Homework

Look at the Space Group P21/c (#14). This is the most common space group for small molecules.

1. No protein has ever been found to crystallize in this space group. Why is that?

2. Someone reports a crystal in P21/c with Z=1. Is this possible? Why or why not.

3. What is the symmetry of the special positions in this space group?

Lesson 11: Adding Translation

- Define pure translation within a cell—centering
- Combine translation with other symmetry operations to produce a new operations
  - Rotation + translation = screw axis
  - Reflection + translation = glide plane

Cell Centering

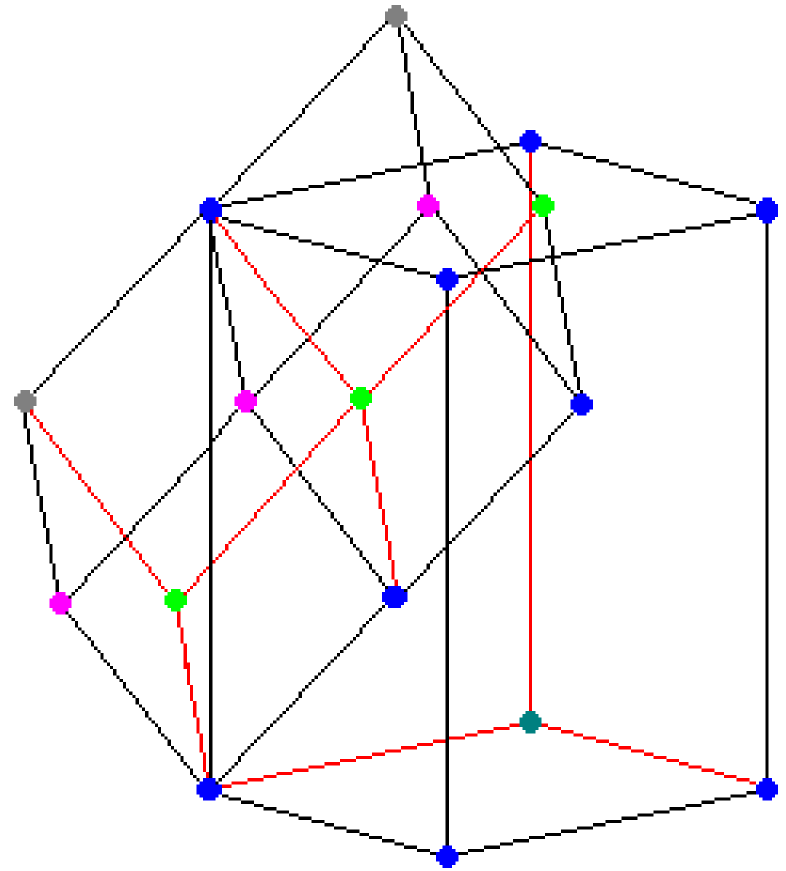
- Remember cell centering is used to increase the symmetry of a unit cell.
- Centering involves adding one or more purely translational operations.
- The result is that one or more fragments in the unit cell are related by a translation.
- Note-- this does NOT mean there is a fragment situated about a certain point.

Centering Types

- Centering is indicated by a capital letter at the start of the H-M cell name.
- Face Centering
  - A centering (0, ½, ½)(so x,y,z = x,½+y,½+z for every point)
  - B centering (½, 0, ½)
  - C centering (½, ½, 0)
  - F centering – A+B+C centering (Face centered)
- Body Centering
  - I centering –(½, ½, ½) (Body Centered)
- No Centering P for primitive

Rhombohedral Centering

- It is always possible to take a rhombohedral cell (a=b=c $\alpha=\beta=\gamma$) and convert it to a hexagonal cell (a=b $\alpha=\beta=90,\gamma=120$).
- The hexagonal cell will have 3 times the volume and be rhomohedral centered—R
- (2/3, 1/3, 1/3) (1/3, 2/3, 2/3)
- Today rhombohedral cells are always reported in their hexagonal form.



Screw Axes

- The screw axis is a combination of rotation and translation.
- Translation is always along the line that is the rotation axis
- Since neither rotation or translation change one enantiomer into the other, this symmetry operation can be present in optically active crystals.

Screw Axes are a combination of rotation axes and translations.

The symbols are:

2_1 3_1 3_2 4_1 4_2 4_3

6_1 6_2 6_3 6_4 6_5

The symbols are of the form

X_y

$$X_y$$

The rotation is $\frac{360}{X}$ degrees.

The translation is $\frac{y}{X}$ units

along the screw axis.

This direction is determined by the location in the H-M name as we saw last time. $Pmm2_1$ implies the screw is along c.

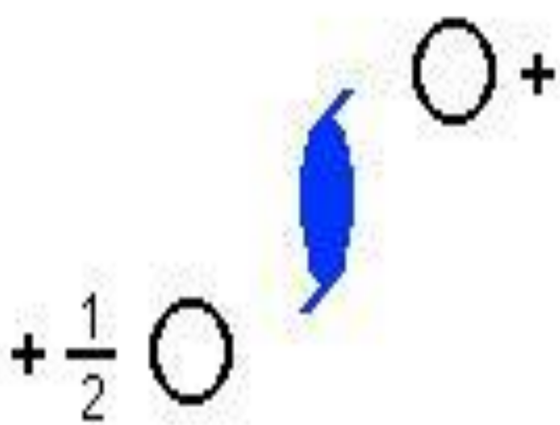
A two-fold screw axis, 2_1,

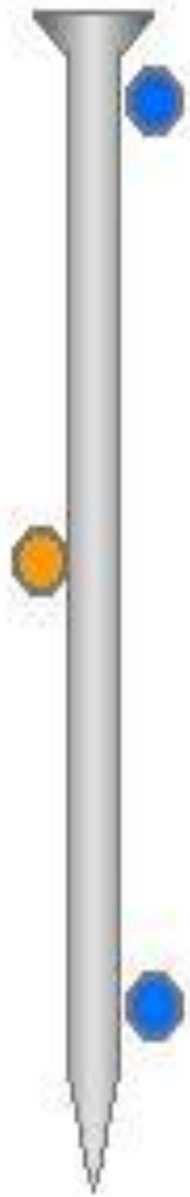
refers to a rotation of

$\frac{360}{2}$ or 180 degrees,

combined with a translation of

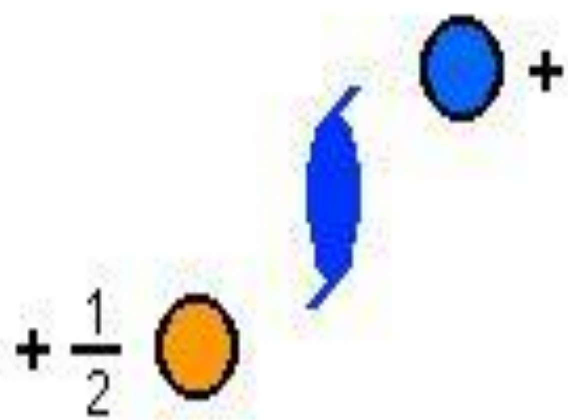
$\frac{1}{2}$ along the screw axis.

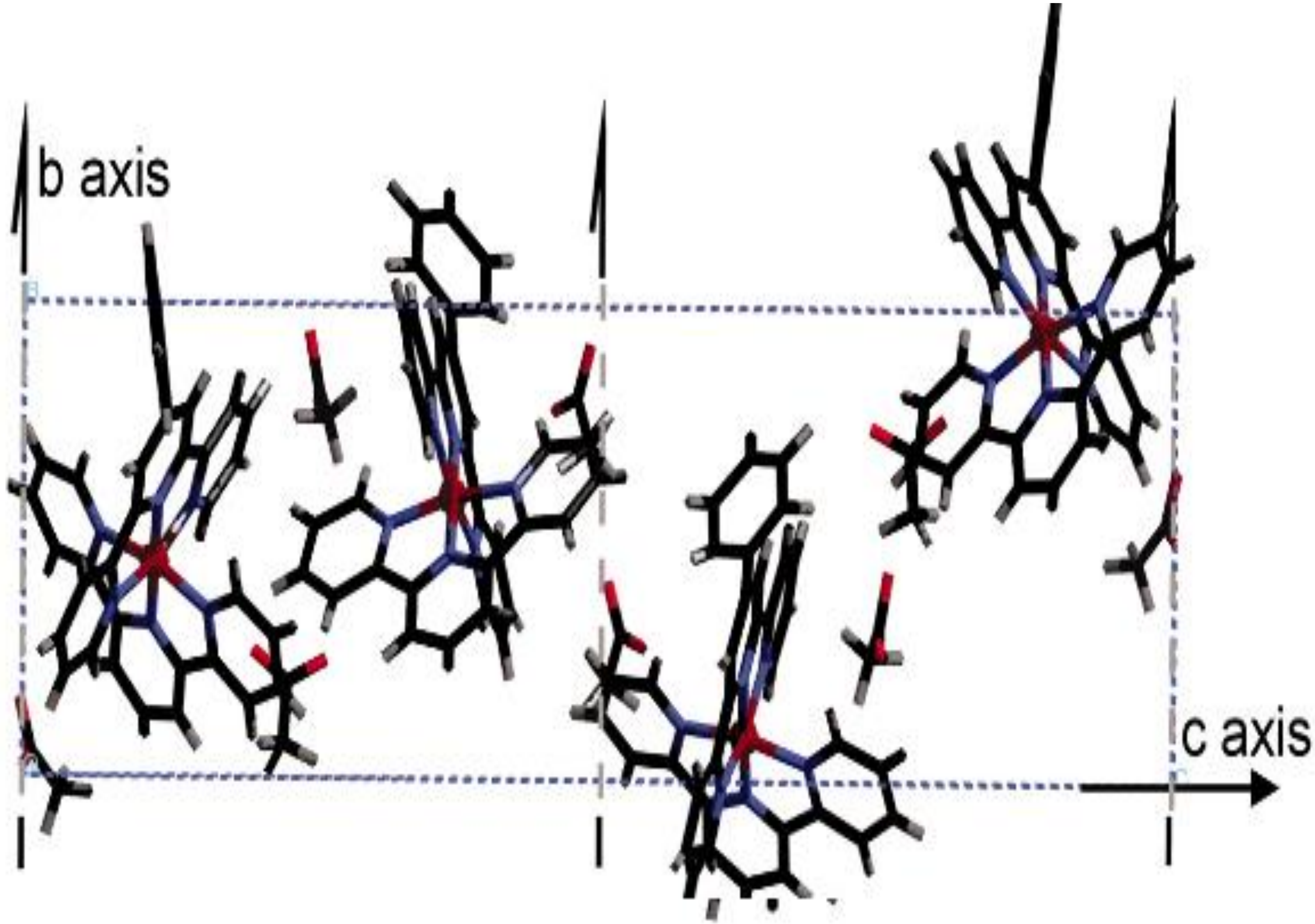




$+\frac{1}{2}$ indicates translation of $+\frac{1}{2}$ normal to the plane of the page

(2_1 is read two sub one)




b axis
c axis

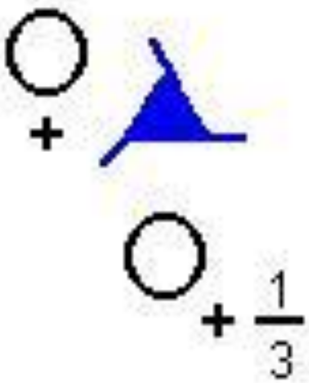
A three-fold screw axis, 3_1 ,

refers to a rotation of

$\frac{360}{3}$ or 120 degrees,

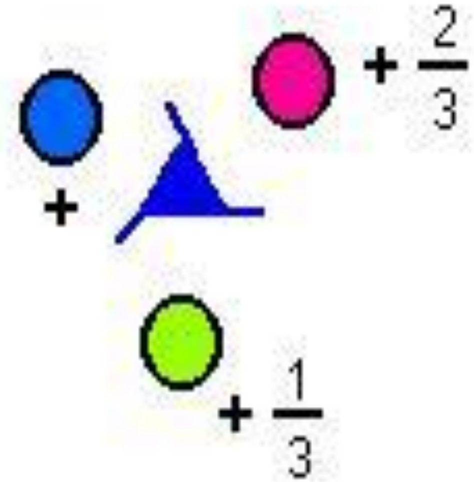
combined with a translation of

$\frac{1}{3}$ along the screw axis.



A second operation of the 3_1 results in the object translated by $+\frac{2}{3}$ along the screw axis.

(3_1 is read three sub one)



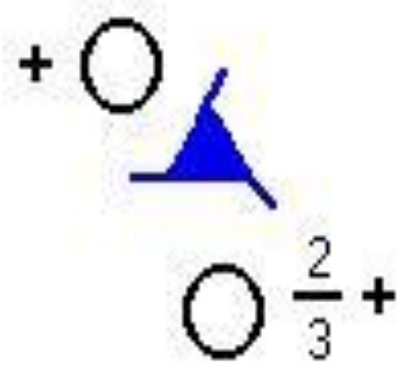
A three-fold screw axis, 3_2,

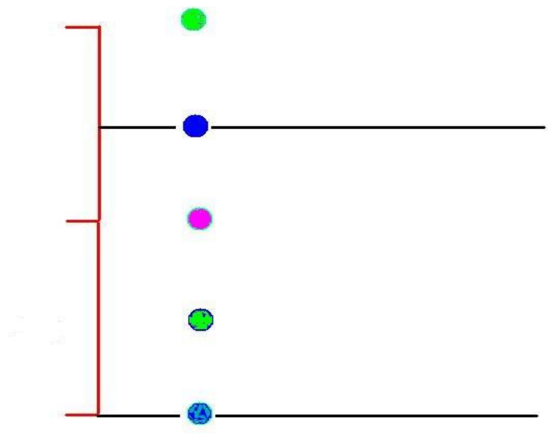
refers to a rotation of

$\frac{360}{3}$ or 120 degrees,

combined with a translation of

$\frac{2}{3}$ along the screw axis.

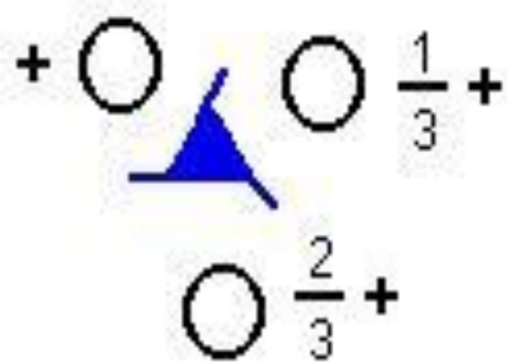




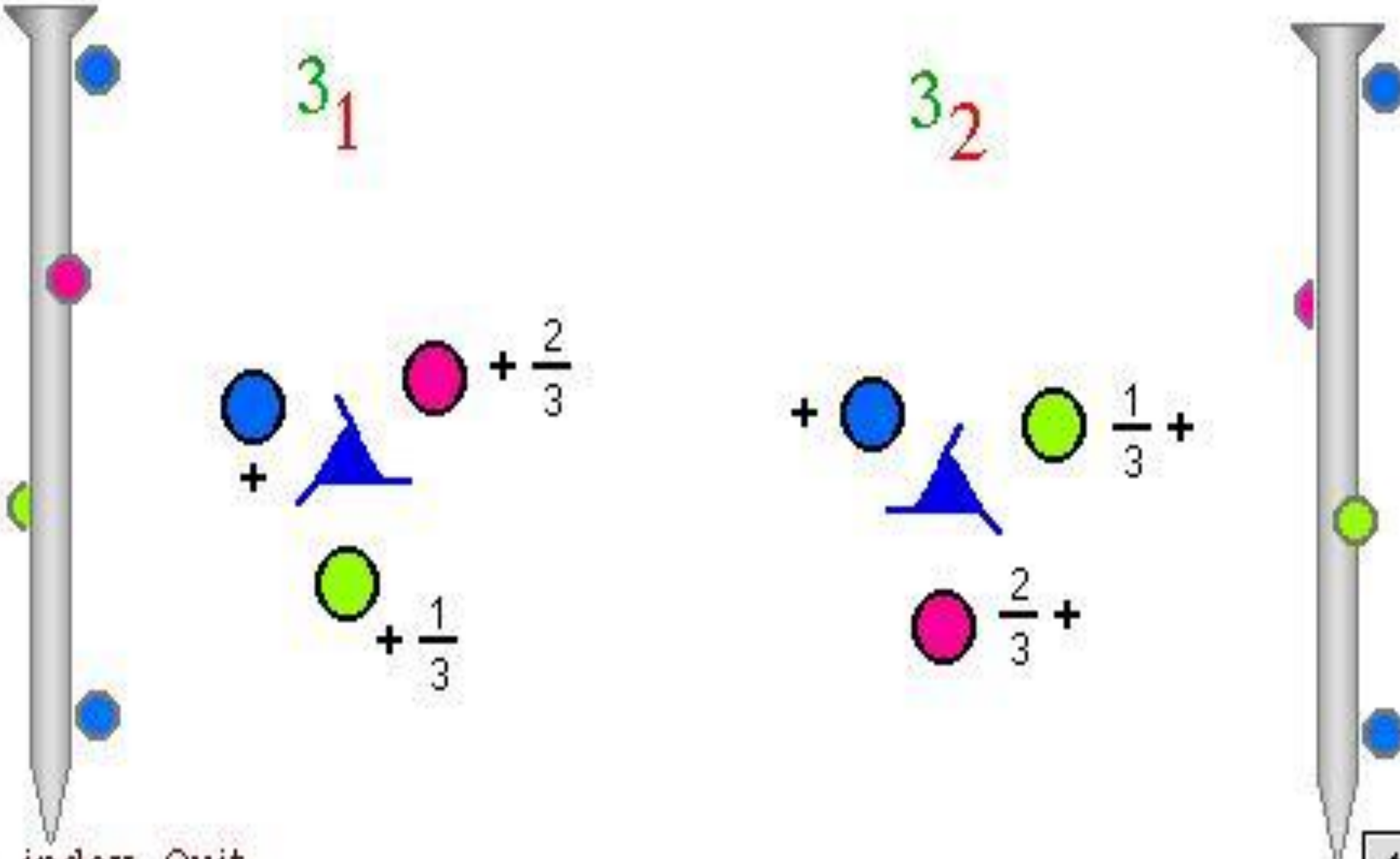
A translation by 2/3 generates a point at 1/3

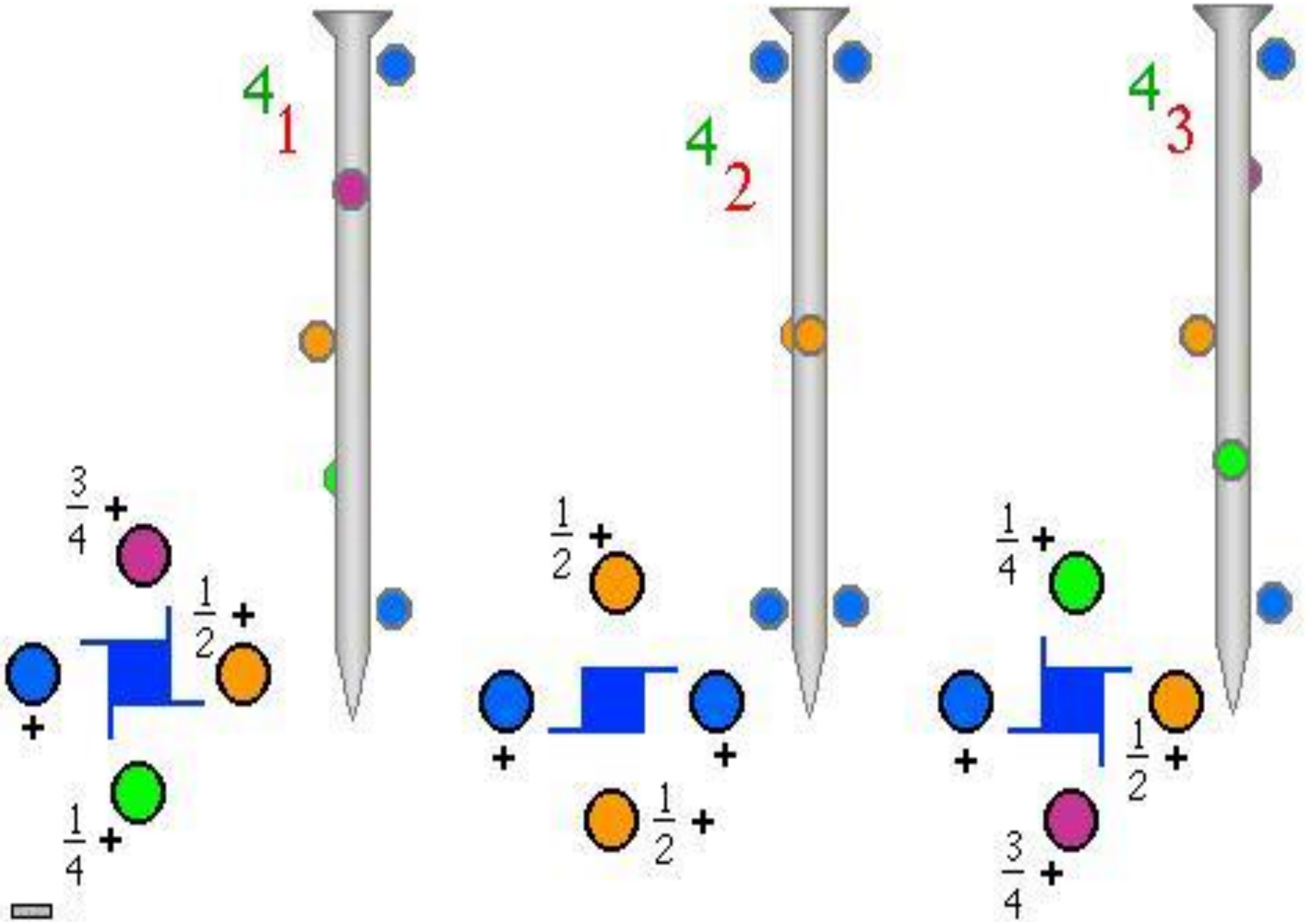
A second operation of the 3_2 results in the object translated by $+\frac{2}{3}$ along the screw axis.

(3_2 is read three sub two)

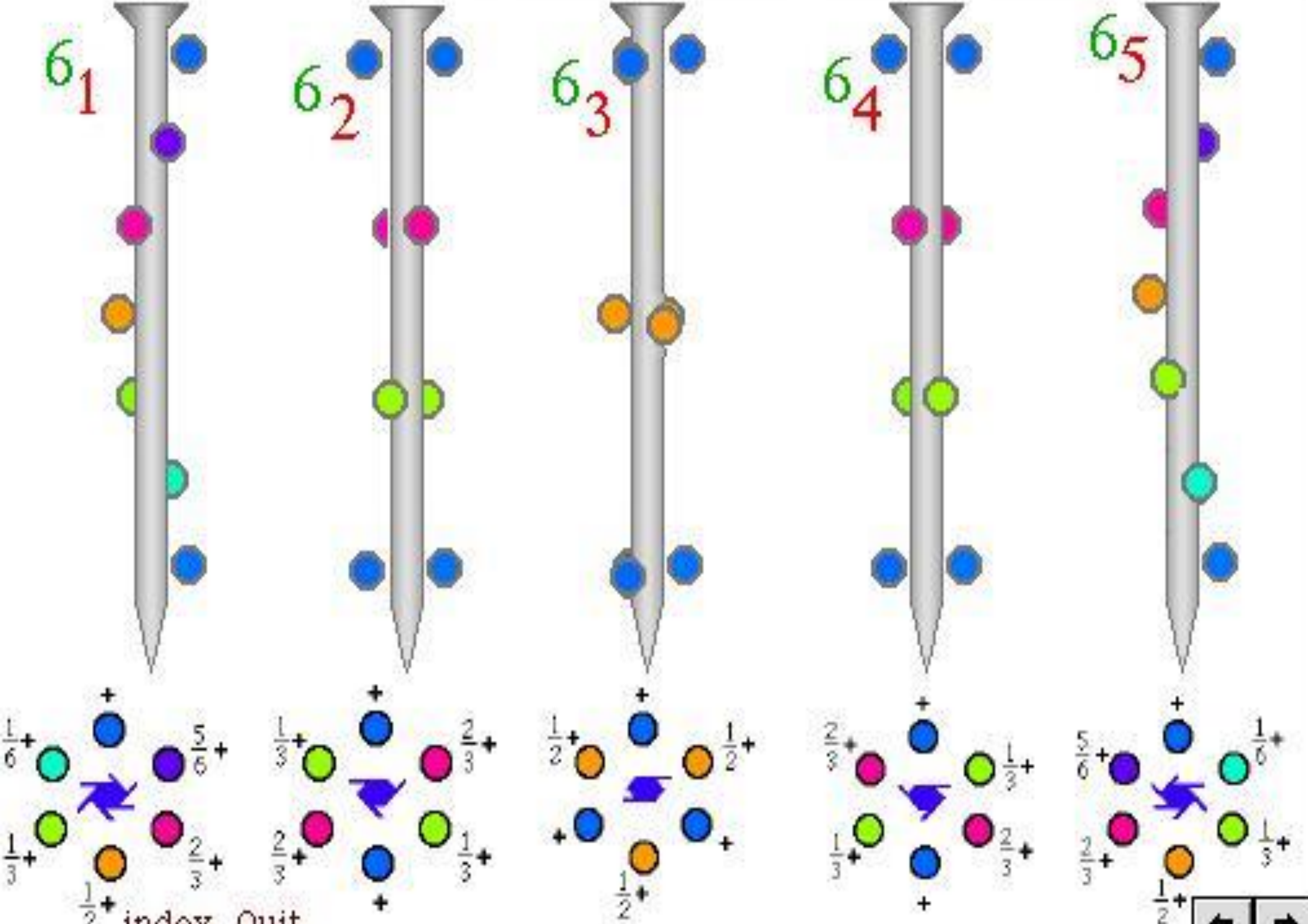


Notice the result is a set of that
that screws that turn in opposite directions.





4_1
4_2
4_3
$\frac{3}{4}$ +
$\frac{1}{2}$ +
$\frac{1}{4}$ +
$\frac{1}{2}$ +
$\frac{1}{2}$ +
$\frac{1}{4}$ +
$\frac{1}{2}$ +
$\frac{3}{4}$ +



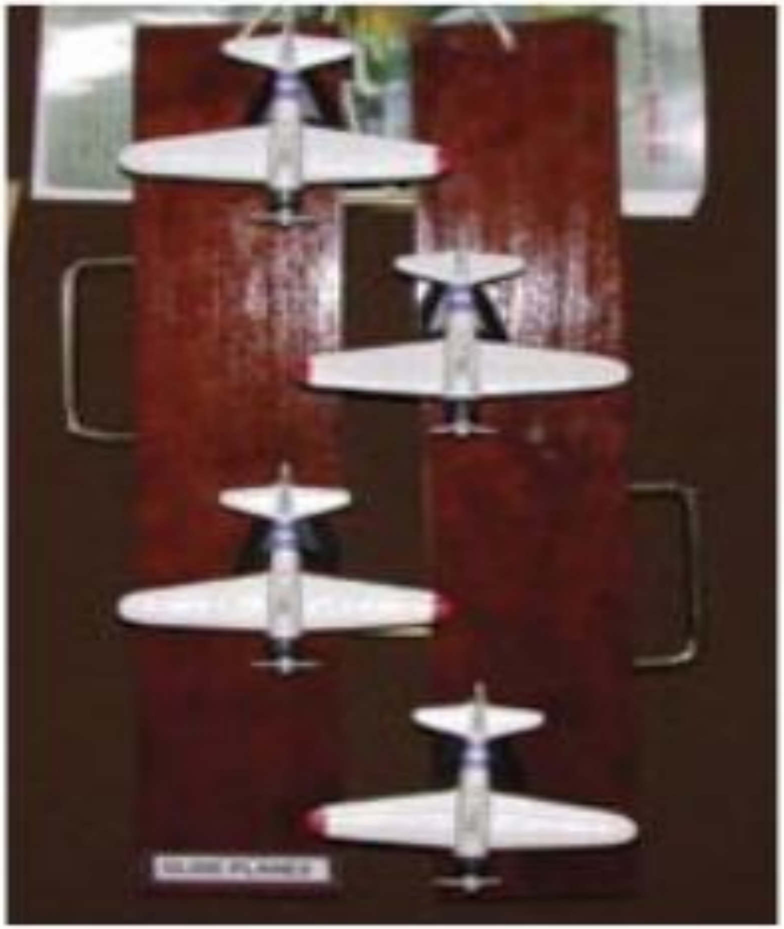
6_1
6_2
6_3
6_4
6_5
+ $\frac{5}{6}$+ $\frac{2}{3}$+ $\frac{1}{2}$+ $\frac{1}{3}$+ $\frac{1}{6}$+
+ $\frac{2}{3}$+ $\frac{1}{3}$+ + $\frac{2}{3}$+ $\frac{1}{3}$+
+ $\frac{1}{2}$+ + $\frac{1}{2}$+ + $\frac{1}{2}$+
+ $\frac{1}{3}$+ $\frac{2}{3}$+ + $\frac{1}{3}$+ $\frac{2}{3}$+
+ $\frac{1}{6}$+ $\frac{1}{3}$+ $\frac{1}{2}$+ $\frac{2}{3}$+ $\frac{5}{6}$+

index Quit

Glide Planes

- A glide plane is a mirror followed by a translation of ½ the length of the vector in the plane of the mirror.
- The translation can be along an axis in the plane (a,b,c) or along the diagonal (n)
- The glide plane is indicated by a lower case letter indicating the direction of translation.
- The axis perpendicular to the plane is found from the position in the H-M symbol
- The translation is always in the mirror plane.
- Since this involves a mirror, it cannot be in optically active crystals.

An example



"*Glide planes*" *from Wally Cordes' ACA poster on teaching cyrstallo-graphy*

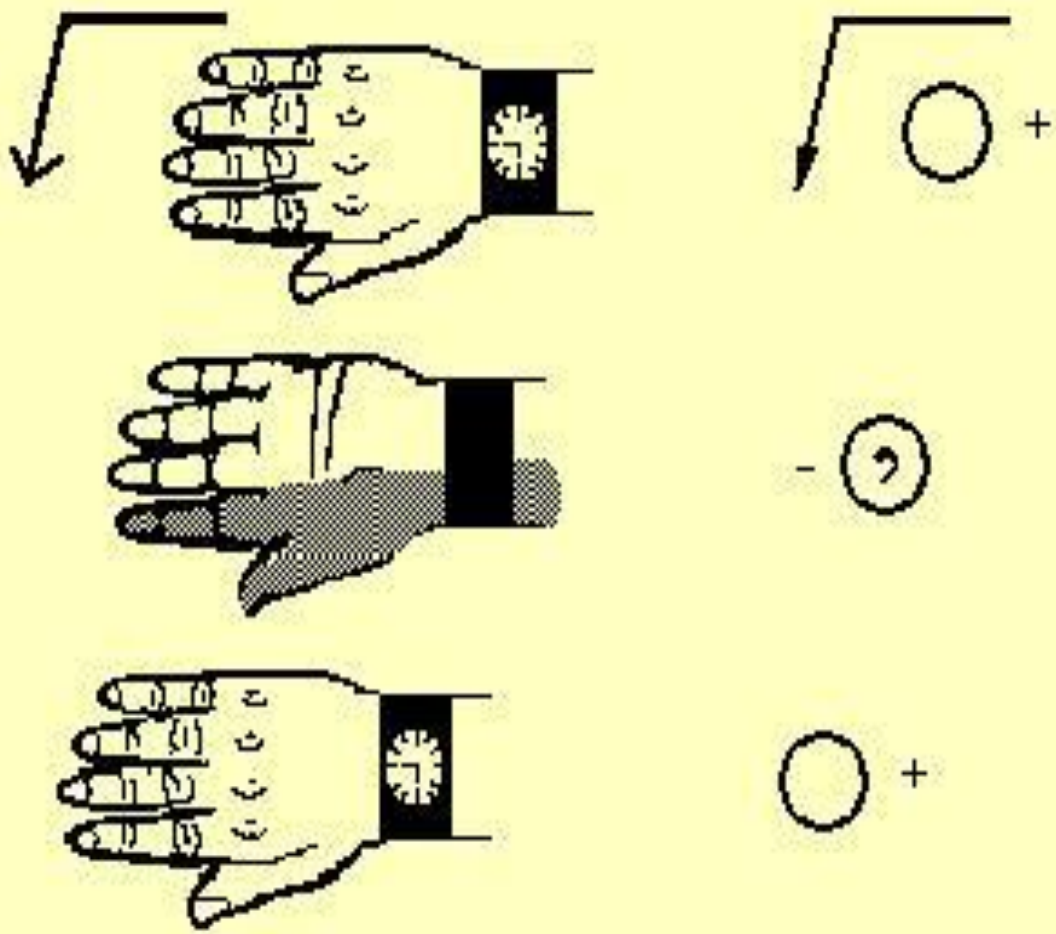
H-M Glide Plane

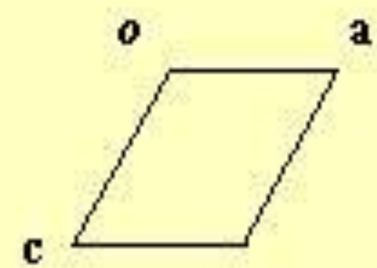
- A letter a, b, c, or n indicates the direction of the translation. The letter n represents a glide along the diagonal
- The location of the symbol in the H-M name indicates what axis is perpendicular to the mirror
- Example Pnma—there is a glide plane with a mirror perpendicular to **a** and a translation in the **bc** diagonal, a mirror perpendicular to **b** and a glide plane perpendicular to **c** with a translation along **a**

Symmetry Elements in 3-Dimensions

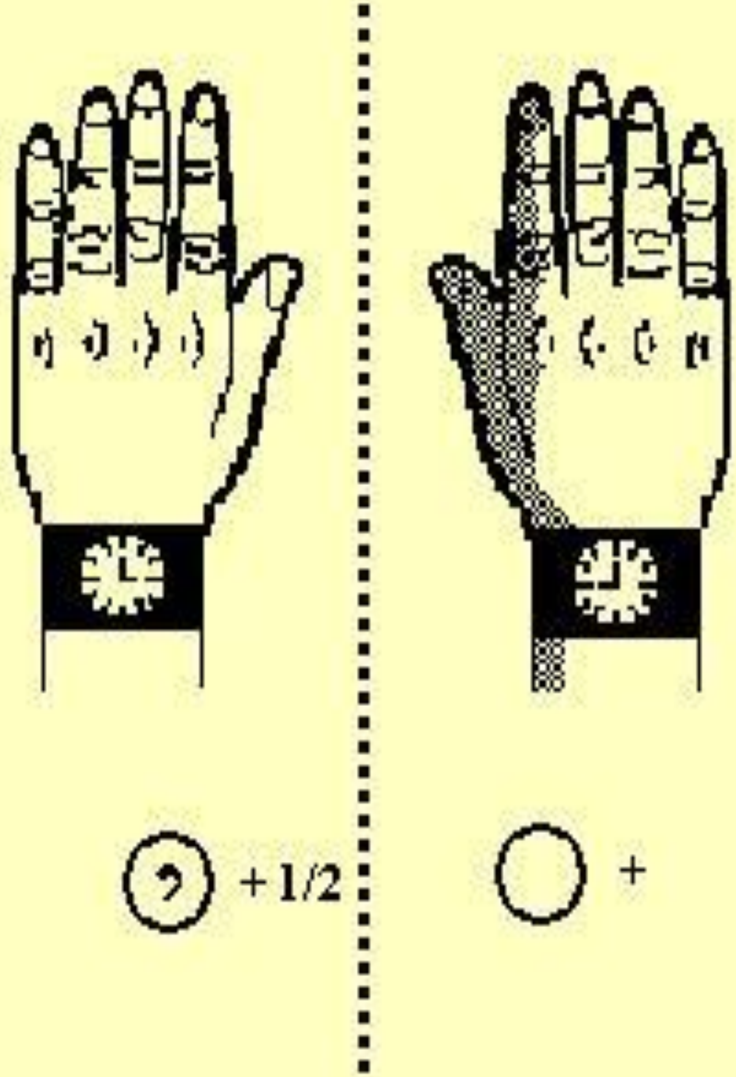
c-Glide

The reflection plane is perpendicular to b, parallel to a, and the translation is along c.



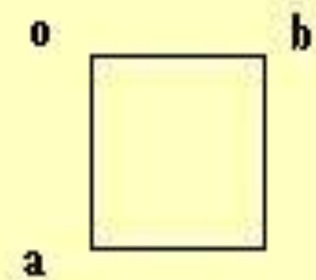


Symmetry Elements in 3-Dimensions



c-Glide

The reflection plane is perpendicular to b, parallel to a, c and the translation is along c.



MAIN

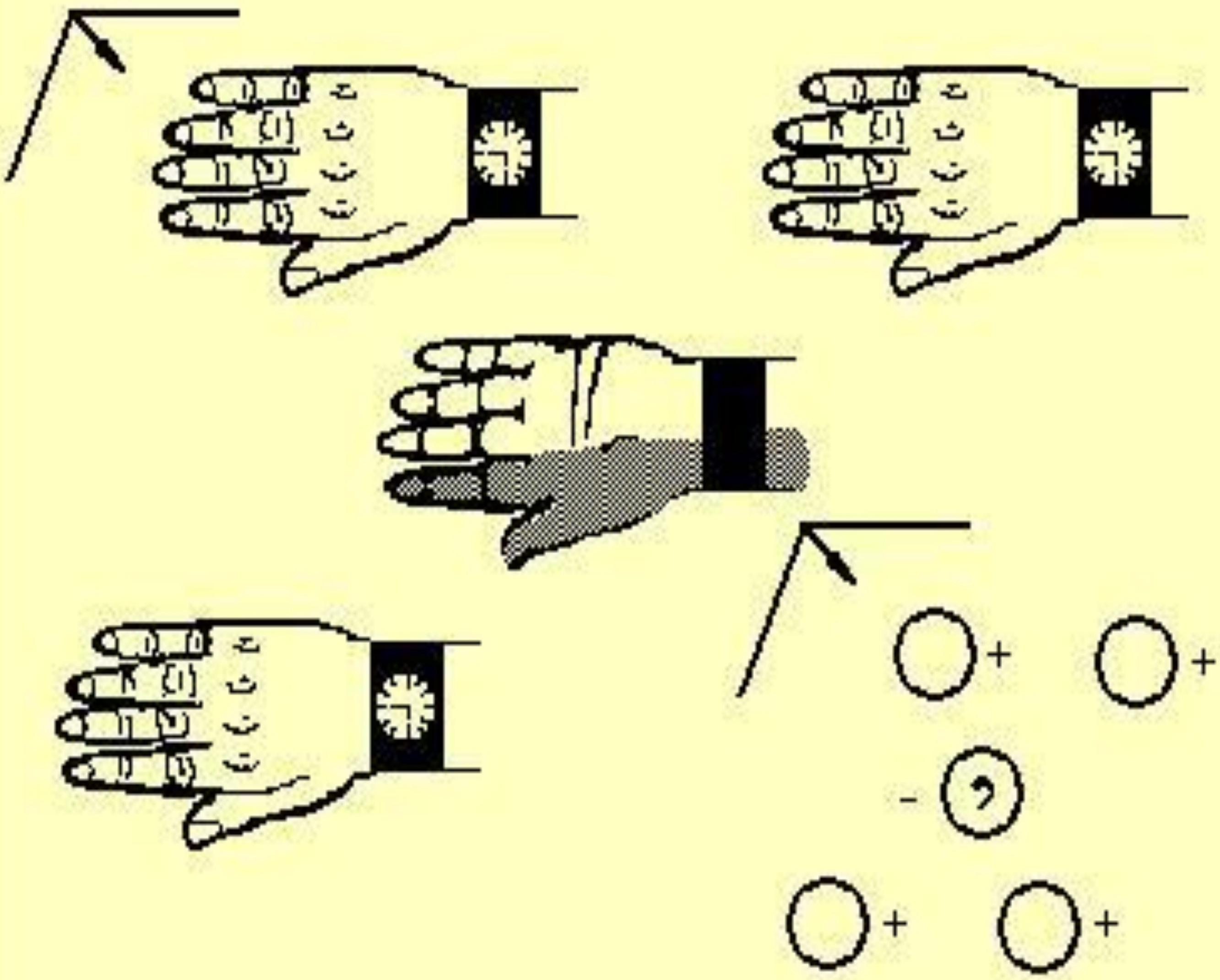
Summary

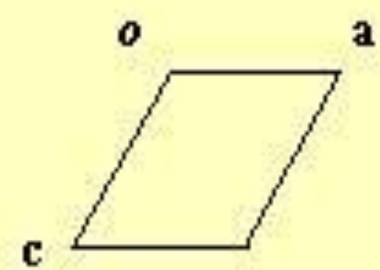
Introduction Page

Symmetry Elements in 3-Dimensions

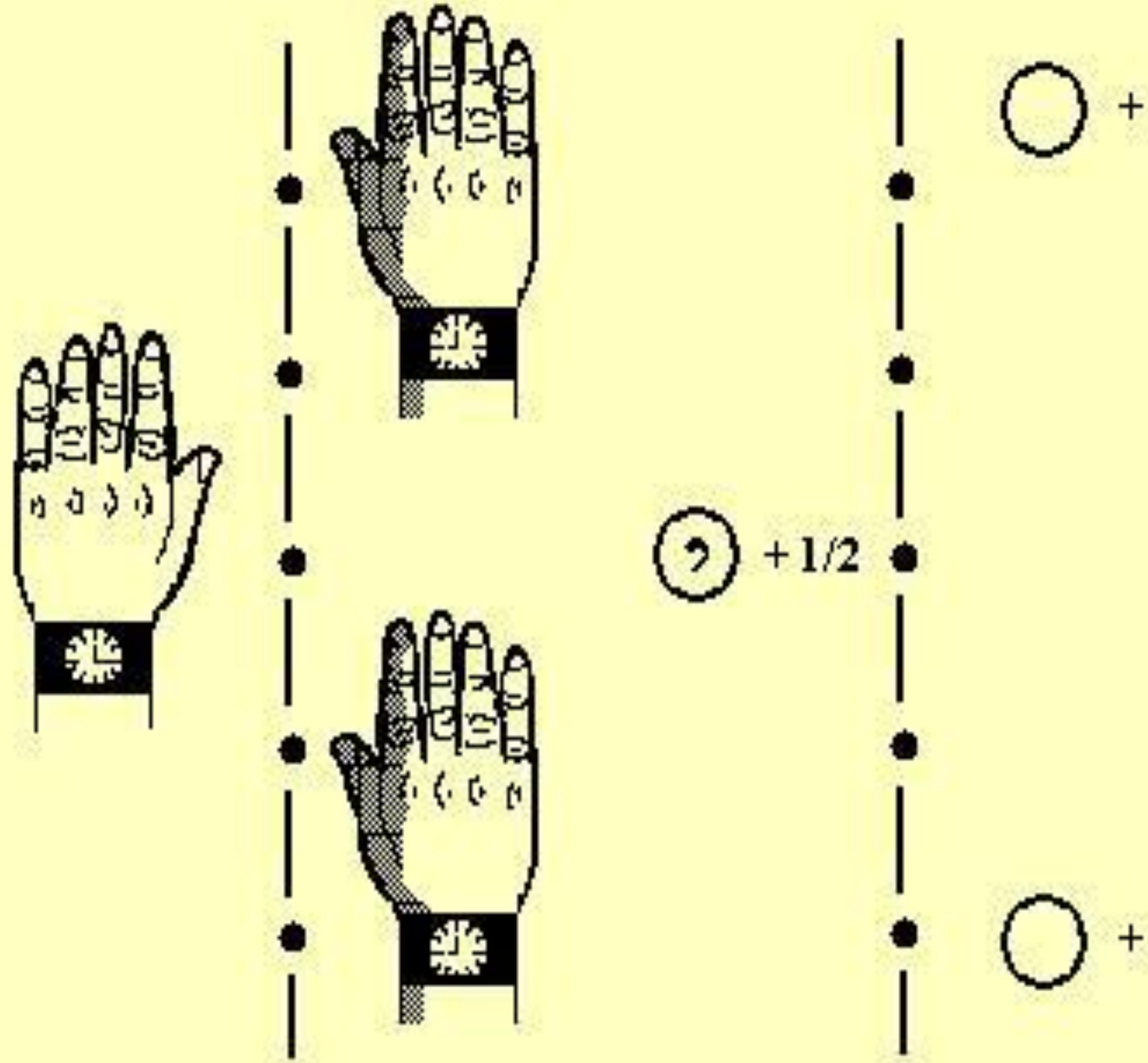
n-Glide

The reflection plane is perpendicular to b, parallel to a, c and the translation is half along a and half along c.



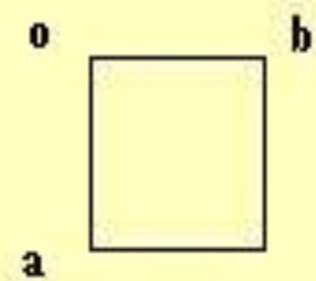


Symmetry Elements in 3-Dimensions



n-Glide

The reflection plane is perpendicular to b, parallel to a, c and the translation is half along a and half along c.



MAIN

Summary

Introduction Page

Diamond Glide

- Symbol d
- Reflection followed by ¼ translation along the diagonal of the mirror plane
- Very Rare—thank goodness

Homework

- Is there anything wrong with the proposed space group Pbac? If so what.
- Is there a difference between 2_1 and 6_3? If so what is it.