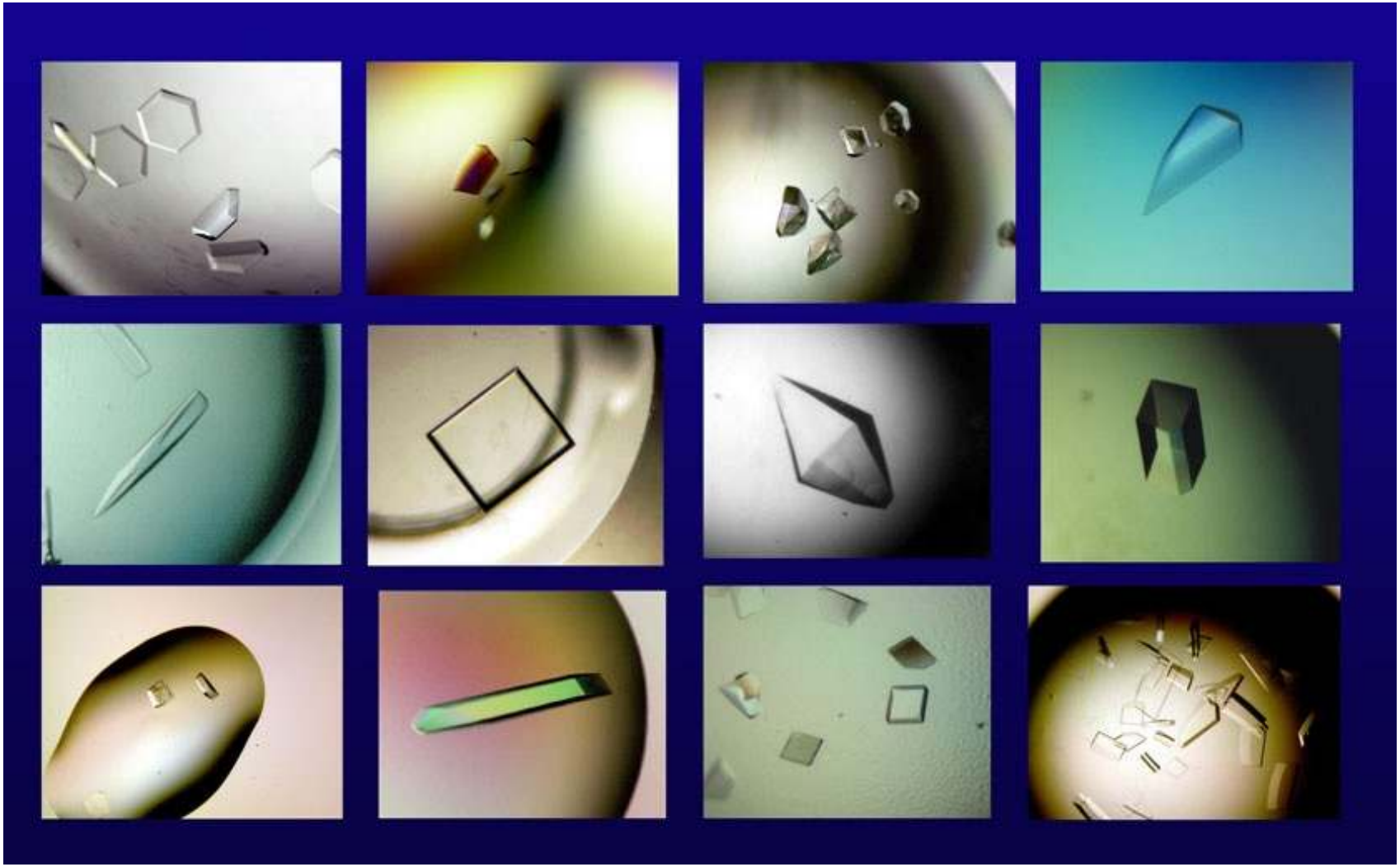
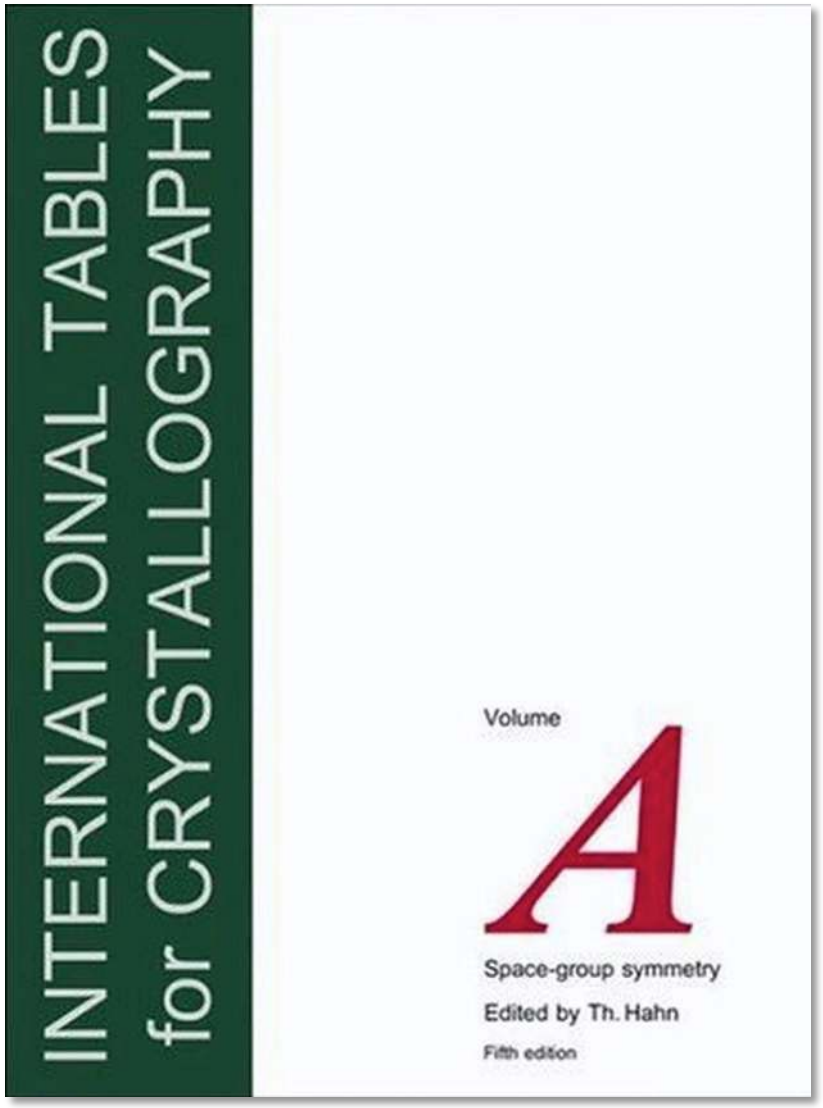
# Introduction to space groups

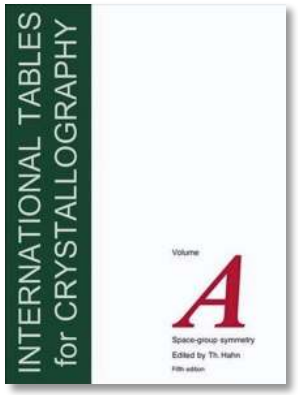
Andrey Lebedev, CCP4





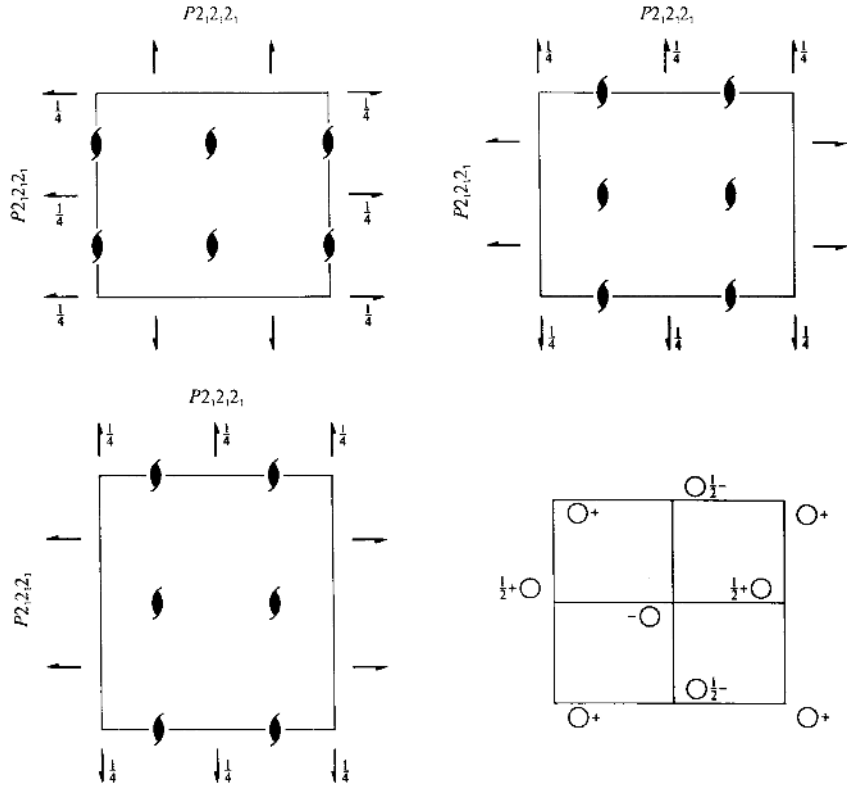

Further referred to as ITC-A

# Space group representation in ITC-A




$P2_12_12_1$ $D_2^4$ 222 Orthorhombic

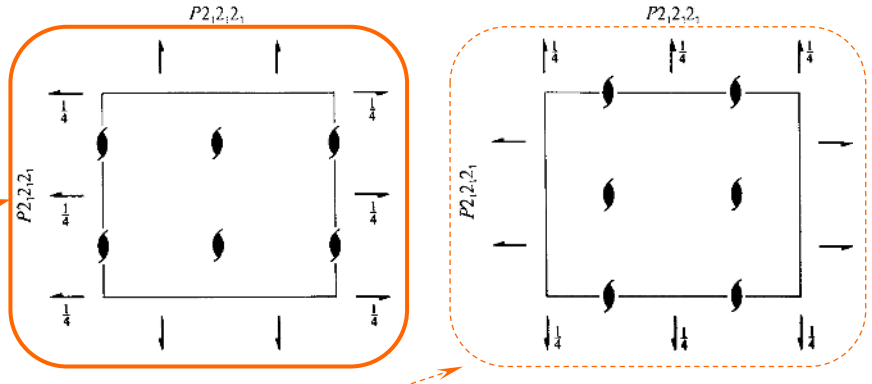
No. 19 $P2_12_12_1$ Patterson symmetry $Pmmm$



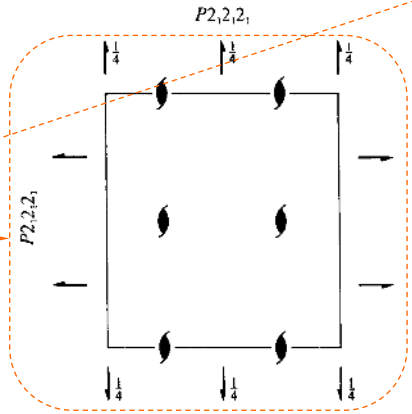
# Space group representation in ITC-A

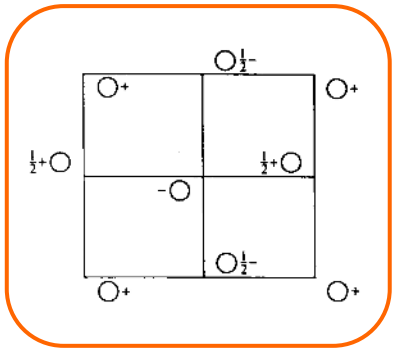
| | | | |
|---|---|---|---|
| $P2_12_12_1$ | $D_2^4$ | 222 | Orthorhombic |
| No. 19 | $P2_12_12_1$ | | Patterson symmetry $Pmmm$ |

Location of symmetry elements




Two other projections are also shown for this space group

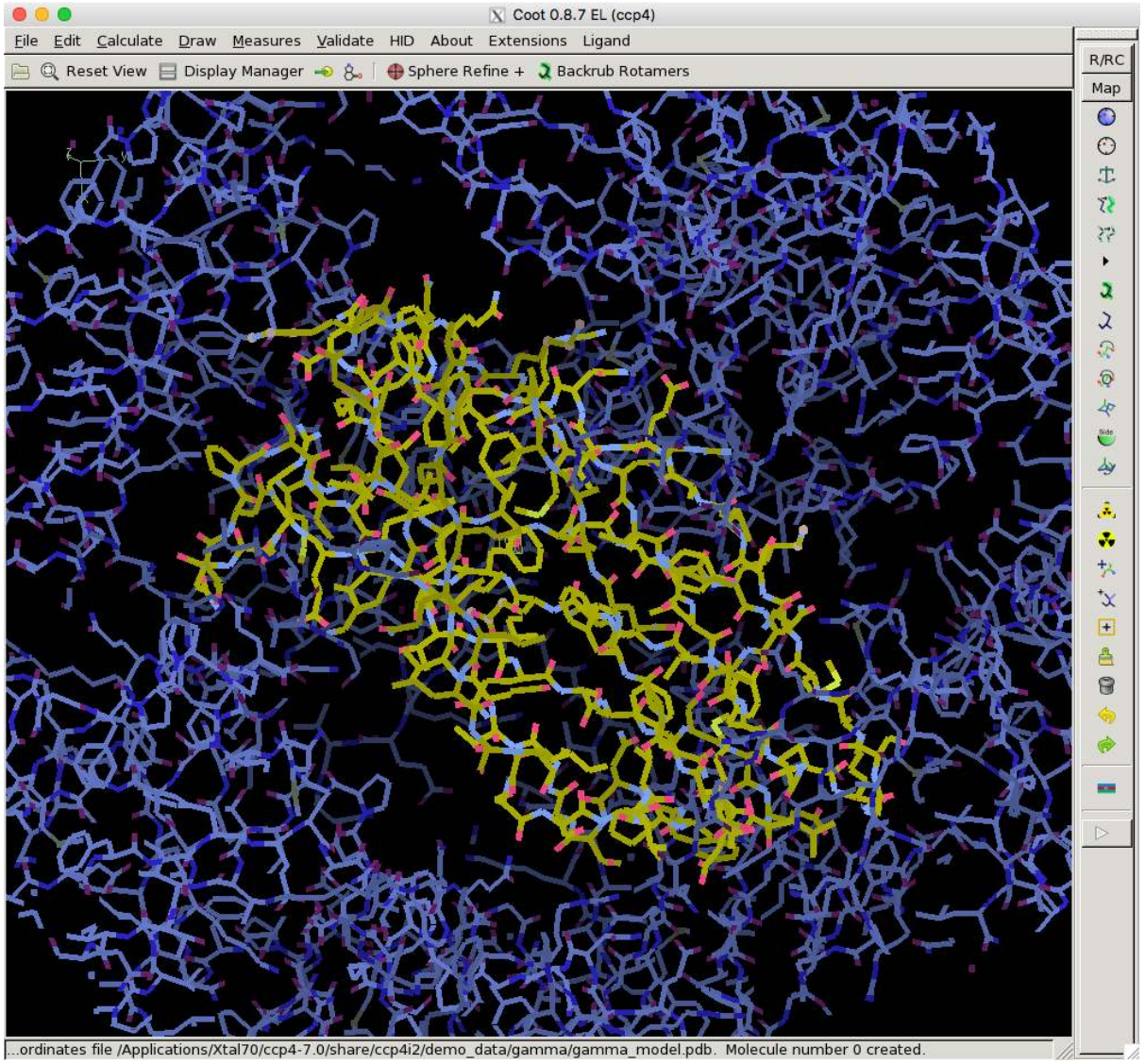


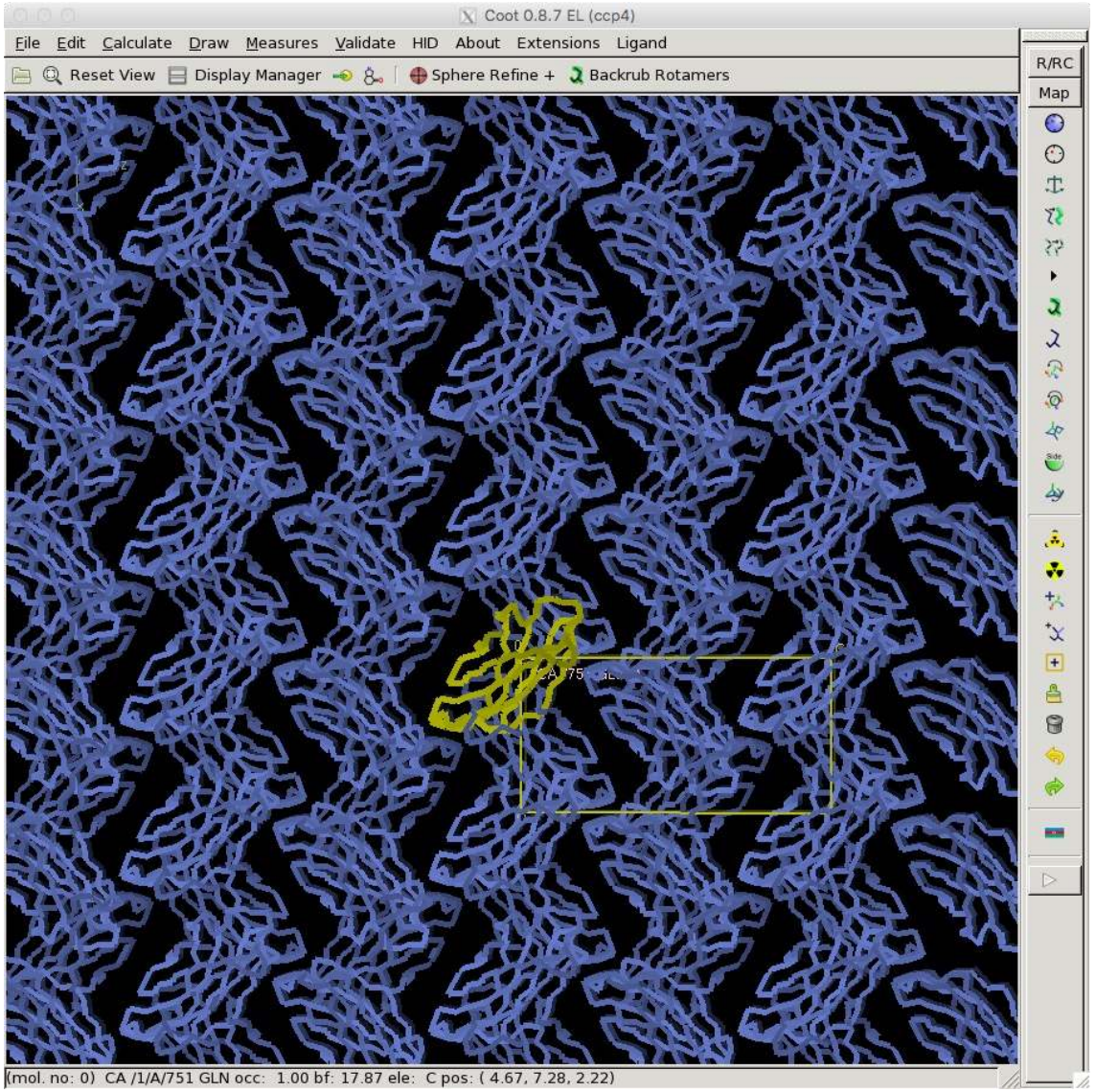
Set of equivalent points in general position.

We will be looking at "molecular wallpaper" instead

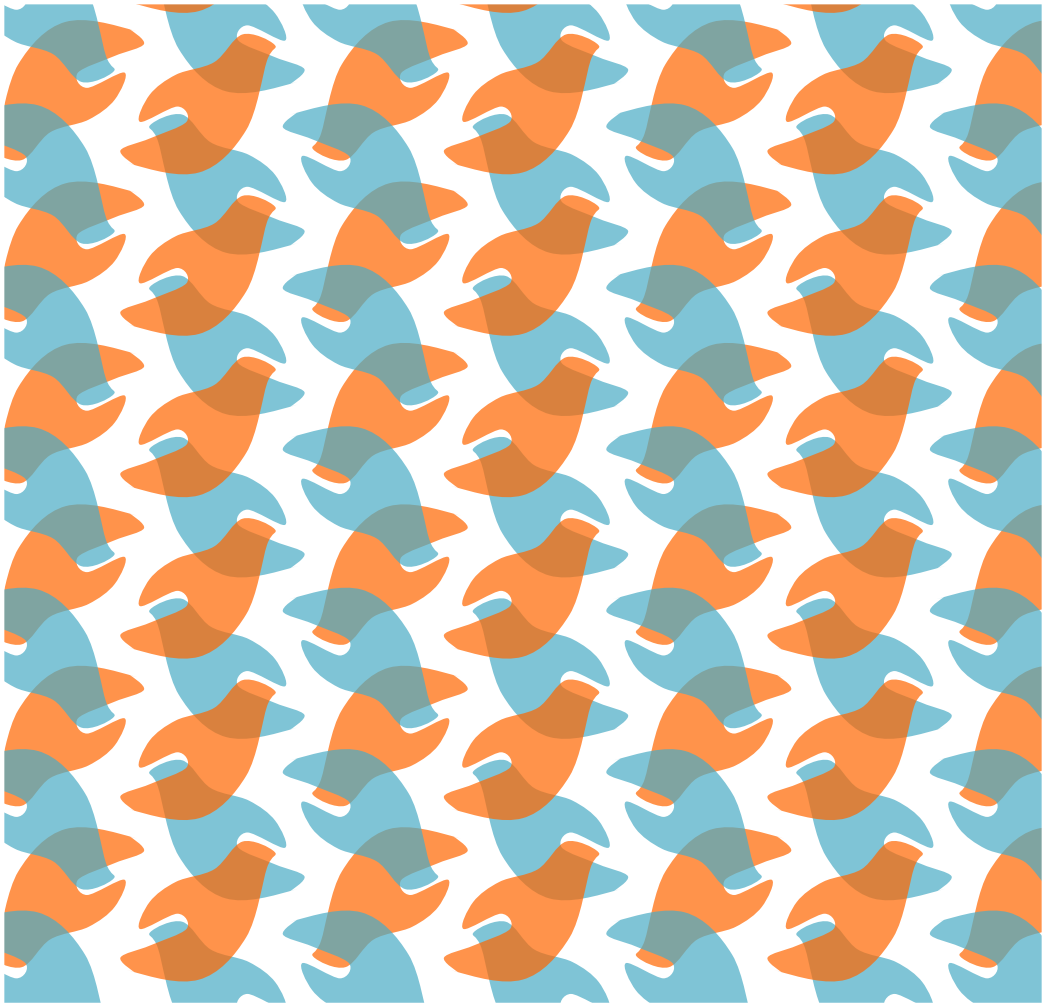
# Examine structure in Coot



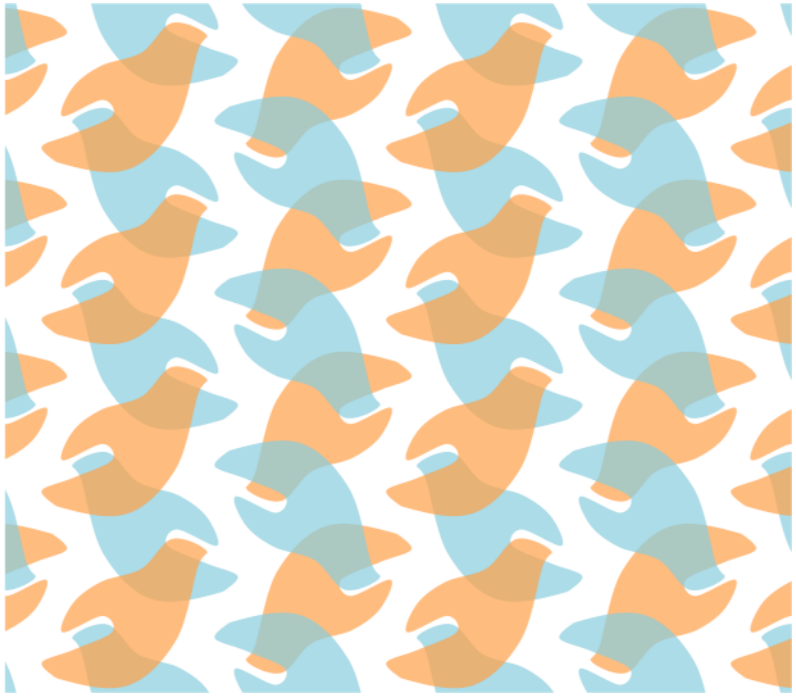
# Symmetry view in Coot



# Simplified representation

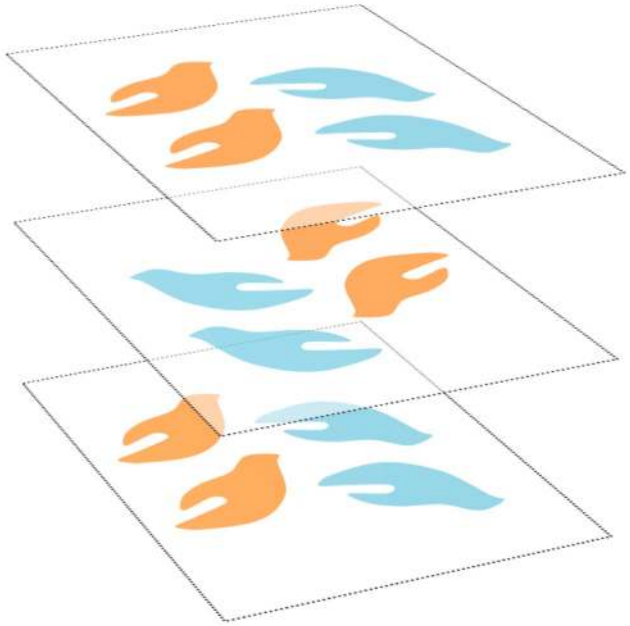


# Simplified representation

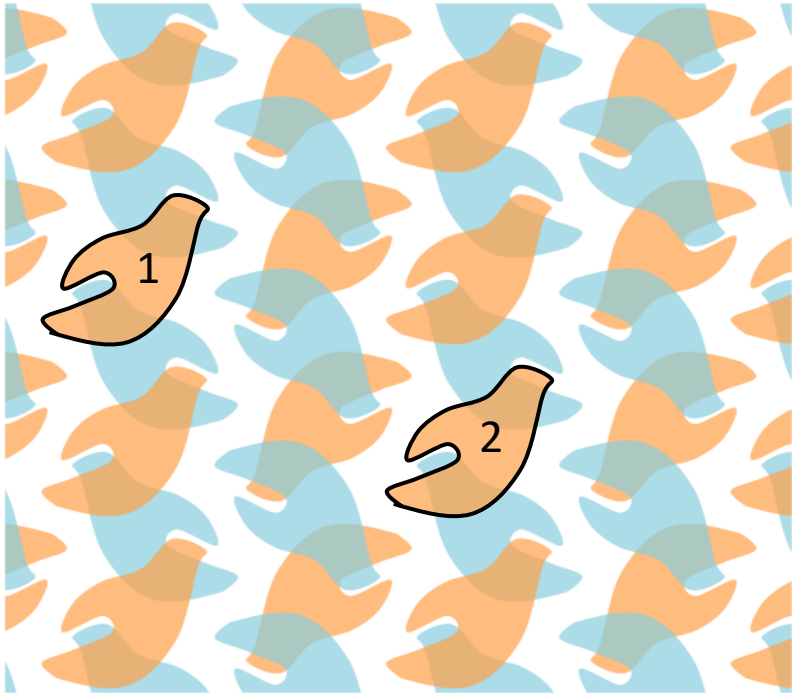


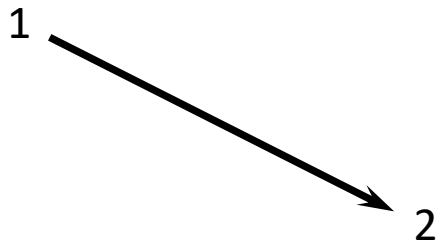
View from the top

There is a third dimension.



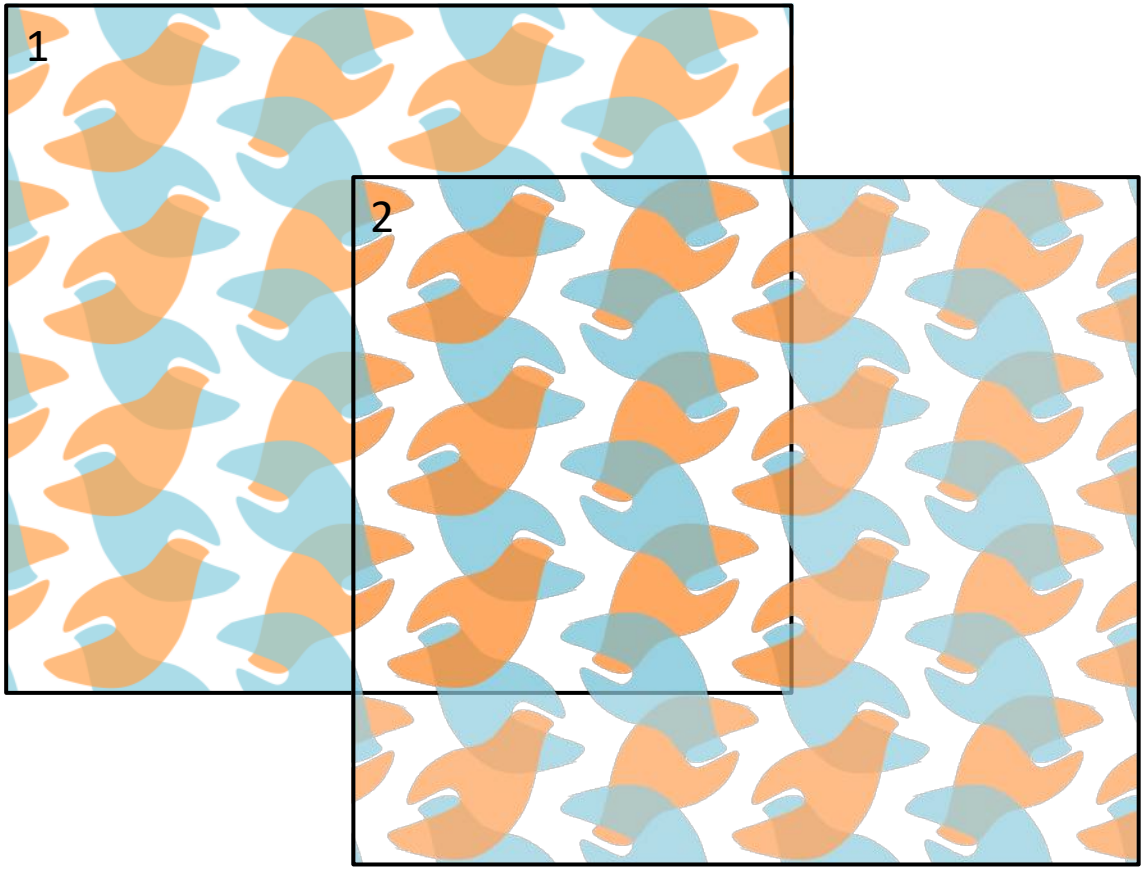
# Translation 1-2

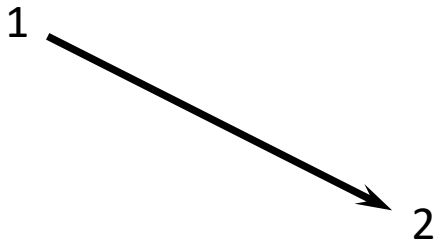



Vector maps 1 -> 2

# Translation 1-2 is global

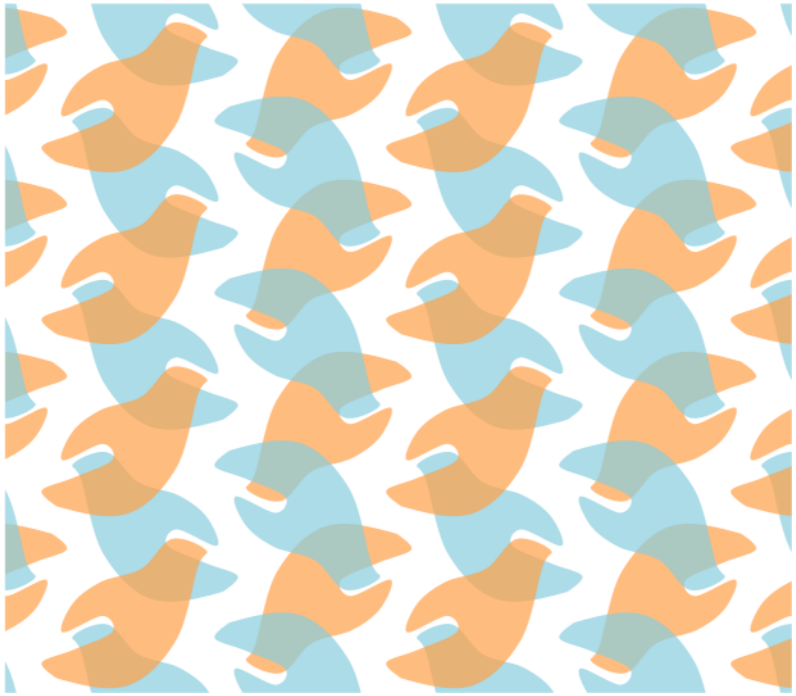


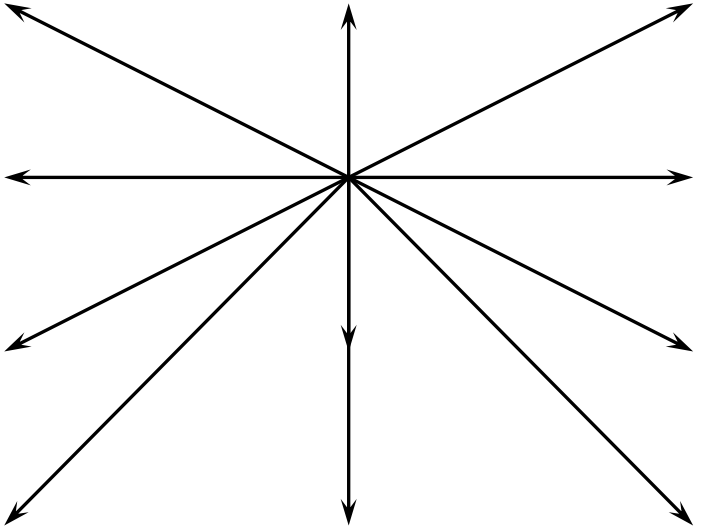




Vector 1->2 maps the whole crystal onto itself:

it defines a crystallographic operation

# All translations form an infinite group

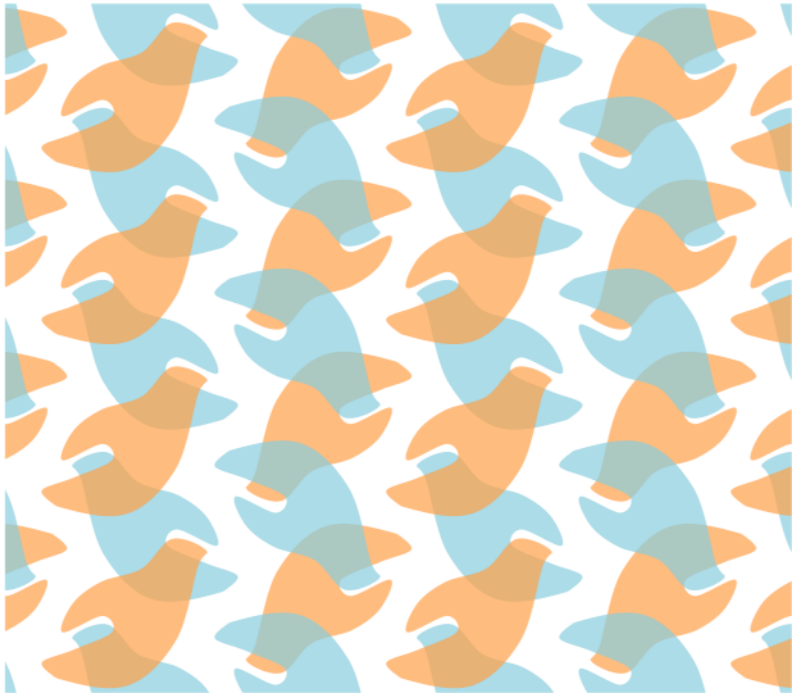


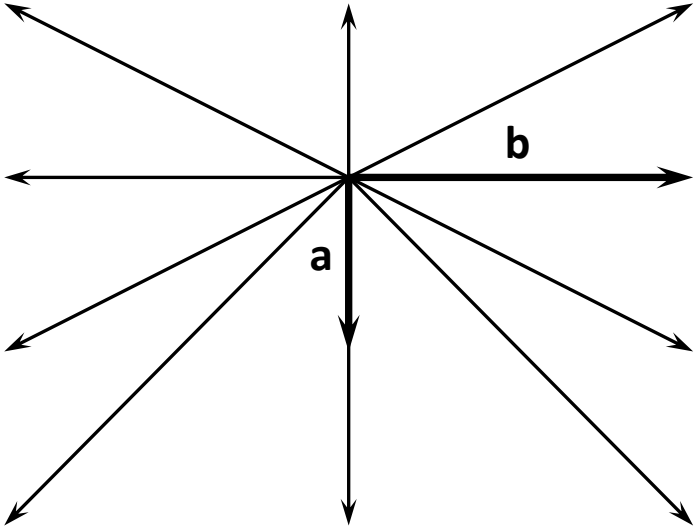


An infinite group (over vector sum):

- inverse translations included
- sum of any two vectors from the group belongs to the group

# Basis vectors

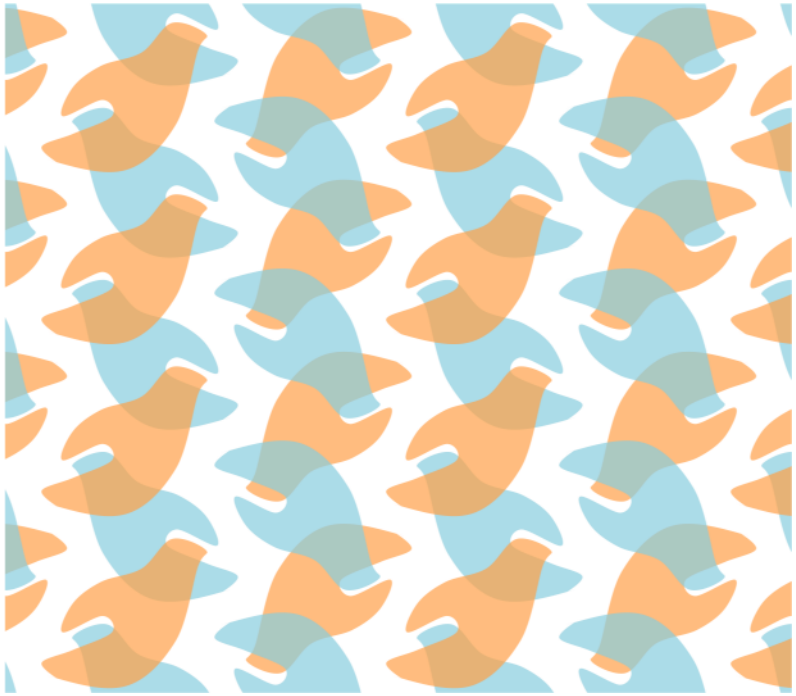


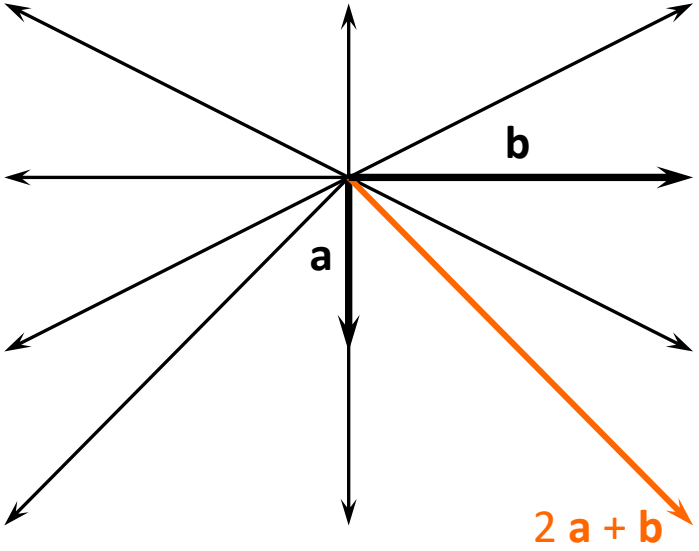



All the translations that map the crystal onto itself can be produced from a basis set: **a**, **b**, **c**

(**c** is perpendicular to the plane)

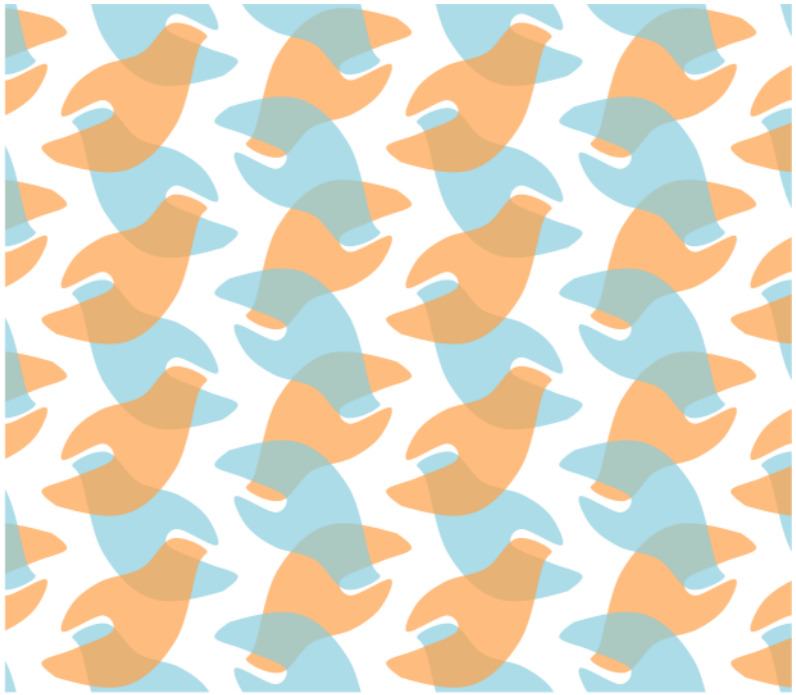
# Basis vectors

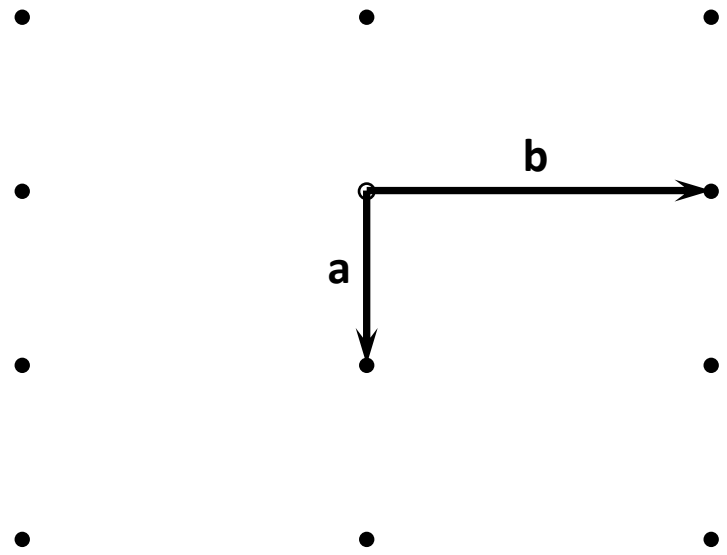





For example, the highlighted vector is expressed as 2 **a** + **b**.

# Lattice

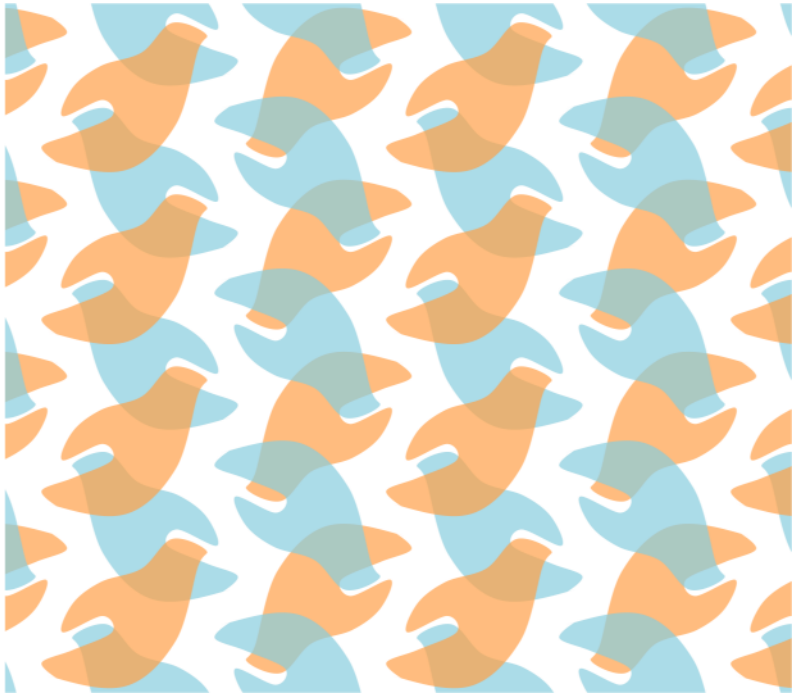


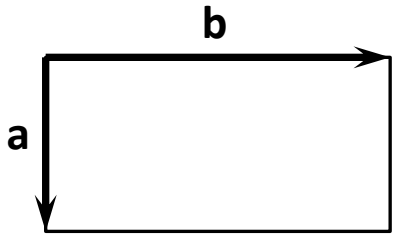



All the crystallographic translations can be represented as a lattice.

Translations, crystal lattice and unit cell live in a separate space. Coordinates in that space do not define coordinates of atoms but relation between equivalent atoms

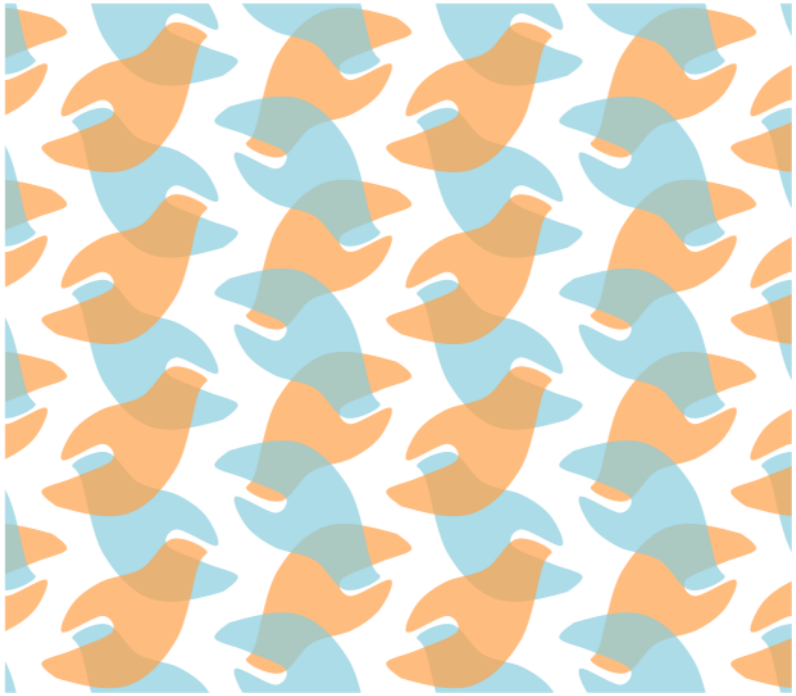
# Unit cell

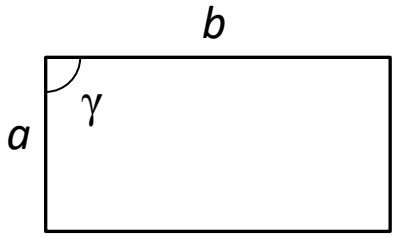





A compact representation of translational symmetry and base vectors.

# Unit cell

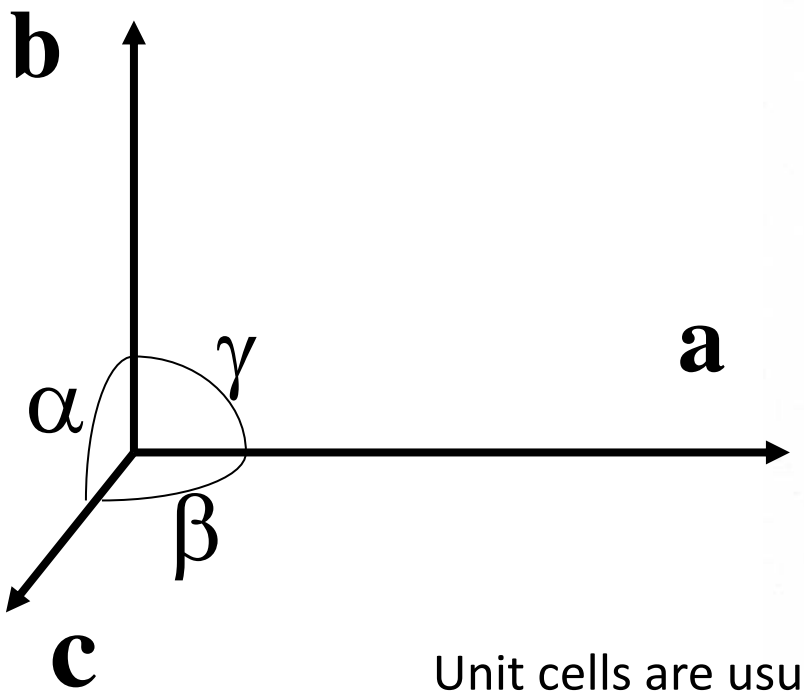


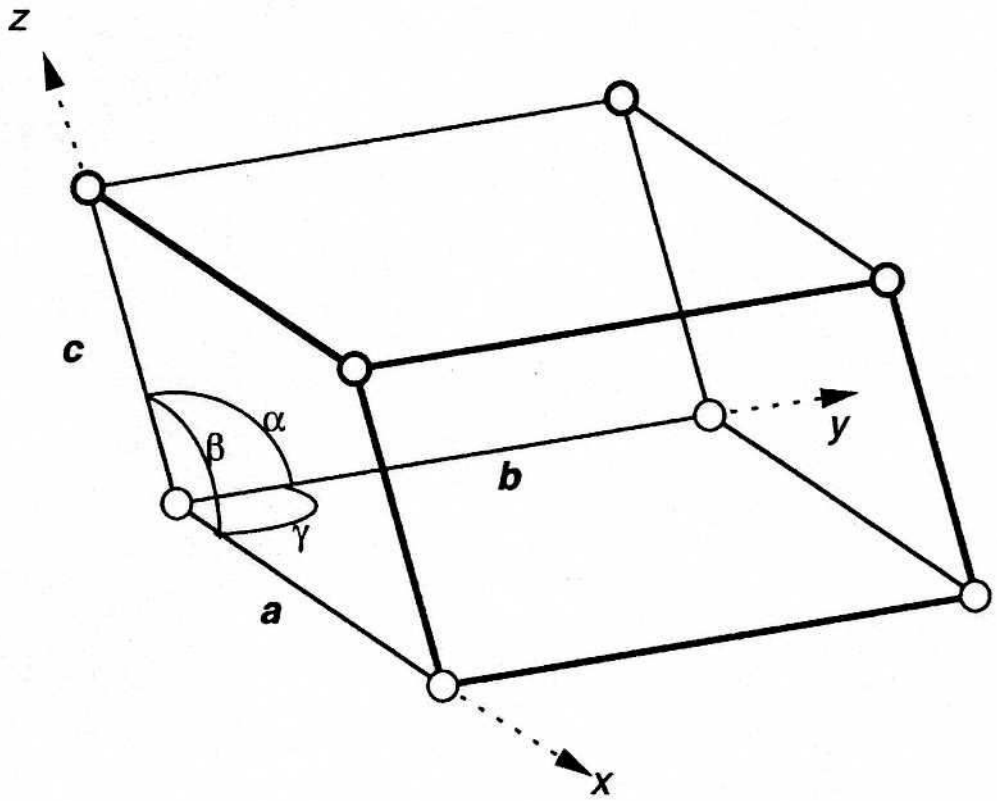



Can be fully characterised by six numbers
(the third dimension is not shown here)

# Unit cell parameters (3D view)

Translation symmetry is defined by three base vectors **a**, **b**, and **c**.

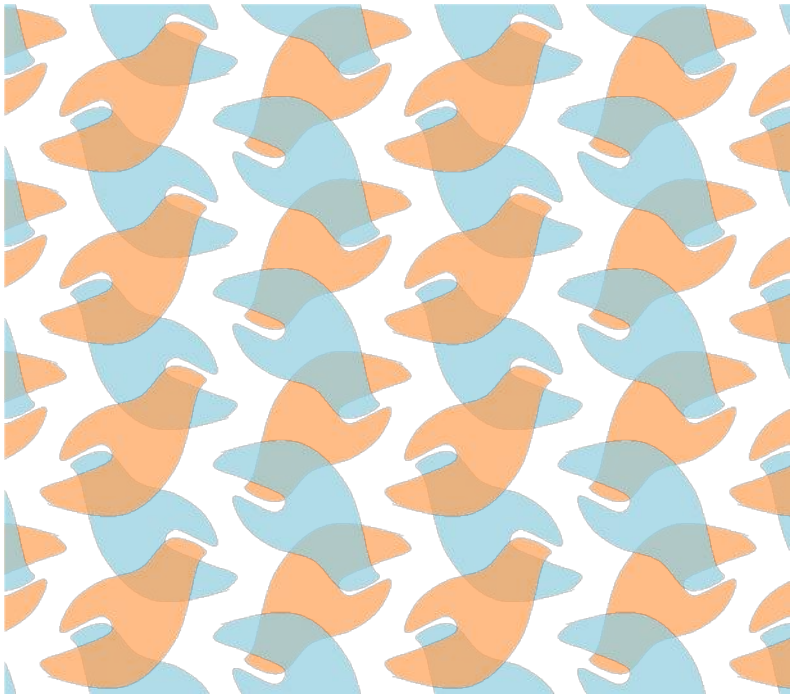


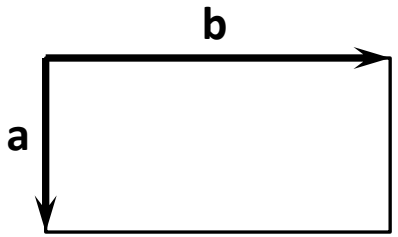




Unit cells are usually defined in terms of the *lengths* of these vectors and angles between them. For example,

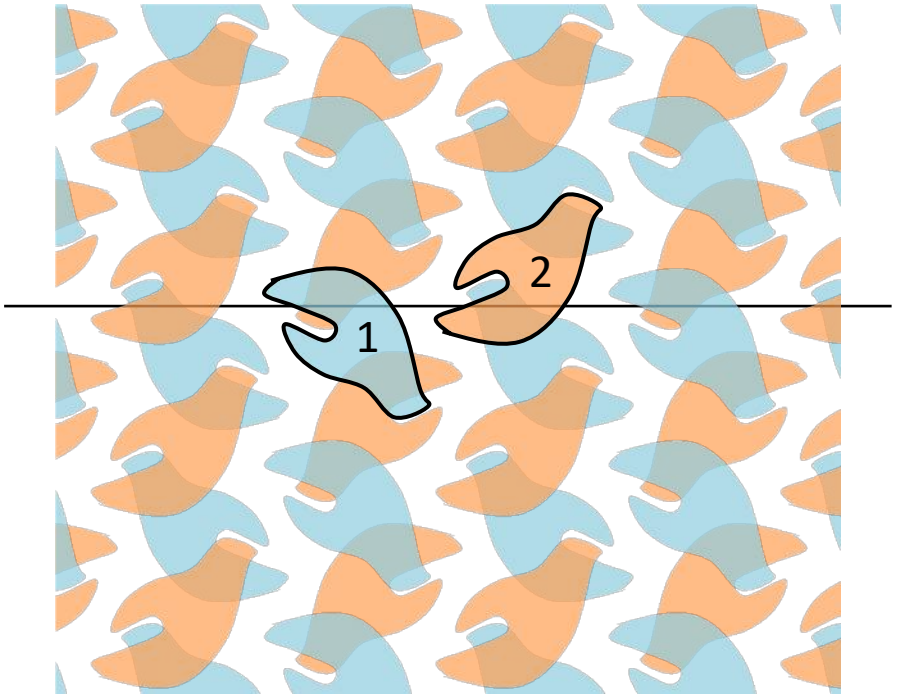
a=94.2Å, b=72.6Å, c=30.1Å, $\alpha$=90°, $\beta$=102.1°, $\gamma$=90°.

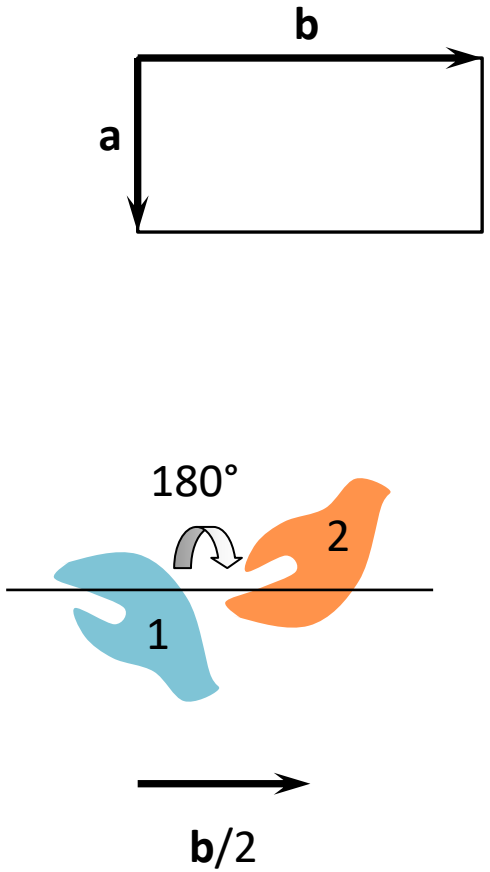
# Back to example



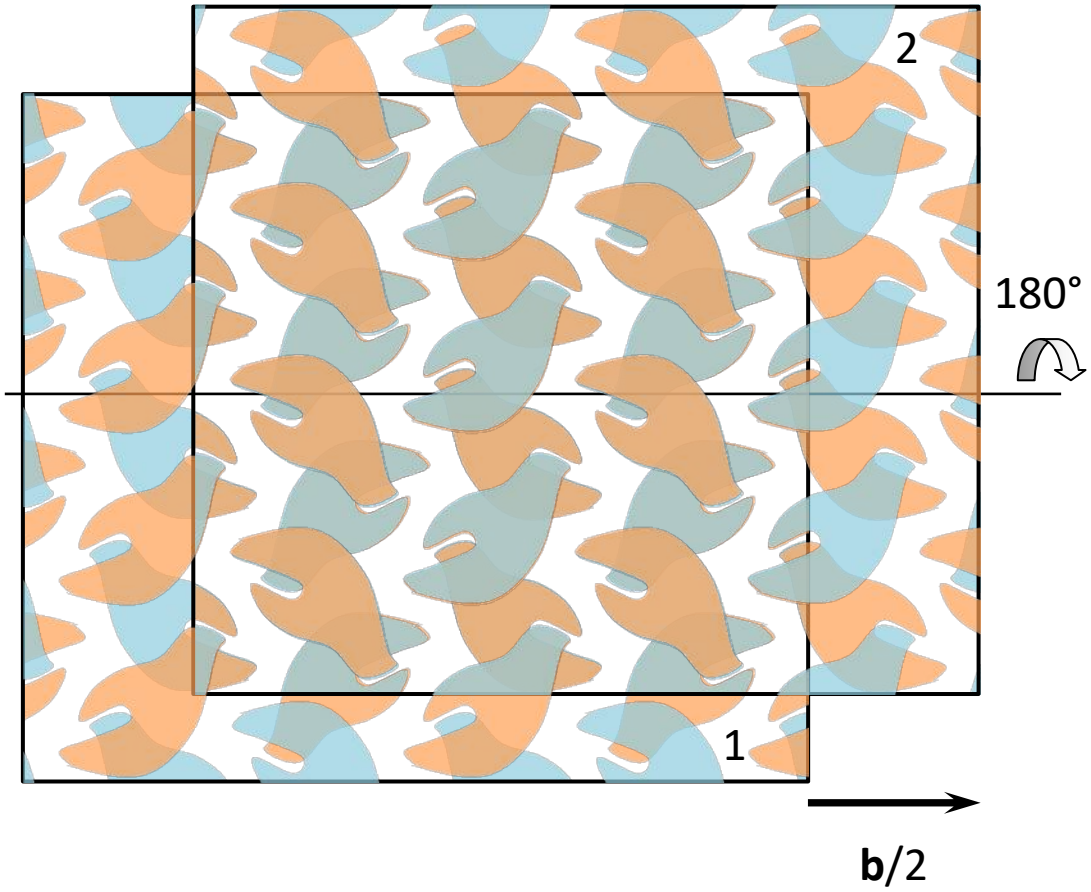


# Screw rotation



# Screw rotation axis





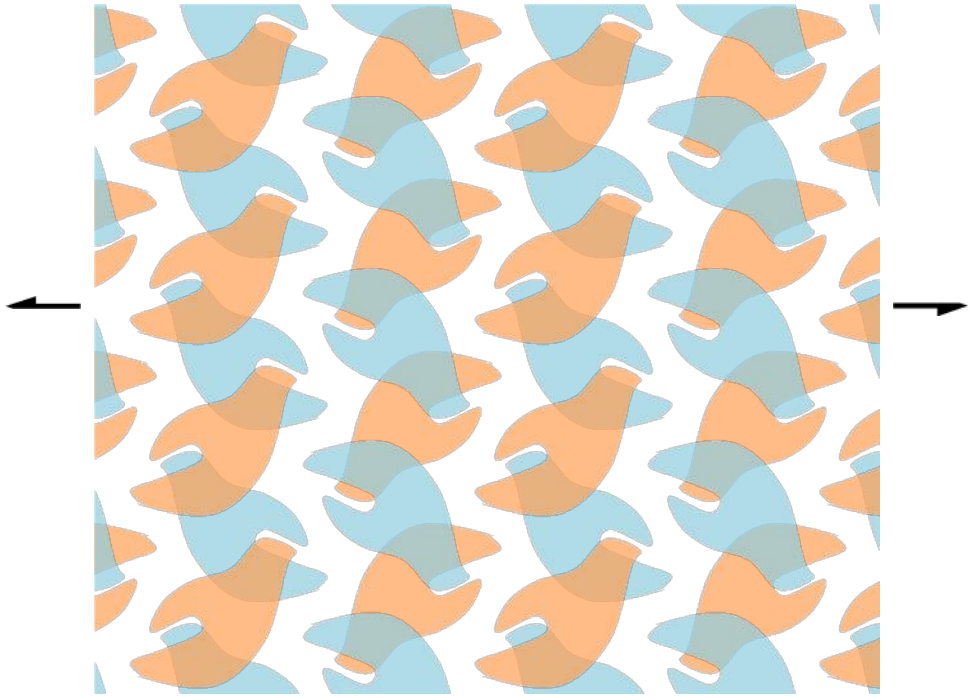
Operation 1->2 maps the whole crystal onto itself:

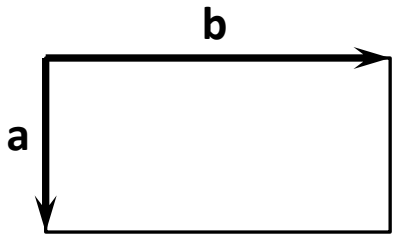
this is a crystallographic operation

The axis is a crystallographic symmetry element,

it can be mapped into the structure

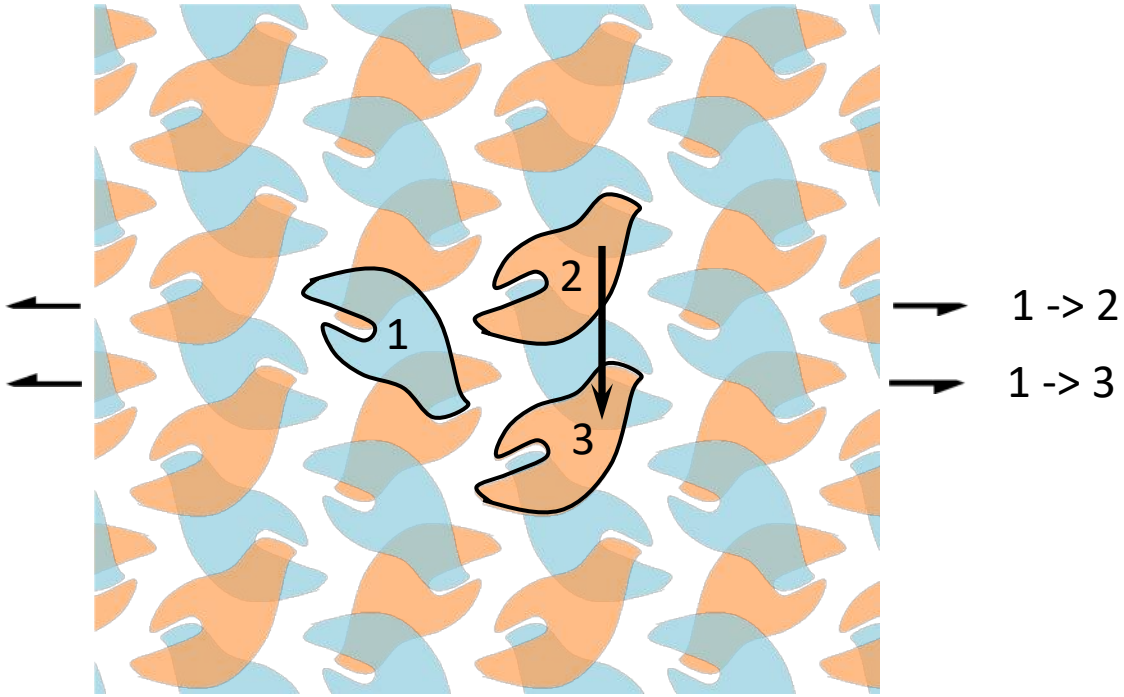
# Screw rotation - symbol

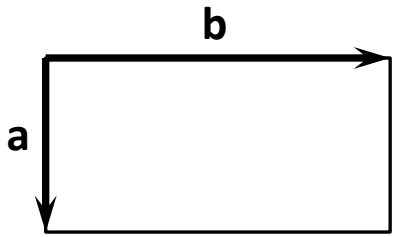





$2_1$ (plane of figure):

# Screw rotation - repeats

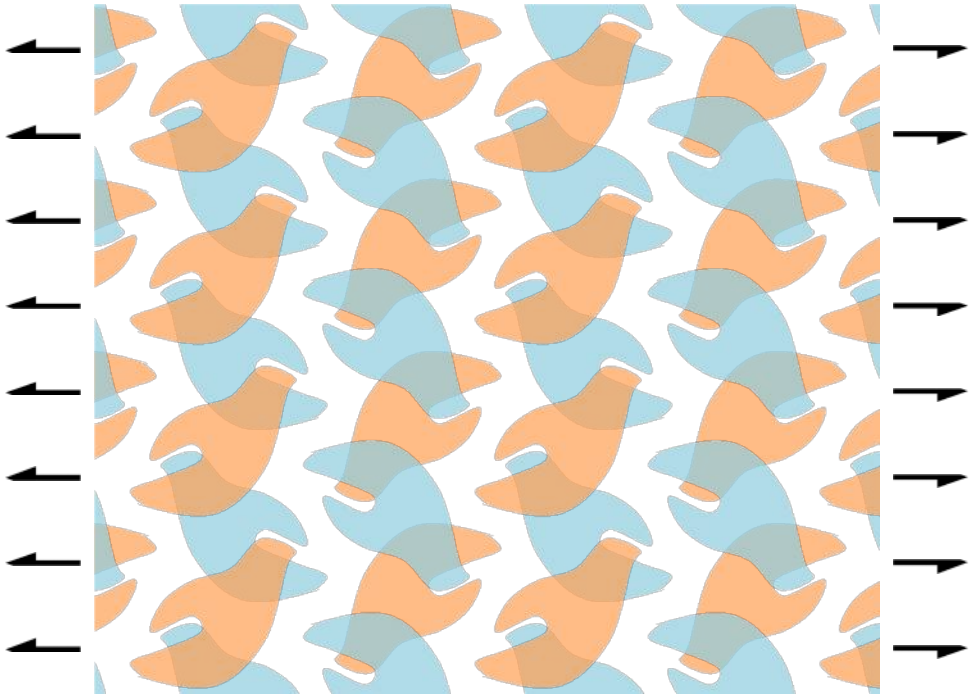



action of top axis
×
translation **a**
=
action of bottom axis

(elements of a group)

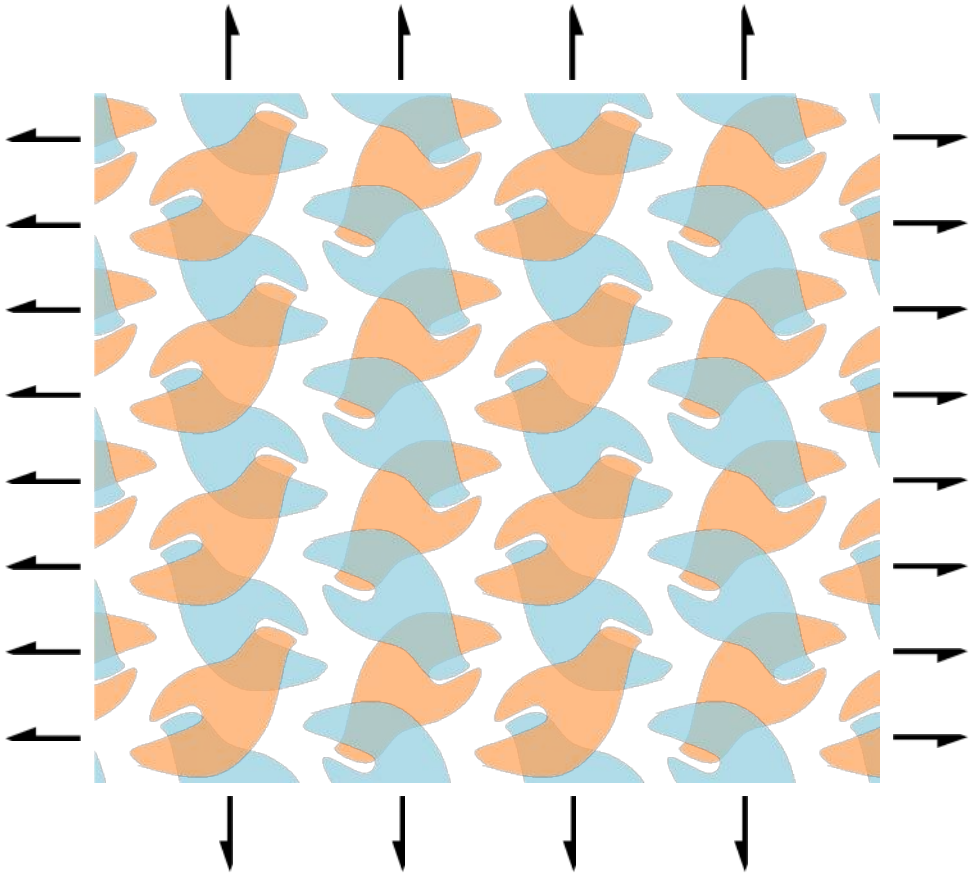
# Screw rotation 1 - repeats

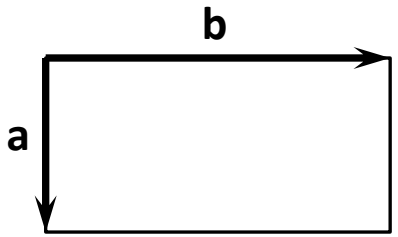



$2_1$ (plane of figure): ← →

Also repeated in 3d dimension with offset of ½ **c**

# Screw rotations parallel to **a** and **b**

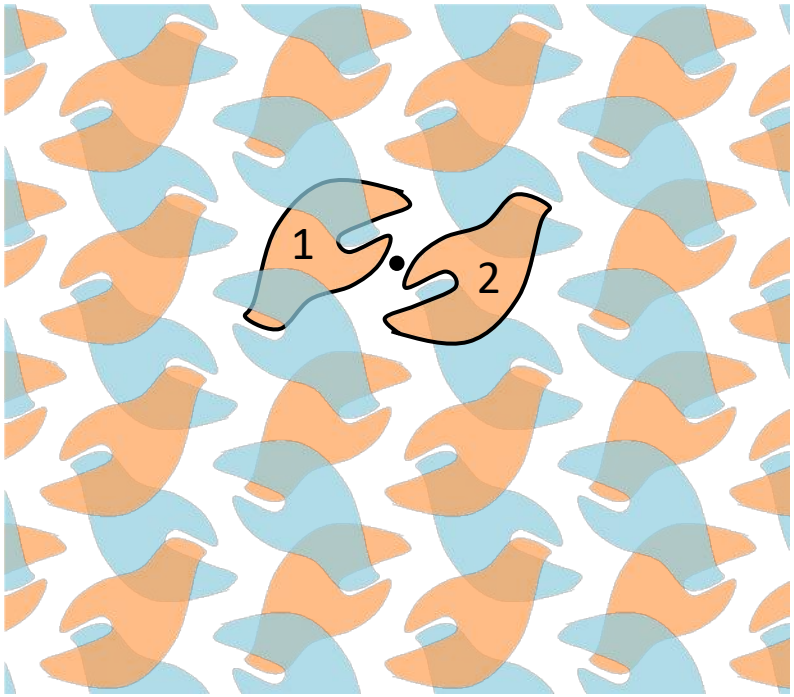


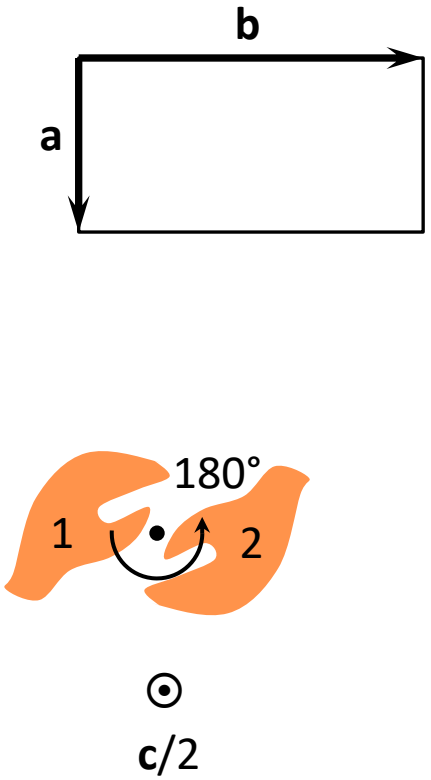



$2_1$ (plane of figure): ← →

Series of $2_1$ axes offset by
½ unit cell from each other.

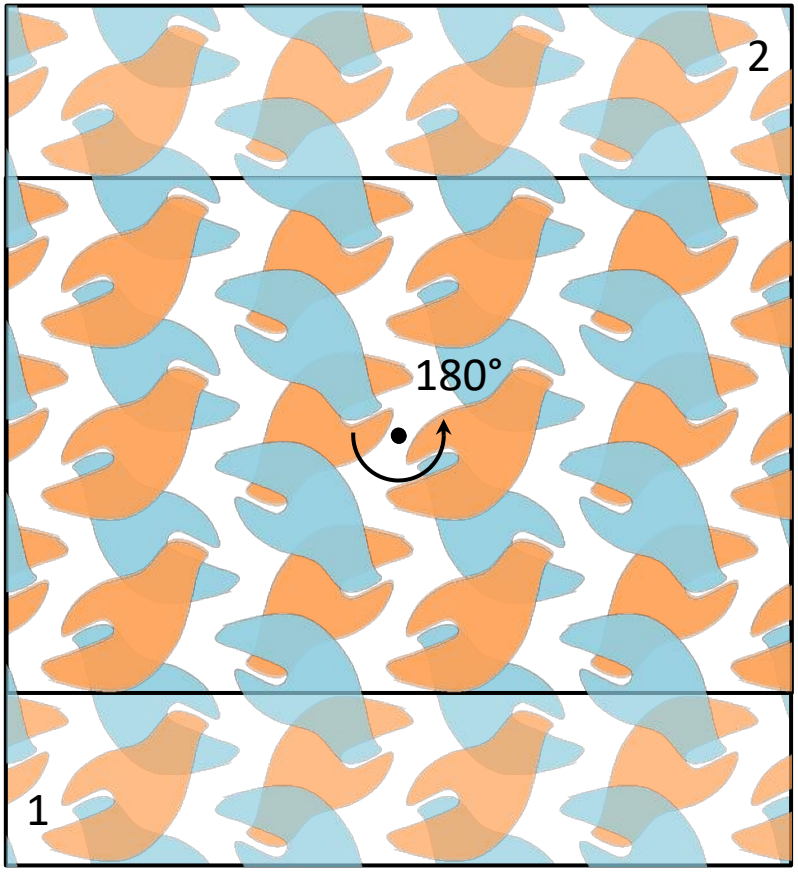
# Screw rotation – into plane



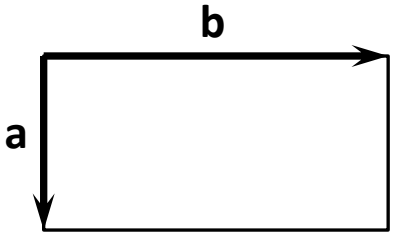




A rotation of 180° with a translation of ½ unit cell from the figure.

# Screw rotation 3 is global




⊙
**c**/2



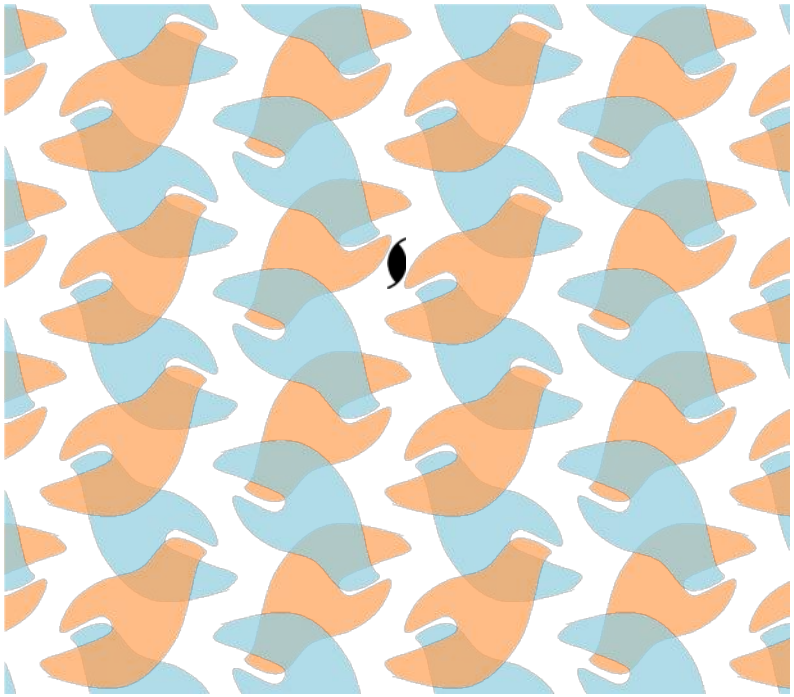

Screw rotation 3 maps the whole crystal onto itself:

this is a crystallographic operation

The rotation axis is a crystallographic symmetry element,

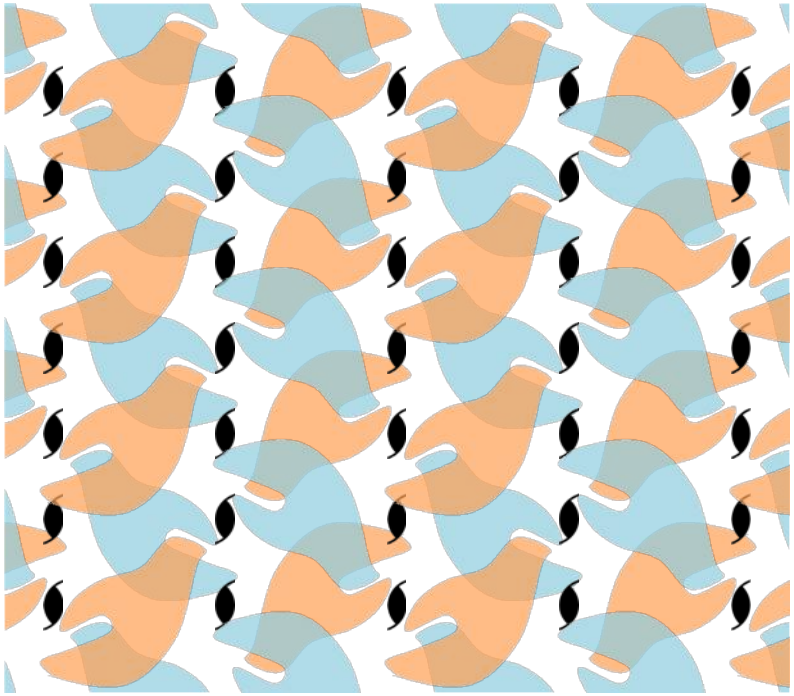
it can be mapped into the structure

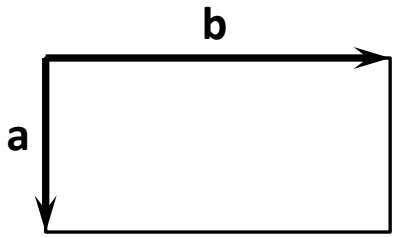
# Screw rotation 3 - symbol




$2_1$ (along view):

# Screw rotation 3 - repeats

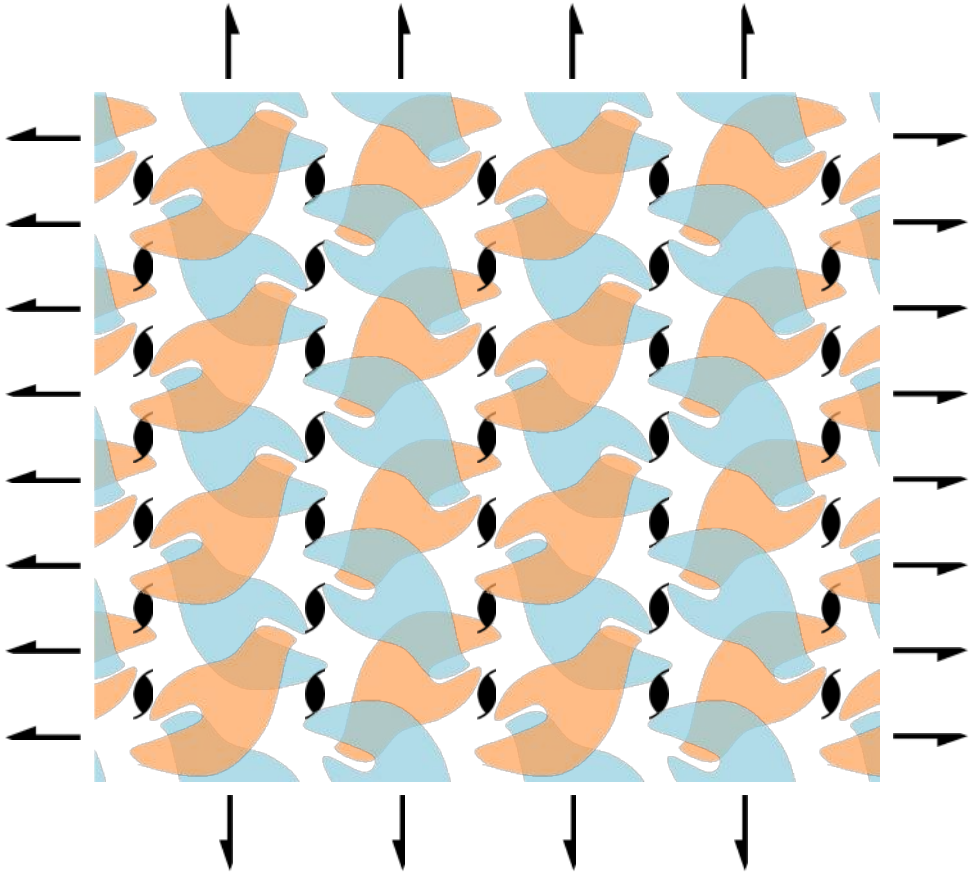


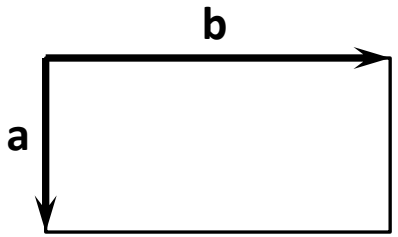



$2_1$ (along view):

As for the in-plane axes, there are repeated axes into the plane

# All axes together



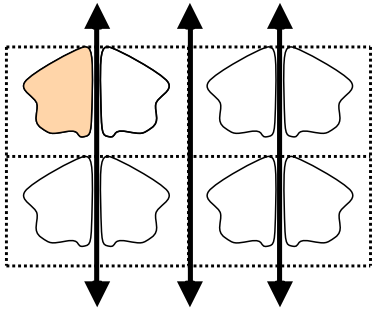



$2_1$ (plane of figure): 

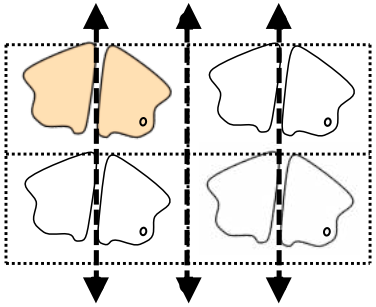
$2_1$ (along view): 

we have built
a space group

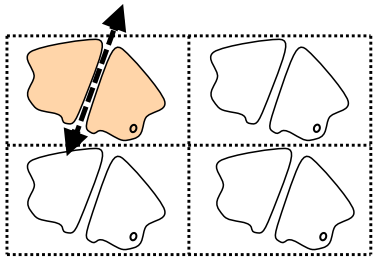
# Crystallographic Symmetry, Pseudosymmetry and Non-Crystallographic Symmetry (NCS)



Crystallographic symmetry
- symmetry is **global** and **exact**

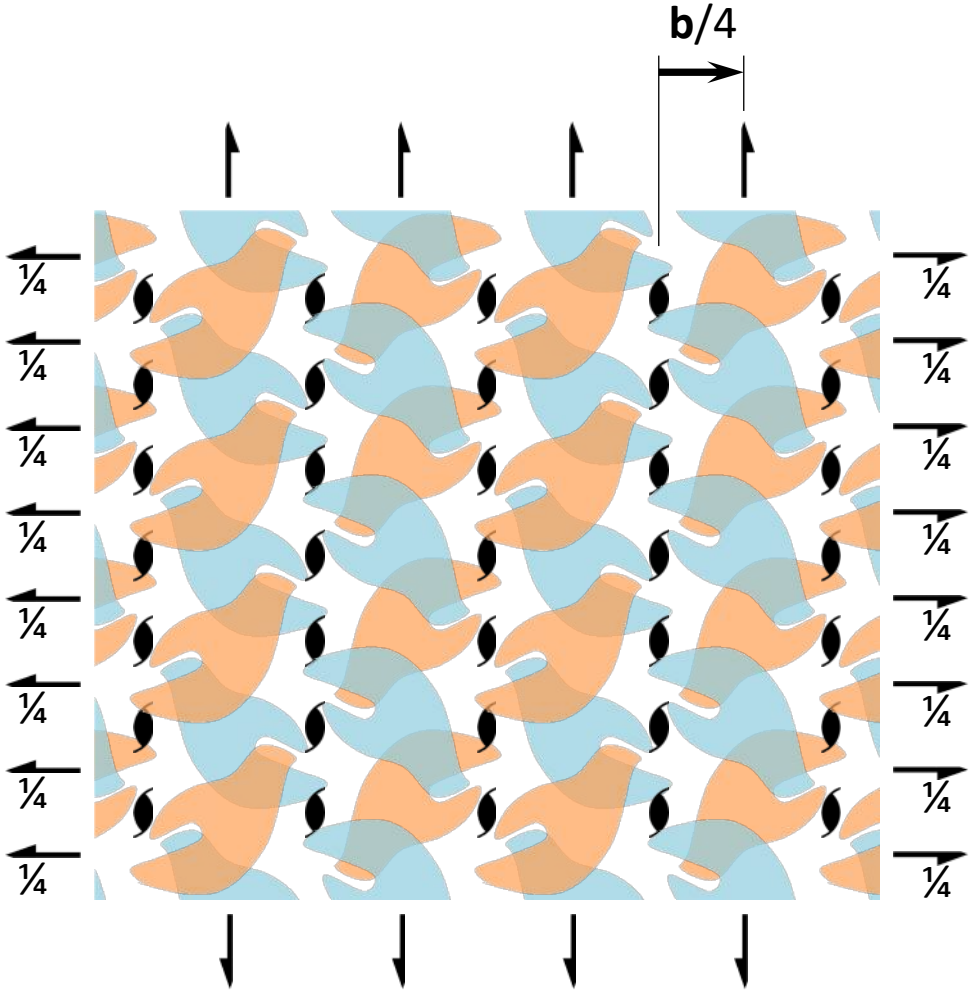


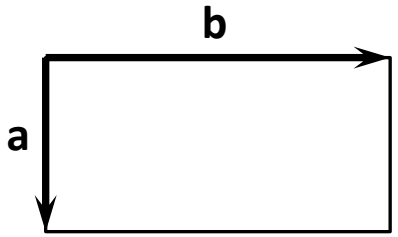
Pseudosymmetry (a limiting case of NCS)
- symmetry is **global** and **approximate**



Generic Non-Crystallographic Symmetry (NCS):
- symmetry is **local** and **approximate**

# Relative positions of axes




$2_1$ (plane of figure):

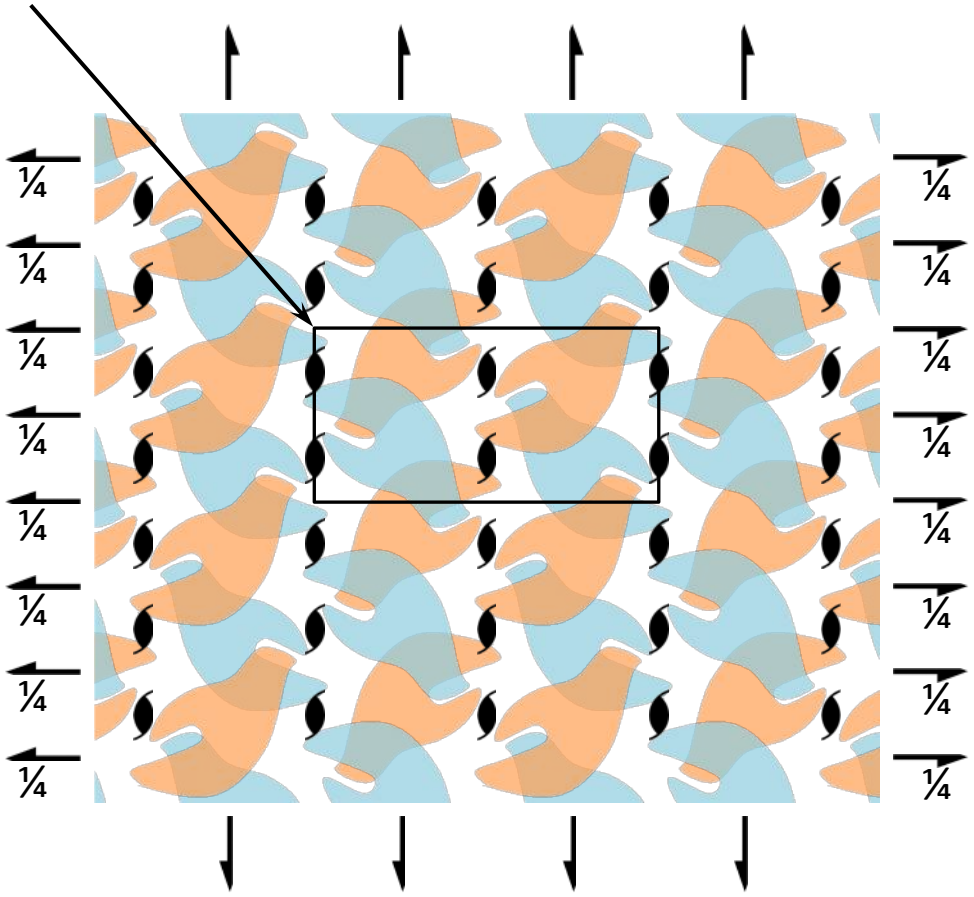
$2_1$ (along view):

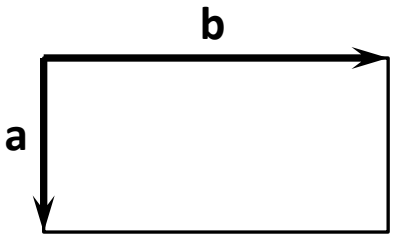
The adjacent axes running in different directions are offset by ¼ of corresponding base vector.

The horizontal ¼ indicates a offset of (½ n + ¼) **c** into the figure.

# Choice of origin is a convention. Notation

The origin (x=0, y=0, z=0)




$2_1$ (plane of figure): ← →

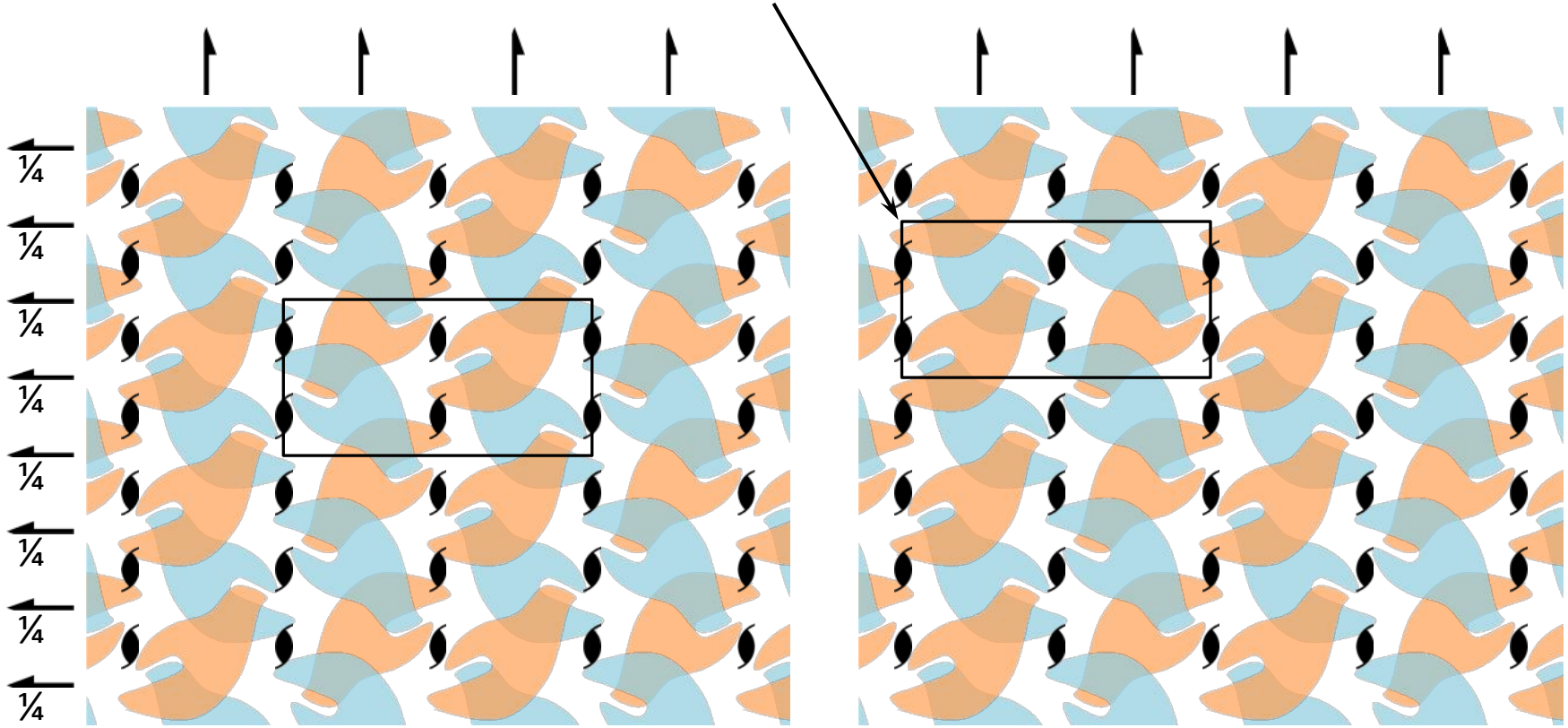
$2_1$ (along view): ʃ

The unit cell placed on picture with symmetry elements means a choice of origin.

is chosen to be equidistant from adjacent axes. Such a choice is a convention.

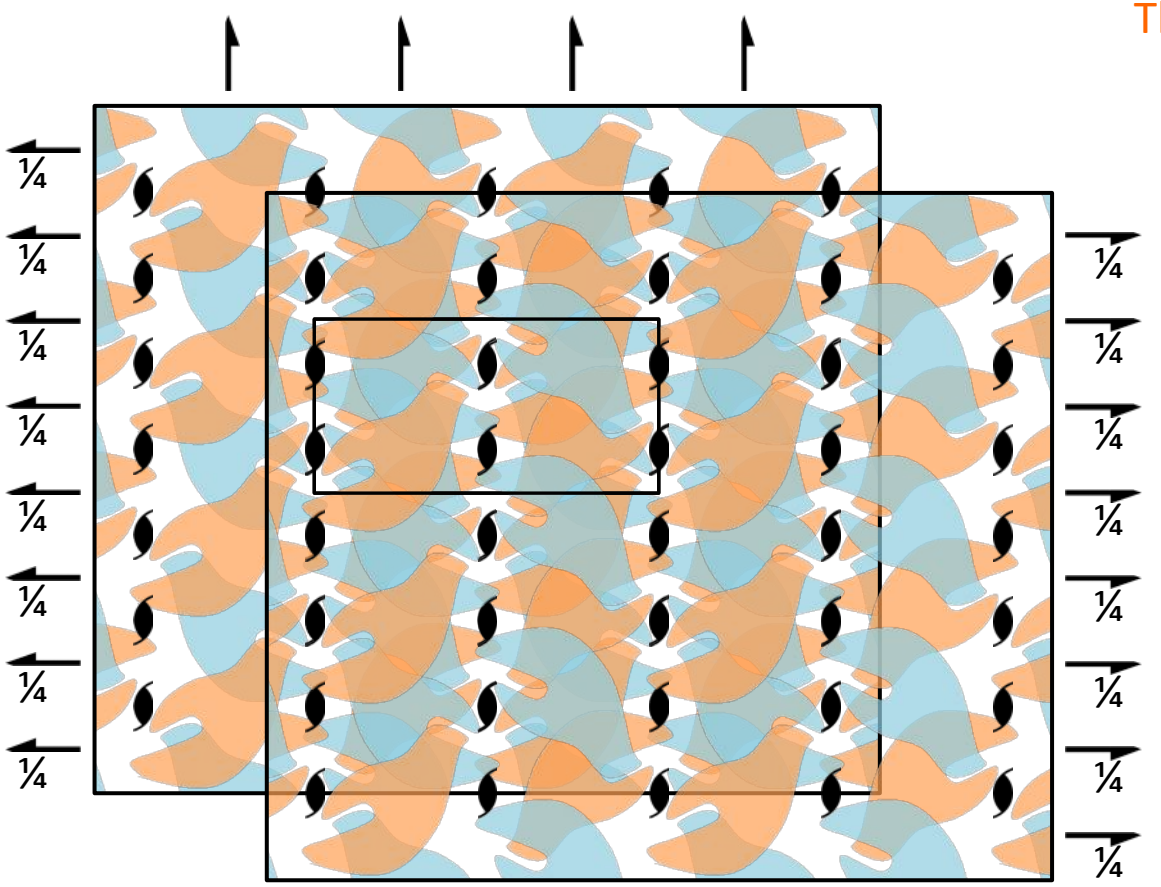
# Alternative origins

Choose a different origin following the same convention (equidistant from adjacent axes)



# Structures "solved in alternative origins"

Superpose two unit cells. Positions of axes match (requirement for convention).



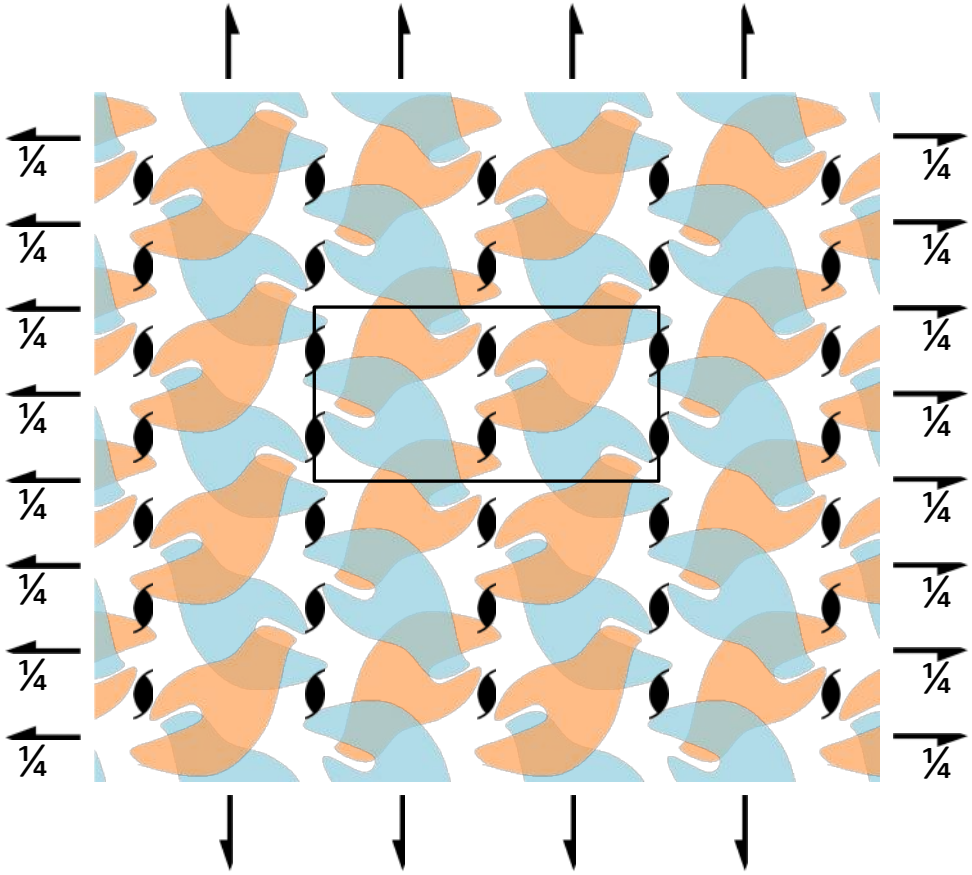

The structures do not match.

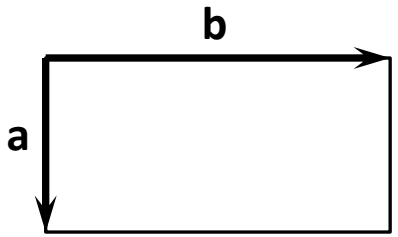
Conventions regarding the choice of crystallographic origin are expressed in terms of position relative to crystallographic axes.

Such a choice is not necessarily unique with respect to the structure.

Be conscious of "alternative" origins when e.g. comparing different MR solutions.

# Complete picture



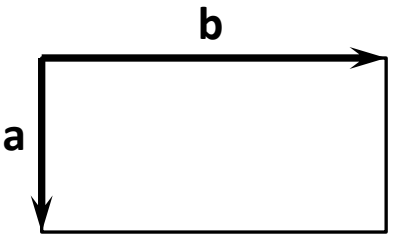

$2_1$ (plane of figure): ← →

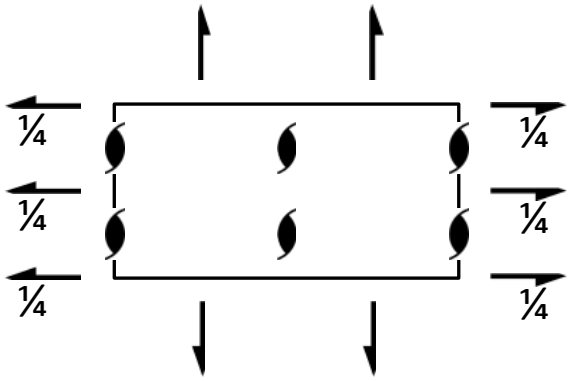
$2_1$ (along view): ❜

# Compact representation

$P2_12_12_1$

No. 19




$2_1$ (plane of figure):

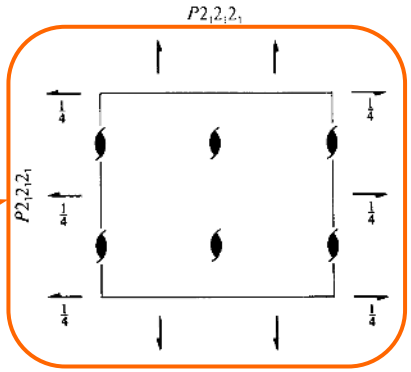
$2_1$ (along view):

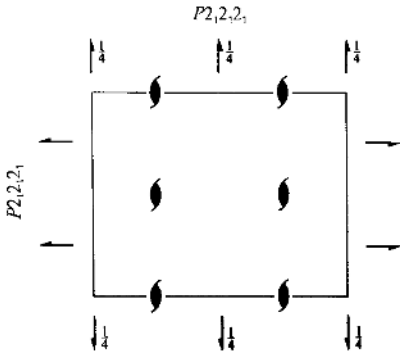
Scheme with symmetry axes -> space group symbol -> more info in International Tables
We will discuss space group symbols a bit later

# Space group representation in ITC-A

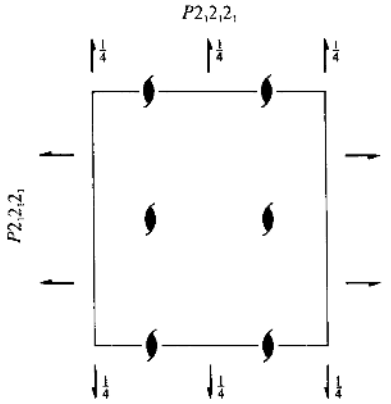
| | | | |
|---|---|---|---|
| $P2_12_12_1$ | $D_2^4$ | 222 | Orthorhombic |
| No. 19 | $P2_12_12_1$ | | Patterson symmetry $Pmmm$ |

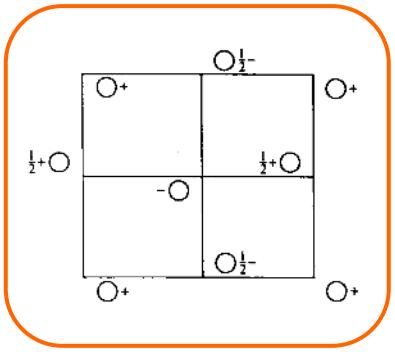
Location of symmetry elements




Two other projections are also shown for this space group




Set of equivalent points in general position.

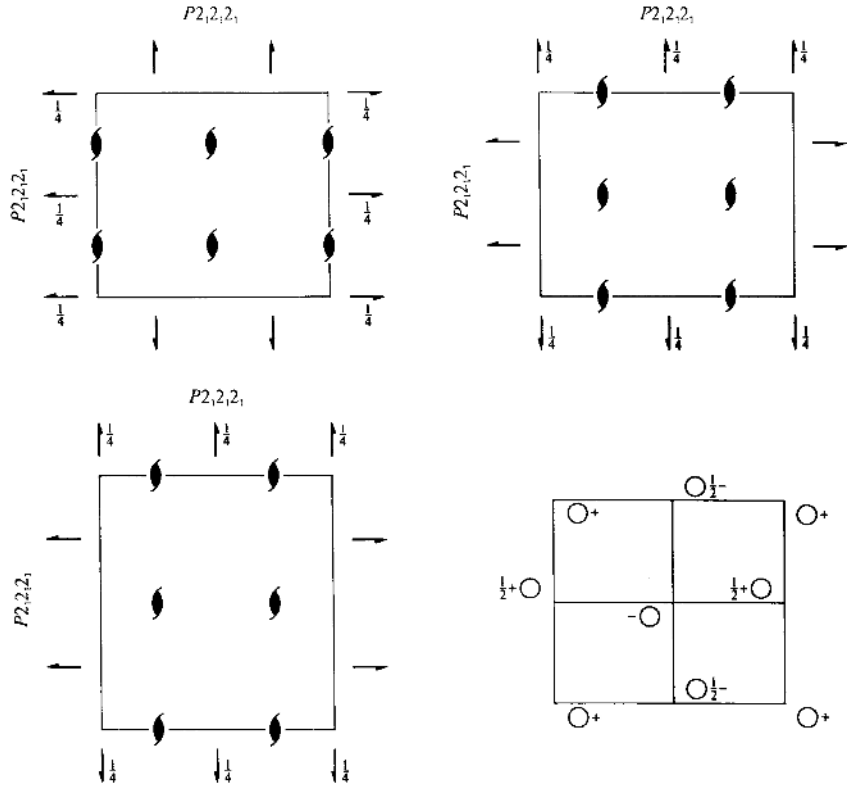
We will be looking at "molecular wallpaper" instead

# Space group representation in ITC-A

Crystal system

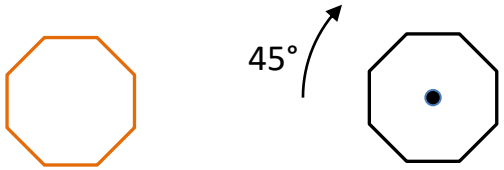
$P2_12_12_1$ $D_2^4$ 222 Orthorhombic

No. 19 $P2_12_12_1$ Patterson symmetry $Pmmm$



# Rotational symmetry

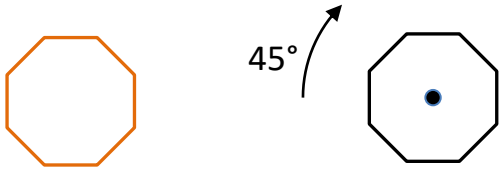
An **N**-fold rotational symmetry implies that if a rotation of 360°/**N** degrees is applied, the transformed object is identical to the original.




This object has **8**-fold rotational symmetry

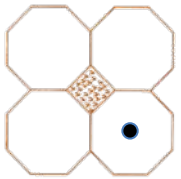
# Rotational symmetry

An **N**-fold rotational symmetry implies that if a rotation of 360°/**N** degrees is applied, the transformed object is identical to the original.

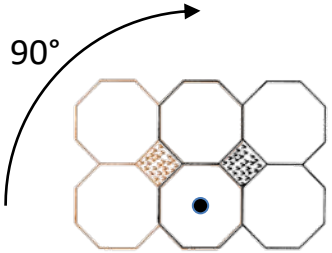



This object has **8**-fold rotational symmetry

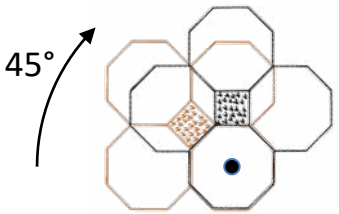
The only rotational symmetries possible in a **crystal** are **2**, **3**, **4** and **6**.



Wallpaper: objects with **8**-fold symmetry



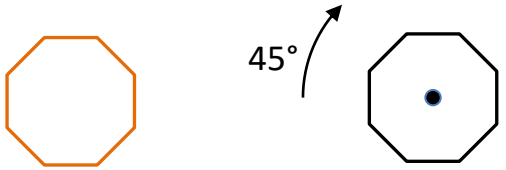

**4**-fold rotational **crystal** symmetry




**8**-fold rotational **crystal** symmetry is **impossible**

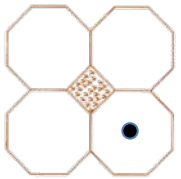
# Rotational symmetry

An **N**-fold rotational symmetry implies that if a rotation of 360°/**N** degrees is applied, the transformed object is identical to the original.

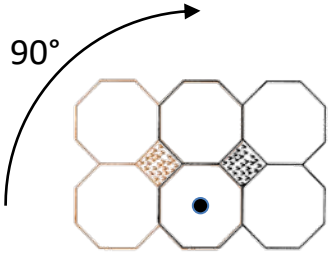



This object has **8**-fold rotational symmetry

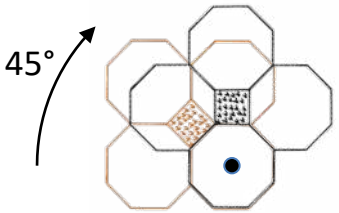
The only rotational symmetries possible in a **crystal** are **2**, **3**, **4** and **6**.



Wallpaper: objects with **8**-fold symmetry




**4**-fold rotational **crystal** symmetry



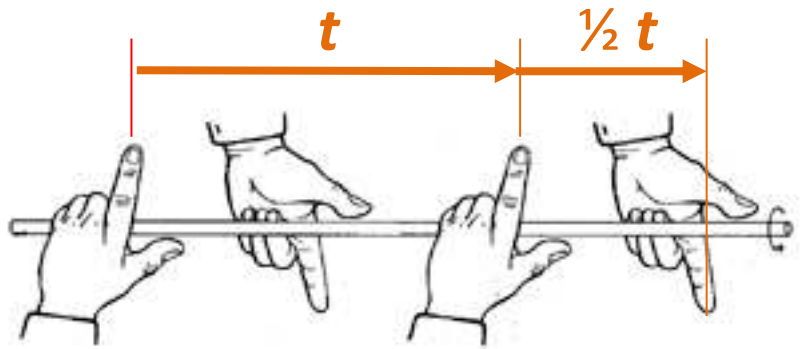

**8**-fold rotational **crystal** symmetry is **impossible**

45° rotation is a **Non-Crystallographic Symmetry** (NCS)

# Screw axes

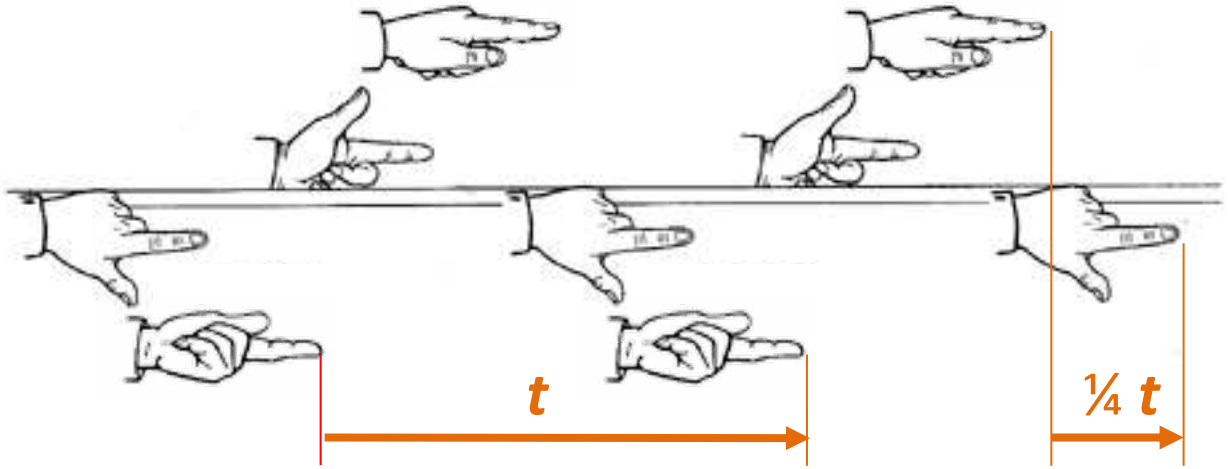
- Rotate clockwise about an axis (1, 2, 3, 4 or 6-fold rotation)
- Translate along this axis by a fraction of the shortest crystallographic translation along the rotation axis

$2_1$




translation of ½ *t* per 180° rotation

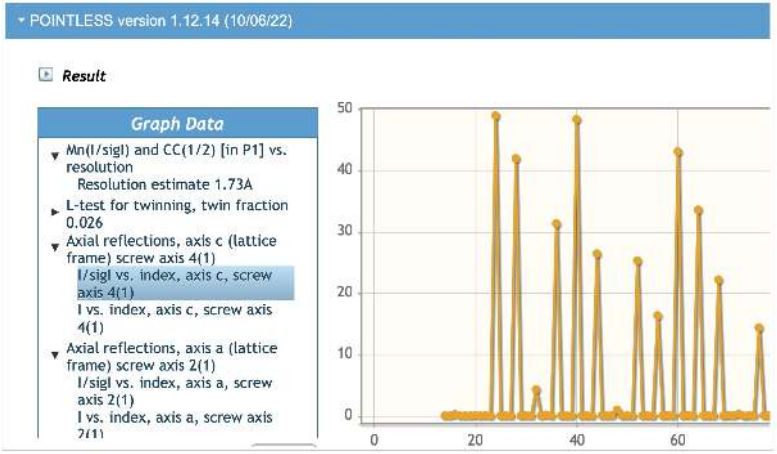
$4_1$



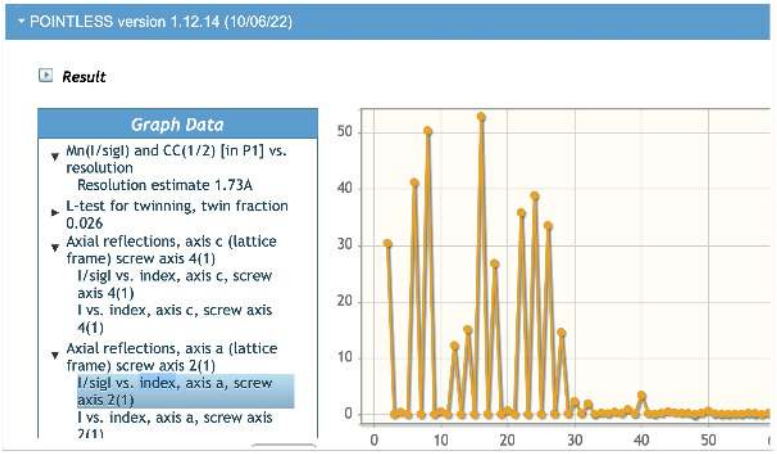

translation of ¼ *t* per 90° rotation

# Screw axes: systematic absences

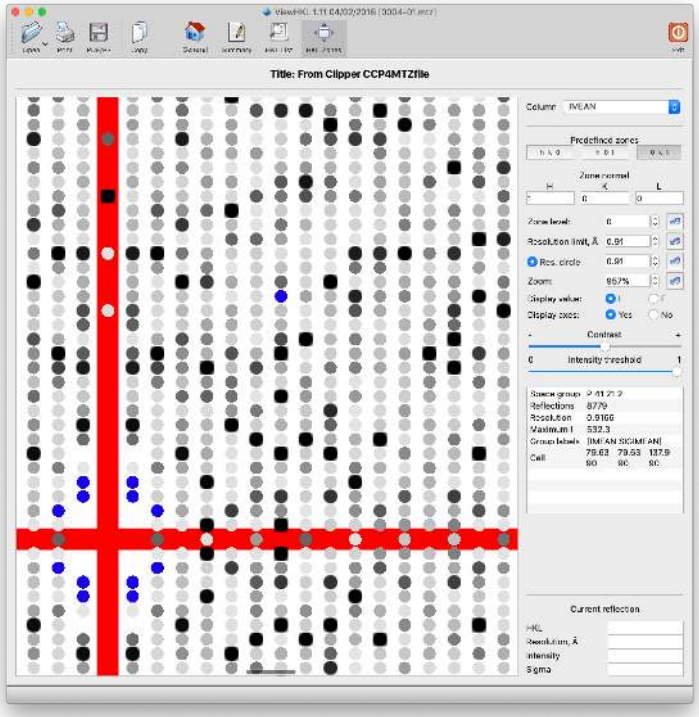
h = k = 0: every fourth l strong: $4_1$ or $4_3$




k = l = 0: every second h strong: $2_1$



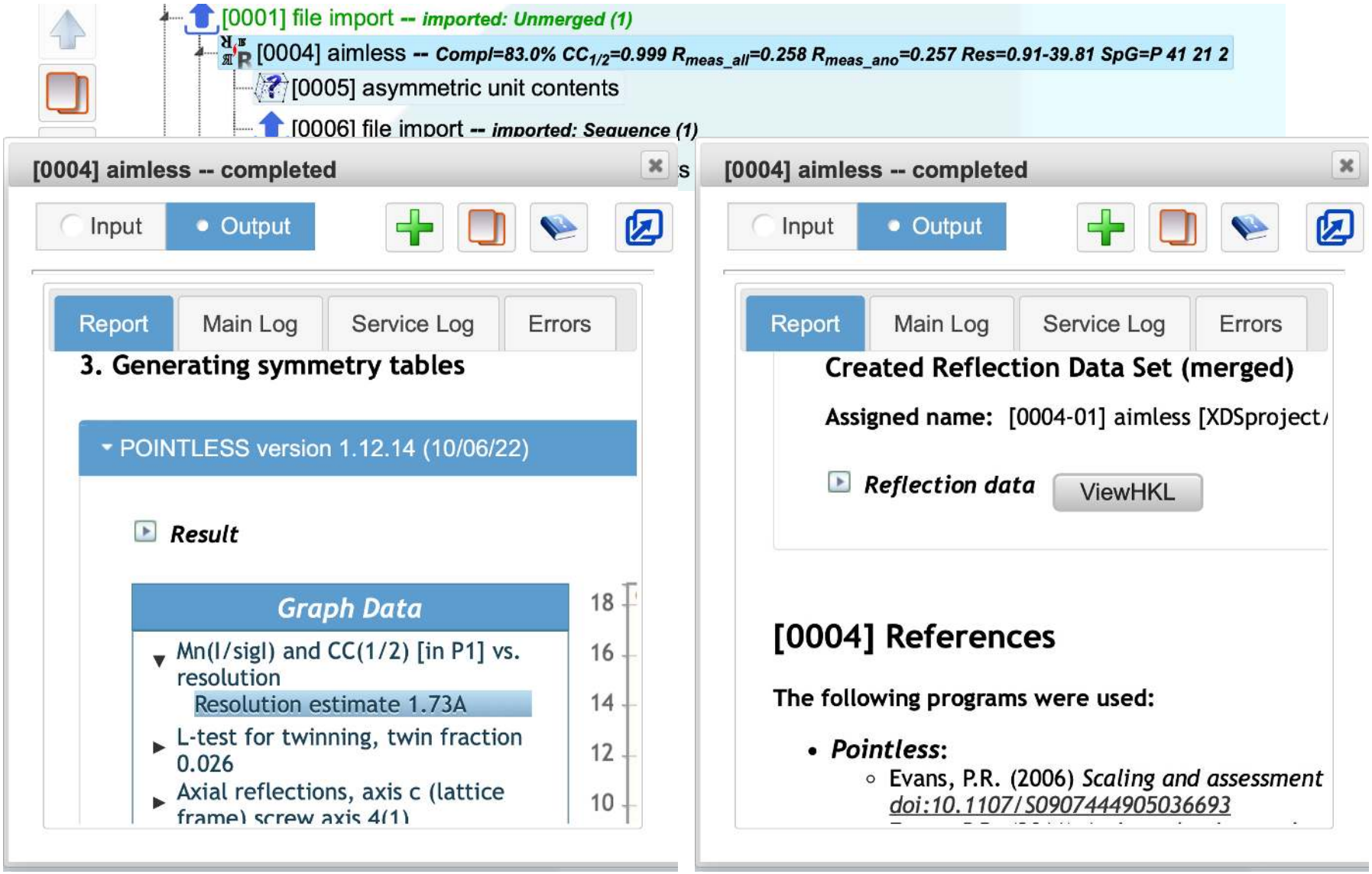

$4_1$ or $4_3$




$2_1$

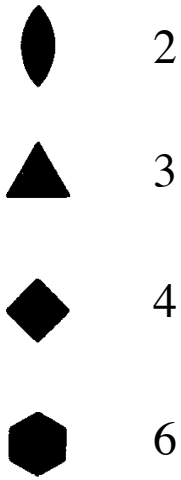
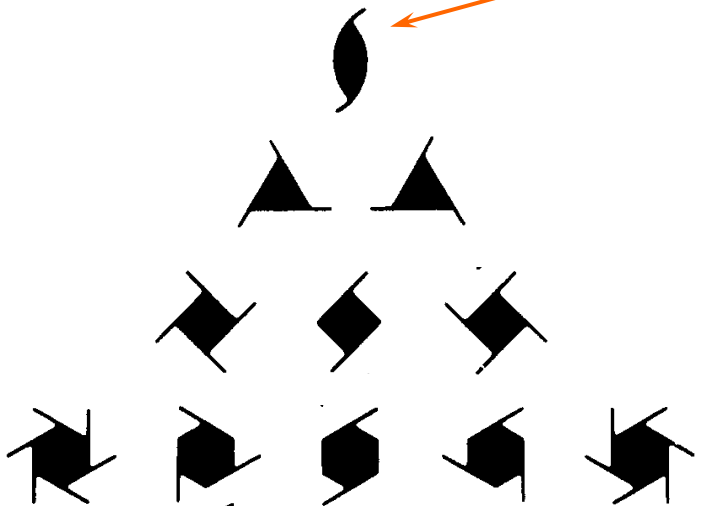
- might not be very clear with noisy data
- enantiomorph not resolved: $P4_12_12$ or $P4_32_12$

# Screw axes: systematic absences: CCP4Cloud



# Symmetry elements allowed in chiral structures

Apart from the identity and translations, macromolecular crystals can only contain the following symmetry elements:

| Proper Rotations | Screw Rotations |
|---|---|
|  2, 3, 4, 6 |  $2_1$, $3_1$, $3_2$, $4_1$, $4_2$, $4_3$, $6_1$, $6_2$, $6_3$, $6_4$, $6_5$ |

$P2_12_12_1$ example

# Symmetry elements disallowed by chiral centres

Small molecules also face other symmetry operations

- Mirror plane **m**
- Glide planes **a**, **b**, **c**, **n** or **d**: reflection across plane followed by translation parallel to plane along **a**, **b**, **c**, **face diagonal** or **body diagonal**, respectively
- Rotation – inversion $\bar{1}, \bar{3}, \bar{4}, \bar{6}$: a rotation $\bar{1}$ followed by inversion

# Space groups

- All possible combinations of symmetry elements => 230 space groups
- Because protein and nucleic acid molecules are chiral, there are only 65 “biological” space groups.
- Space groups are divided on 7 crystal system based on
  - the presence of  symmetry elements of a certain order (6, 4, 3, 2)
  - the number of different orientations of these elements

# Crystal Systems

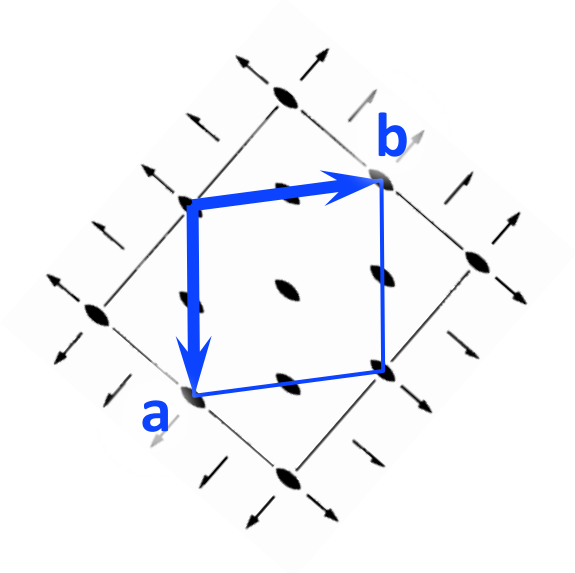
| **Crystal System** | **Characteristic symmetry elements** | Convention | Bravais lattices | Constraints on unit cell parameters |
|---|---|---|---|---|
| 1. Triclinic | Translations only | | 1. Primitive (*P*) | $\alpha = \gamma = 90°$ |
| 2. Monoclinic | 2-fold axes, all parallel | along **b** | 2. Primitive (*P*)<br>3. Base-Centered (*C*) | $\alpha = \gamma = 90°$ |
| 3. Orthorhombic | 2-fold axes in three perpendicular directions<br>(example) | along **a**, **b** and **c** | 4. Primitive (*P*)<br>5. Base-Centered (*C*)<br>6. Body-Centered (*I*)<br>7. Face-Centered (*F*) | $\alpha = \beta = \gamma = 90°$ |
| 4. Tetragonal | 4-fold axes, all parallel | along **c** | 8. Primitive (*P*)<br>9. Body-Centered (*I*) | $a = b$<br>$\alpha = \beta = \gamma = 90°$ |
| 5. Trigonal | 3-fold axes, all parallel | along **c** | 10. Primitive (*P*)<br>11. Rhombohedral (*R* / *H*) | $a = b$<br>$\alpha = \beta = 90°;\ \gamma = 120°$ |
| 6. Hexagonal | 6-fold axes, all parallel | along **c** | 10. Primitive (*P*) | $a = b$<br>$\alpha = \beta = 90°;\ \gamma = 120°$ |
| 7. Cubic | 3-fold axes in four different orientations | along body diagonals | 12. Primitive (*P*)<br>13. Body-Centered (*I*)<br>14. Face-Centered (*F*) | $a = b = c$<br>$\alpha = \beta = \gamma = 90°$ |

# Crystal Systems

| **Crystal System** | **Characteristic symmetry elements** | **Convention** | **Bravais lattices** | **Constraints on unit cell parameters** |
|---|---|---|---|---|
| 1. Triclinic | Translations only | | 1. Primitive (*P*) | $\alpha = \gamma = 90°$ |
| 2. Monoclinic | 2-fold axes, all parallel | along **b** | 2. Primitive (*P*)<br>3. Base-Centered (*C*) | $\alpha = \gamma = 90°$ |
| 3. Orthorhombic | 2-fold axes in three perpendicular directions | along **a**, **b** and **c** | 4. Primitive (*P*)<br>5. Base-Centered (*C*)<br>6. Body-Centered (*I*)<br>7. Face-Centered (*F*) | $\alpha = \beta = \gamma = 90°$ |
| 4. Tetragonal | 4-fold axes, all parallel | along **c** | 8. Primitive (*P*)<br>9. Body-Centered (*I*) | $a = b$<br>$\alpha = \beta = \gamma = 90°$ |
| 5. Trigonal | 3-fold axes, all parallel | along **c** | 10. Primitive (*P*)<br>11. Rhombohedral (*R* / *H*) | $a = b$<br>$\alpha = \beta = 90°;\ \gamma = 120°$ |
| 6. Hexagonal | 6-fold axes, all parallel | along **c** | 10. Primitive (*P*) | $a = b$<br>$\alpha = \beta = 90°;\ \gamma = 120°$ |
| 7. Cubic | 3-fold axes in four different orientations | along body diagonals | 12. Primitive (*P*)<br>13. Body-Centered (*I*)<br>14. Face-Centered (*F*) | $a = b = c$<br>$\alpha = \beta = \gamma = 90°$ |

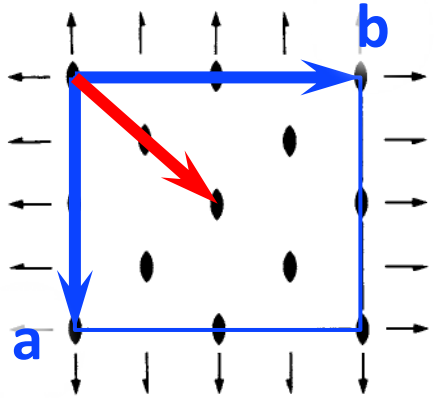
# *C*222: an example of a centred cell

If we were using
a primitive cell




2-fold axes are along face diagonals (non-conventional crystal setting)

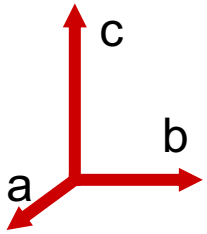
<u>Standard</u> setting;
C means additional translation ½ (**a** + **b**)

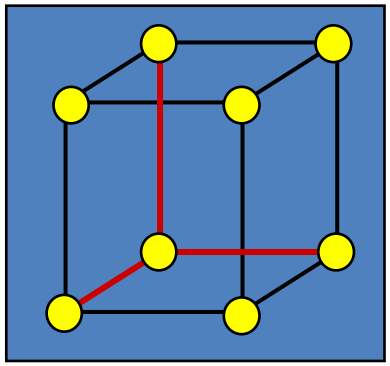



2-fold axes are along **a**, **b** and **c** (conventional setting)

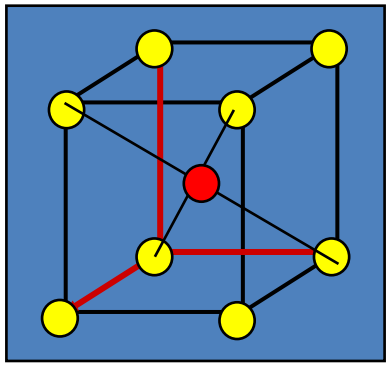
# Centred unit cells in pictures

Our convention dictates that direction(s) of rotation axes define **a**, **b** and **c**
As a result, the crystal lattice of some space groups contains "additional" nodes (red) that represent "additional" translations

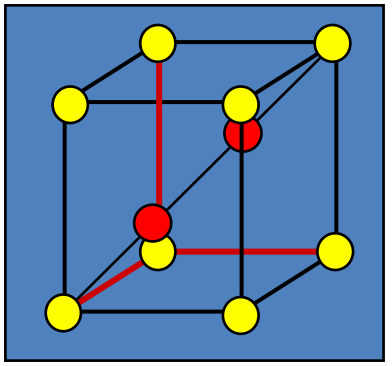


P – Primitive

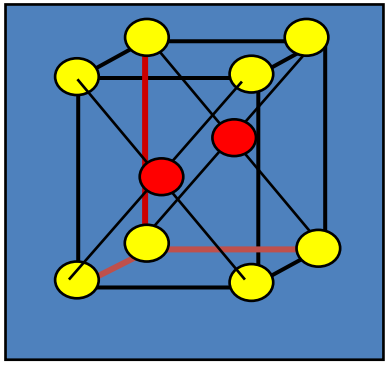


I – Body centred



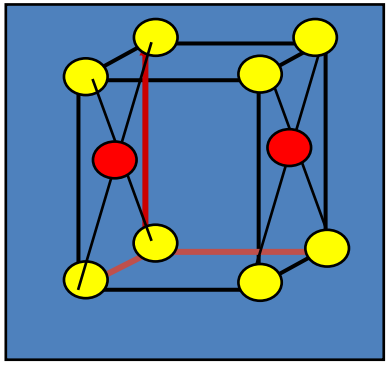
H – Hexagonal

(non-standard)

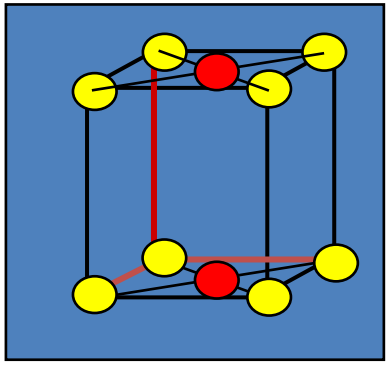


A – Face centred (A)

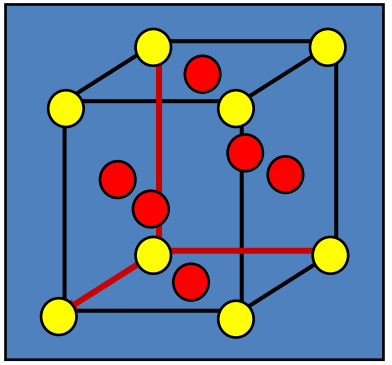
(non-standard)



B – Face centred (B)



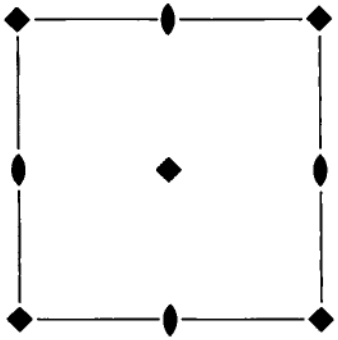
C – Face centred (C)



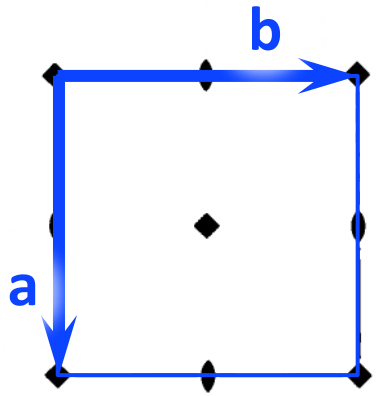
F – Face centred (all)

# *C*4: an example of a redundant space group symbol

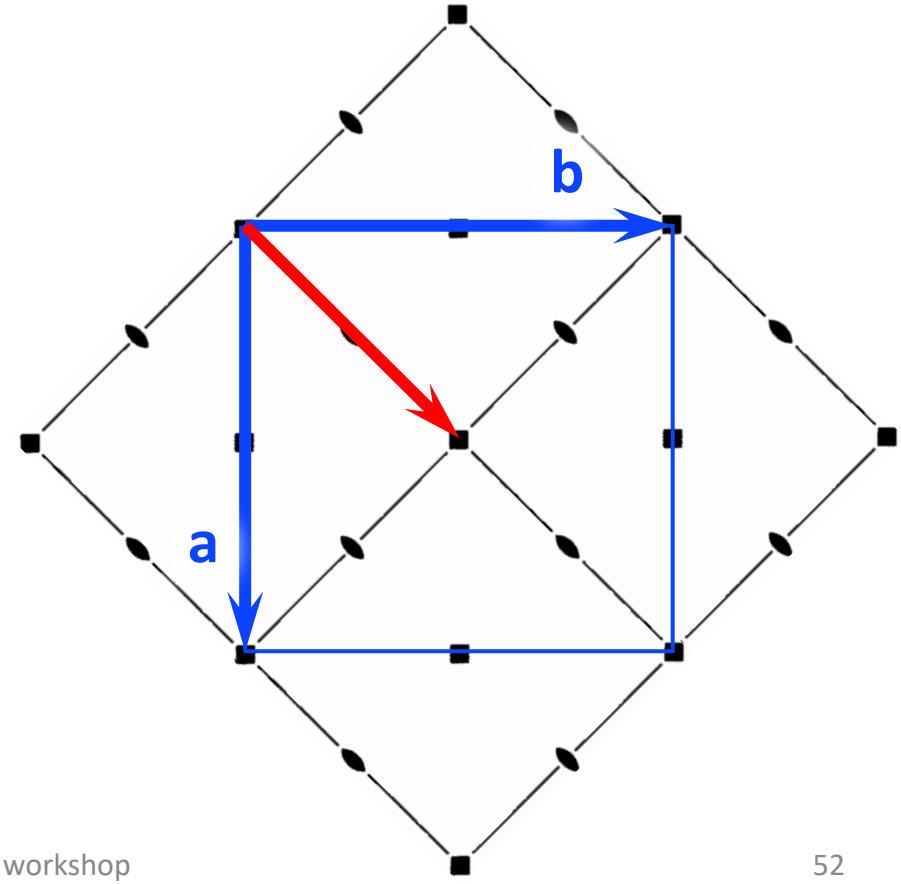
*P*4
as presented in the International Tables for Crystallography



and with base vectors shown




*C*4
This is just a different setting obtained
- by rotation 45° and
- redefining base vectors
- additional translation (**a** + **b**)/ 2



# Bravais lattices

- 7 crystal systems, combined with some of the centring types (P, C, I, F or H) give 14 Bravais lattices

- Not included:
  - impossible combinations (*e.g. A*4)
  - redundant combinations (*e.g. P*4 is kept, C4 is excluded)

# Crystal Systems

| **Crystal System** | **Characteristic symmetry elements** | **Convention** | **Bravais lattices** | **Constraints on unit cell parameters** |
|---|---|---|---|---|
| 1. Triclinic | Translations only | | 1. Primitive (*P*) | $\alpha = \gamma = 90°$ |
| 2. Monoclinic | 2-fold axes, all parallel | along **b** | 2. Primitive (*P*)<br>3. Base-Centered (*C*) | $\alpha = \gamma = 90°$ |
| 3. Orthorhombic | 2-fold axes in three perpendicular directions | along **a**, **b** and **c** | 4. Primitive (*P*)<br>5. Base-Centered (*C*)<br>6. Body-Centered (*I*)<br>7. Face-Centered (*F*) | $\alpha = \beta = \gamma = 90°$ |
| 4. Tetragonal | 4-fold axes, all parallel | along **c** | 8. Primitive (*P*)<br>9. Body-Centered (*I*) | $a = b$<br>$\alpha = \beta = \gamma = 90°$ |
| 5. Trigonal | 3-fold axes, all parallel | along **c** | 10. Primitive (*P*)<br>11. Rhombohedral (*R* / *H*) | $a = b$<br>$\alpha = \beta = 90°;\ \gamma = 120°$ |
| 6. Hexagonal | 6-fold axes, all parallel | along **c** | 10. Primitive (*P*) | $a = b$<br>$\alpha = \beta = 90°;\ \gamma = 120°$ |
| 7. Cubic | 3-fold axes in four different orientations | along body diagonals | 12. Primitive (*P*)<br>13. Body-Centered (*I*)<br>14. Face-Centered (*F*) | $a = b = c$<br>$\alpha = \beta = \gamma = 90°$ |

# Crystal Systems

| **Crystal System** | **Characteristic symmetry elements** | **Convention** | **Bravais lattices** | **Constraints on unit cell parameters** |
|---|---|---|---|---|
| 1. Triclinic | Translations only | | 1. Primitive (*P*) | $\alpha = \gamma = 90°$ |
| 2. Monoclinic | 2-fold axes, all parallel | along **b** | 2. Primitive (*P*)<br>3. Base-Centered (*C*) | $\alpha = \gamma = 90°$ |
| 3. Orthorhombic | 2-fold axes in three perpendicular directions | along **a**, **b** and **c** | 4. Primitive (*P*)<br>5. Base-Centered (*C*)<br>6. Body-Centered (*I*)<br>7. Face-Centered (*F*) | $\alpha = \beta = \gamma = 90°$ |
| 4. Tetragonal | 4-fold axes, all parallel | along **c** | 8. Primitive (*P*)<br>9. Body-Centered (*I*) | $a = b$<br>$\alpha = \beta = \gamma = 90°$ |
| 5. Trigonal | 3-fold axes, all parallel | along **c** | 10. Primitive (*P*)<br>11. Rhombohedral (*R* / *H*) | $a = b$<br>$\alpha = \beta = 90°;\ \gamma = 120°$ |
| 6. Hexagonal | 6-fold axes, all parallel | along **c** | 10. Primitive (*P*) | $a = b$<br>$\alpha = \beta = 90°;\ \gamma = 120°$ |
| 7. Cubic | 3-fold axes in four different orientations | along body diagonals | 12. Primitive (*P*)<br>13. Body-Centered (*I*)<br>14. Face-Centered (*F*) | $a = b = c$<br>$\alpha = \beta = \gamma = 90°$ |

# Crystal Systems

| **Crystal System** | **Characteristic symmetry elements** | **Convention** | **Bravais lattices** | **Constraints on unit cell parameters** |
|---|---|---|---|---|
| 1. Triclinic | Translations only | | 1. Primitive (*P*) | $\alpha = \gamma = 90°$ |
| 2. Monoclinic | 2-fold axes, all parallel | along **b** | 2. Primitive (*P*)<br>3. Base-Centered (*C*) | $\alpha = \gamma = 90°$ |
| 3. Orthorhombic | 2-fold axes in three perpendicular directions | along **a**, **b** and **c** | 4. Primitive (*P*)<br>5. Base-Centered (*C*)<br>6. Body-Centered (*I*)<br>7. Face-Centered (*F*) | $\alpha = \beta = \gamma = 90°$ |
| 4. Tetragonal | 4-fold axes, all parallel | along **c** | 8. Primitive (*P*)<br>9. Body-Centered (*I*) | $a = b$<br>$\alpha = \beta = \gamma = 90°$ |
| 5. Trigonal | 3-fold axes, all parallel | along **c** | 10. Primitive (*P*)<br>11. Rhombohedral (*R* / *H*) | $a = b$<br>$\alpha = \beta = 90°;\ \gamma = 120°$ |
| 6. Hexagonal | 6-fold axes, all parallel | along **c** | 10. Primitive (*P*) | $a = b$<br>$\alpha = \beta = 90°;\ \gamma = 120°$ |
| 7. Cubic | 3-fold axes in four different orientations | along body diagonals | 12. Primitive (*P*)<br>13. Body-Centered (*I*)<br>14. Face-Centered (*F*) | $a = b = c$<br>$\alpha = \beta = \gamma = 90°$ |

# Space group representation in ITC-A

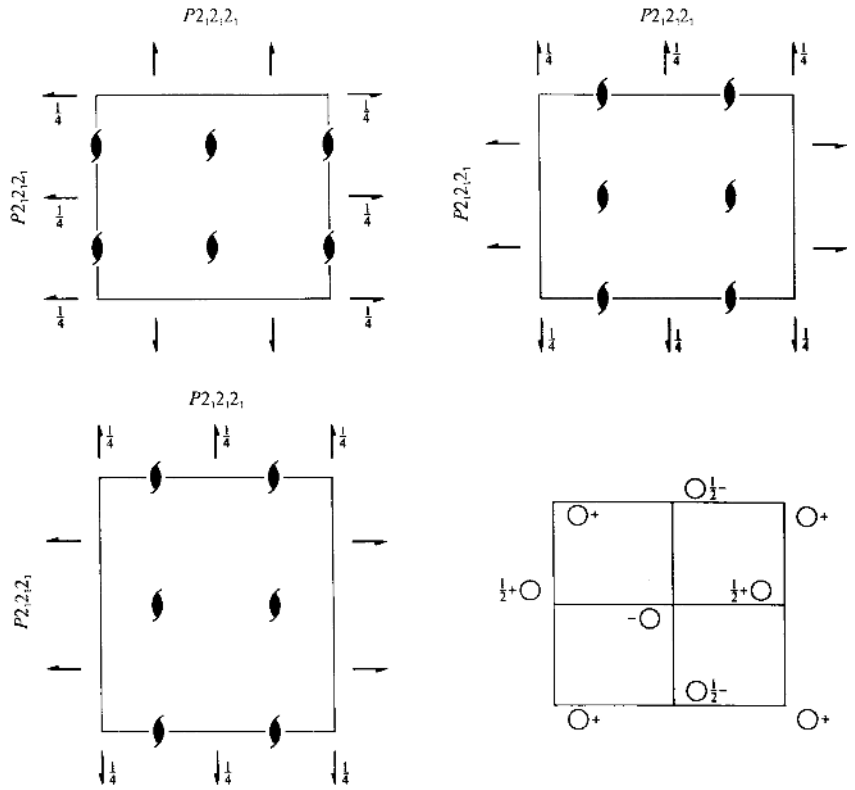
(Short) Hermann-Mauguin symbol

(Extended) Hermann-Mauguin symbol

$P2_12_12_1$ $D_2^4$ 222 Orthorhombic

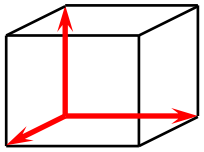
No. 19 $P2_12_12_1$

Patterson symmetry $Pmmm$



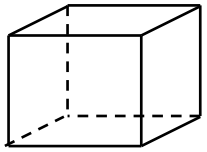
# Triclinic *P* 1

Lattice type



***P***

"1" means no symmetry operations except for translations



**1**

No constraints on
*a*, *b*, *c*, α, β, γ

# Monoclinic

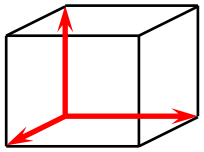
*P* 2 *P* $2_1$
*C* 2

Standard HM symbols: **papers**

*P* 1 2 1 *P* 1 $2_1$ 1
*C* 1 2 1

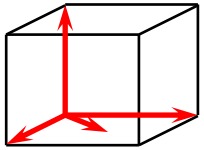
Extended HM symbols: **PDB**

Lattice type



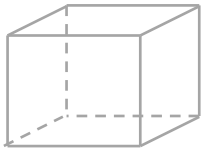
***P***

or

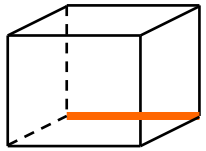


***C***

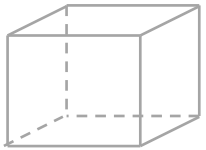
**Directions** and **orders** of axes



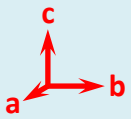
**1**



**$2_x$**



**1**



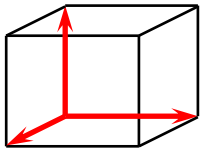

2-fold axes, all parallel

α = γ = 90°

# Orthorhombic

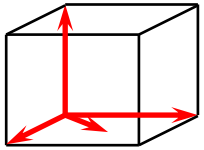
| | | | |
|---|---|---|---|
| $P\,2\,2\,2$ | $P\,2\,2\,2_1$ | $P\,2_1\,2_1\,2$ | $P\,2_1\,2_1\,2_1$ |
| $C\,2\,2\,2$ | $C\,2\,2\,2_1$ | | |
| $I\,2\,2\,2$ | | | $I\,2_1\,2_1\,2_1$ |
| $F\,2\,2\,2$ | | | |

Lattice type



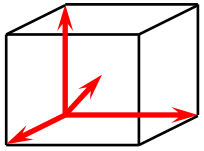
***P***

or



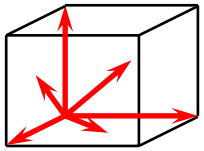
***C***

or



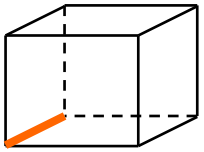
***I***

or

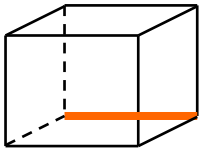


***F***

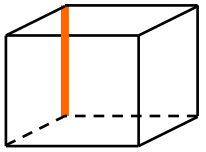
**Directions** and **orders** of axes



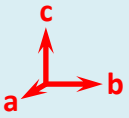
$\mathbf{2_x}$



$\mathbf{2_x}$



$\mathbf{2_x}$




2-fold axes in three perpendicular directions

$\alpha = \beta = \gamma = 90°$

# Orthorhombic

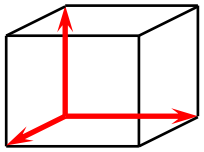
$P\,2\,2\,2$ $P\,2\,2\,2_1$ $P\,2_12_12$ $P\,2_12_12_1$ example

$C\,2\,2\,2$ $C\,2\,2\,2_1$

$I\,2\,2\,2$ $I\,2_12_12_1$

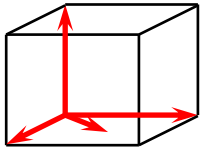
$F\,2\,2\,2$

Lattice type



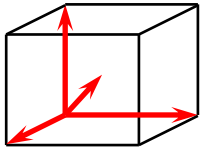
***P***

or



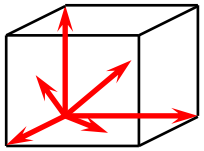
***C***

or



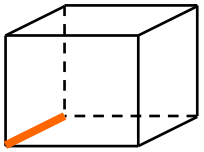
***I***

or

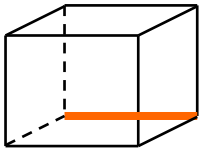


***F***

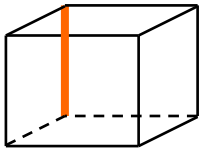
**Directions** and **orders** of axes



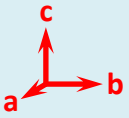
**$2_x$**



**$2_x$**



**$2_x$**



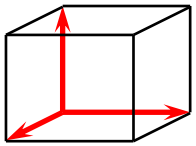

2-fold axes in three perpendicular directions

$\alpha = \beta = \gamma = 90°$

# Tetragonal

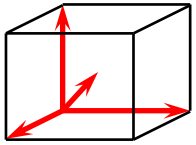
| | | | | | | | |
|---|---|---|---|---|---|---|---|
| *P* 4 $2_1$2 | *P* $4_1$$2_1$2 | *P* $4_2$$2_1$2 | *P* $4_3$$2_1$2 | | *P*4 | *P*$4_1$ | *P*$4_2$ | *P*$4_3$ |
| *P* 4 2 2 | *P* $4_1$2 2 | *P* $4_2$2 2 | *P* $4_3$ 2 2 | | | | | |
| *I* 4 2 2 | *I* $4_1$2 2 | | | | *I* 4 | *I* $4_1$ | | |

Lattice type



***P***

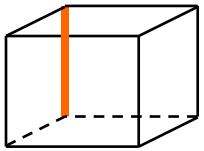
or



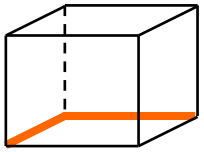
***I***

**Directions** and **orders** of axes

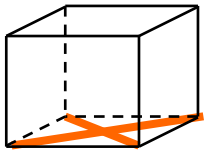
or



**$4_x$**

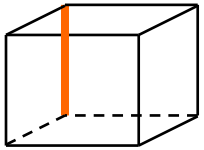


**$2_y$**

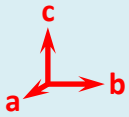


**2**

or



**$4_x$**




4-fold axes along **c**

$\alpha = \beta = \gamma = 90°$

$a = b$

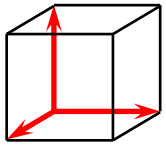
# Cubic

*P* 4 3 2 $P\,4_1 3\,2$ $P\,4_2 3\,2$ $P\,4_3 3\,2$ *P* 2 3 $P\,2_1 3$

*I* 4 3 2 $I\,4_1 3\,2$ *I* 2 3 $I\,2_1 3$

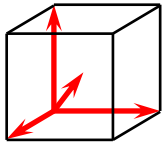
*F* 4 3 2 $F\,4_1 3\,2$ *F* 2 3

Lattice type



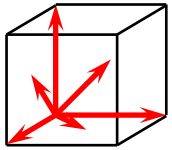
***P***

or



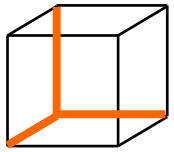
***I***

or

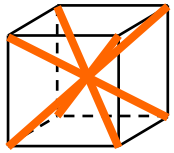


***F***

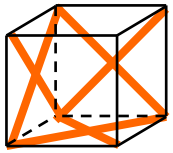
**Directions** and **orders** of axes



**$4_x$**

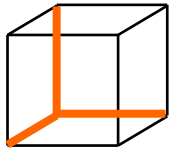


**3**

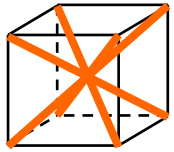


**2**

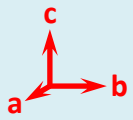
or



**$2_x$**



**3**




3-fold axes parallel to the body diagonals

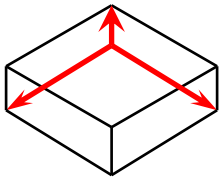
$\alpha = \beta = \gamma = 90°$

$a = b = c$

# Trigonal - P

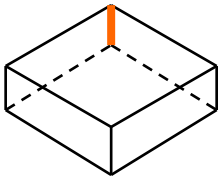
*P* 3 2 1 *P* $3_1$2 1 *P* $3_2$2 1 *P*3 *P*$3_1$ *P*$3_2$
*P* 3 1 2 *P* $3_1$1 2 *P* $3_2$1 2

Lattice type

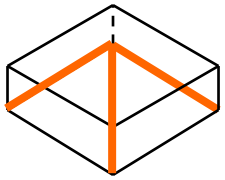


***P***

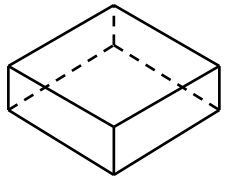
**Directions** and **orders** of axes



**$3_x$**

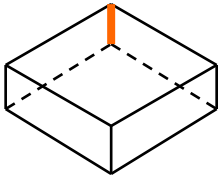


**2**

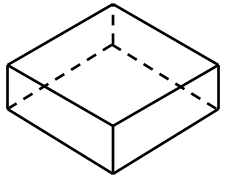


**1**

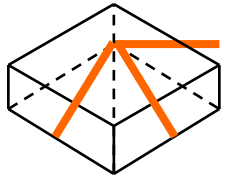
or



**$3_x$**

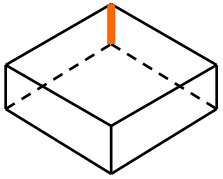


**1**

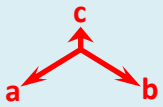


**2**

or



**$3_x$**




3-fold axes along **c**

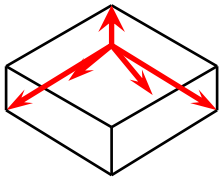
α = β = 90° γ = 120°  *a* = *b*

# Trigonal - H

*H* 3 2

*H*3

Lattice type

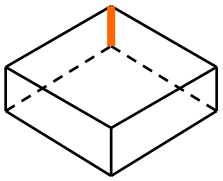


***H***

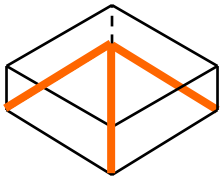
or

Rhombohedral setting ***R*** is an alternative to setting ***H***

**Directions** and **orders** of axes

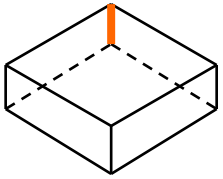


**3**

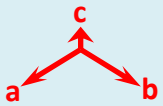


**2**

or



**3**




3-fold axes along **c**

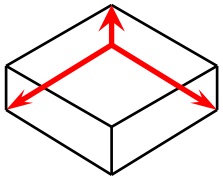
$\alpha = \beta = 90°$ $\gamma = 120°$ $a = b$

# Hexagonal

*P* 6 2 2 *P* $6_1$2 2 *P* $6_2$2 2 *P* $6_3$2 2 *P* $6_5$2 2 *P* $6_4$2 2

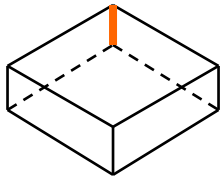
*P*6 *P*$6_1$ *P*$6_2$ *P*$6_3$ *P*$6_5$ *P*$6_4$

Lattice type

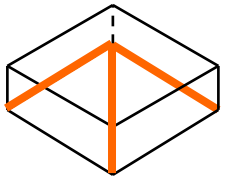


***P***

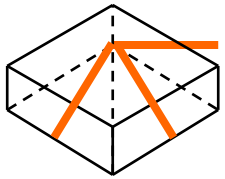
**Directions** and **orders** of axes



**$6_x$**

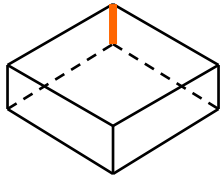


**2**

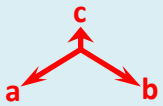


**2**

or



**$6_x$**




6-fold axes along **c**

α = β = 90° γ = 120°  *a* = *b*

# Ones

| | |
|---|---|
| ~~*P* 1 1 1~~ | *P* 1 |
| *P* 1 2 1 | *P* 2 |
| ~~*P* 4 1 1~~ | *P* 4 |
| ~~*P* 3 1 1~~ | *P* 3 |
| *P* 3 2 1 | ~~*P* 3 2~~ |
| *P* 3 1 2 | ~~*P* 3 2~~ |

# Subscripts

P43212 P 43 21 2 P 4(3) 2(1) 2 $P4_32_12$

# Symmetry based setting vs. lattice based setting: *C*2

Symmetry based setting: $\alpha = \gamma = 90°$ *C* 1 2 1

Lattice based setting: $\alpha = \gamma = 90°$, $\beta < 120°$ *C* 1 2 1 or *I* 1 2 1

- the same space group
- different crystal setting

# Symmetry based setting vs. lattice based setting: primitive orthorhombic

| | | | |
|---|---|---|---|
| Symmetry based setting: | $\alpha = \beta = \gamma = 90°$ | $P\ 2\ 2\ 2_1$ | $P\ 2_1 2_1 2$ |
| Lattice based setting: | $\alpha = \beta = \gamma = 90°$<br>$a < b < c$ | $P\ 2\ 2\ 2_1$<br>$P\ 2\ 2_1 2$<br>$P\ 2_1 2\ 2$ | $P\ 2_1 2_1 2$<br>$P\ 2_1 2\ 2_1$<br>$P\ 2\ 2_1 2_1$ |

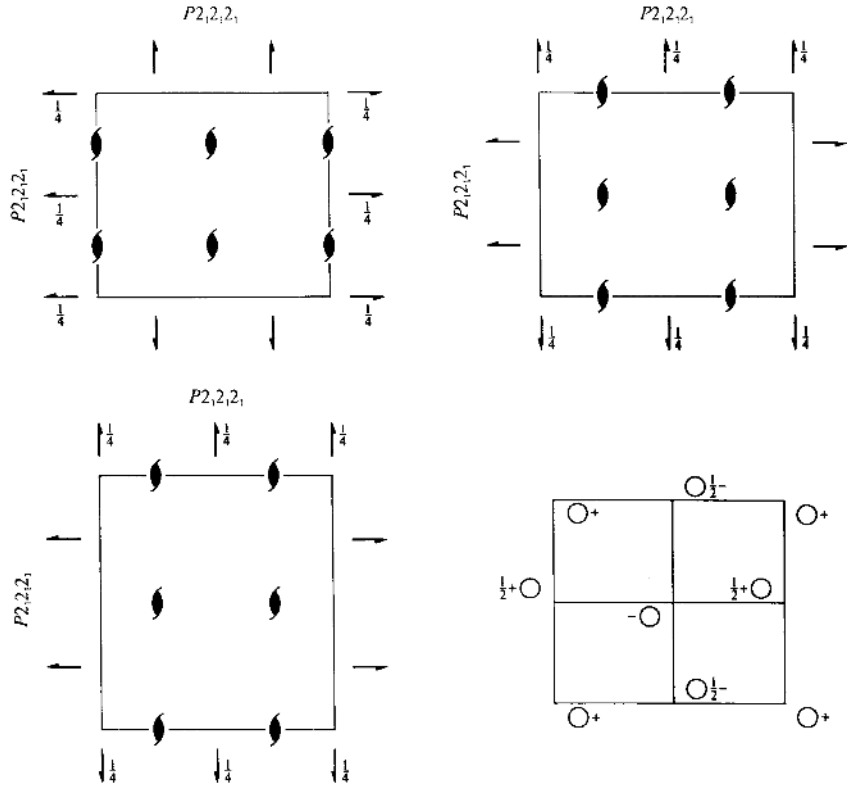
each of the two columns:
- the same space group
- different crystal setting

# Space group representation in ITC-A

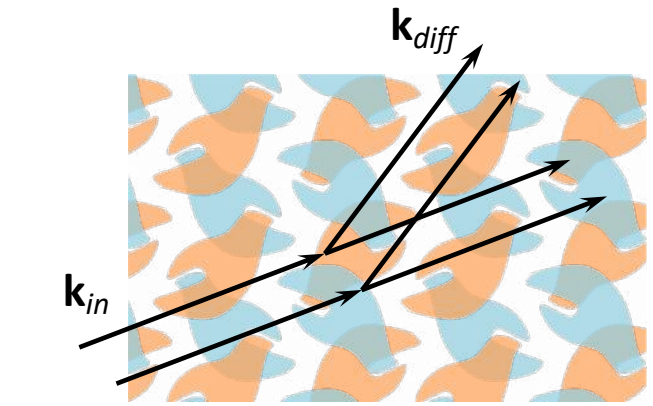
Crystal Class
(point group)

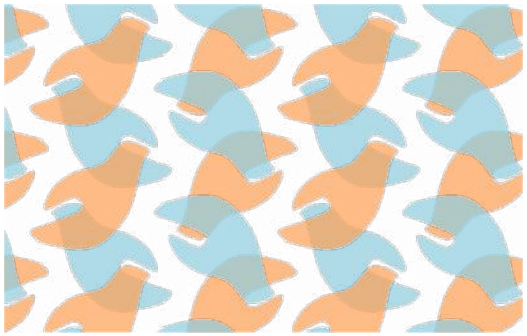
$P2_12_12_1$ $D_2^4$ 222 Orthorhombic

No. 19 $P2_12_12_1$ Patterson symmetry $Pmmm$

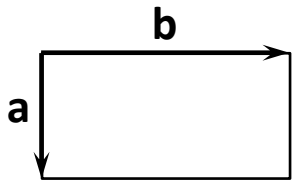


# Conventional diffraction scheme

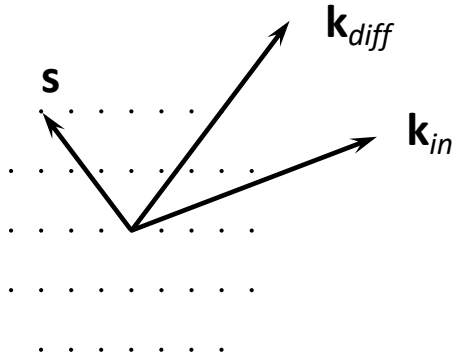


real space




Bragg planes




reciprocal space

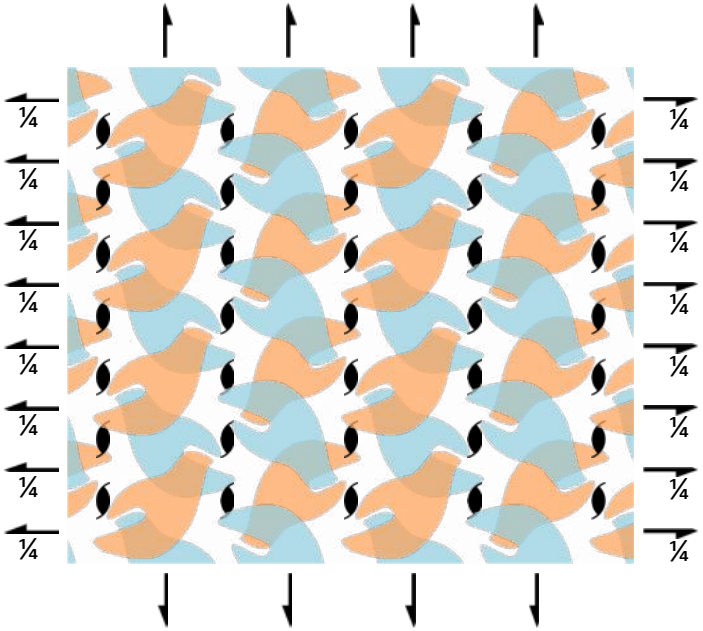
# Symmetry of intensities

The concept of reciprocal lattice is based on angular relations between the incident beam and the Bragg planes. Therefore:

- Reciprocal lattice rotates together with crystal
- However, reciprocal lattice is not translated together with crystal

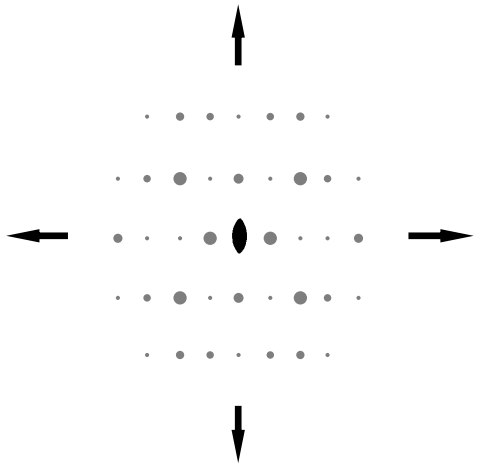
# Symmetry of intensities

real space




All axes of the same order and in the same direction are "merged" together

reciprocal space



to give an element of a point group.

# Symmetry of intensities

*Real space*

Crystal structure

Space group operation

The same crystal structure

*Reciprocal space*

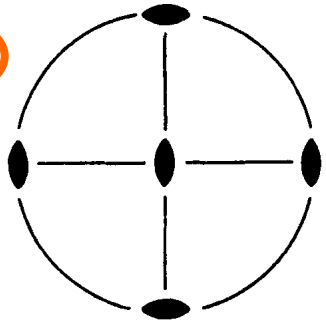
Intensities at Bragg points

Strip any translation component from the space group operation:
Point group operation

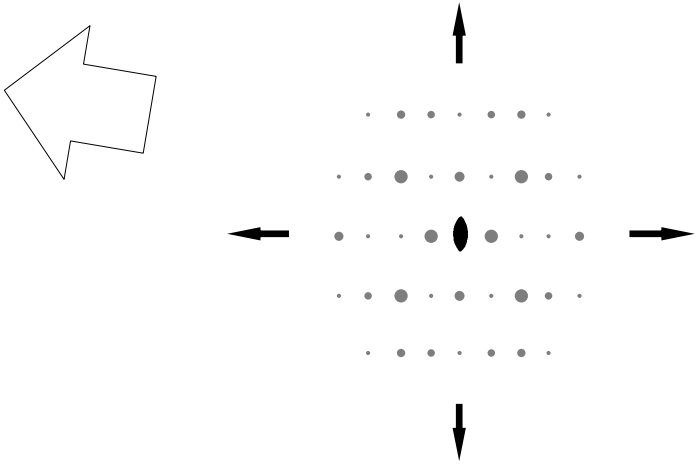
The same set of intensities (within σ)

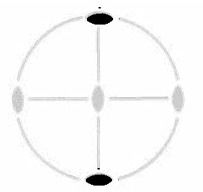
# Point group scheme

222

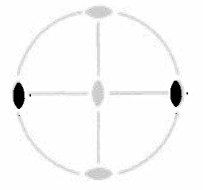


reciprocal space

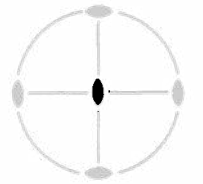




vertical 2-fold axis



horizontal 2-fold axis

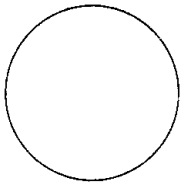


2-fold axis into plane

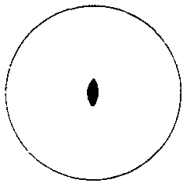
# The point groups that can exist in protein crystals

If it helps view as sphere

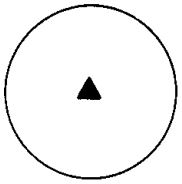
1



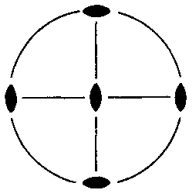
2



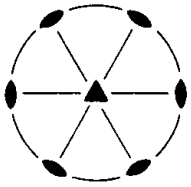
3



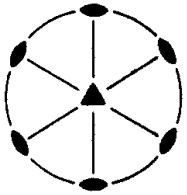
222



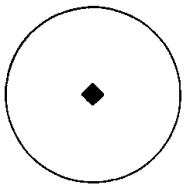
321



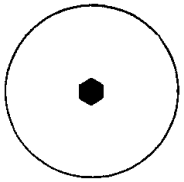
312



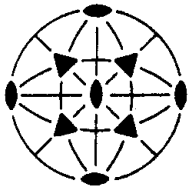
4



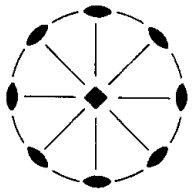
6



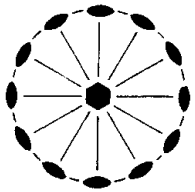
23



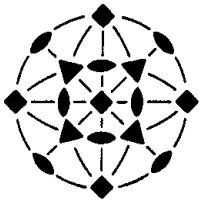
422



622

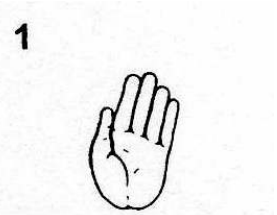


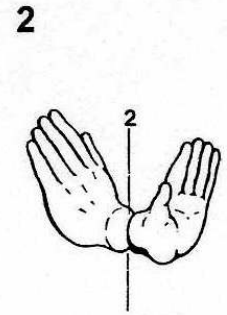
432

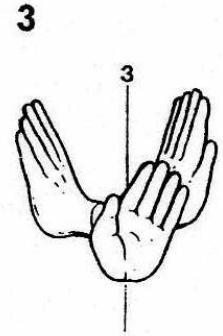


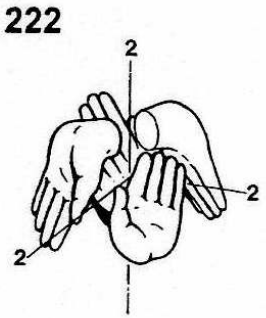
# The point groups that can exist in protein crystals

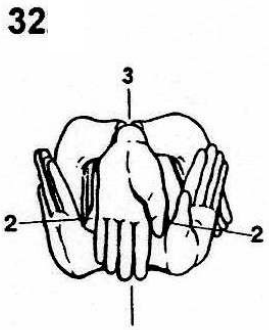
maybe an easier representation

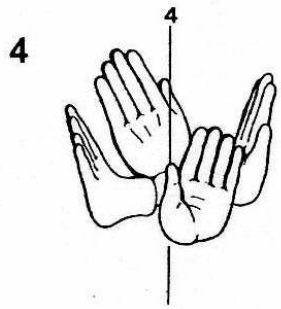


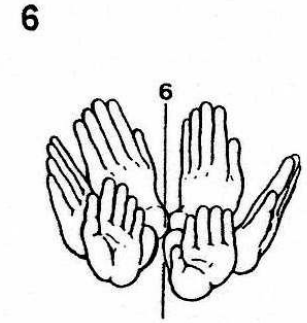



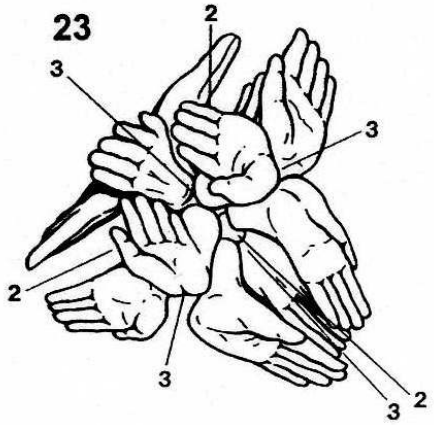



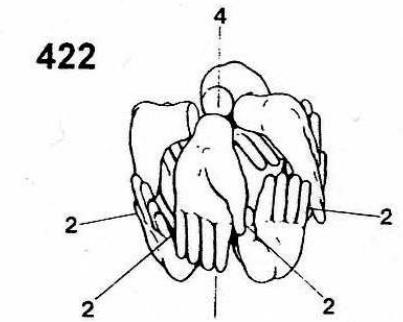



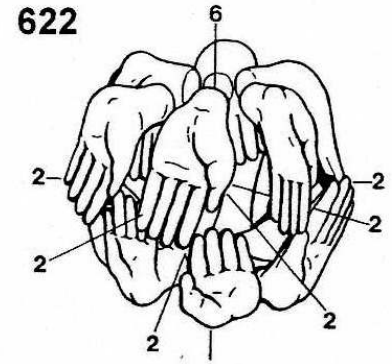



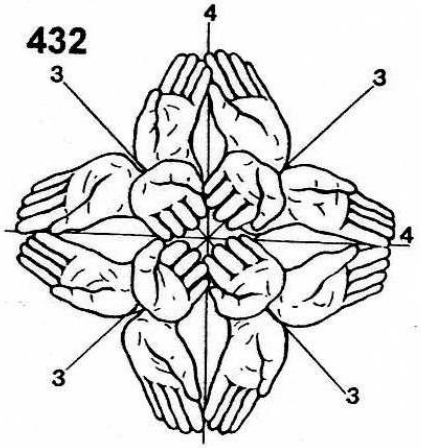



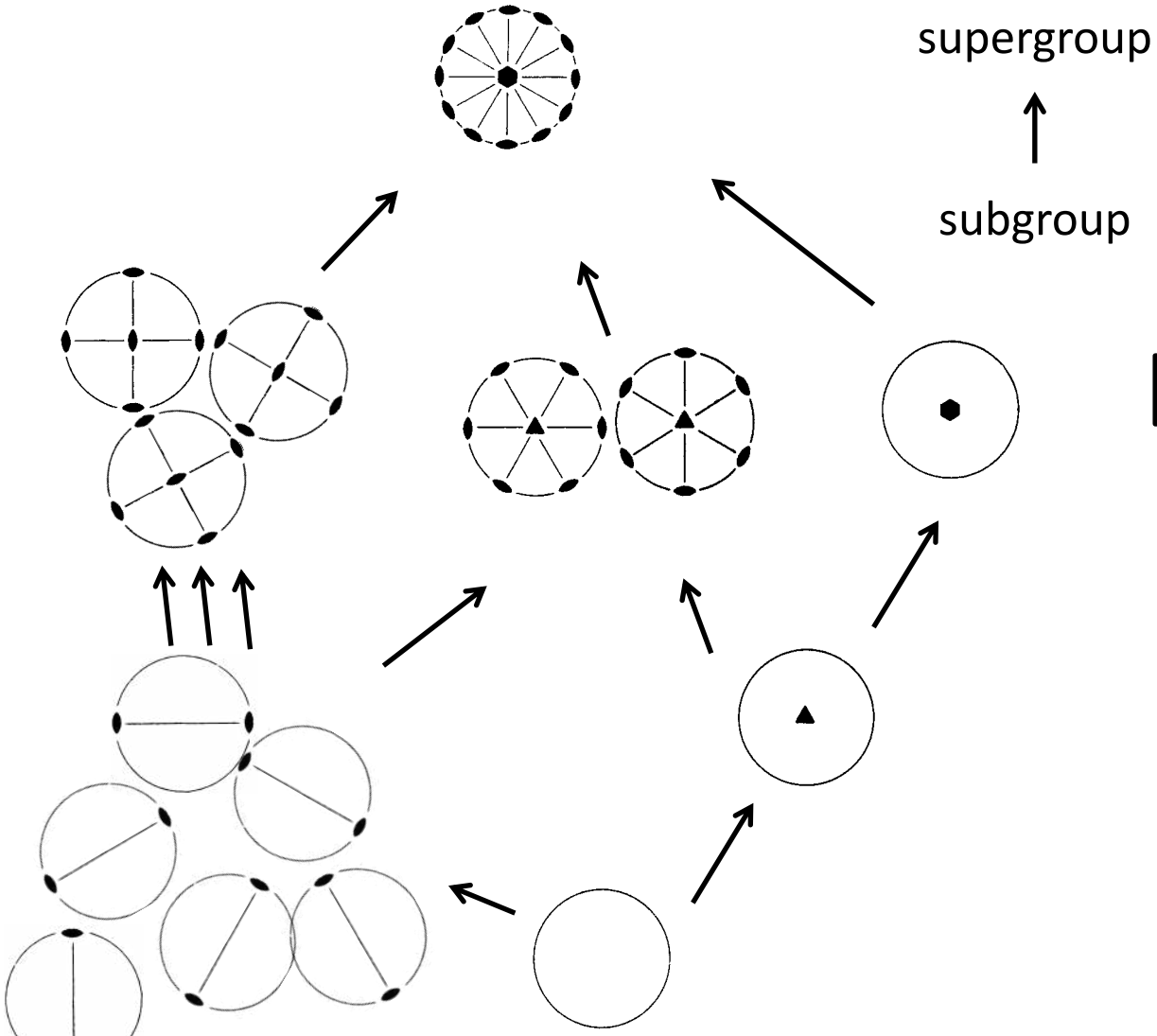



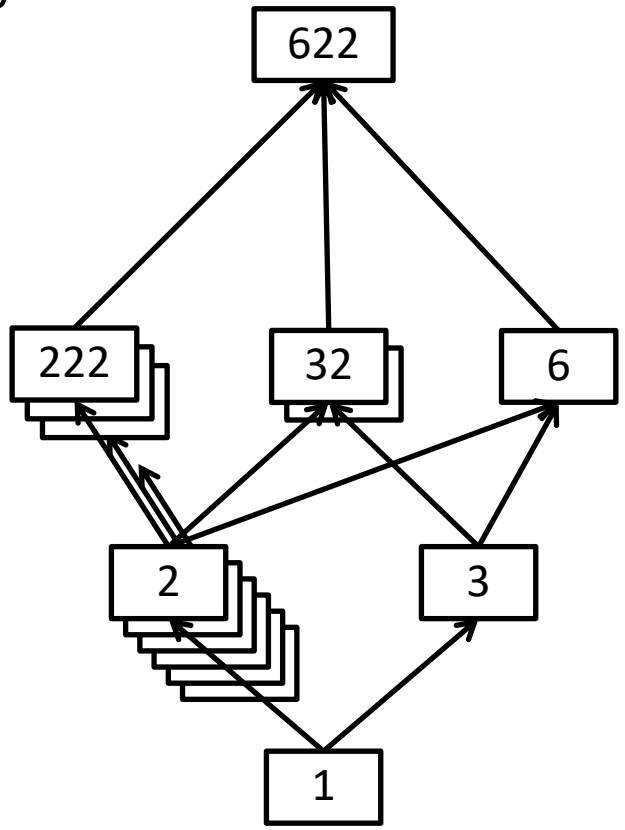
# Subgroups of the point group 622



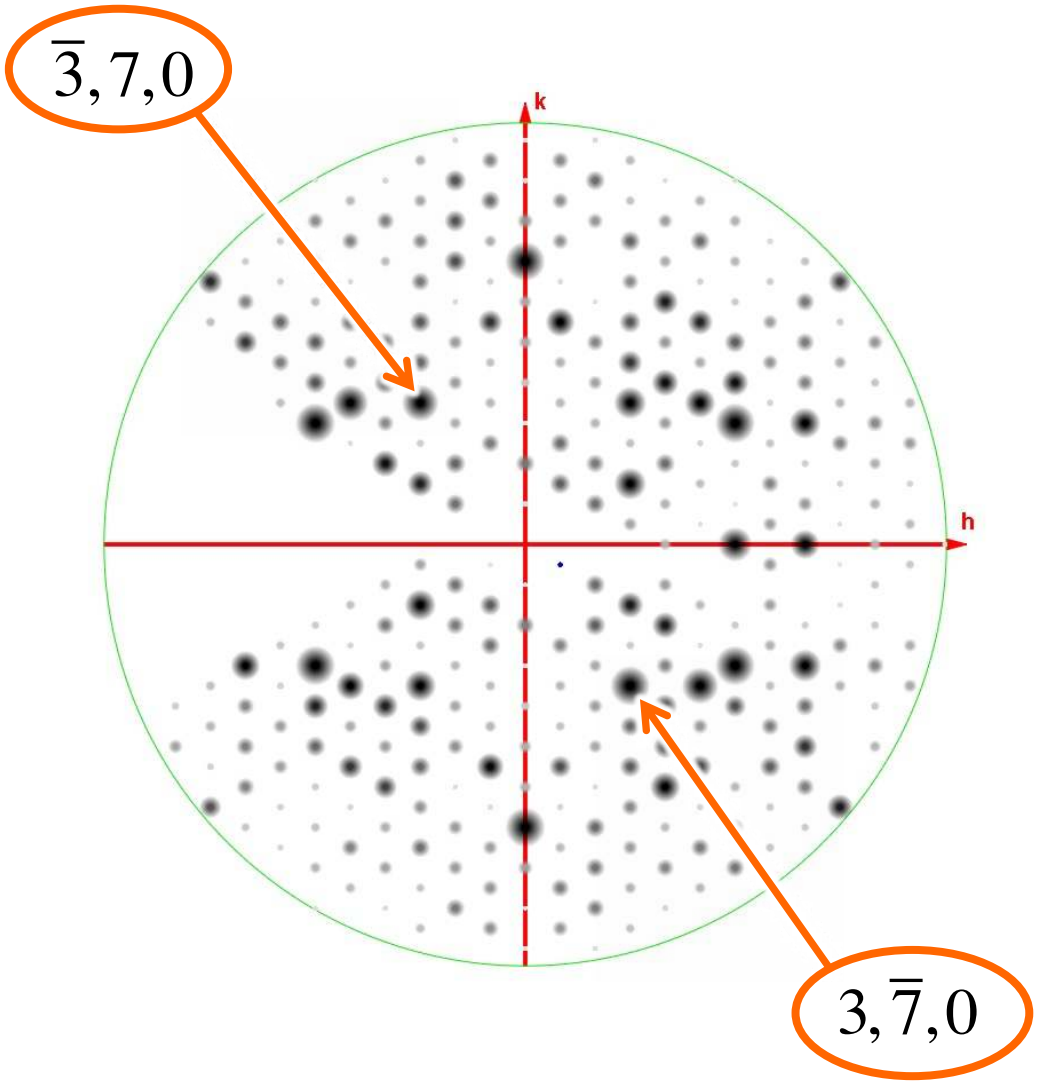
supergroup

↑

subgroup



# Friedel's law




(no anomalous signal)

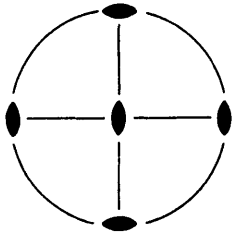
$$I\left(\overline{3},7,0\right) = I\left(3,\overline{7},0\right)$$

# Point group and Laue group

+ inversion =

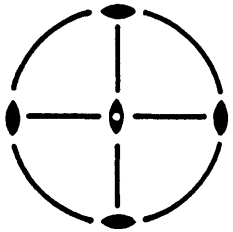
*Crystal point group*

222



*Laue point group*

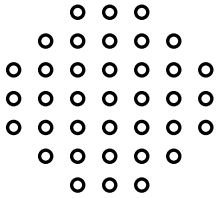
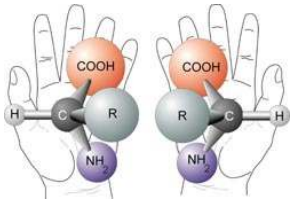
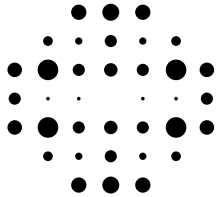
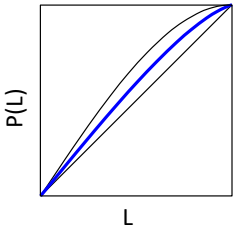
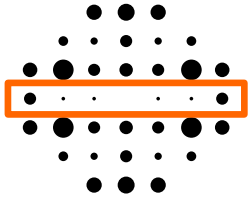
m m m

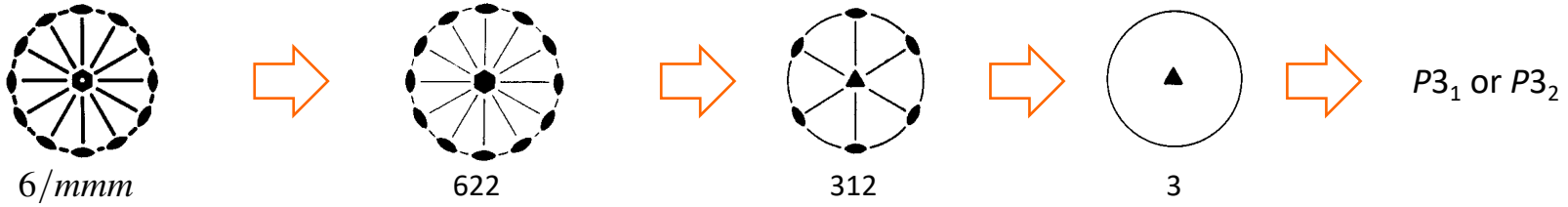


# The eleven Laue point groups or crystal classes

| Crystal system | Laue point group<br>experiment<br>(no anomalous data) | Non-centrosymmetric point groups belonging to the Laue point group | | |
|---|---|---|---|---|
| Cubic | $m3m$<br>$m3$ | 432<br>23 | $\bar{4}3m$ | |
| Tetragonal | $4/mmm$<br>$4/m$ | 422<br>4 | $4mm$<br>$\bar{4}$ | $\bar{4}2m$ |
| Orthorhombic | $mmm$ | 222 | $mm2$ | |
| Trigonal | $3m$<br>3 | 32<br>3 | $3m$ | |
| Hexagonal | $6/mmm$<br>$6/m$ | 622<br>6 | $6mm$<br>$\bar{6}$ | $\bar{6}m2$ |
| Monoclinic | $2/m$ | 2 | $m$ | |
| Triclinic | $\bar{1}$ | 1 | | |

# Space group assignment (*e.g. Pointless*)

| Reciprocal space lattice (positions of reflections) | Mirror symmetry is <u>not</u> allowed in biological macromolecules | Intensities of reflections | Twinning test | Intensities of axial reflections |
|---|---|---|---|---|
|  |  |  |  |  |




| Lattice point group | Highest possible crystal point group | Approximate point group of diffraction | Possible crystal point group | Possible crystal space group(s) |
|---|---|---|---|---|

User: decision making, structure solution, final space group assignment

# End

(Short) Hermann-Mauguin symbol

$P2_12_12_1$

No. 19

(Extended) Hermann-Mauguin symbol

$D_2^4$

$P2_12_12_1$

Crystal Class (point group)

222

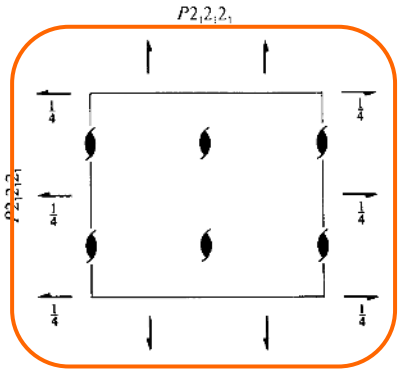
Crystal system

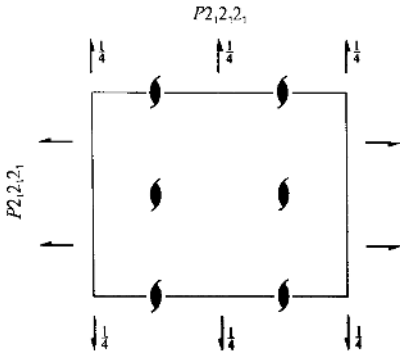
Orthorhombic

Patterson symmetry $Pmmm$

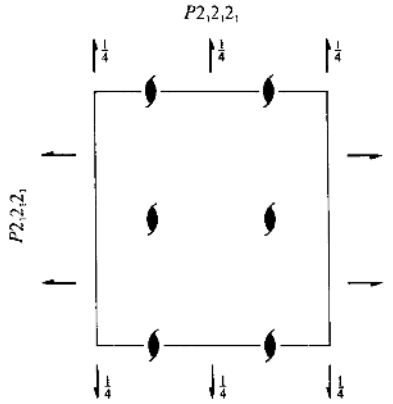
Patterson symmetry

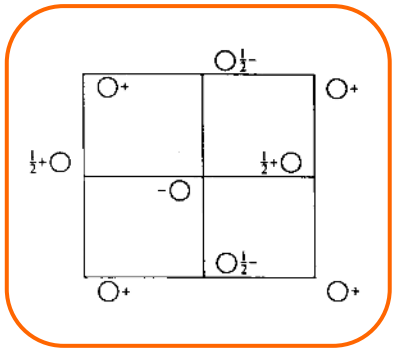
Location of symmetry elements




Two other projections are also shown for this space group



Set of equivalent points in general position.

We were looking at "molecular wallpaper" instead