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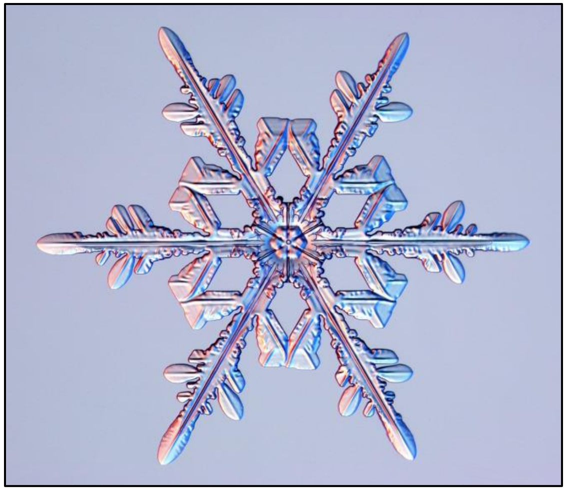
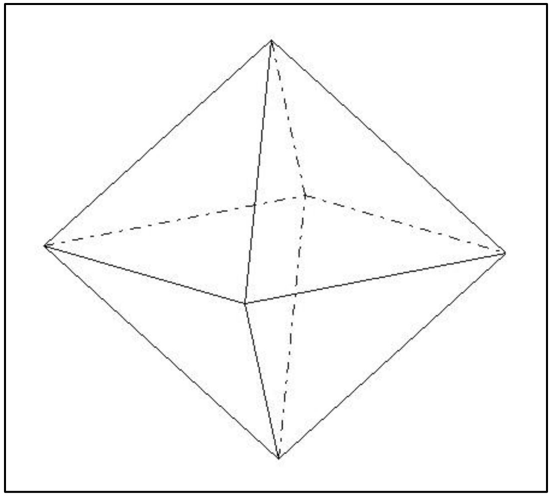
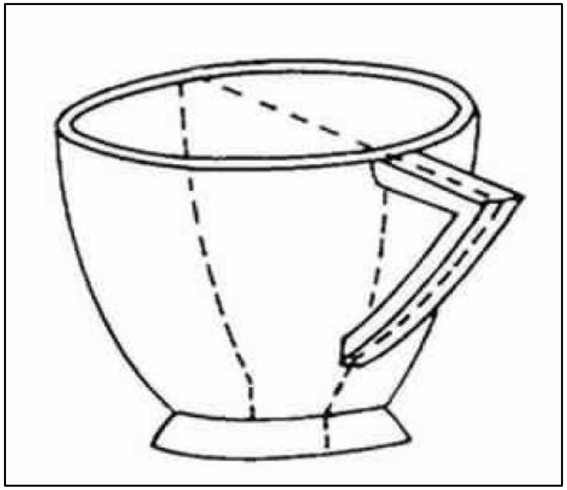
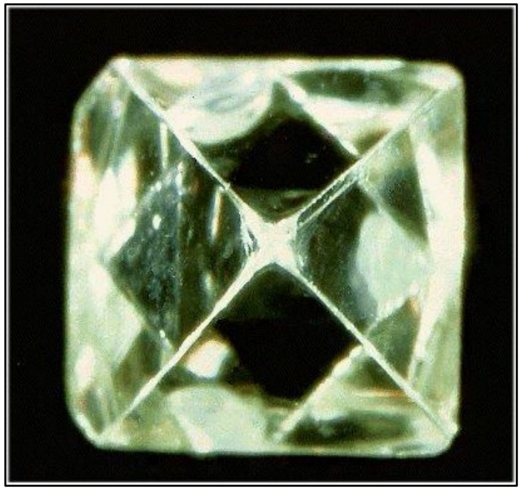
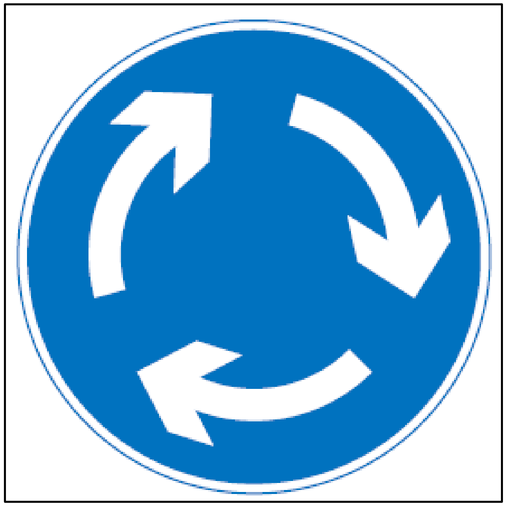
Lecture course on crystallography, 2015

Lecture 5: Symmetry in crystallography

What is symmetry?

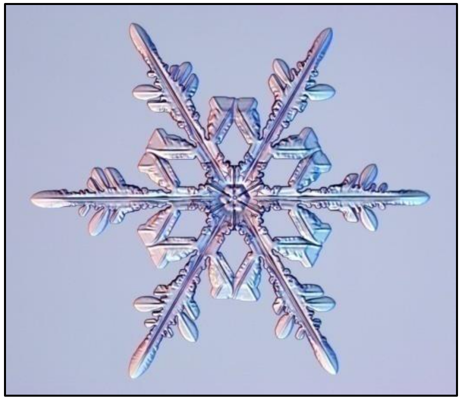
Symmetry ***is a property of an object to stay*** ***unchanged (invariant)*** ***after*** ***certain type of movement*****.**



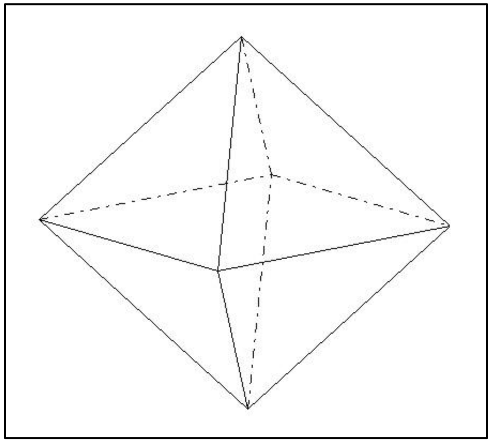





Symmetry operation

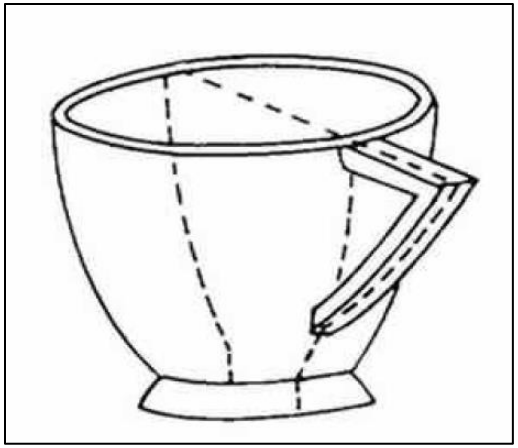
***Symmetry operation* is the movement which keeps the object unchanged**



Rotation by 60 degrees



Rotation by 90 degrees around the vertical axis



Reflection in the plane through the middle

"Unchanged" means it is not possible to distinguish two objects from any kind of physical experiments

Types of symmetry operation

According to the type of movement there are different types of symmetry operations

1. Point symmetry: AT LEAST one point is fixed during the movement of the object

- ***Rotation***
- ***Reflection***
- ***Inversion***
- ***Combination of any above***

2. Space symmetry: no points are fixed during the movement of the object

- ***Translation (lattice translation)***
- ***Combination of translation and any kind of point symmetry operations***

Rotational symmetry

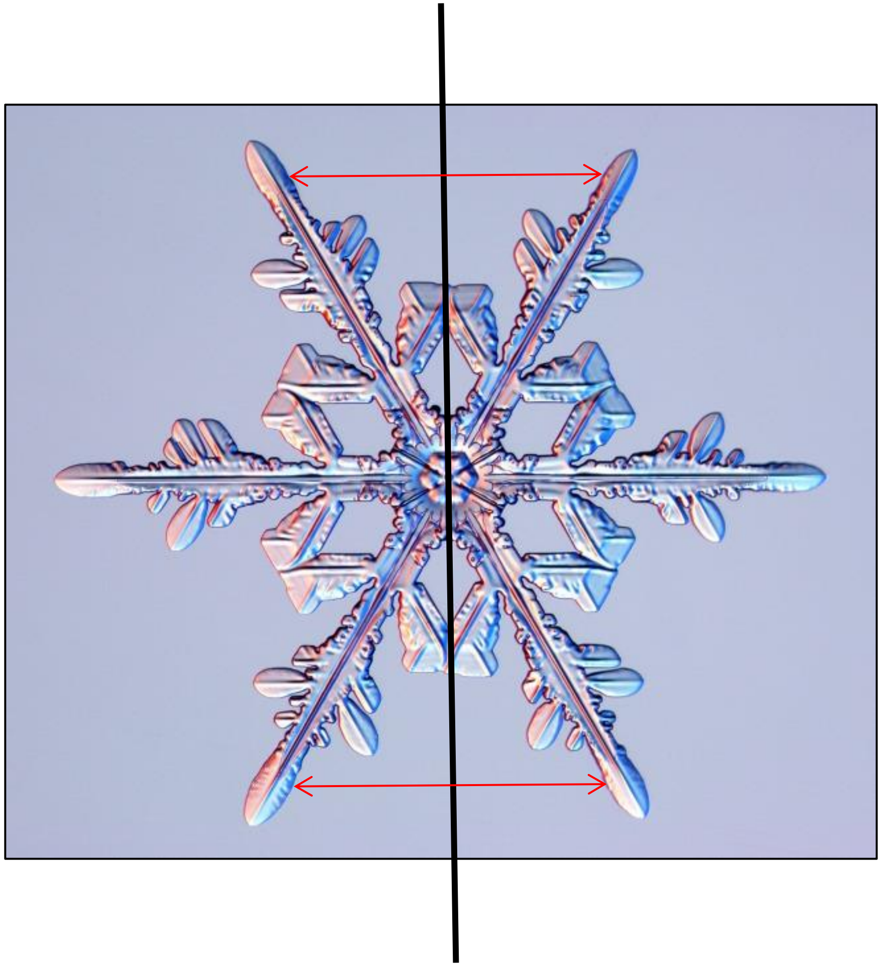
Movement: rotation around selected direction by the angle α. The axis of rotation (symmetry element) is referred to n-FOLD SYMMETRY AXIS with n=360 / α. This symmetry is designated as "n"

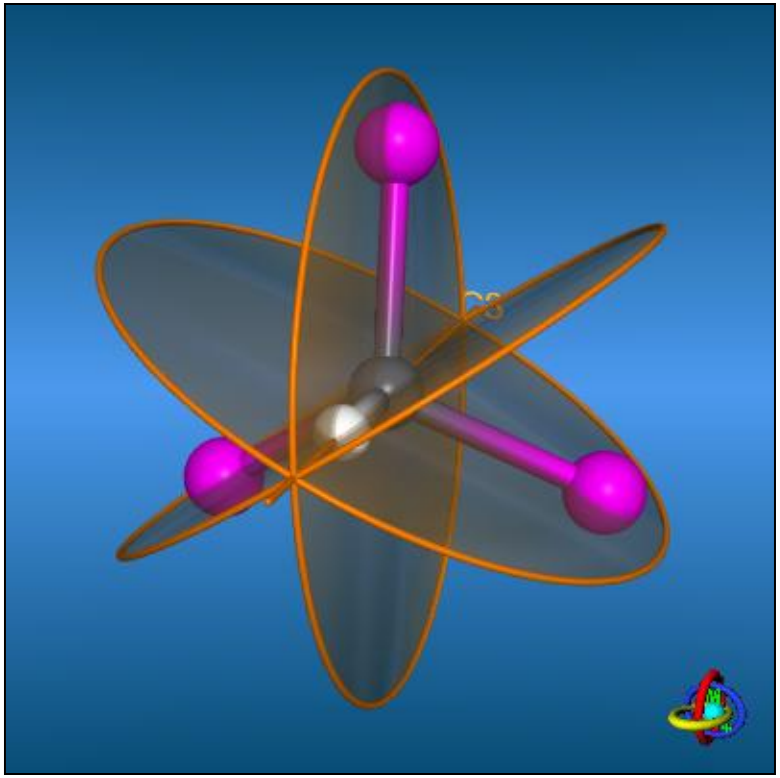
Vertically oriented symmetry axis

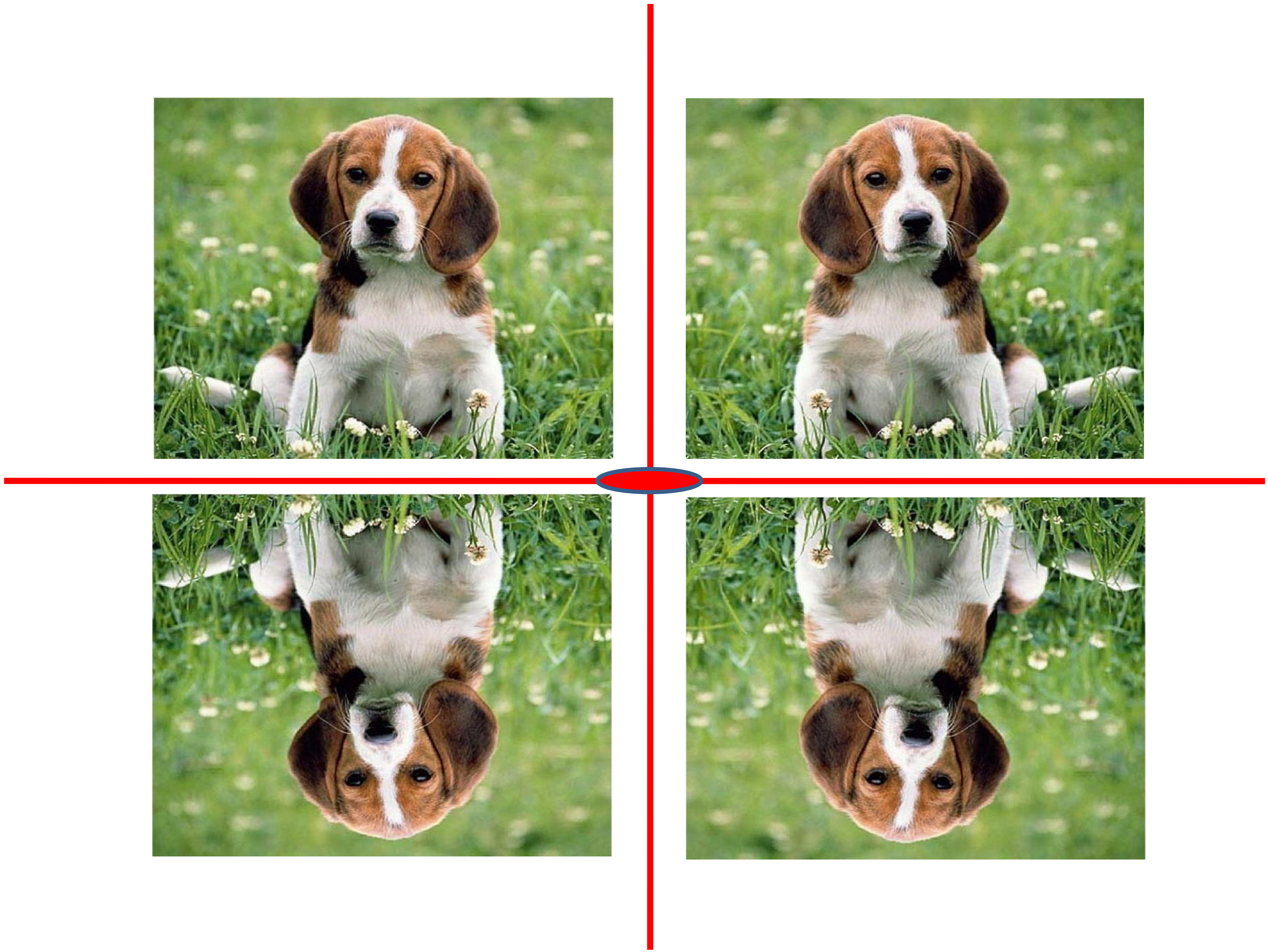
4 (α = 90 deg) *5 (α =72 deg)* *6 (α = 60 deg)*

Reflection symmetry

Movement: reflection in the mirror. Each point is replaced by its mirror reflection. The mirror is referred to as MIRROR PLANE and is designated by "m".



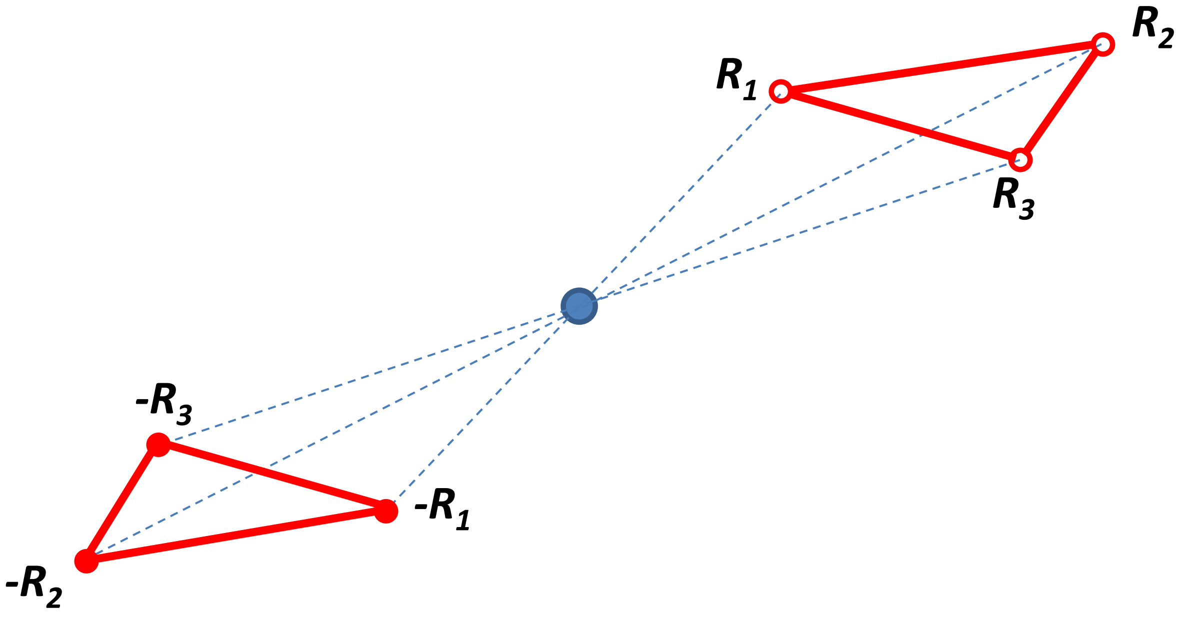




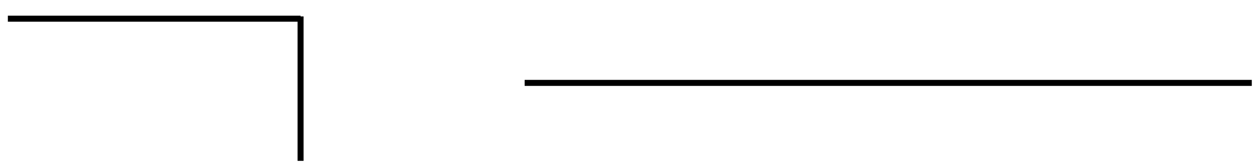
Inversion symmetry

Movement: inversion relative to the origin (centre of inversion). Each point is replaced by the inverted one.

X Y Z ↔ -X -Y -Z

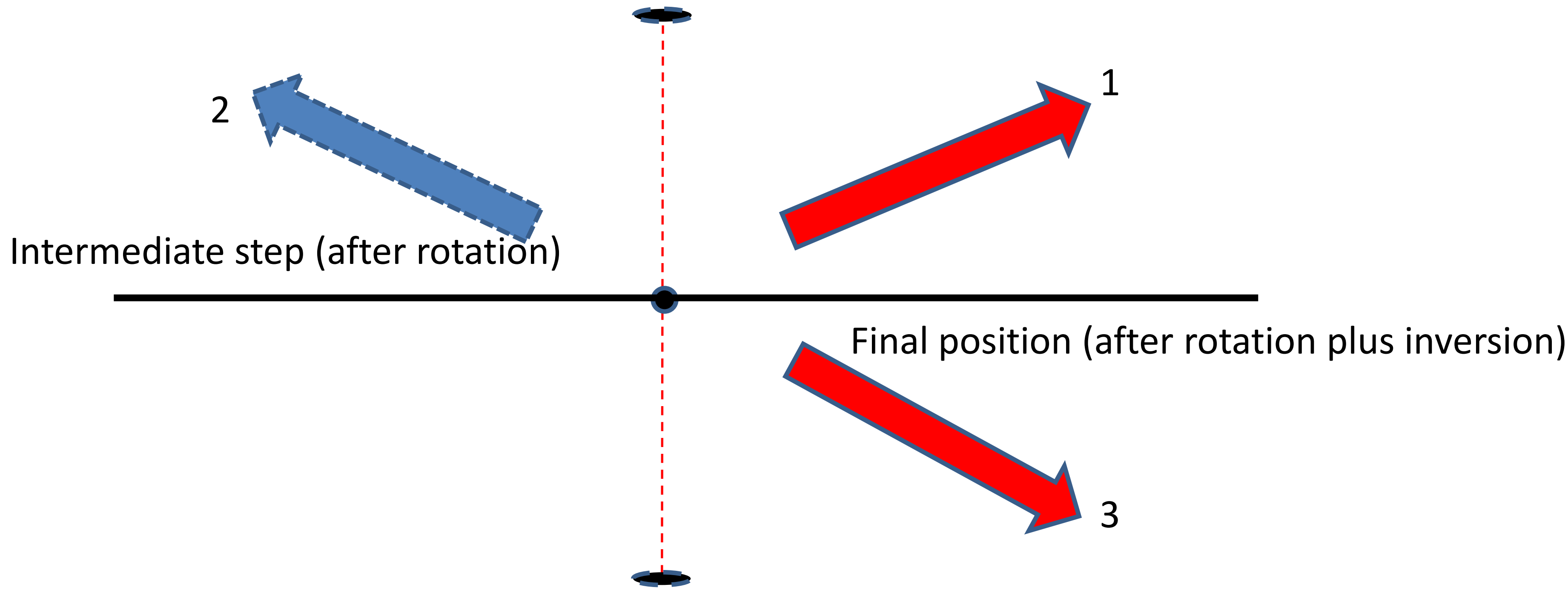


Designation of the symmetry axes and mirror

n	*Designation of an axis*
2	
3	
4	
6	
m	

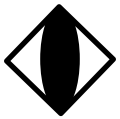
2-fold rotoinversion axis

It is possible to combine some symmetry operations. As an example combination of rotation and inversion gives the symmetry associated with the rotoinversion.

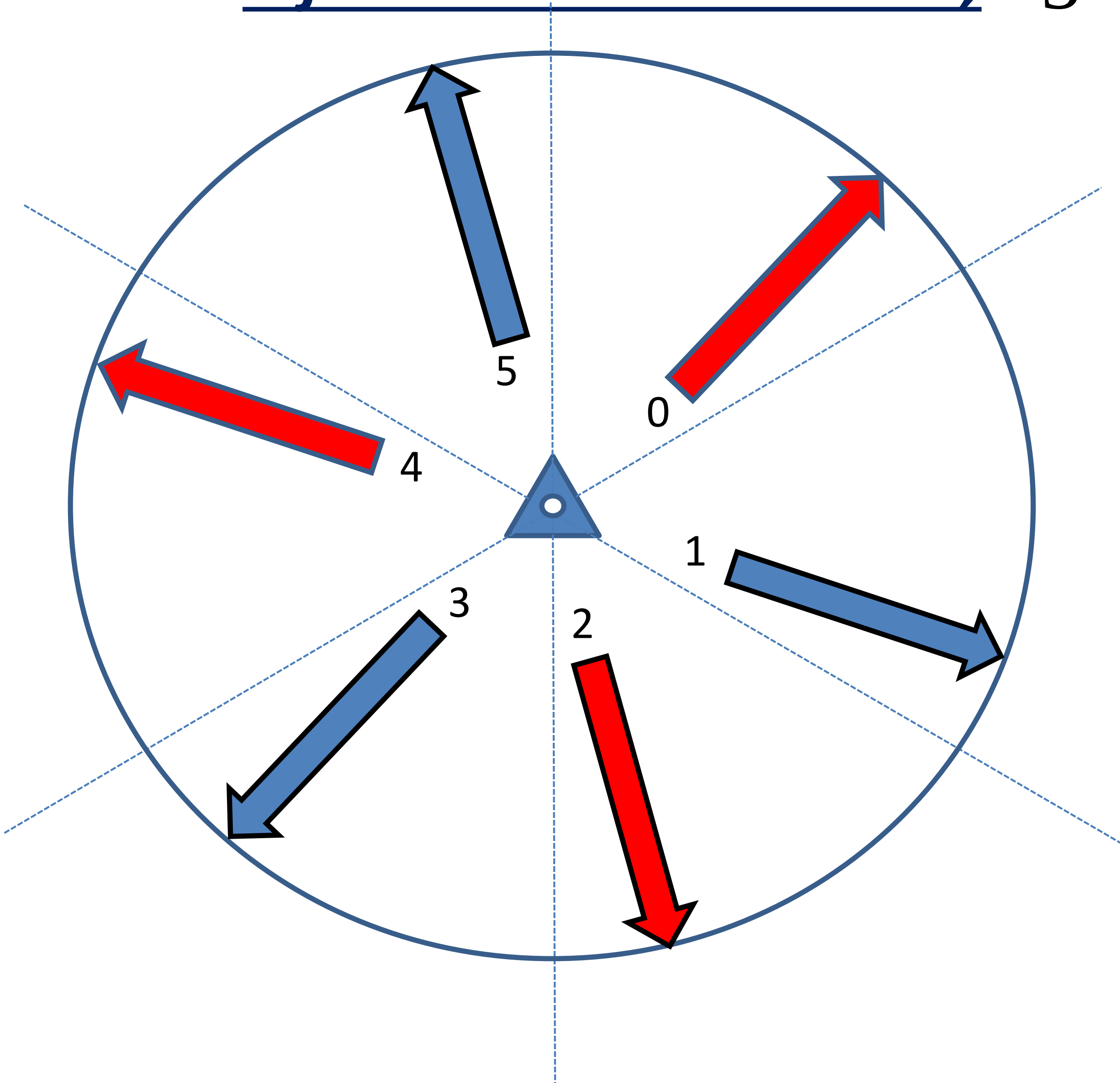


2-fold rotoinversion axis is equivalent to the mirror plane perpendicular to the axis

Designation of the rotoinversion axes

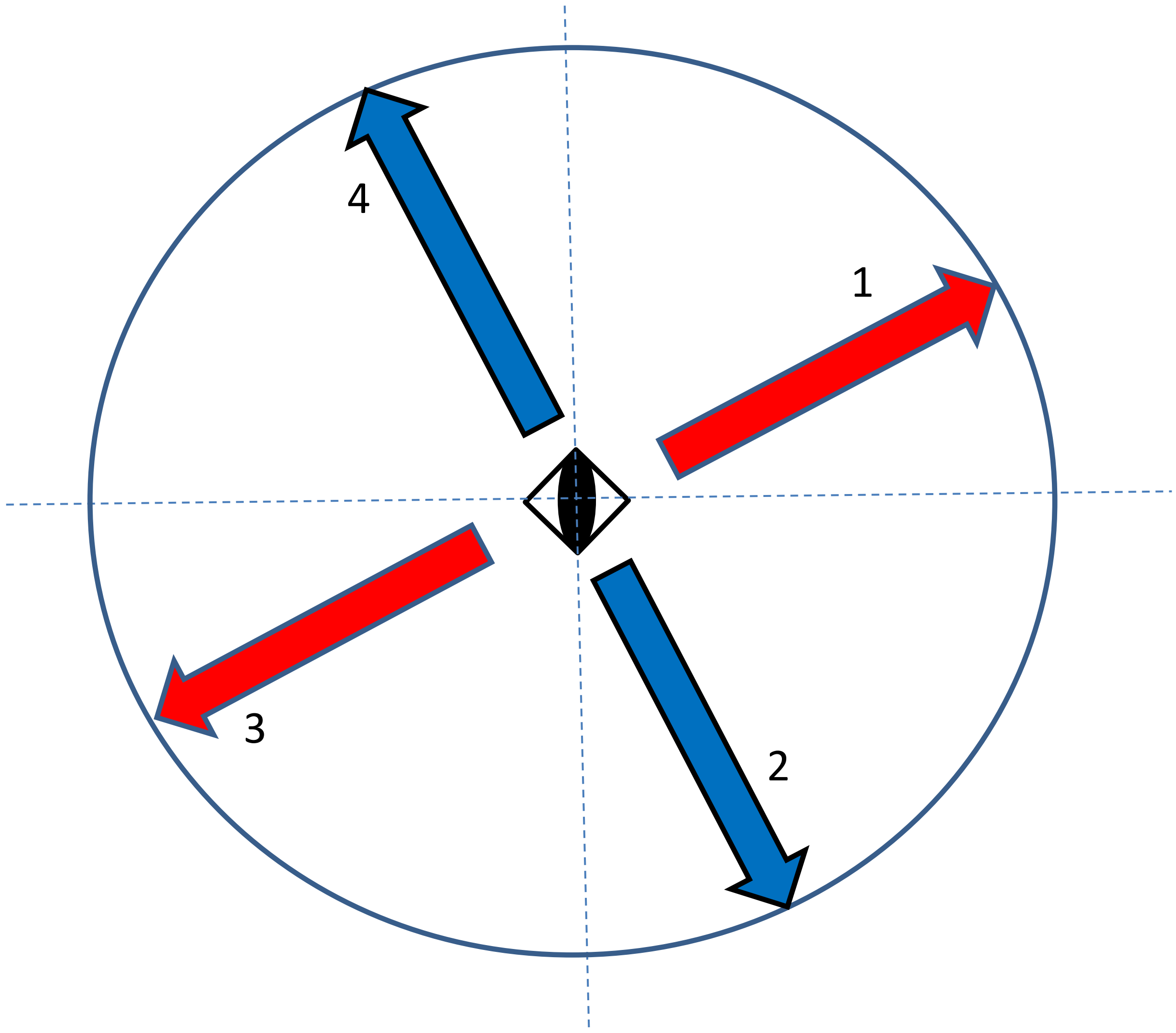
n	*Designation of an axis*
$\bar{2} \equiv m$	
$\bar{3}$	
$\bar{4}$	
$\bar{6}$	

3-fold rotoinversion axis, $\bar{3}$

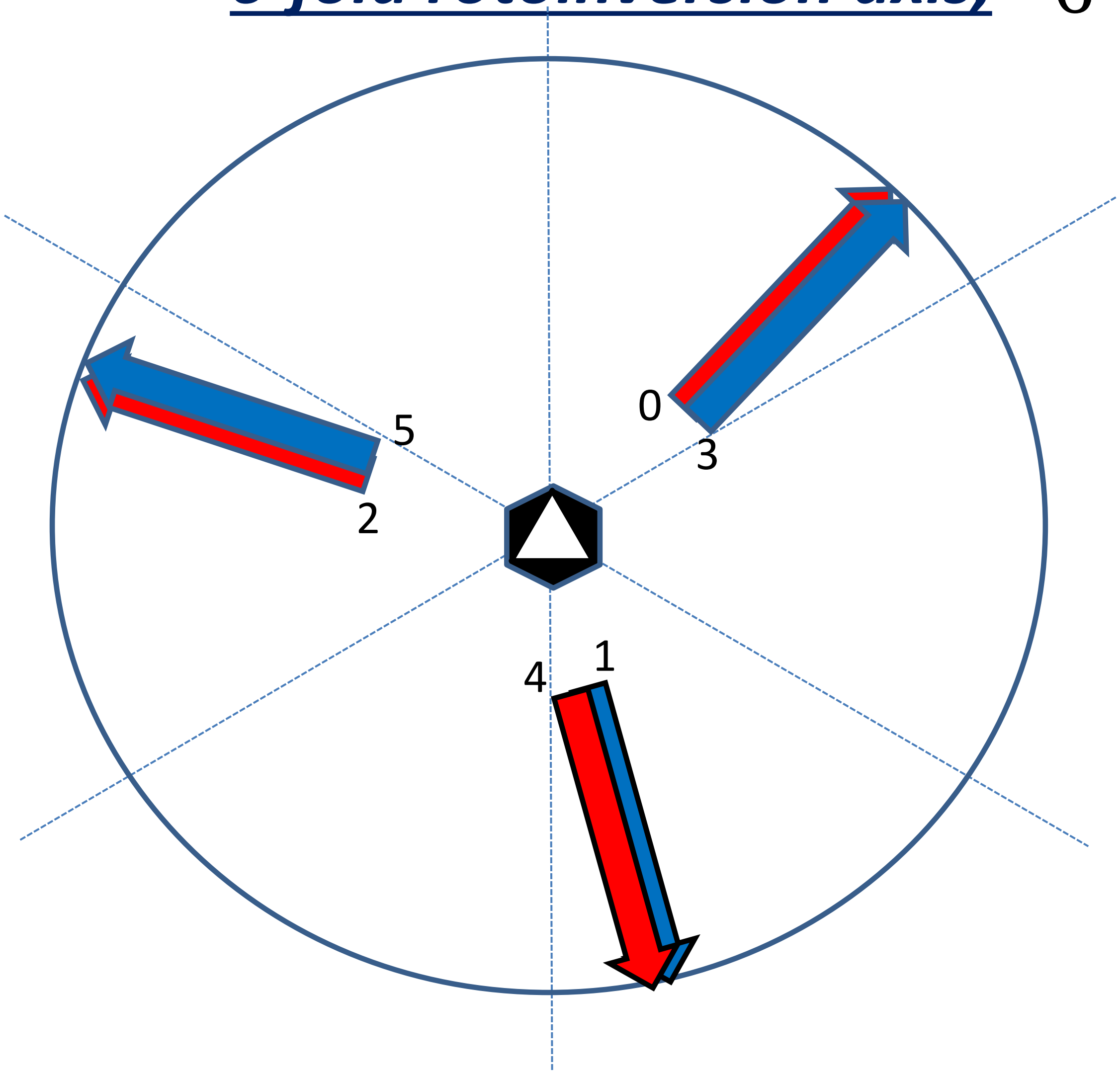


3-fold rotoinversion axis is equivalent to independent existence of 3 fold axis and inversion

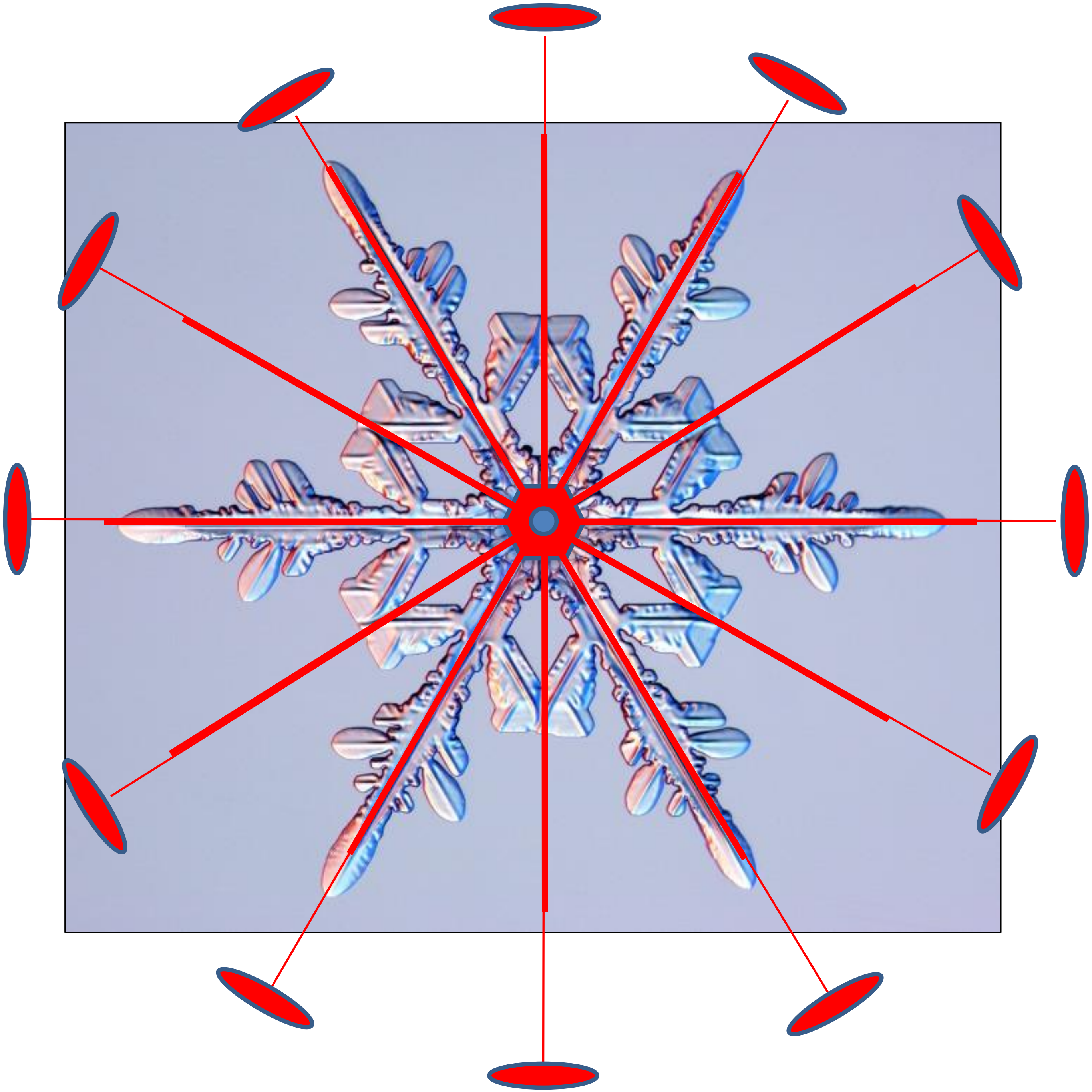
4-fold rotoinversion axis, $\bar{4}$



6-fold rotoinversion axis, $\bar{6}$

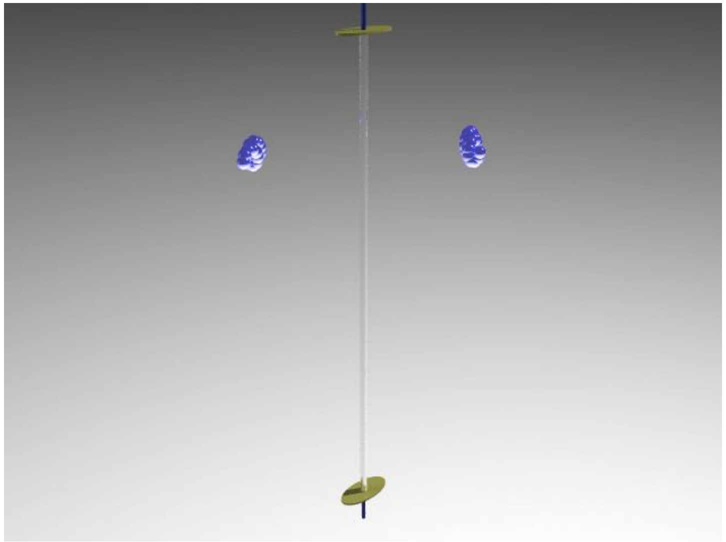


6-fold rotoinversion axis is equivalent to independent existence of 3 fold axis and mirror plane

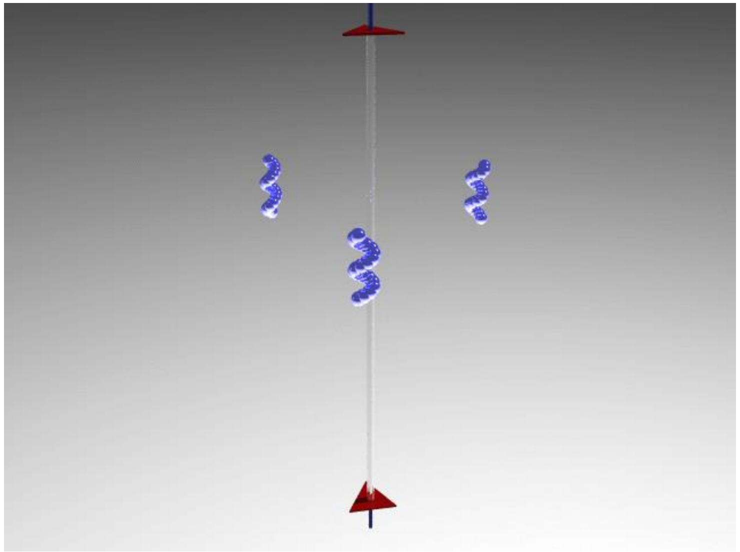


Further demonstration of symmetry

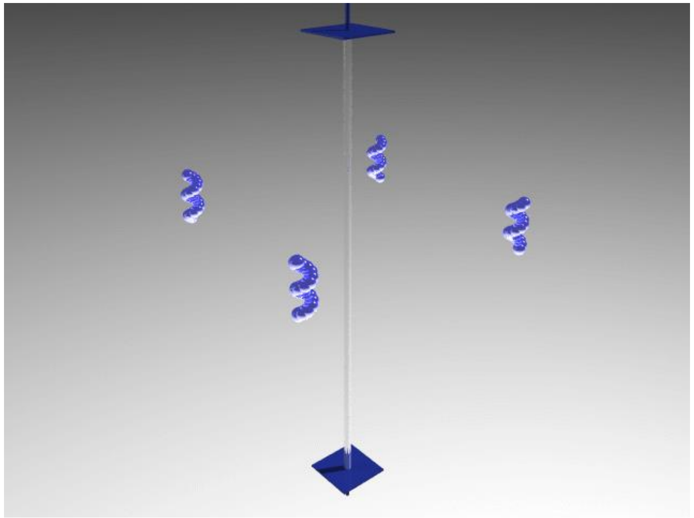
2 fold axis



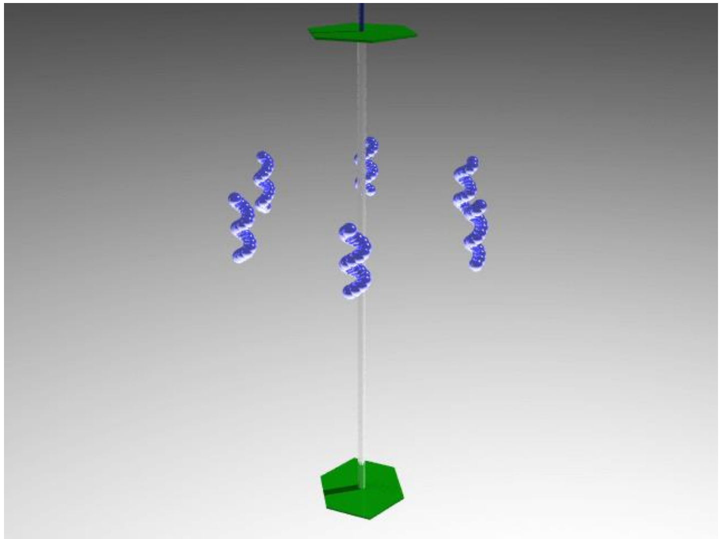
3 fold axis



4 fold axis

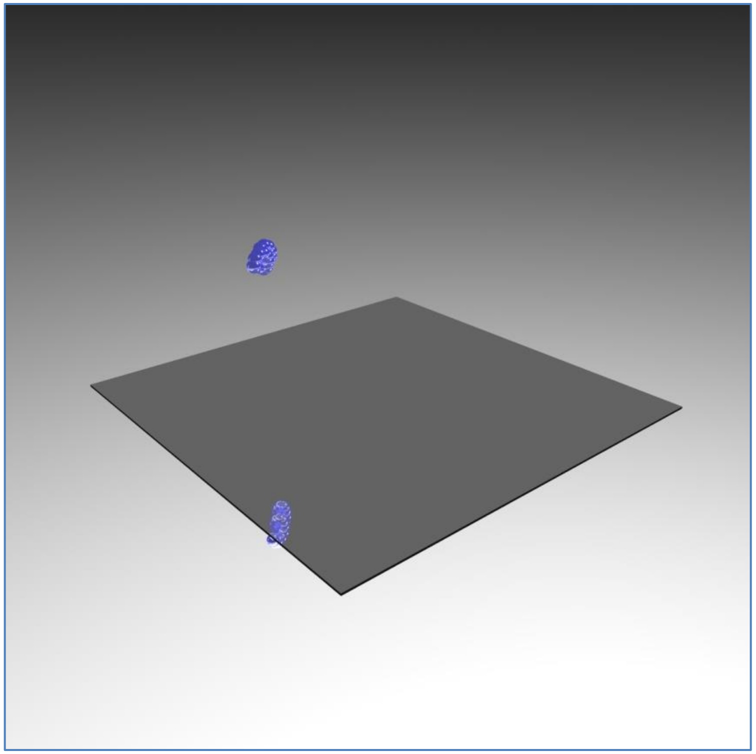


6 fold axis

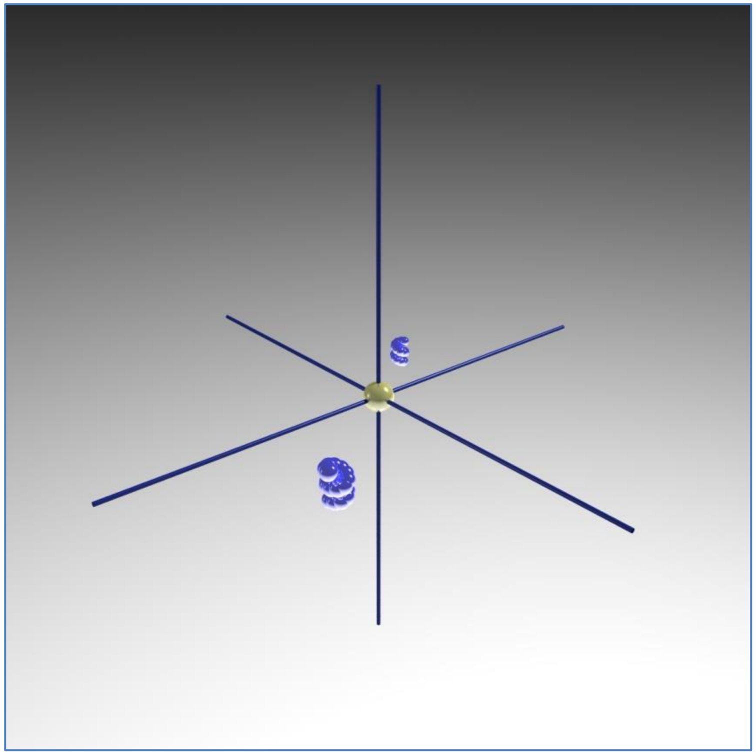


Further demonstration of symmetry

Mirror plane

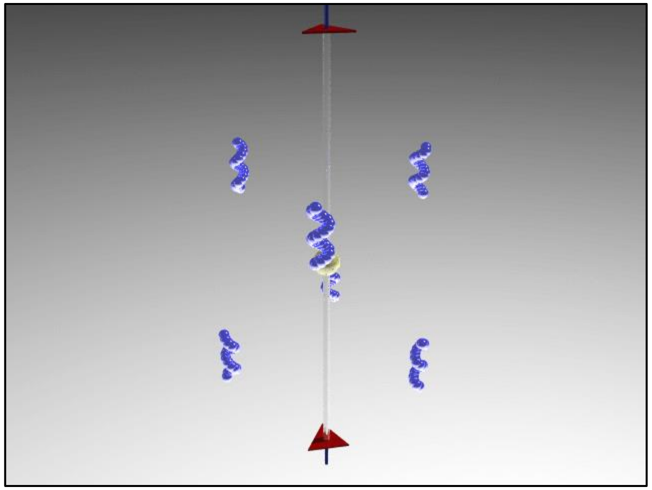


Centre of inversion

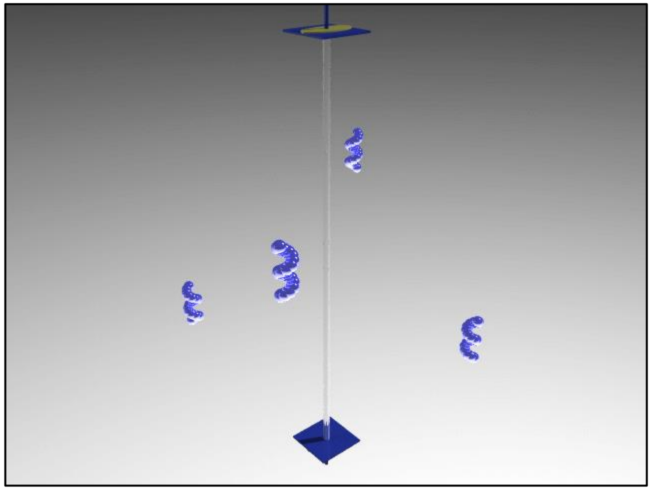


Further demonstration of symmetry

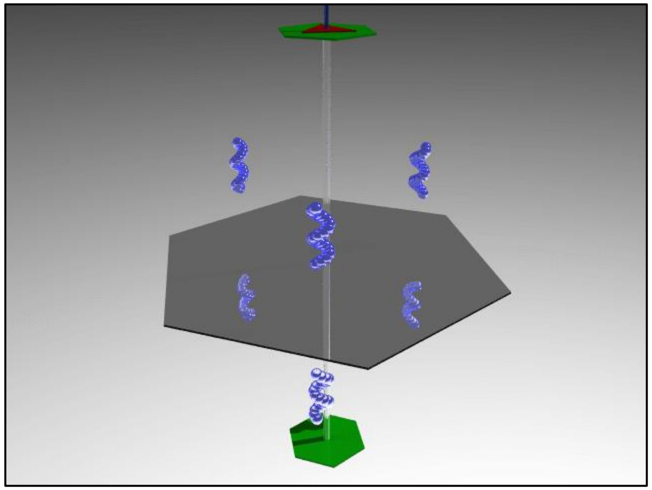
3 fold rotoinversion axis



4 fold rotoinversion axis

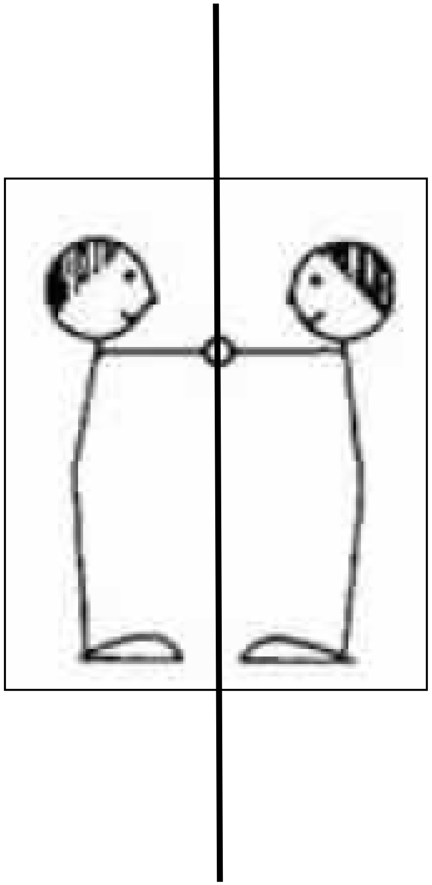


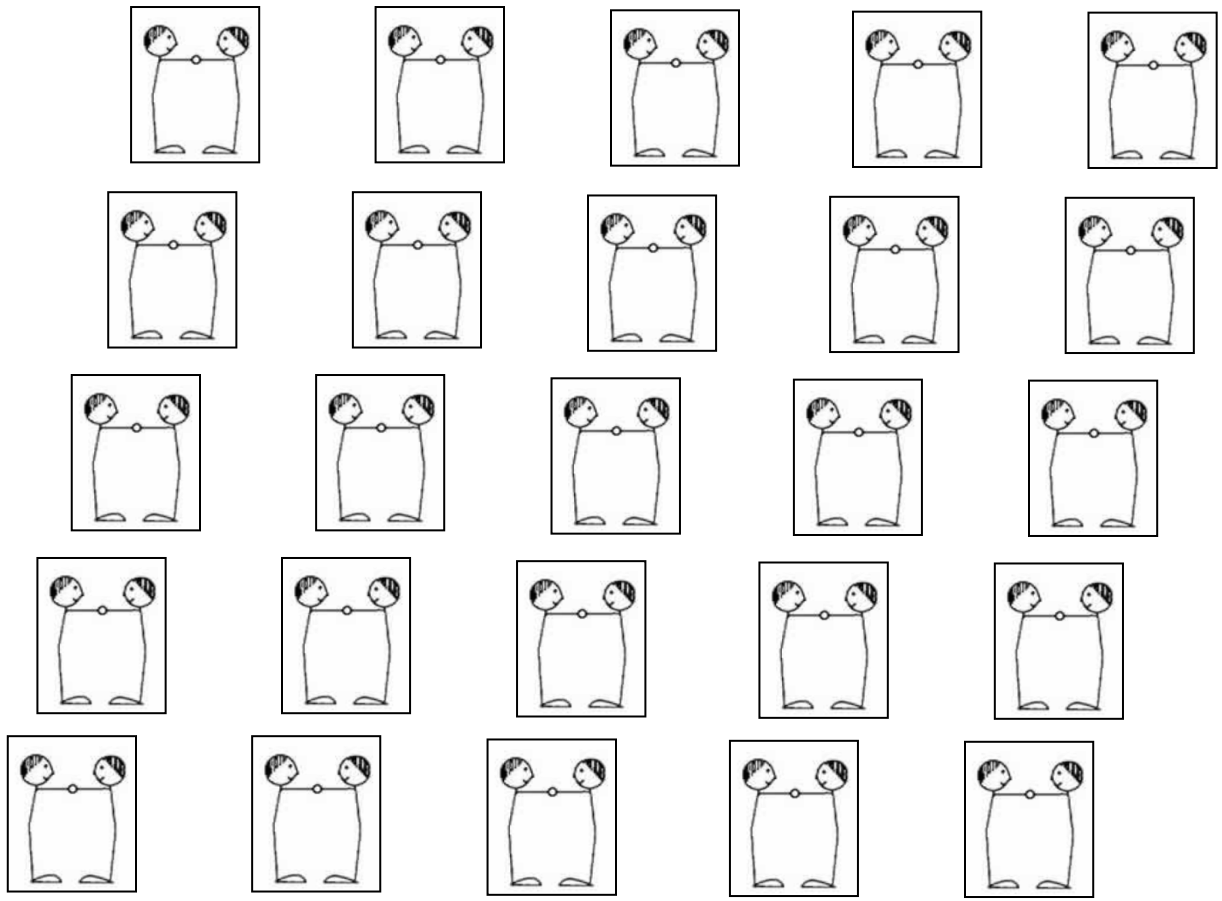
6 fold rotoinversion axis

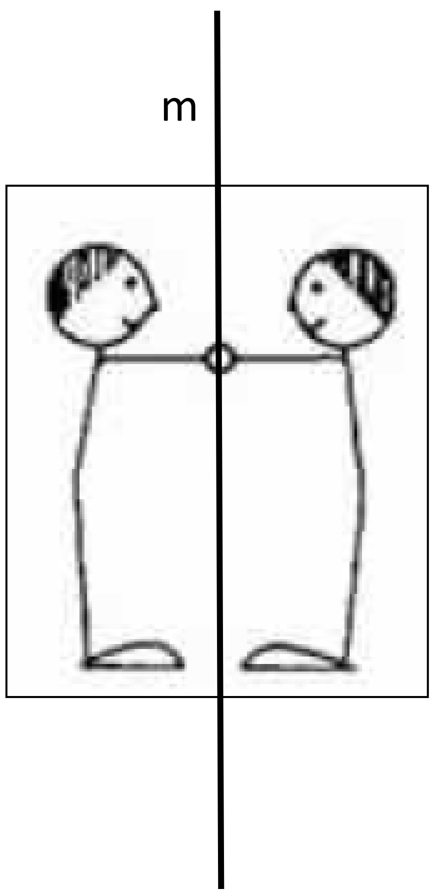


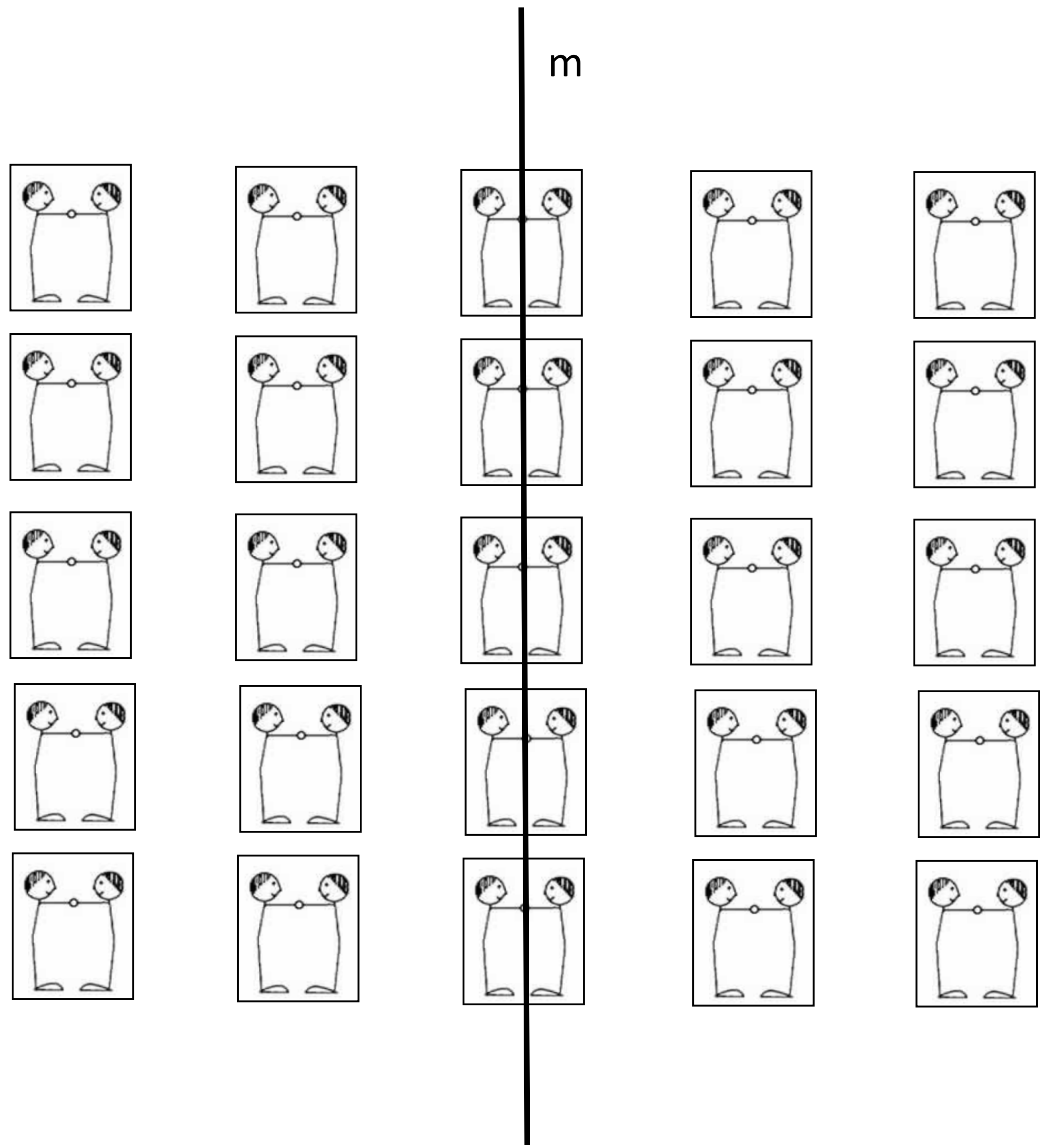
Crystal lattice as a symmetry operation

The main feature of the 3D structure of a crystalline solid is lattice periodicity. A crystals DOES NOT HAVE TO have any of the symmetry described above, however it MUST sustain the periodic structure / long range order. The structure of a crystal must be described by the unit cell and crystal lattice. Consider a unit cell and crystal lattice






m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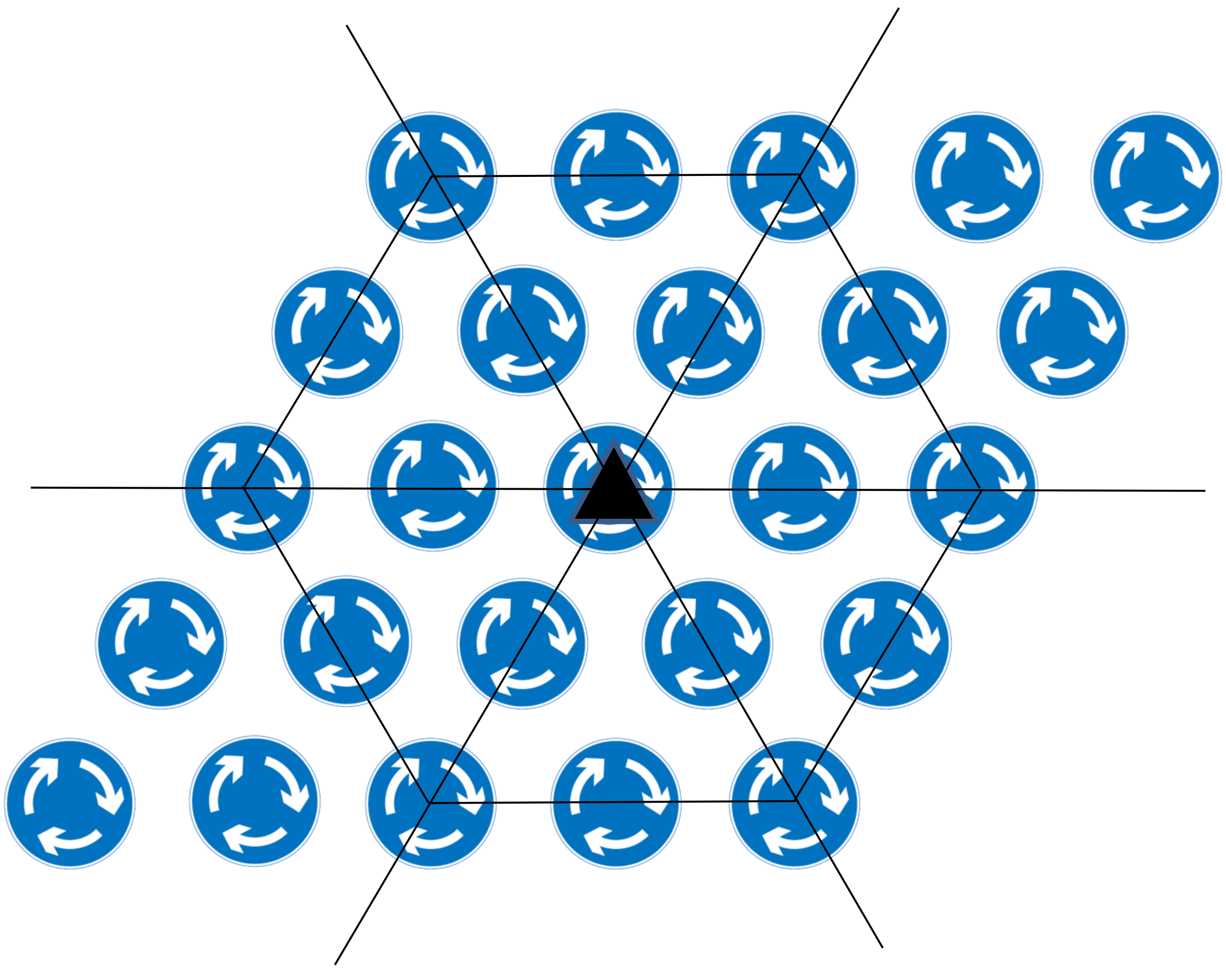


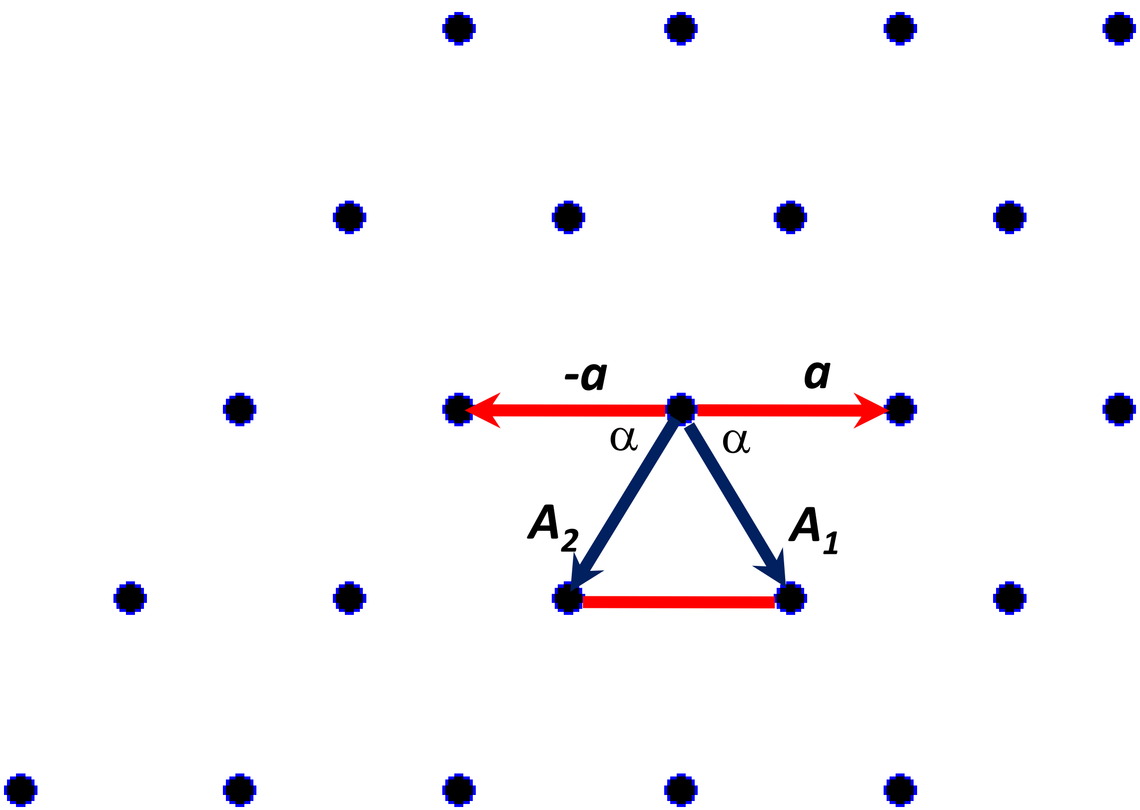
CRYSTAL → UNIT CELL + CRYSTAL LATTICE

SYMMETRY of CRYSTAL → SYMMETRY of UNIT CELL * SYMMETRY of CRYSTAL LATTICE

The are no RESTRICTIONS on the SYMMETRY OF a UNIT CELL. There are however a certain restriction on the symmetry of the lattice. Therefore holding the long range (3D periodicity) order puts the natural restriction on the possible symmetry of a crystal

<u>*MAIN THEOREM of CRYSTALLOGRAPHY*</u>

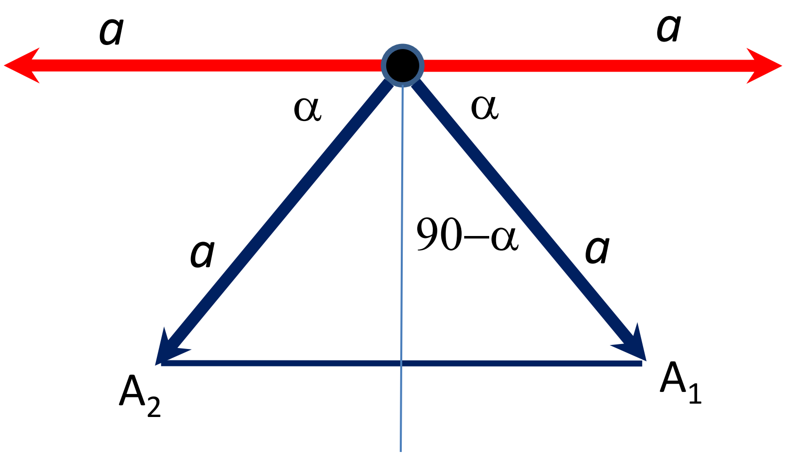
The only possible ROTATIONAL SYMMETRIES accepted by a crystal lattice are 1,2,3,4 and 6



We consider the lattice vector, ***a*** and suppose there is a symmetry axis of the order n=360/α. The two lattice vectors $\boldsymbol{A}_1$ and $\boldsymbol{A}_2$ are obtained by rotation by the α of ***a*** and ***–a*** in two opposite directions. If the rotation is the symmetry operation then $\boldsymbol{A}_1$, $\boldsymbol{A}_2$ and $\boldsymbol{A}_2$-$\boldsymbol{A}_1$ are also the lattice vectors. However according to the construction $\boldsymbol{A}_2$-$\boldsymbol{A}_1$ is parallel to ***a.*** That means the following condition must be hold:

$$A_2A_1 = \mathrm{N}^* a$$

where N is integer number



According to the construction

$A_1A_2 = 2\ a \sin(90 - \alpha) = 2\ a \cos\alpha$,

Therefore

$\cos\alpha = N / 2$.

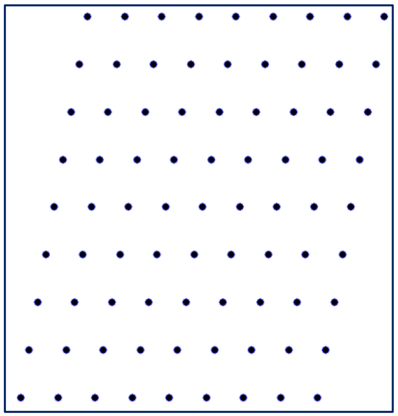
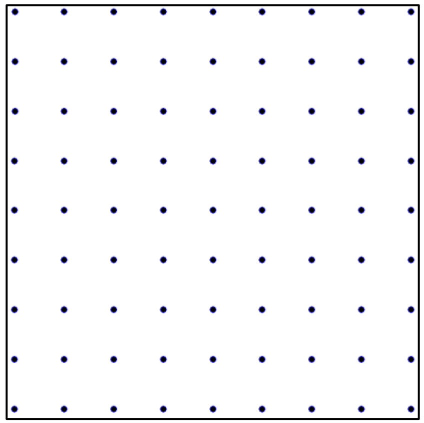
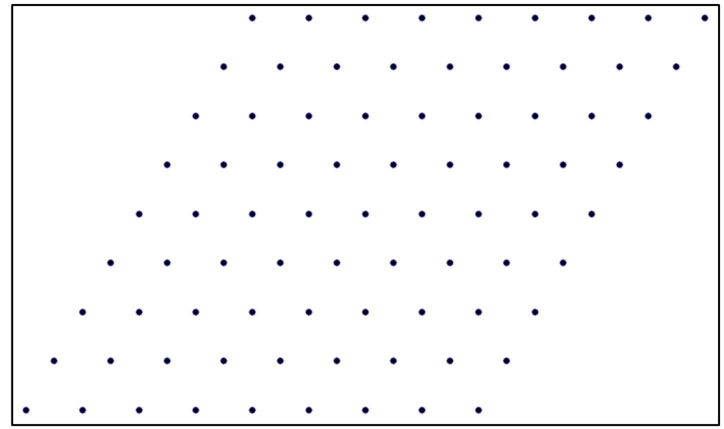
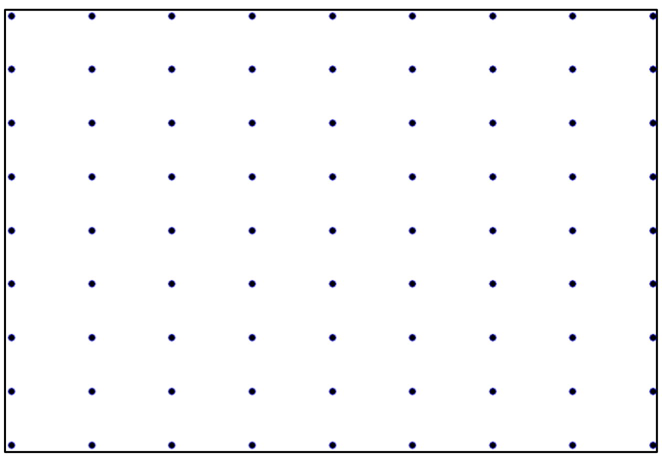
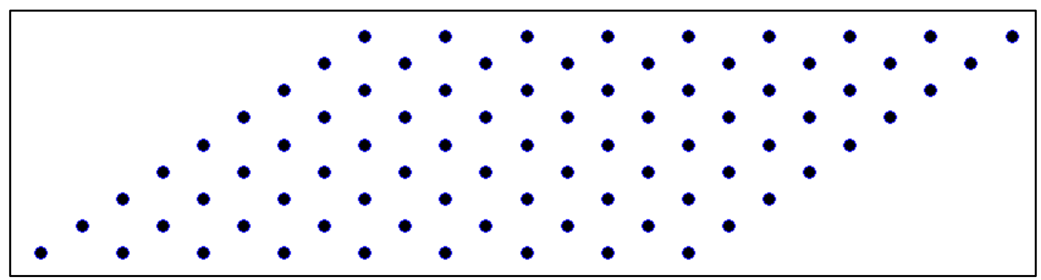
As $|\cos\alpha| <= 1$ there are a few possibilities only

N	cos α	α, deg	Order of symmetry axis	
-2	*-1*	*180*	*2*	
-1	*-0.5*	*120*	*3*	
0	*0*	*90*	*4*	
1	*0.5*	*60*	*6*	
2	*1*	*0*	*∞*	

IMPORTANT MESSAGE

The 3D periodicity crystals puts the RESTRICTION on the POSSIBLE SYMMETRY OPERATION of a whole CRYSTAL STRUCTURE. In particular the maximum order of the rotation axis possible in crystals is 6. In addition 5-fold rotational symmetry is forbidden !

Depending on the geometry crystal lattice may sustain different symmetry elements.

According to the symmetry of the LATTICES are all CRYSTAL are subdivided into a CRYSTAL SYSTEMS