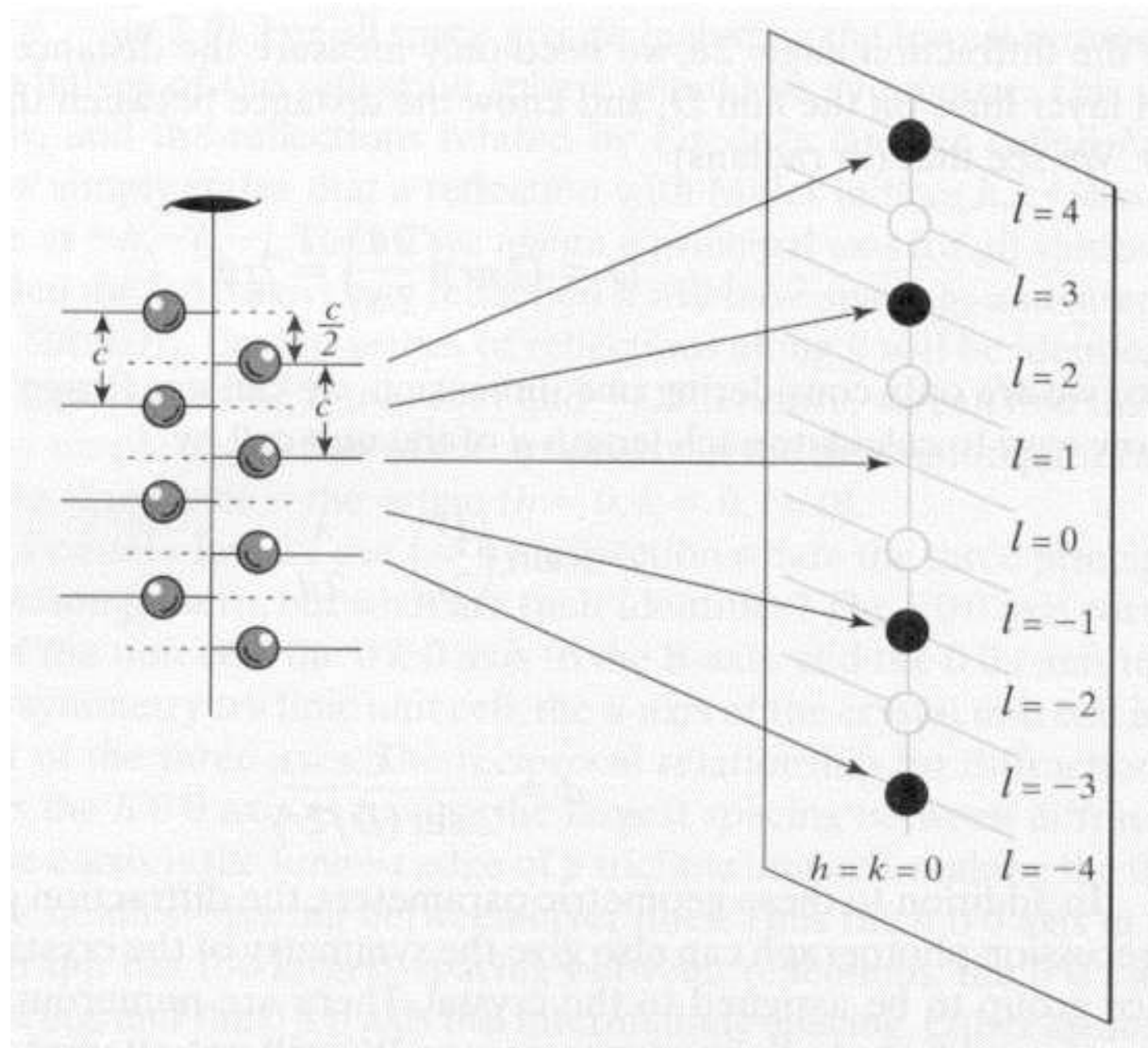
ORIGIN CHOICE 2



Origin at  $\bar{1}$  at  $nnn$ , at  $-\frac{1}{4}, -\frac{1}{4}, -\frac{1}{4}$  from 222

# Reflection Conditions & Systematic Absences





The reflection conditions describe the conditions of occurrence of a reflection (structure factor not systematically zero). There are two types of systematic reflection conditions for diffraction of crystals by radiation:

- *General conditions*
  - *Integral reflection conditions.* The resulting conditions apply to the whole three-dimensional set of reflections  $hkl$ .
  - *Zonal reflection conditions* Glide planes. The resulting conditions apply only to two dimensional sets of reflections, i.e. to reciprocal-lattice nets containing the origin (such as  $hk0$ ,  $h0l$ ,  $0kl$ ,  $hhl$ ). For this reason, they are called zonal reflection conditions.
  - Serial reflection conditions. Screw axes. The resulting conditions apply only to one dimensional sets of reflections, i.e. reciprocal-lattice rows containing the origin (such as  $h00$ ,  $0k0$ ,  $00l$ )..

# General reflection conditions

The **integral reflections** are the general reflection conditions due to the centering of cells.

| Reflection condition (observable reflections)                                          | Centring type of cell                                   | Centering symbol               |
|----------------------------------------------------------------------------------------|---------------------------------------------------------|--------------------------------|
| None                                                                                   | Primitive                                               | $P$<br>$R$ (rhombohedral axes) |
| $h + k = 2n$                                                                           | C-face centred                                          | $C$                            |
| $k + l = 2n$                                                                           | A-face centred                                          | $A$                            |
| $l + h = 2n$                                                                           | B-face centred                                          | $B$                            |
| $h + k + l = 2n$                                                                       | body centred                                            | $I$                            |
| $h + k, h + l$ and<br>$k + l = 2n$ or:<br>$h, k, l$ all odd or<br>All even ('unmixed') | all-face centred                                        | $F$                            |
| $-h + k + l = 3n$                                                                      | rhombohedrally<br>centered, obverse, setting (standard) | $R$ (hexagonal axes)           |
| $h - k + l = 3n$                                                                       | rhombohedrally<br>centred, reverse setting              |                                |
| $h - k = 3n$                                                                           | hexagonally centred                                     | $H$                            |

| <i>Glide planes</i><br>symbol | Concerned orientation | reflections | reflection conditions<br>(observable reflections) |                                    |
|-------------------------------|-----------------------|-------------|---------------------------------------------------|------------------------------------|
| <b>a</b>                      | (010)                 | h0l         | $h = 2n$                                          | <i>zonal reflection conditions</i> |
|                               | (001)                 | hk0         | $h = 2n$                                          |                                    |
| <b>b</b>                      | (100)                 | 0kl         | $k = 2n$                                          |                                    |
|                               | (001)                 | hk0         | $k = 2n$                                          |                                    |
| <b>c</b>                      | (100)                 | 0kl         | $l = 2n$                                          |                                    |
|                               | (010)                 | h0l         | $l = 2n$                                          |                                    |
|                               | (110)                 | hhl         | $l = 2n$                                          |                                    |
|                               | (1-100)               | hh.l        | $l = 2n$                                          |                                    |
|                               | (11-20)               | hh.l        | $l = 2n$                                          |                                    |
| <b>d</b>                      | (100)                 | 0kl         | $k+l = 4n \text{ (k,l=2n)}$                       |                                    |
|                               | (010)                 | h0l         | $h+l = 4n \text{ (h,l=2n)}$                       |                                    |
|                               | (001)                 | hk0         | $h+k = 4n \text{ (h,k=2n)}$                       |                                    |
|                               | (110)                 | hhl         | $2h+l = 4n$                                       |                                    |
| <b>n</b>                      | (100)                 | 0kl         | $k+l = 2n$                                        |                                    |
|                               | (010)                 | h0l         | $h+l = 2n$                                        |                                    |
|                               | (001)                 | hk0         | $h+k = 2n$                                        |                                    |

# Positions

Multiplicity,  
Wyckoff letter,  
Site symmetry

Coordinates

$(0,0,0)+ (\frac{1}{2},\frac{1}{2},\frac{1}{2})+$

Reflection conditions

General:

$hkl : h+k+l=2n$

$hk0 : h+k=2n$

$0kl : k+l=2n$

$hhl : l=2n$

$00l : l=2n$

$h00 : h=2n$

Special: as above, plus

$0kl : k=2n$

no extra conditions

no extra conditions

no extra conditions

$hkl : l=2n$

no extra conditions

$hkl : l=2n$

$hkl : l=2n$

no extra conditions

no extra conditions

|    |          |         |                                        |                                                    |                                        |                                                    |
|----|----------|---------|----------------------------------------|----------------------------------------------------|----------------------------------------|----------------------------------------------------|
| 16 | <i>k</i> | 1       | (1) $x,y,z$<br>(5) $\bar{x},y,\bar{z}$ | (2) $\bar{x},\bar{y},z$<br>(6) $x,\bar{y},\bar{z}$ | (3) $\bar{y},x,z$<br>(7) $y,x,\bar{z}$ | (4) $y,\bar{x},z$<br>(8) $\bar{y},\bar{x},\bar{z}$ |
| 8  | <i>j</i> | . . 2   | $x,x+\frac{1}{2},\frac{1}{4}$          | $\bar{x},\bar{x}+\frac{1}{2},\frac{1}{4}$          | $\bar{x}+\frac{1}{2},x,\frac{1}{4}$    | $x+\frac{1}{2},\bar{x},\frac{1}{4}$                |
| 8  | <i>i</i> | . 2 .   | $x,0,\frac{1}{2}$                      | $\bar{x},0,\frac{1}{2}$                            | $0,x,\frac{1}{2}$                      | $0,\bar{x},\frac{1}{2}$                            |
| 8  | <i>h</i> | . 2 .   | $x,0,0$                                | $\bar{x},0,0$                                      | $0,x,0$                                | $0,\bar{x},0$                                      |
| 8  | <i>g</i> | . . 2   | $x,x,0$                                | $\bar{x},\bar{x},0$                                | $\bar{x},x,0$                          | $x,\bar{x},0$                                      |
| 8  | <i>f</i> | 2 . .   | $0,\frac{1}{2},z$                      | $\frac{1}{2},0,z$                                  | $0,\frac{1}{2},\bar{z}$                | $\frac{1}{2},0,\bar{z}$                            |
| 4  | <i>e</i> | 4 . .   | $0,0,z$                                | $0,0,\bar{z}$                                      |                                        |                                                    |
| 4  | <i>d</i> | 2 . 2 2 | $0,\frac{1}{2},\frac{1}{4}$            | $\frac{1}{2},0,\frac{1}{4}$                        |                                        |                                                    |
| 4  | <i>c</i> | 2 2 2 . | $0,\frac{1}{2},0$                      | $\frac{1}{2},0,0$                                  |                                        |                                                    |
| 2  | <i>b</i> | 4 2 2   | $0,0,\frac{1}{2}$                      |                                                    |                                        |                                                    |
| 2  | <i>a</i> | 4 2 2   | $0,0,0$                                |                                                    |                                        |                                                    |

**Generators selected**  $(1); t(1,0,0); t(0,1,0); t(0,0,1); t(\frac{1}{2}, \frac{1}{2}, 0); (2); (3)$

## Positions

Multiplicity,  
Wyckoff letter,  
Site symmetry

Coordinates

$(0,0,0) + (\frac{1}{2}, \frac{1}{2}, 0) +$

Reflection conditions

General:

$hkl : h + k = 2n$

$0kl : k = 2n$

$h0l : h = 2n$

$hk0 : h + k = 2n$

$h00 : h = 2n$

$0k0 : k = 2n$

Special: as above, plus

no extra conditions

no extra conditions

$hkl : h = 2n$

no extra conditions

no extra conditions

8  $f$  1 (1)  $x, y, z$  (2)  $\bar{x}, \bar{y}, z$  (3)  $x, \bar{y}, z$  (4)  $\bar{x}, y, z$

4  $e$   $m..$   $0, y, z$   $0, \bar{y}, z$

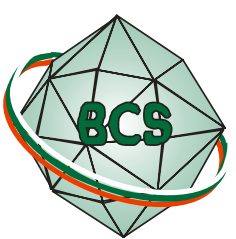
4  $d$   $.m.$   $x, 0, z$   $\bar{x}, 0, z$

4  $c$   $..2$   $\frac{1}{4}, \frac{1}{4}, z$   $\frac{1}{4}, \frac{3}{4}, z$

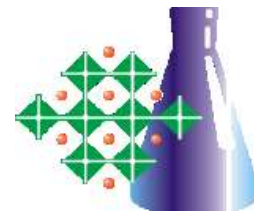
2  $b$   $mm2$   $0, \frac{1}{2}, z$

2  $a$   $mm2$   $0, 0, z$

That's all



# International school



## Introduction in Rietveld structure refinement



PANalytical



CRYSTAL  
IMPACT



**Crystal structure and crystal symmetry (crystal systems, unit cell, reciprocal space, reciprocal lattice, systematic absences, Wyckoff positions)**



Sofia, Bulgaria,  
28 September - 3 October 2015



МИНИСТЕРСТВО  
НА ОБРАЗОВАНИЕТО  
И НАУКАТА

## Equivalence of $\bar{2}$ and $m$

