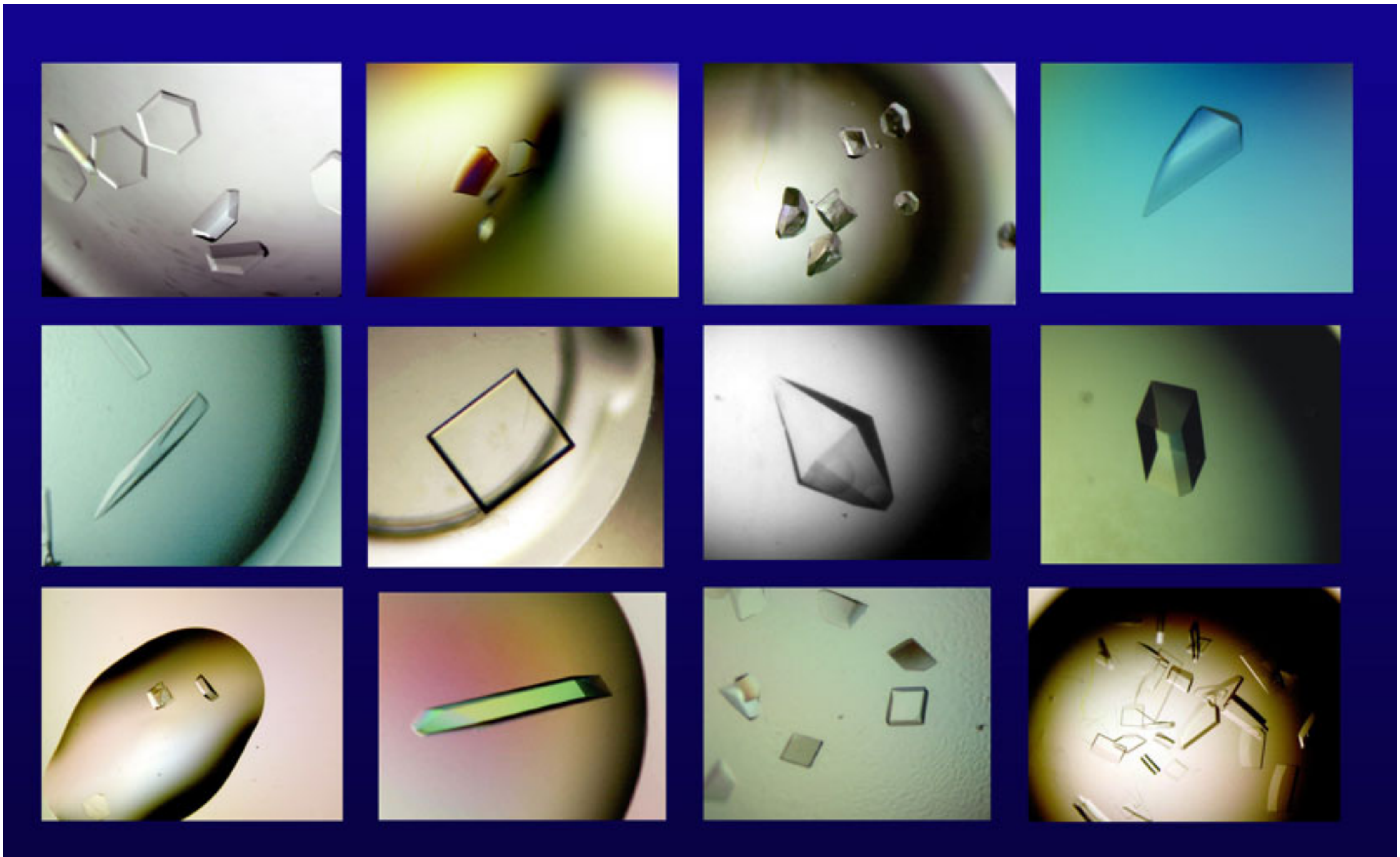
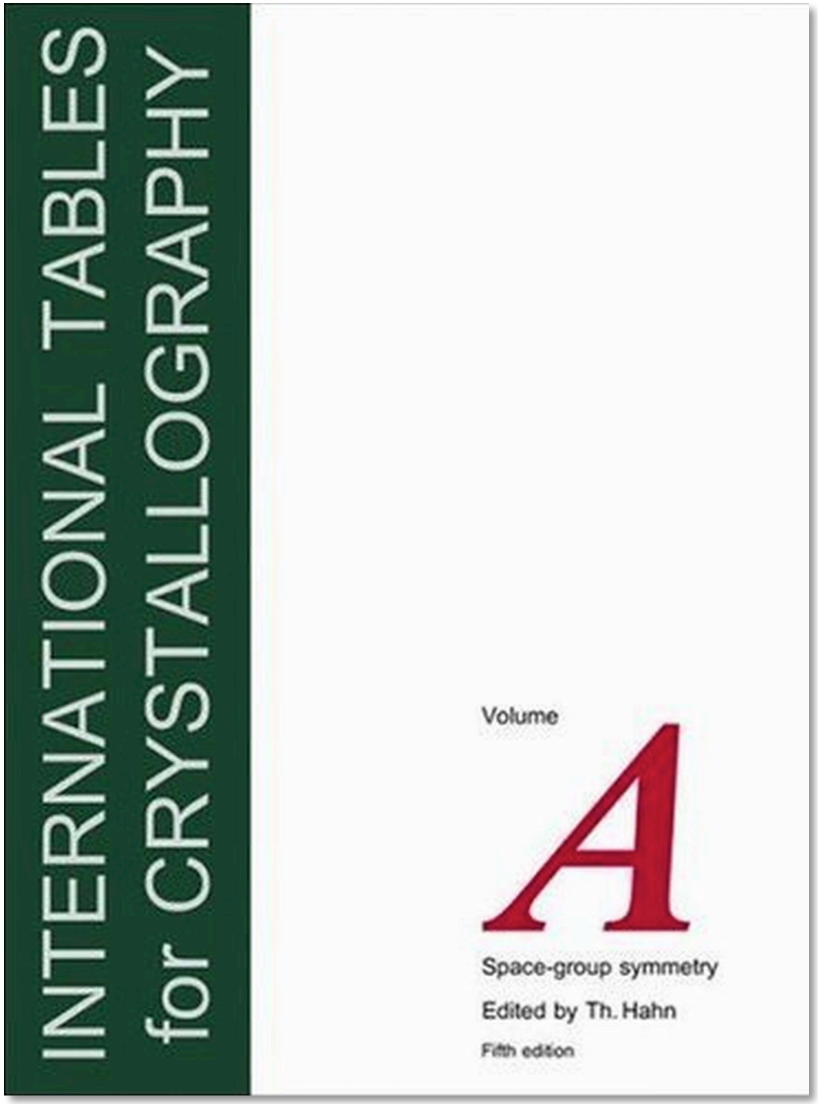
# Introduction to symmetry

Andrey Lebedev, CCP4

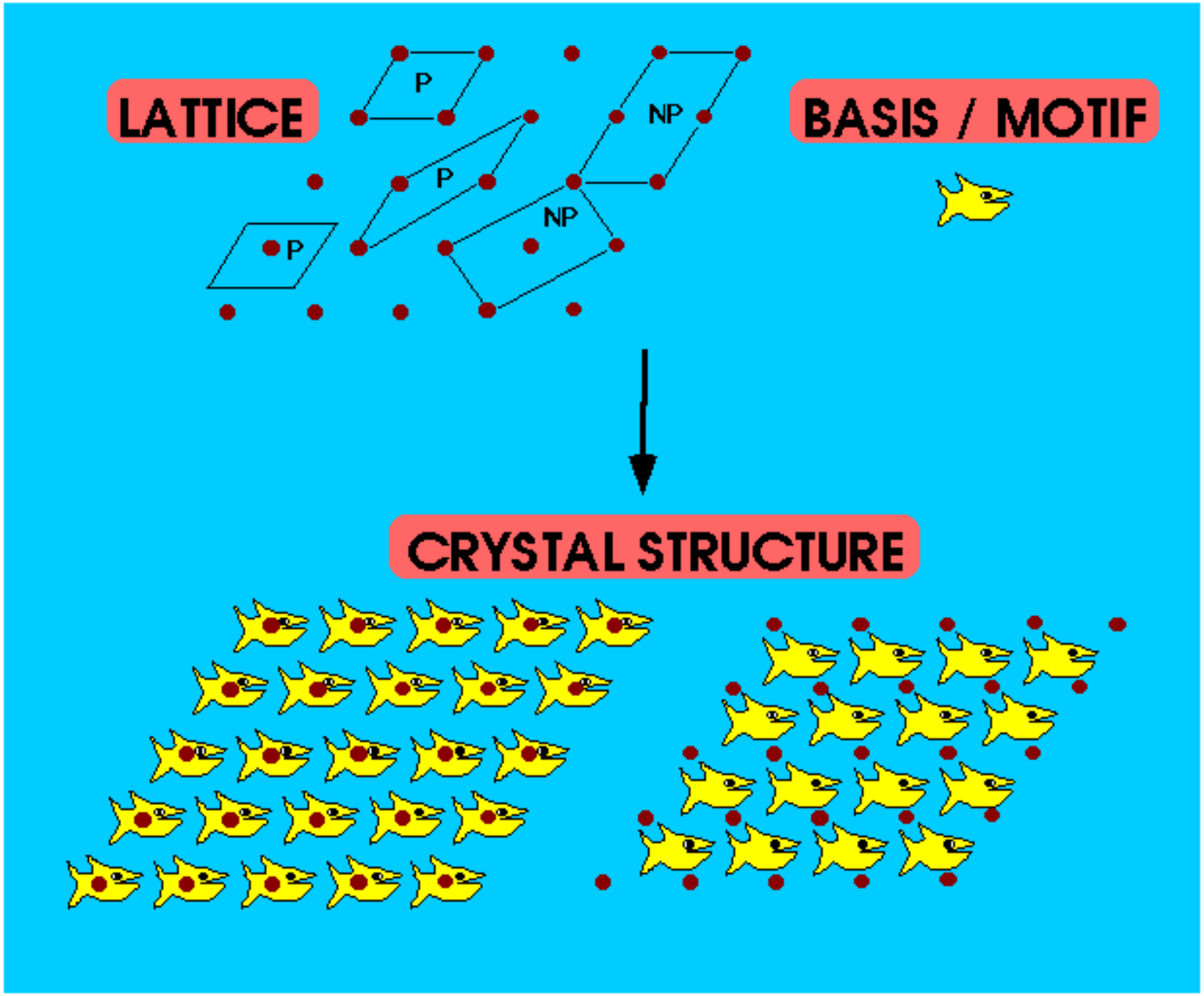


# The Reference

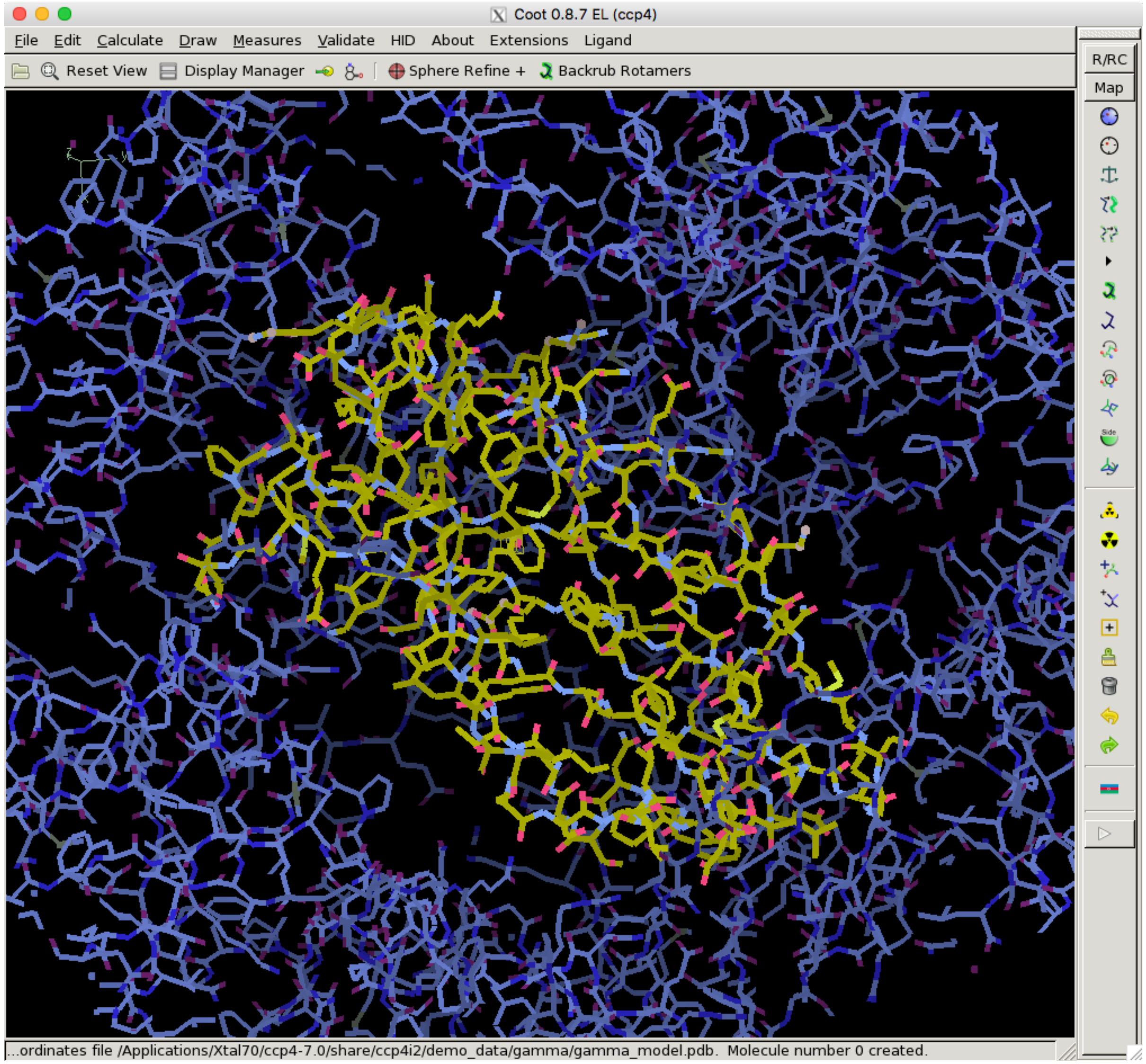


# Crystal: unit cell + lattice

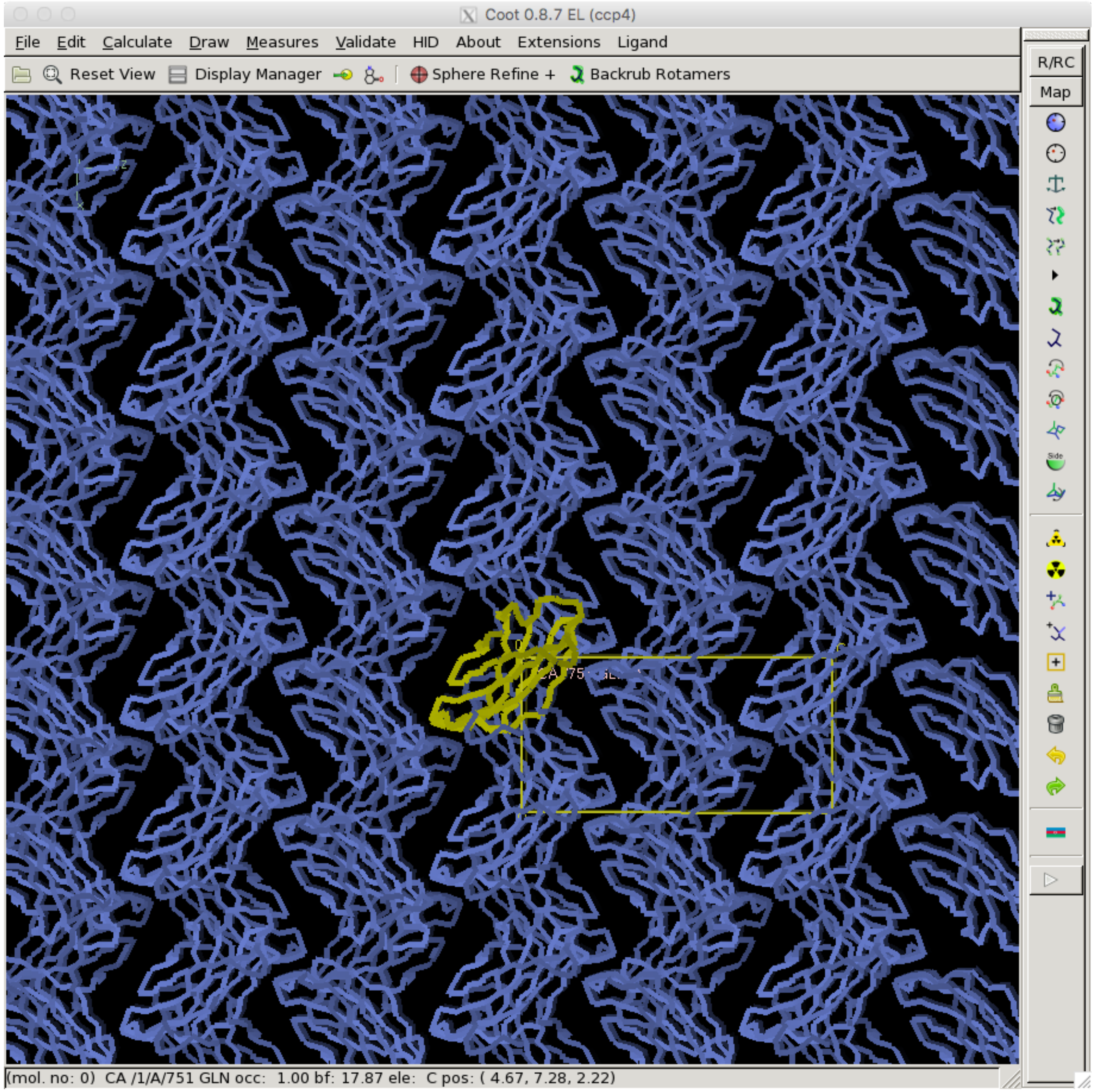
Conventional (constructive) definition of crystal structure.



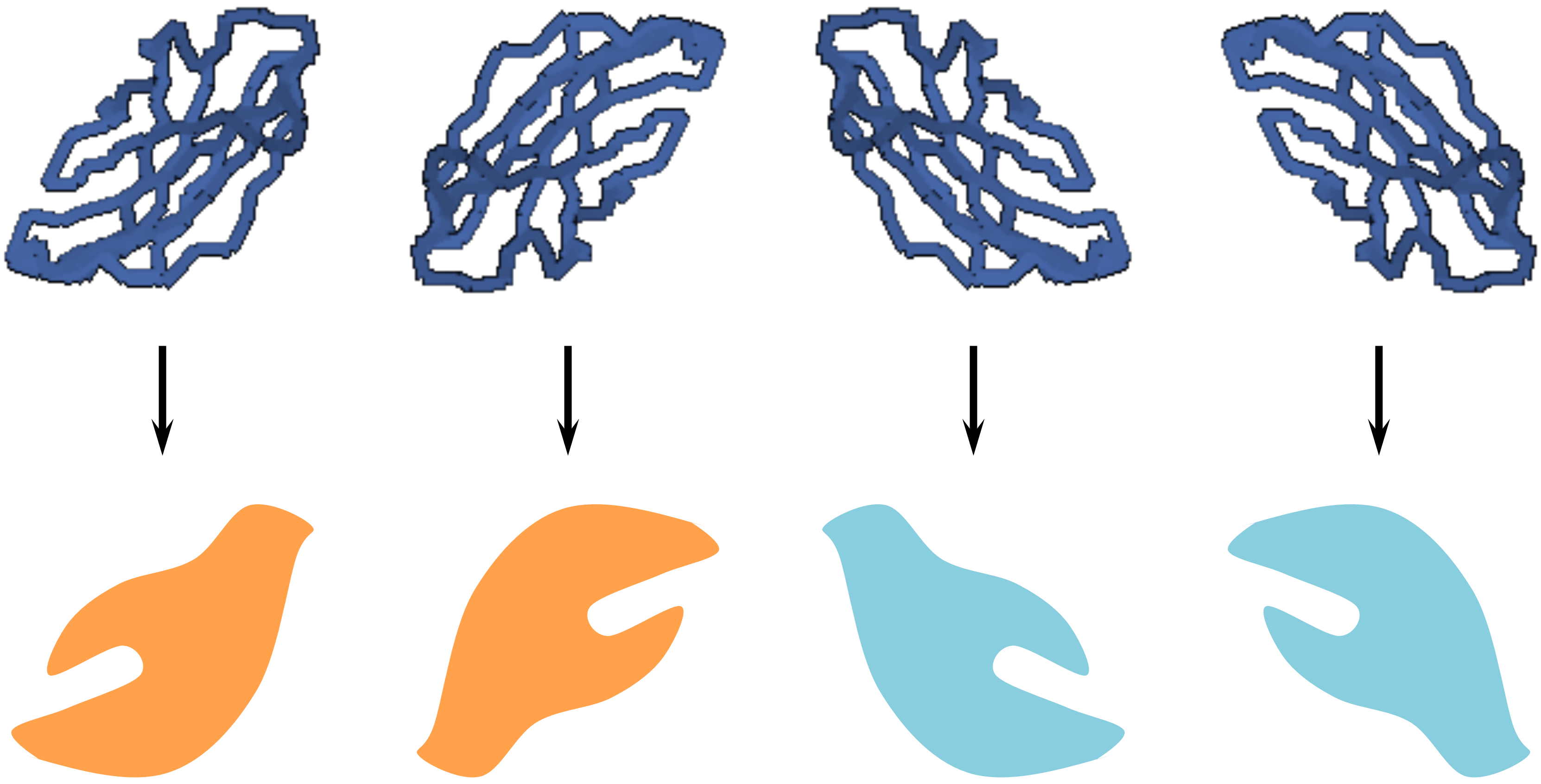
# Good for start? Examine symmetry using Coot



# Symmetry view in Coot

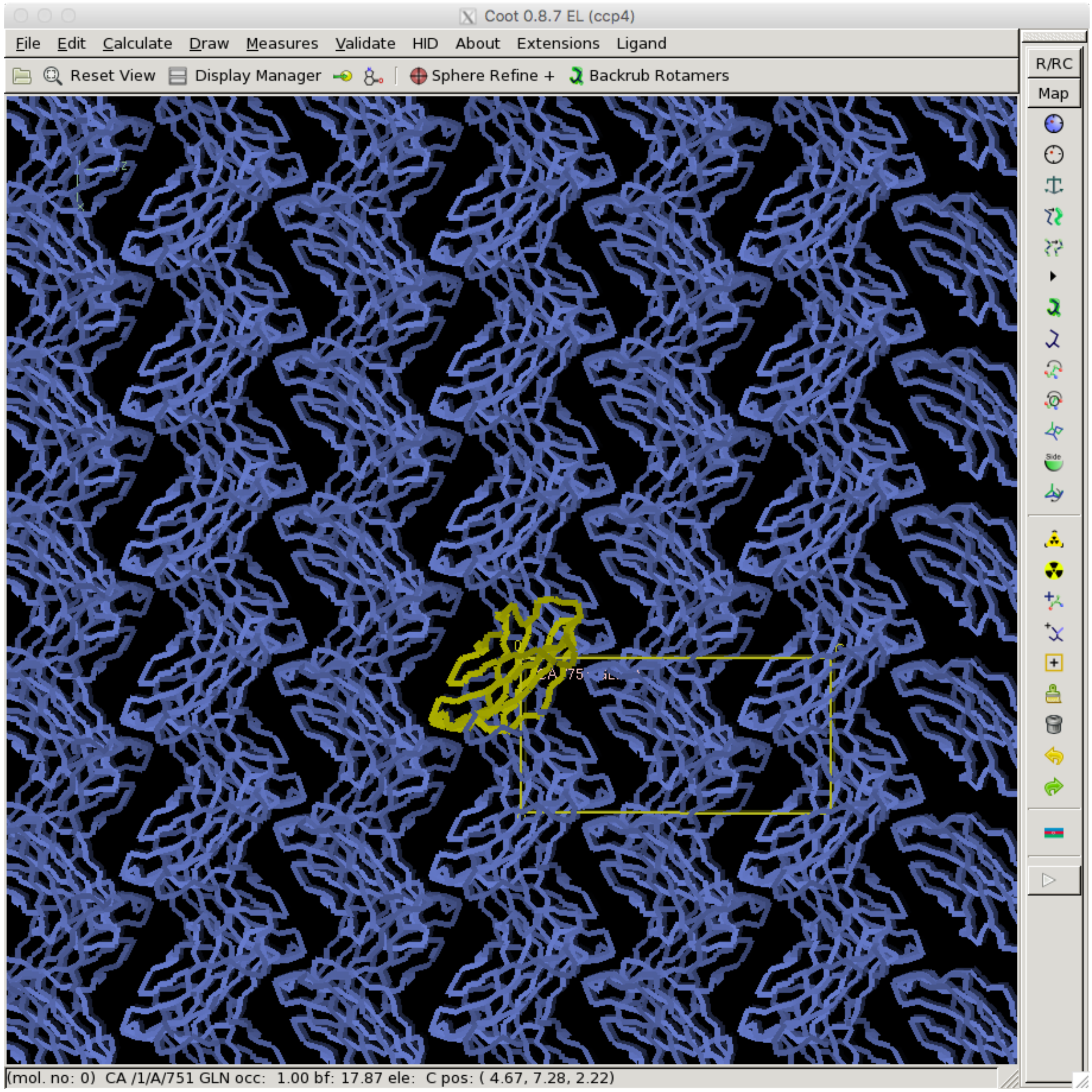


# Simplified representation

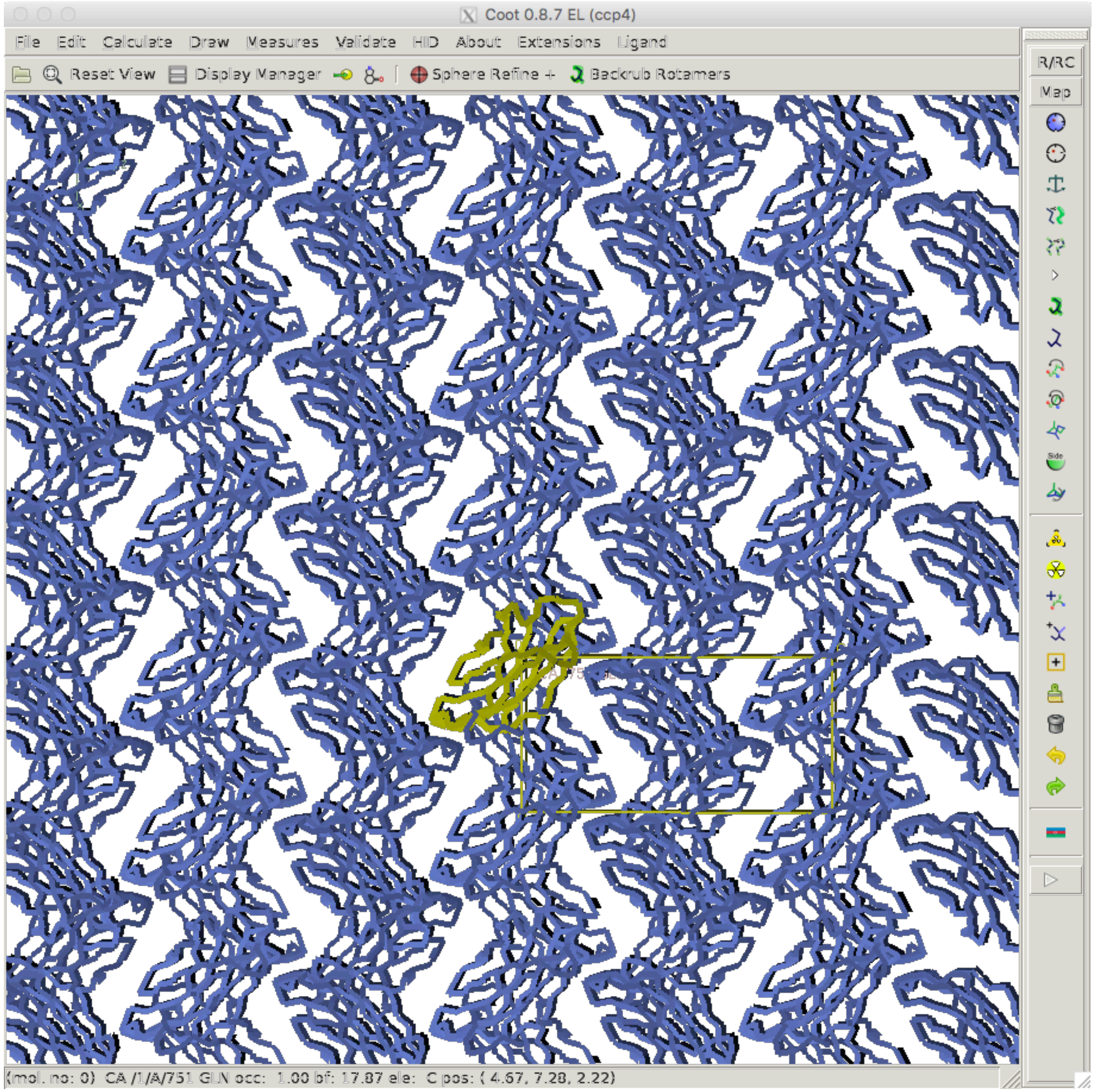


Opposite sides of molecules a denoted with different colours

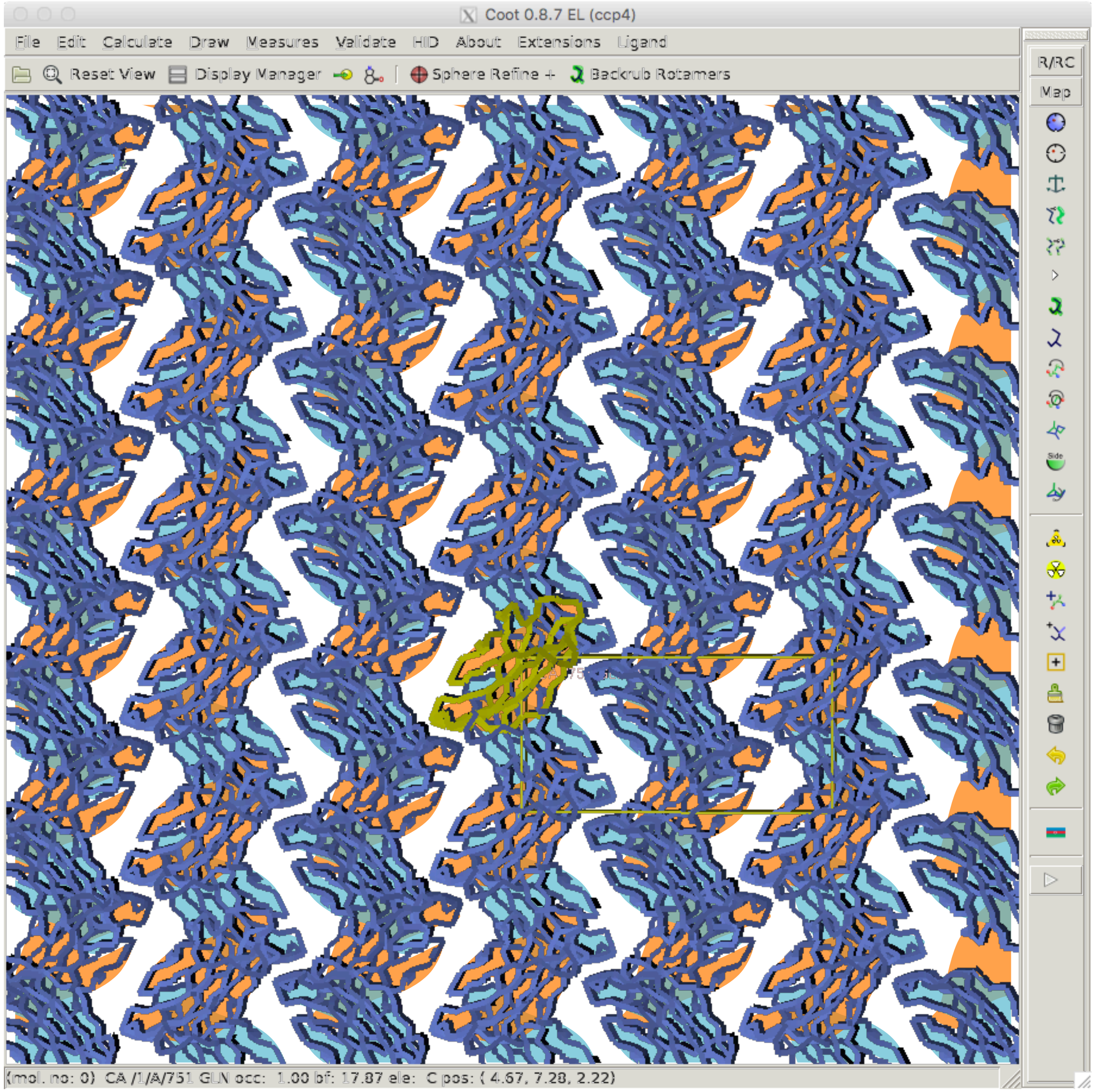
# Simplified representation



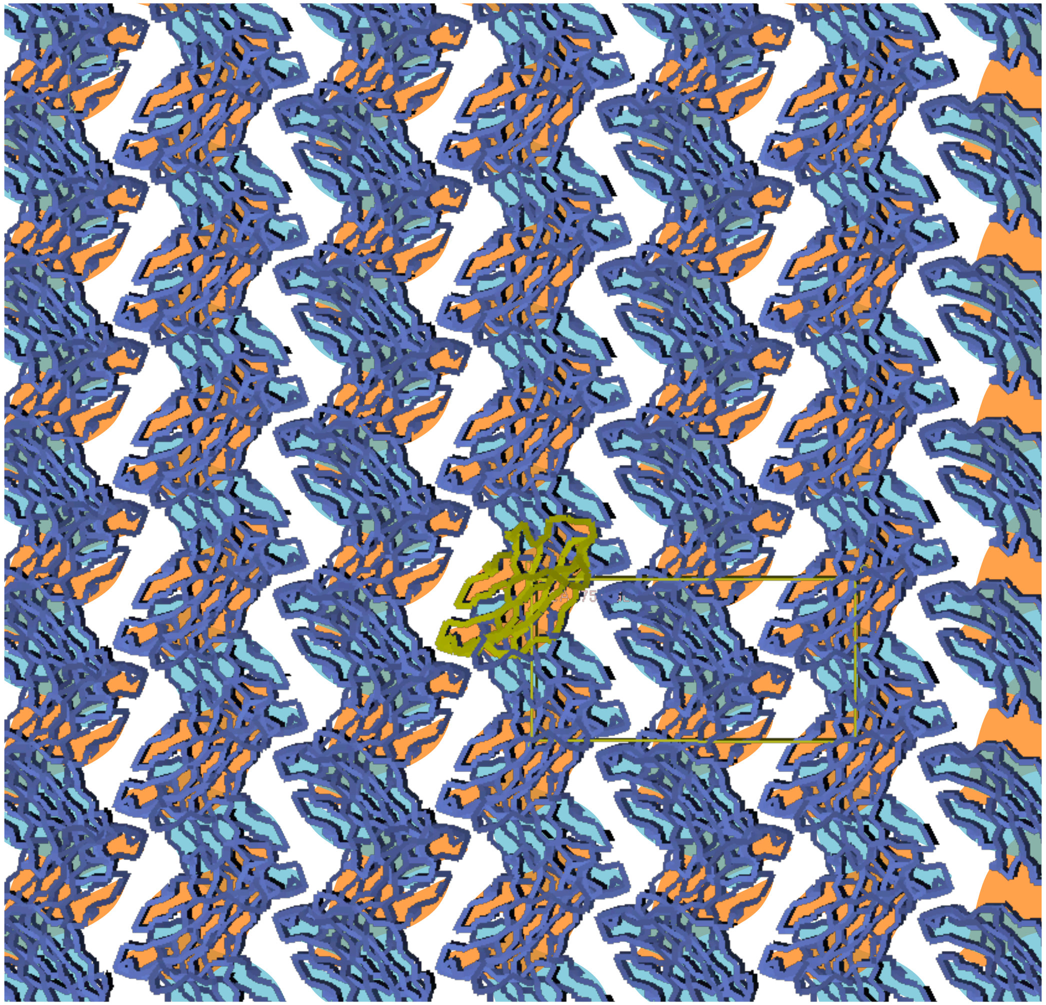
# Simplified representation



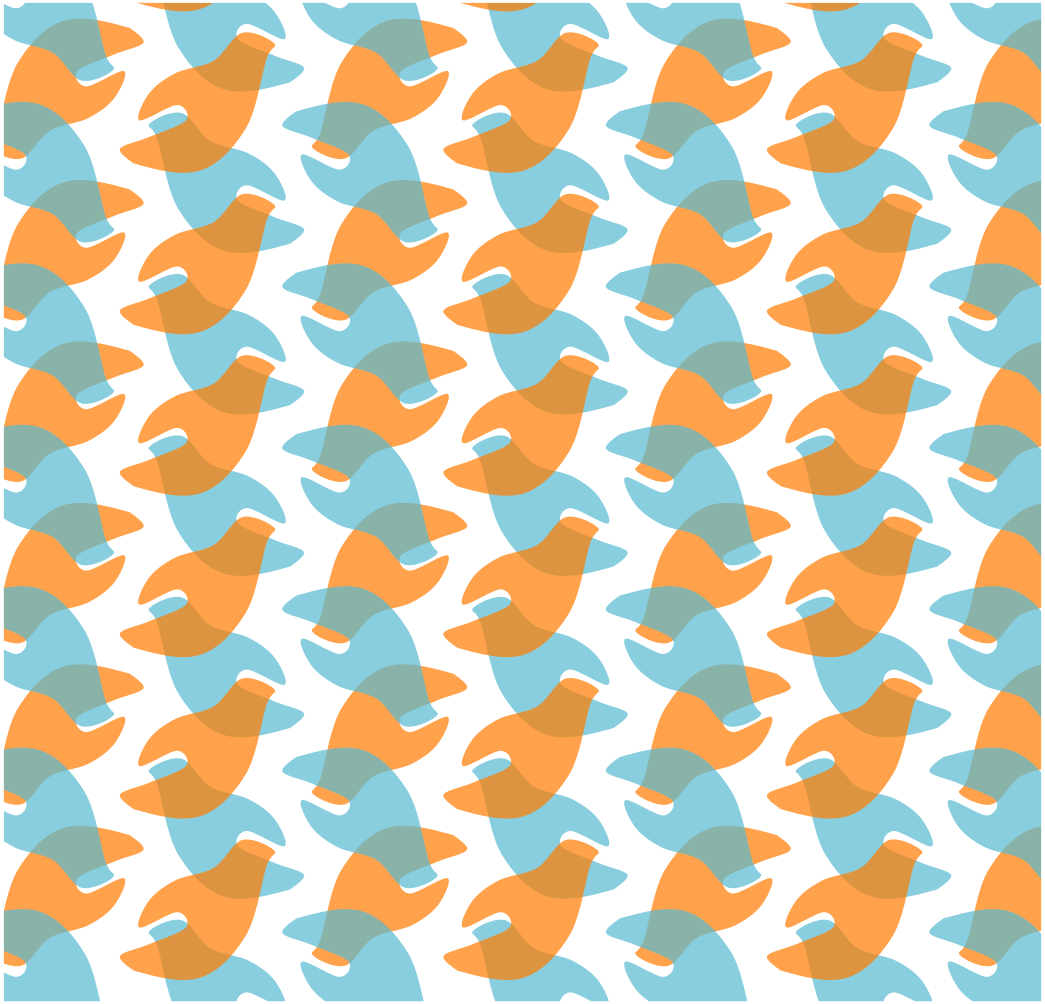
# Simplified representation



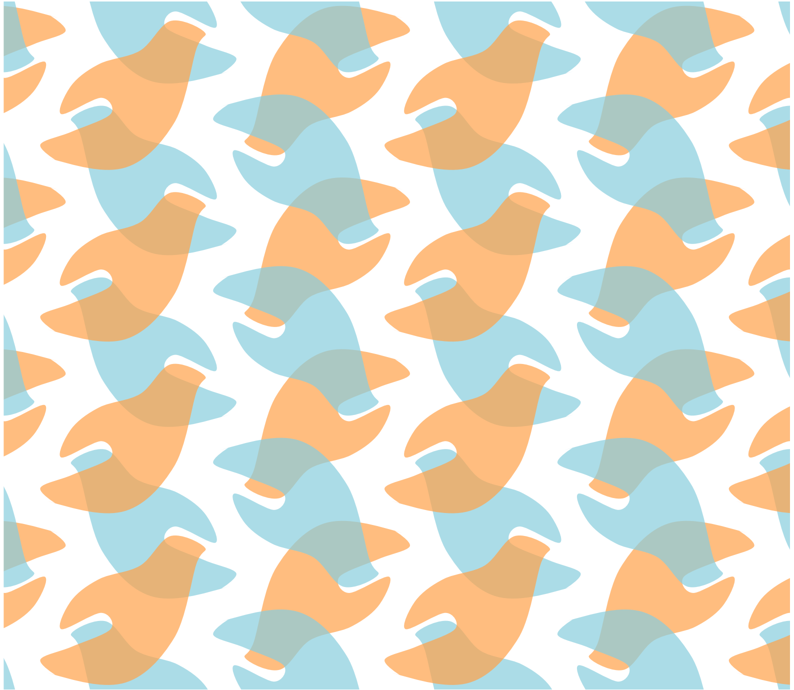
# Simplified representation



# Simplified representation



# Simplified representation



1 2 3 4

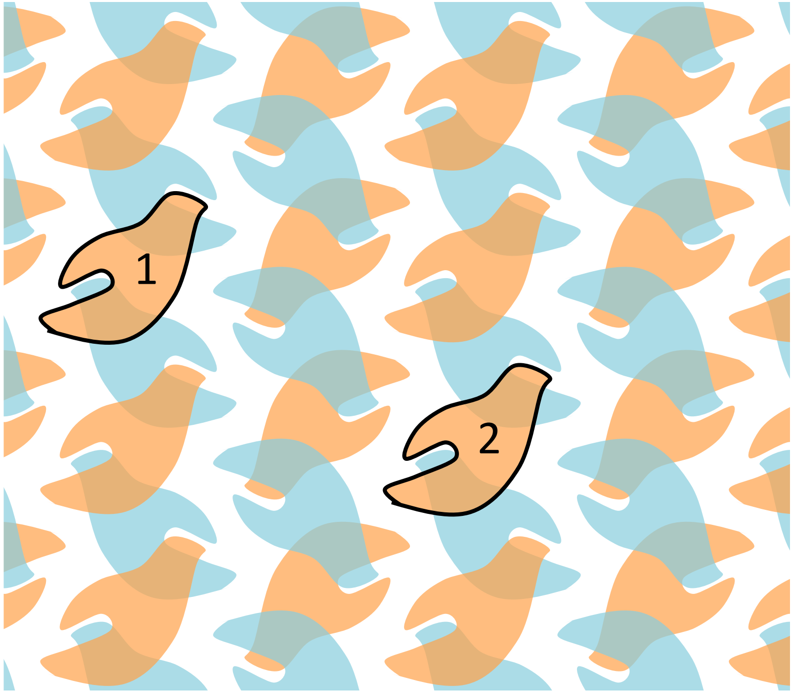
Orange and blue represent opposite sides of molecules

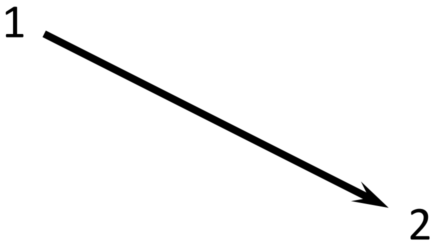
There is the third dimension.

A slice is shown, where

- column 1, 3 : orange-sided molecules on top
- column 2, 4: blue-sided molecules on top
- etc.

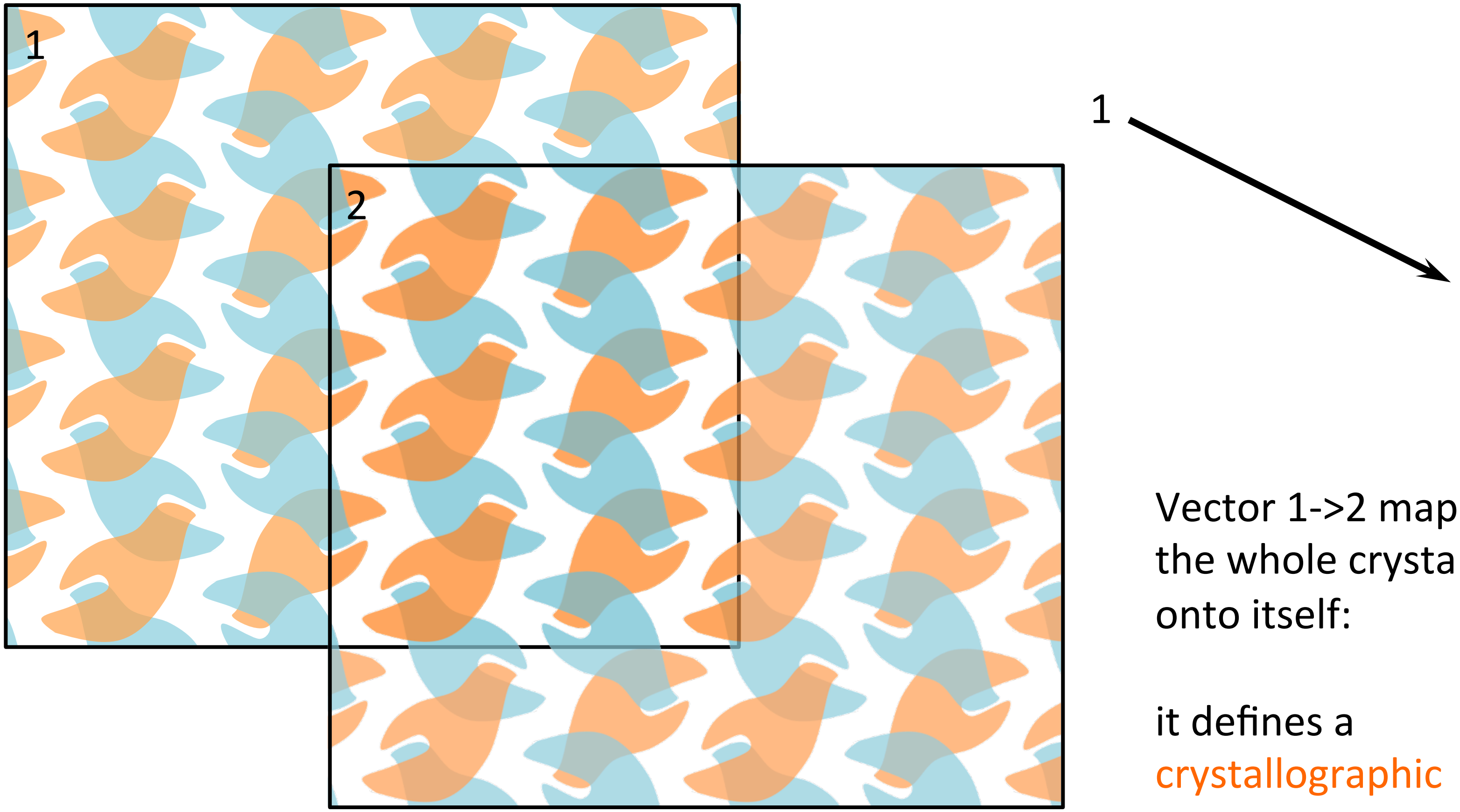
# Translation 1




Vector maps 1 -> 2

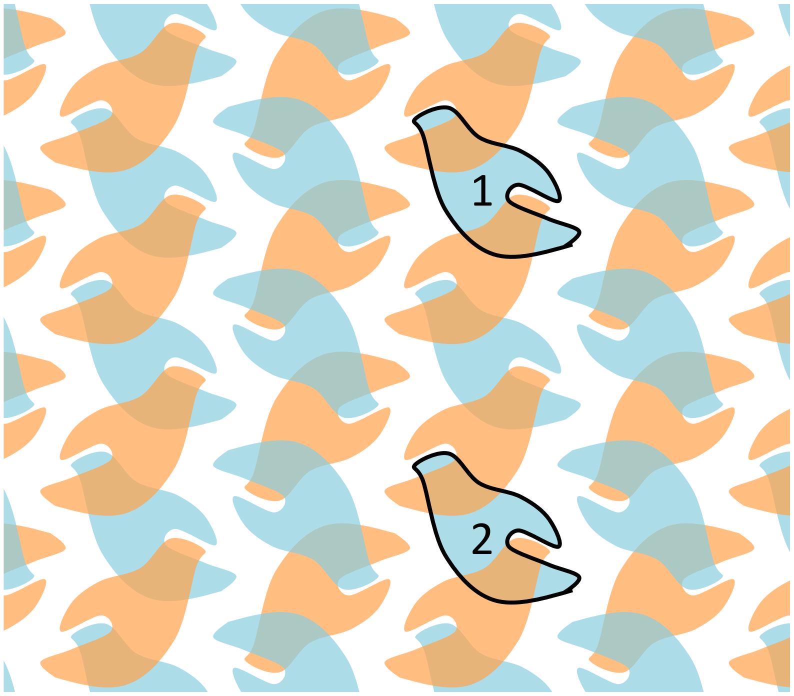
# Translation 1 is global

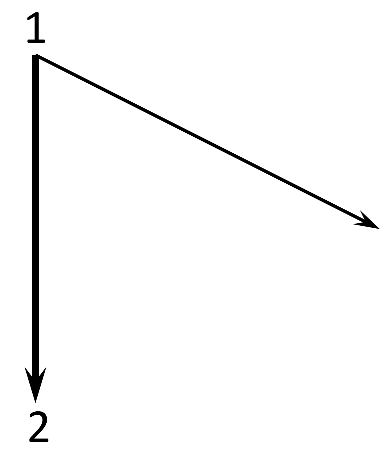



Vector 1->2 maps the whole crystal onto itself:

it defines a crystallographic operation

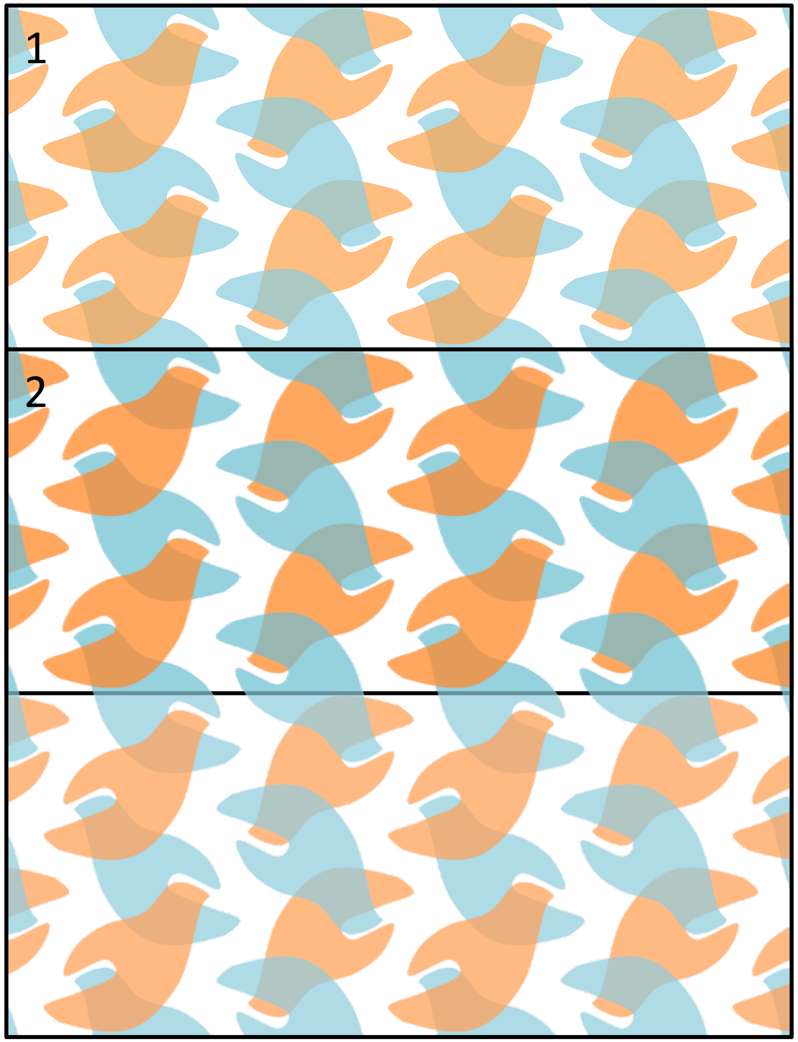
# Translation 2

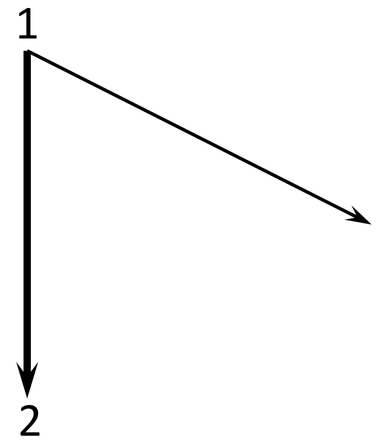



Highlighted vector
maps 1 -> 2

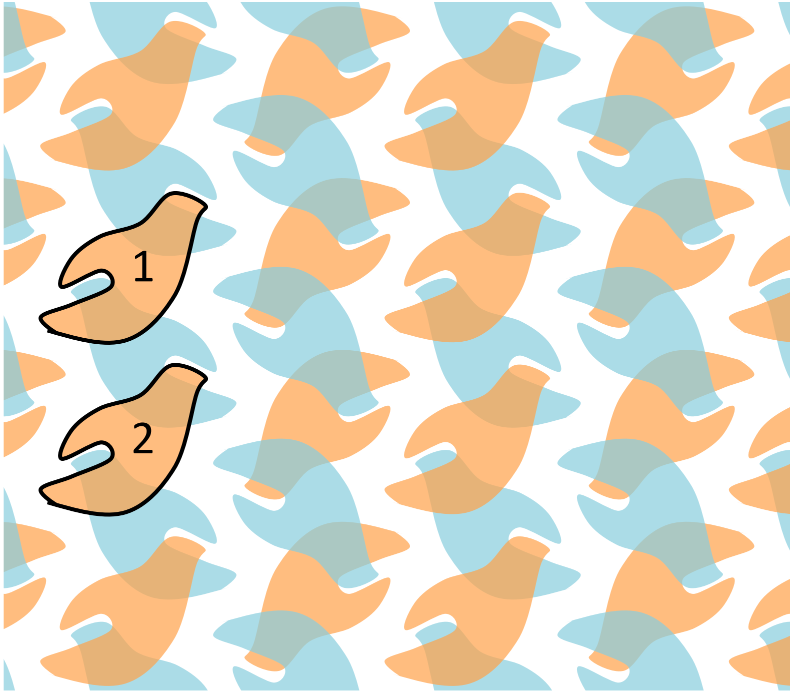
# Translation 2 is global

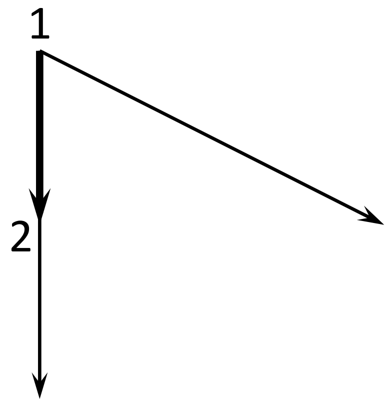



Highlighted vector maps the whole crystal onto itself

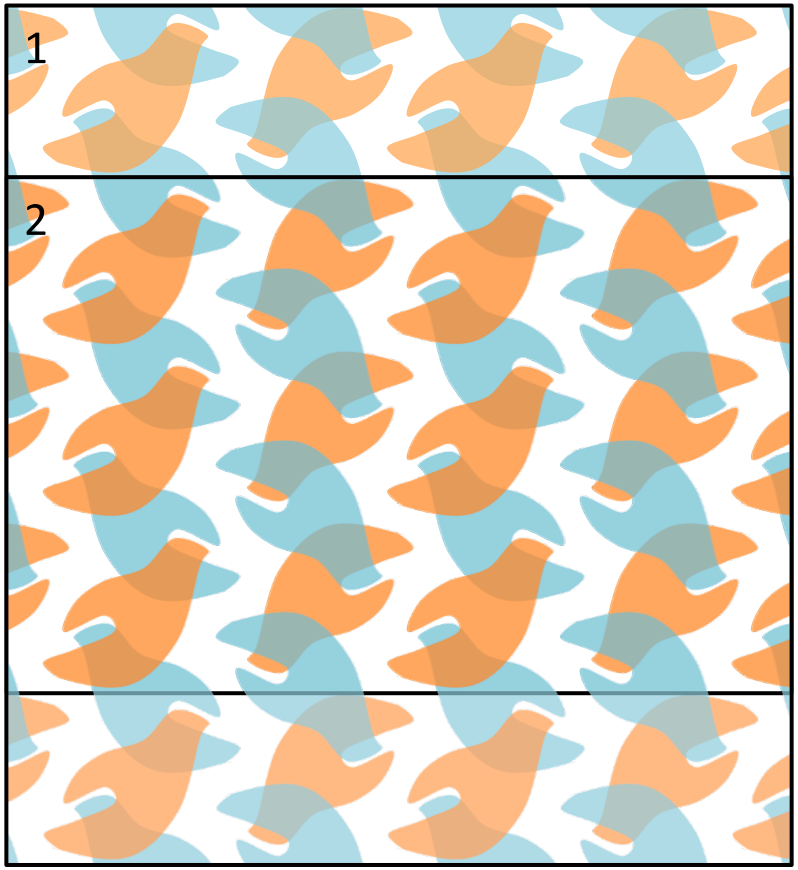
# Translation 3

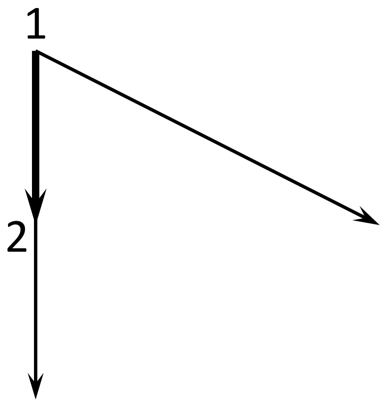



Highlighted vector
maps 1 -> 2

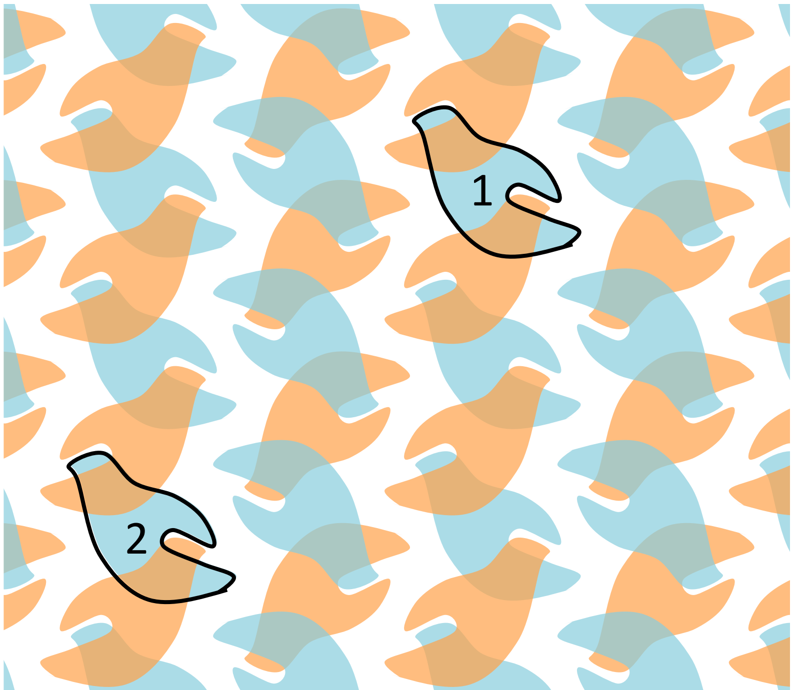
# Translation 3 is global

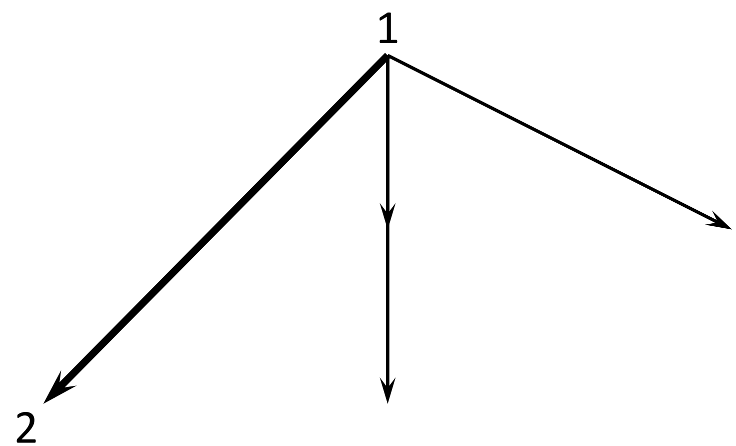



Highlighted vector maps the whole crystal onto itself

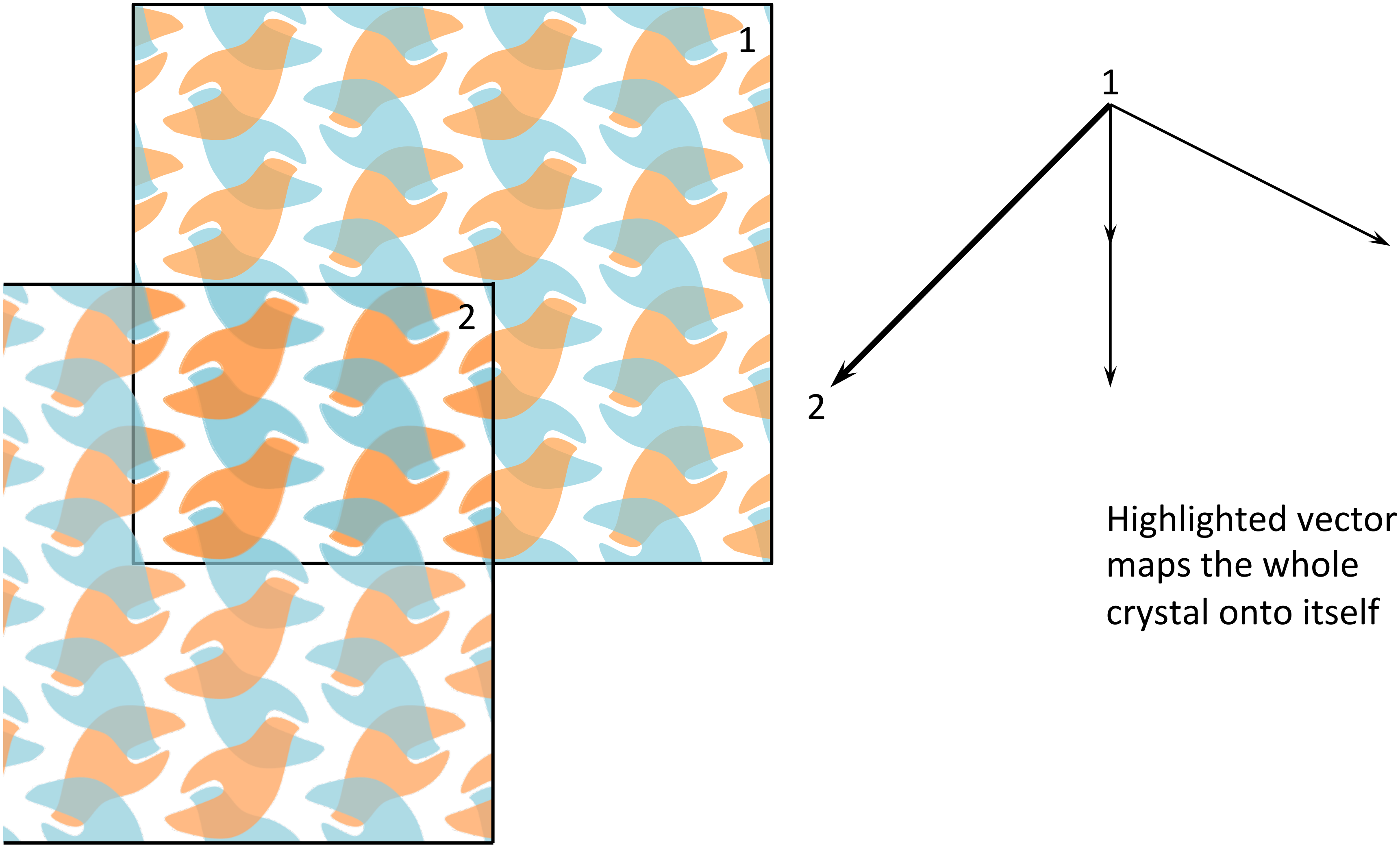
# Translation 4



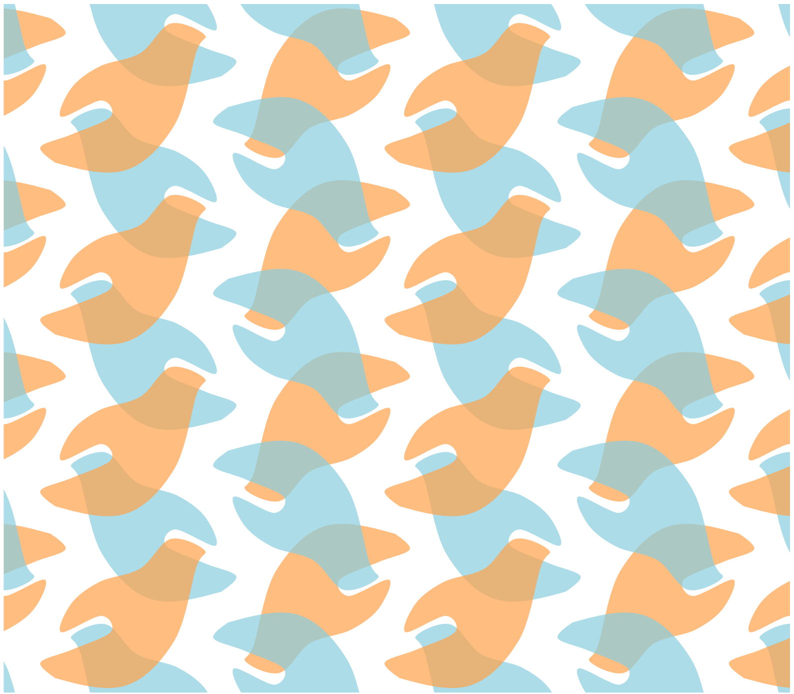

Highlighted vector maps 1 -> 2

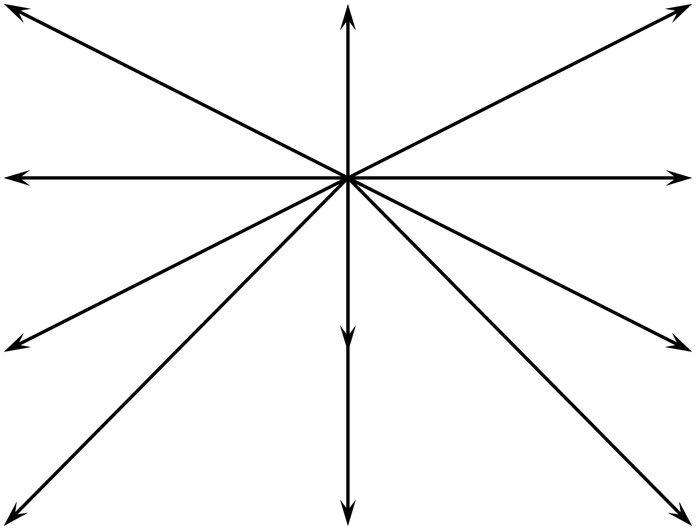
# Translation 4 is global




Highlighted vector maps the whole crystal onto itself

# All translations form an infinite group

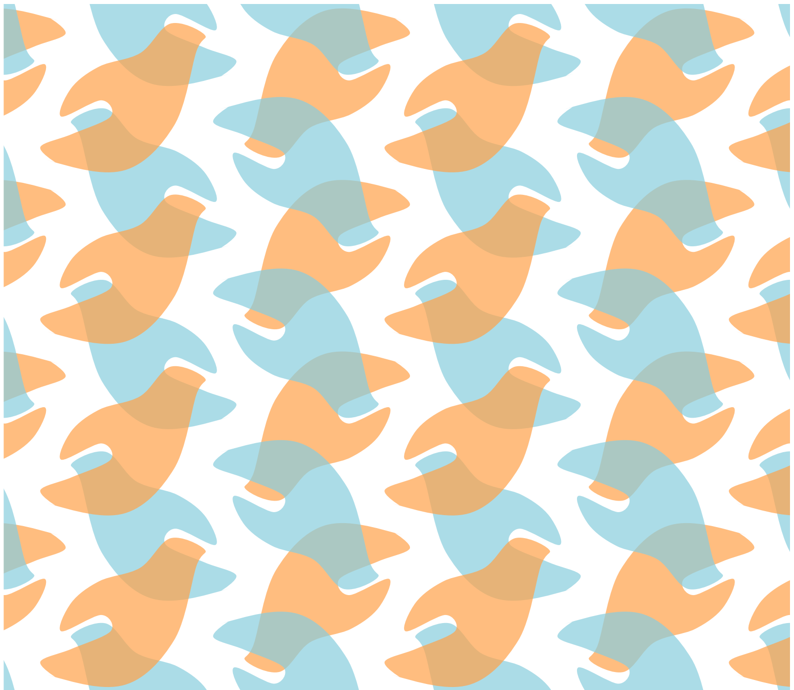


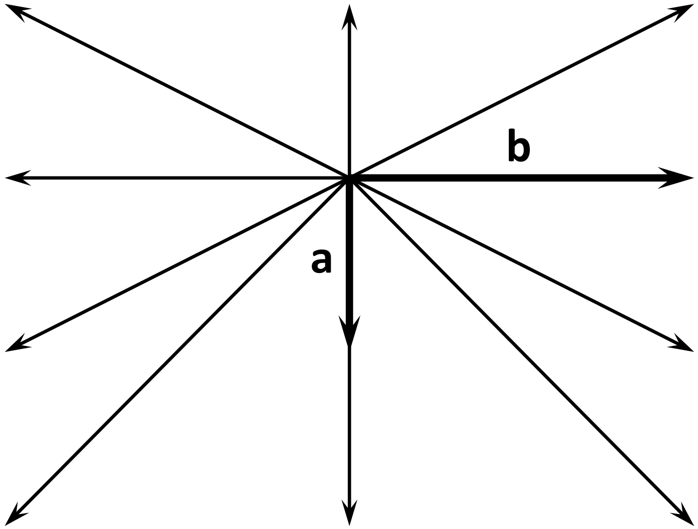


An infinite group (over sum):

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

# Basis set

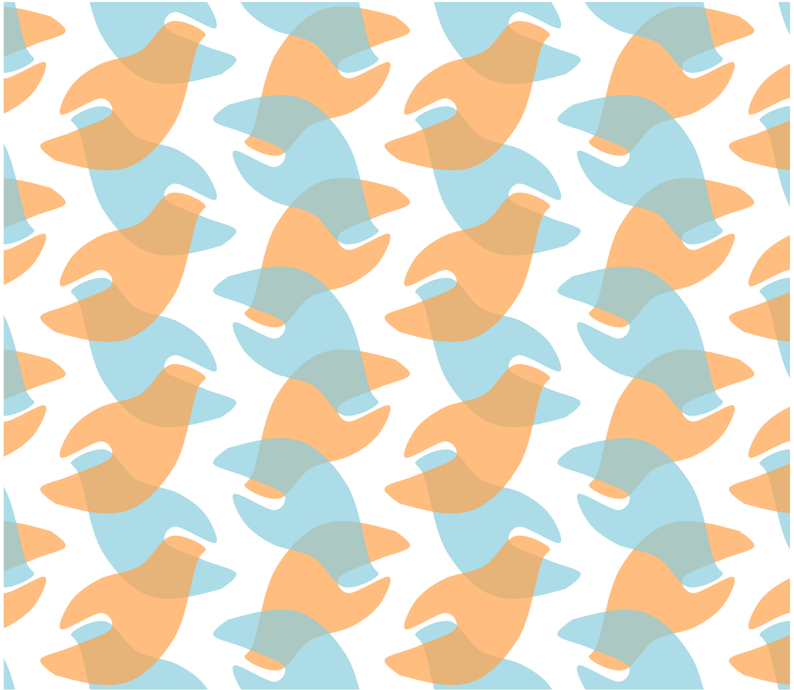


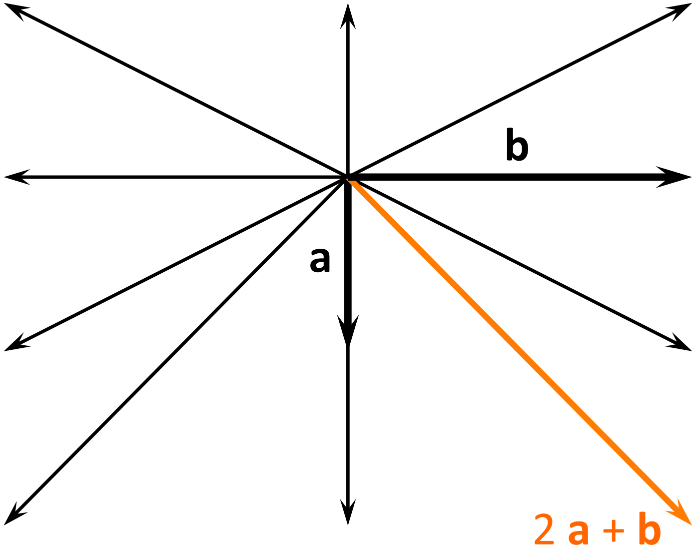



All the translations that map the crystal onto itself can be produced from a basis set: **a**, **b**, **c**

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

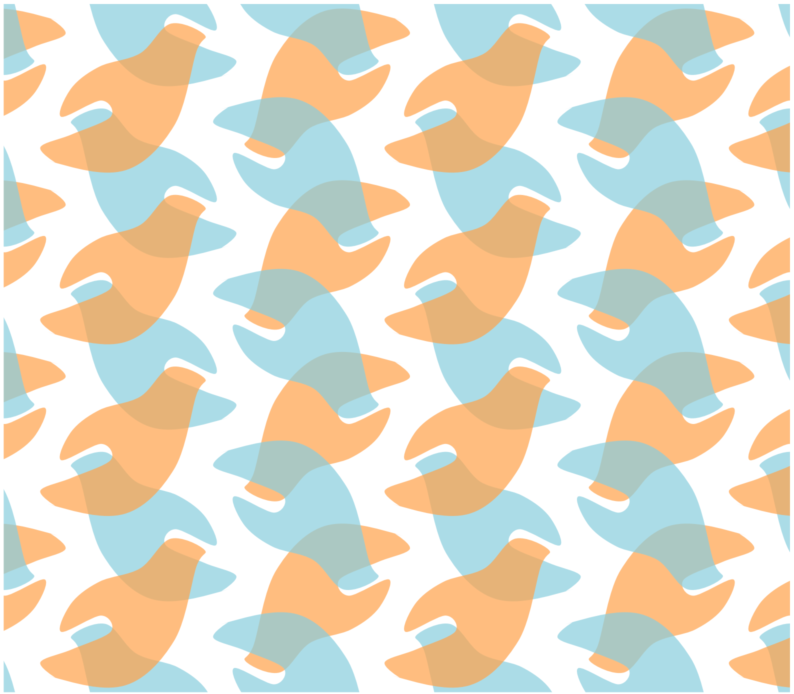
# Basis set

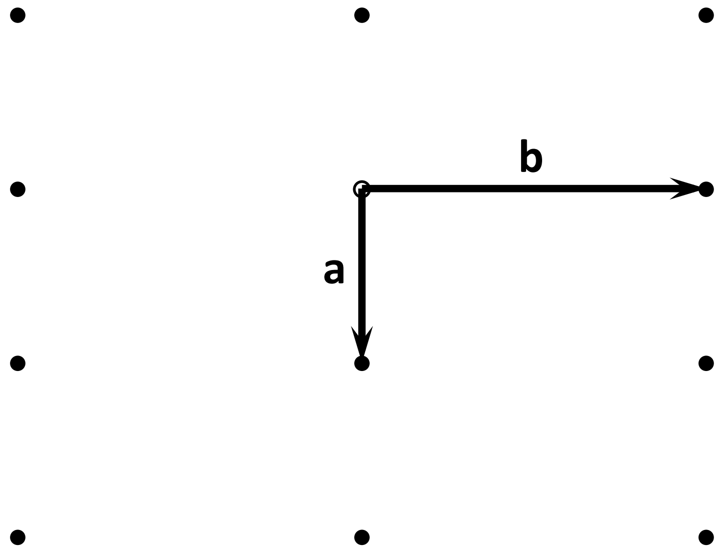





For example, the highlighted vector is expressed as 2 **a** + **b**.

# Lattice

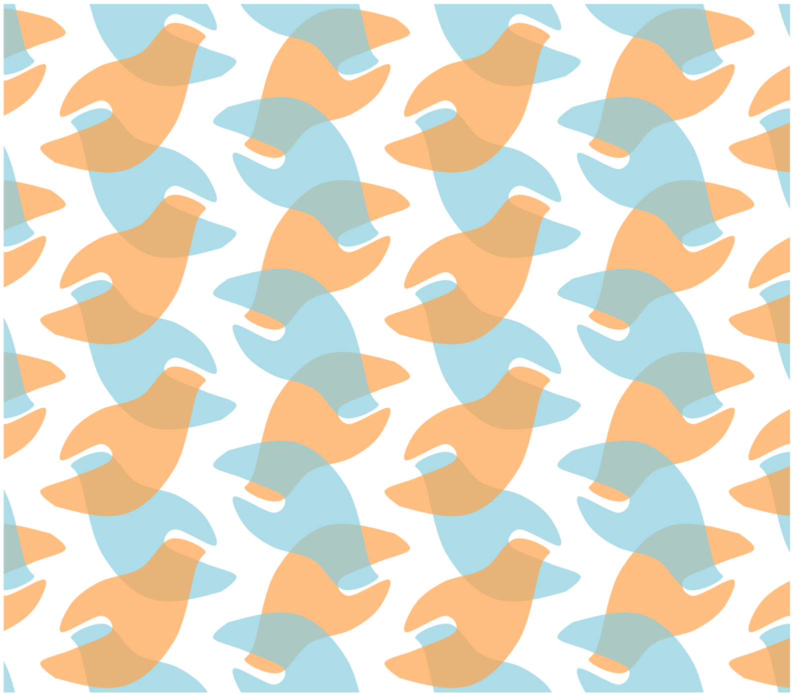


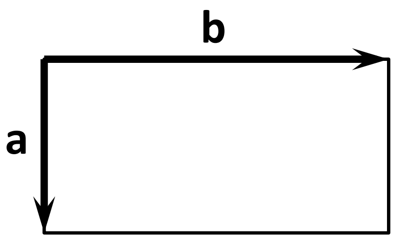



All the crystallographic translations can be represented as a lattice.

Translations live in a separate pace, not connected to crystal (for now)

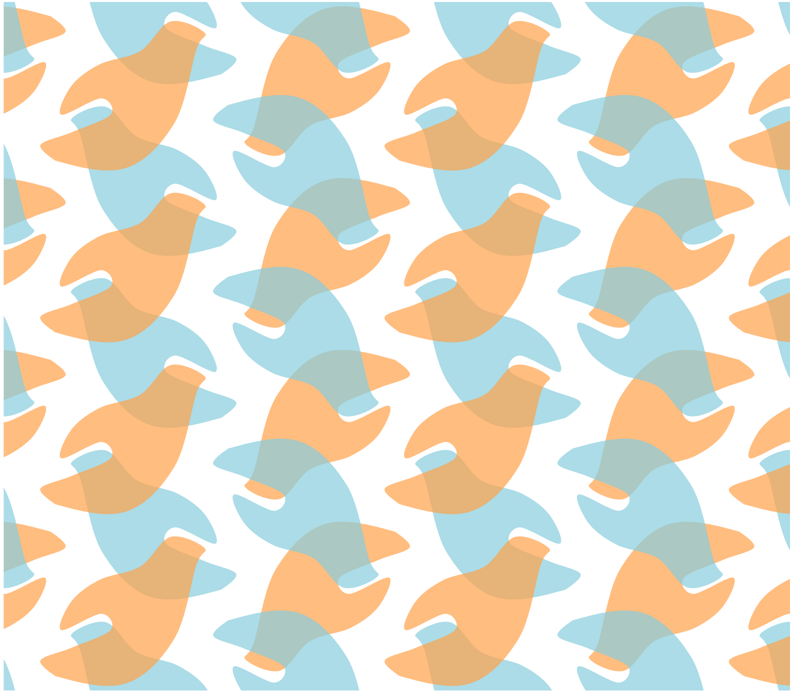
# Unit cell

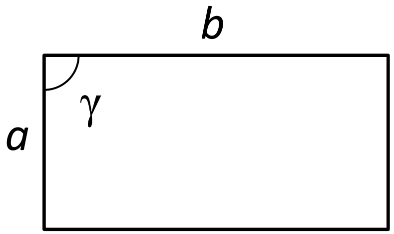





A compact representation of translational symmetry and base vectors.

# Unit cell

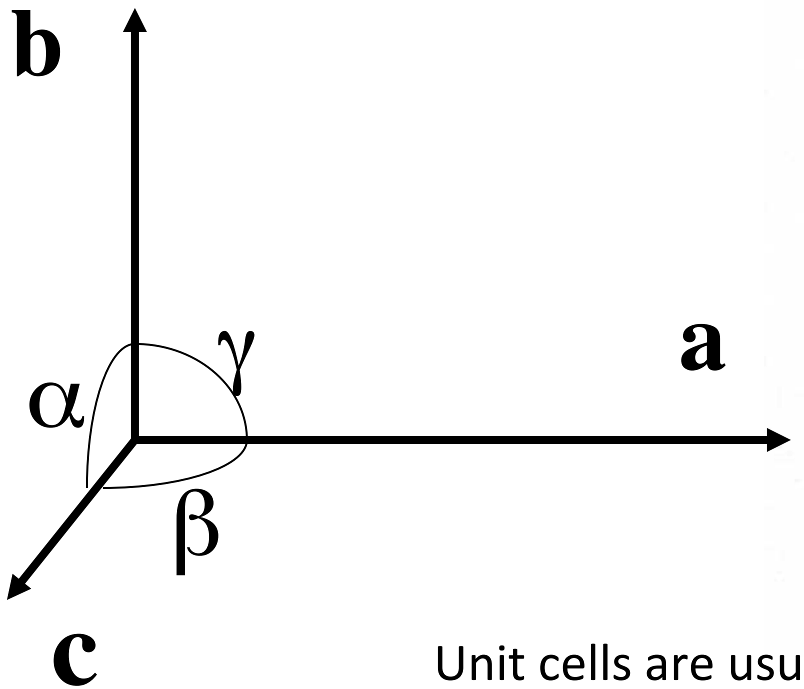


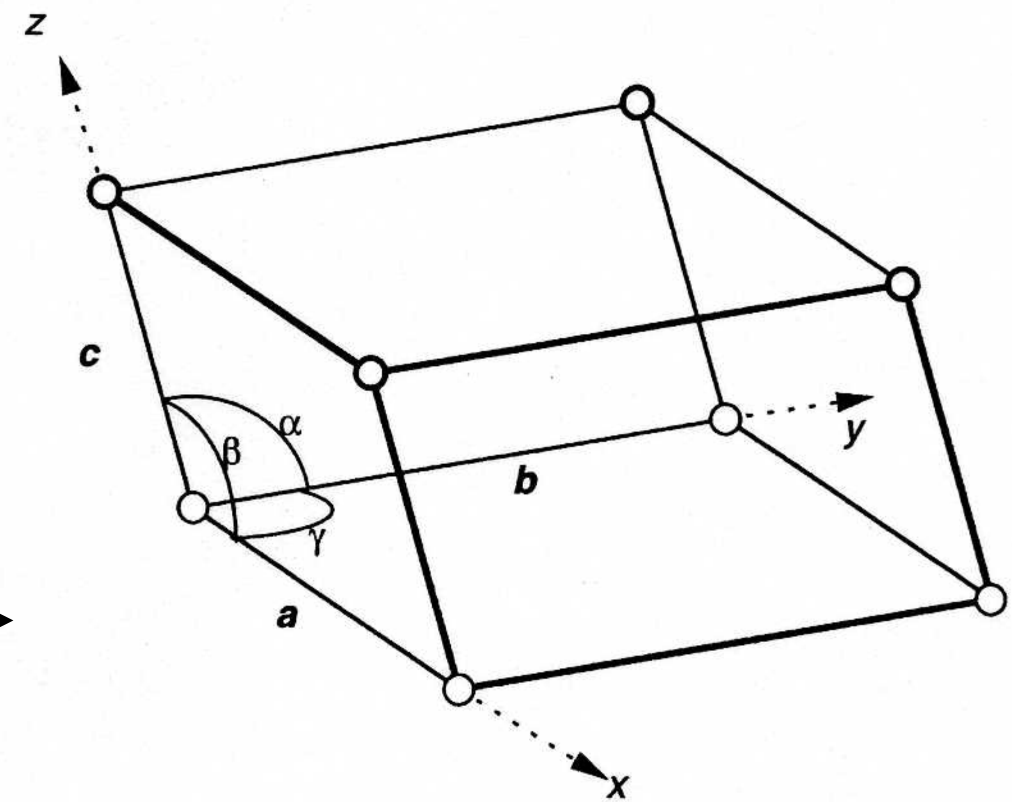



Can be fully characterised by six numbers
(the third dimension is not shown here)

# Unit cell parameters (3D view)

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

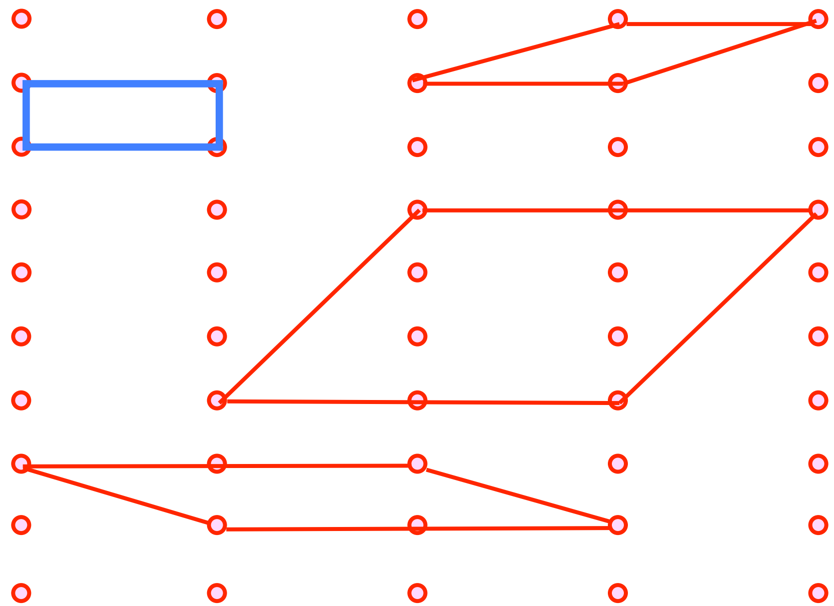



Unit cells are usually defined in terms of the *lengths* of these vectors and angles between them. For example,

a=94.2Å, b=72.6Å, c=30.1Å, α=90°, β=102.1°, γ=90°.

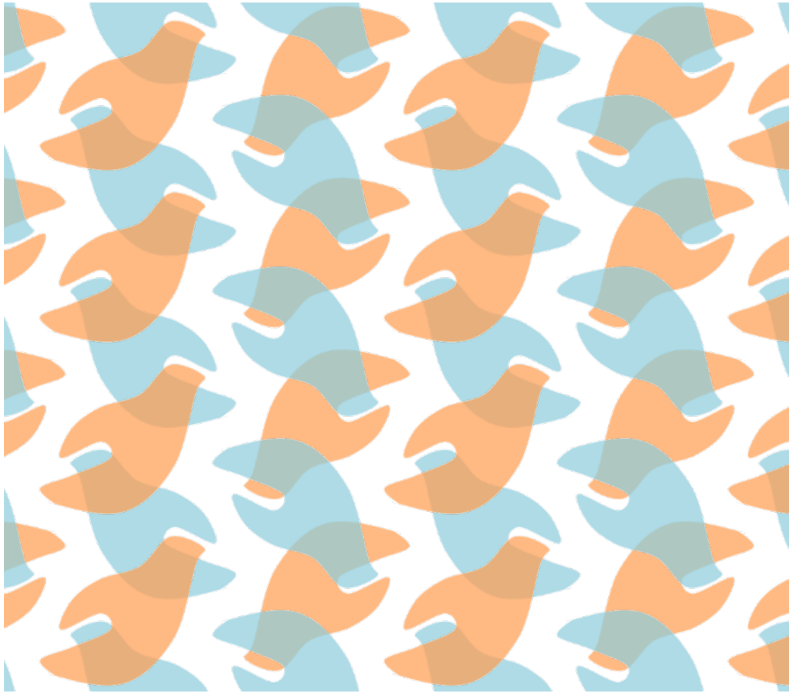
# `Choice of unit cell

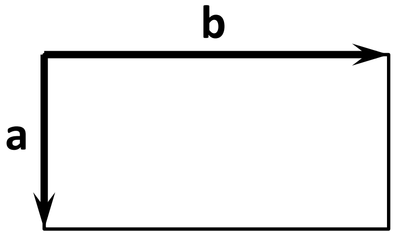


The top two do define all translations = primitive unit cells
The bottom two do NOT define all translations = non-primitive unit cells

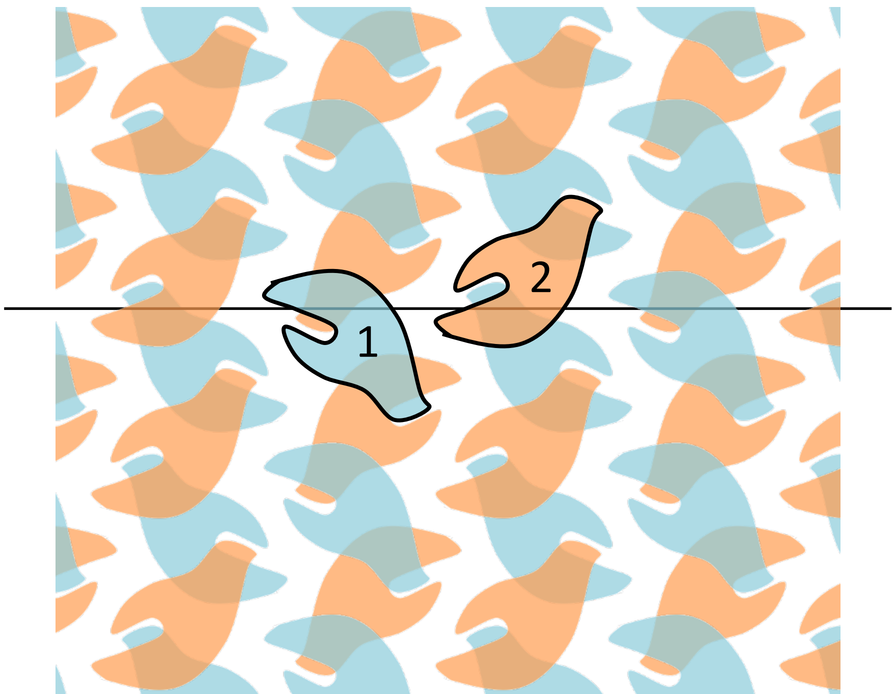
The top left: primitive reduced – the standard for <u>some</u> space groups (including $P2_12_12_1$)

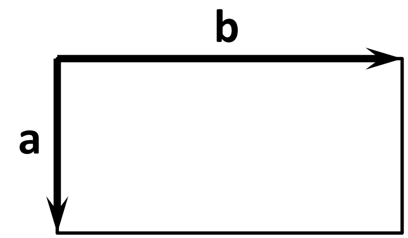
# Back to example

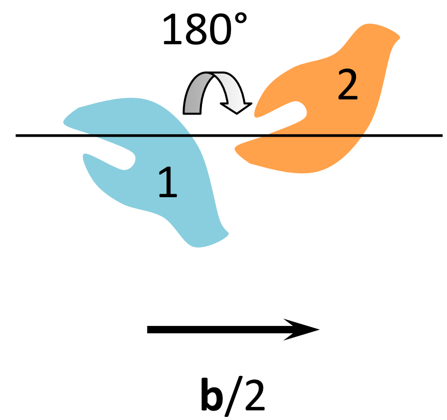




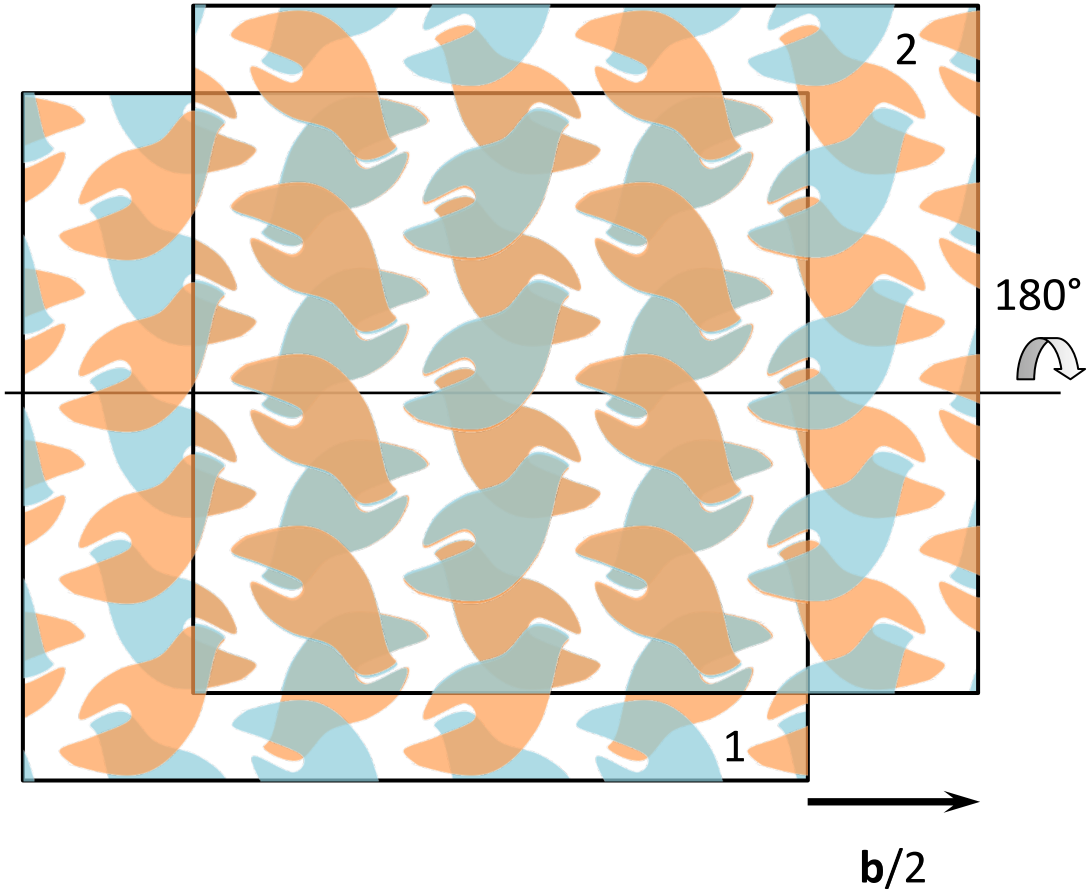
# Screw rotation 1

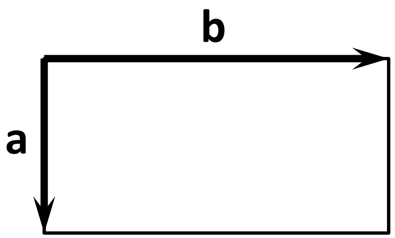


# Screw rotation 1 is global



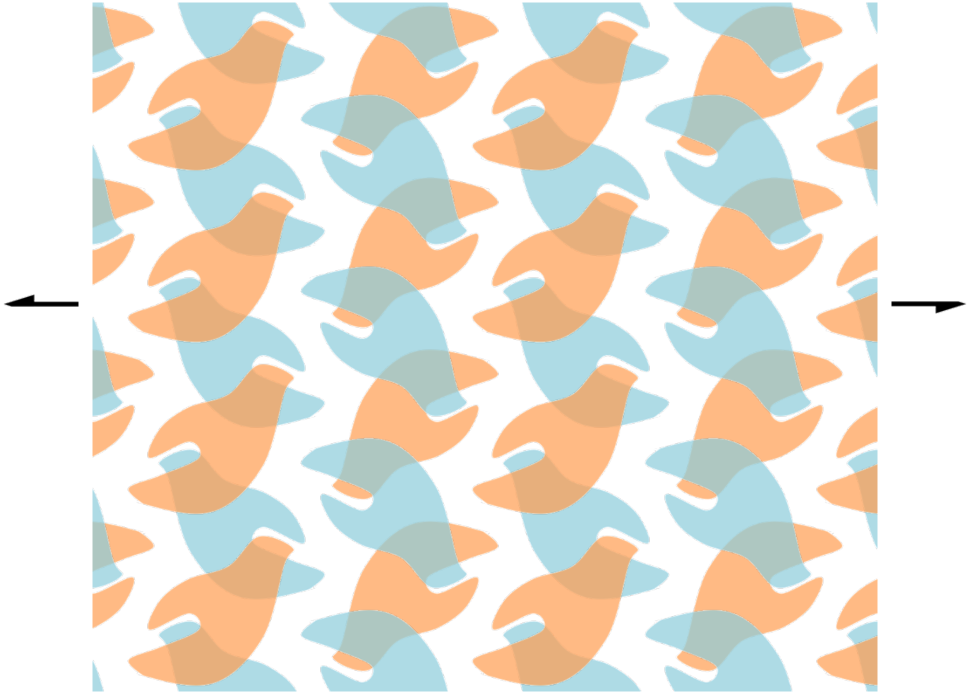

Operation 1->2
maps the whole crystal onto itself:

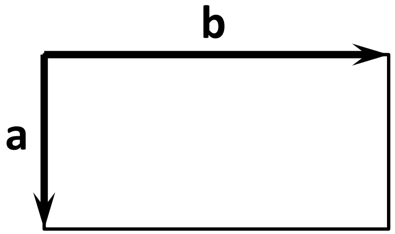
this is a crystallographic operation

The axis is a crystallographic symmetry element,

it can be mapped into the structure

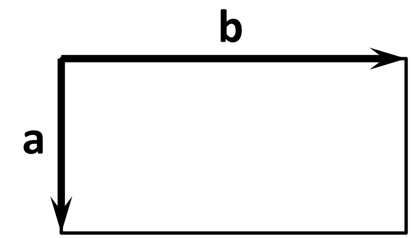
# Screw rotation 1 - symbol

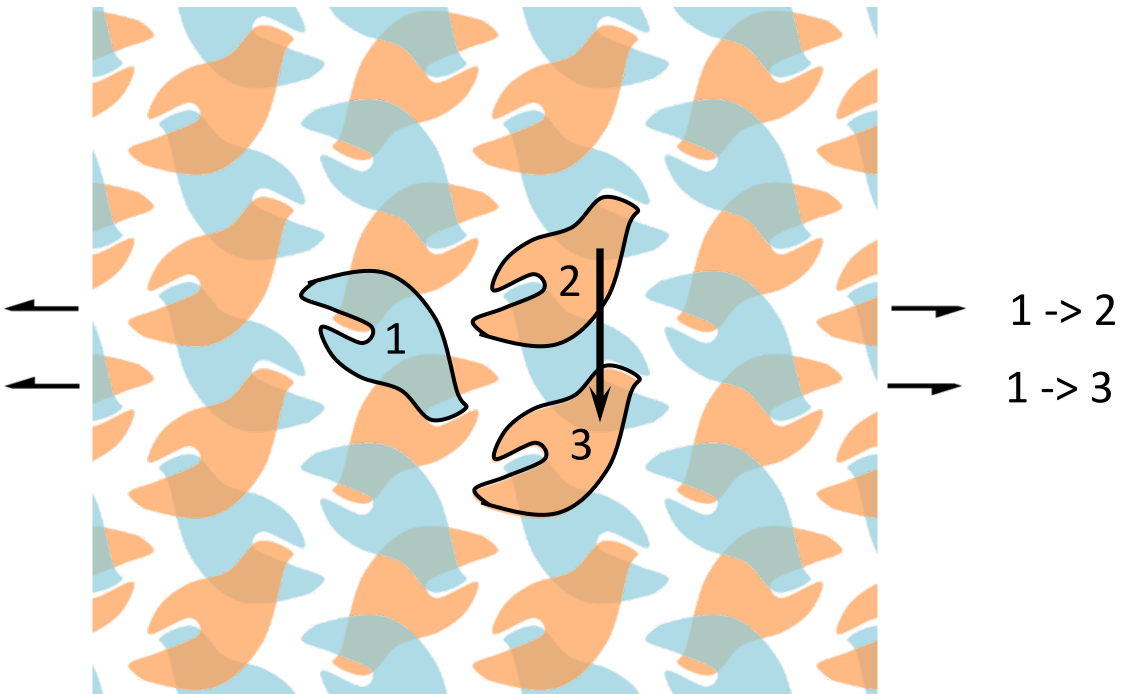





$2_1$ (plane of figure):

# Screw rotation 1 - repeats



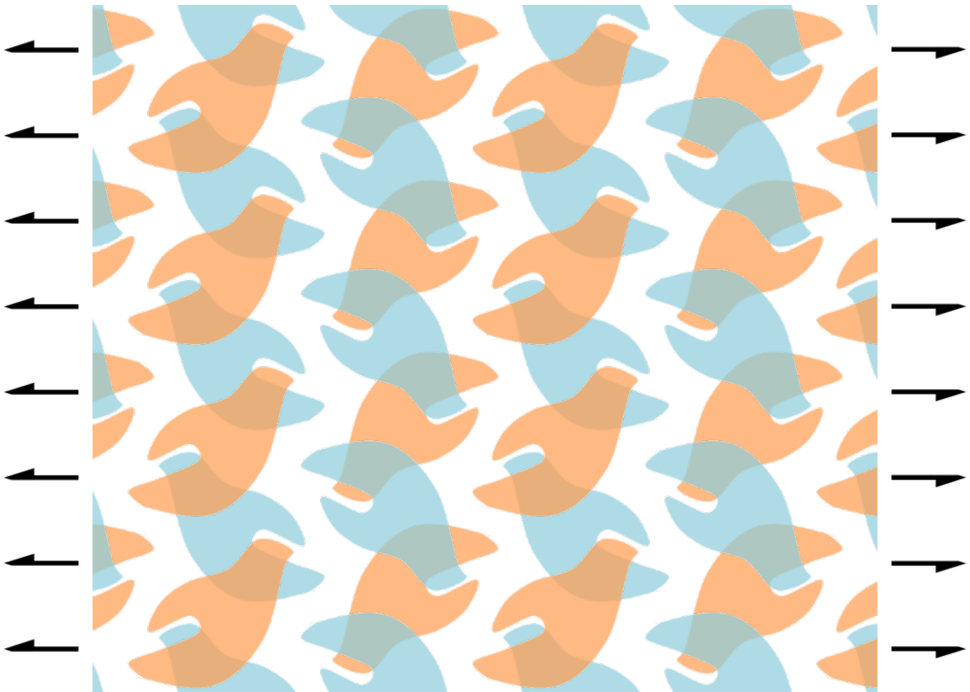



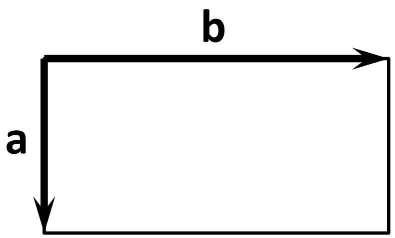

action of top axis
×
translation **a**
=
action of bottom axis

(elements of a group)

The operation on the top axis, combined with translation **a**, can be used to recreate the bottom axis. Here this also means that a rotation/translation offset by ½ **a** is also available.

# Screw rotation 1 - repeats

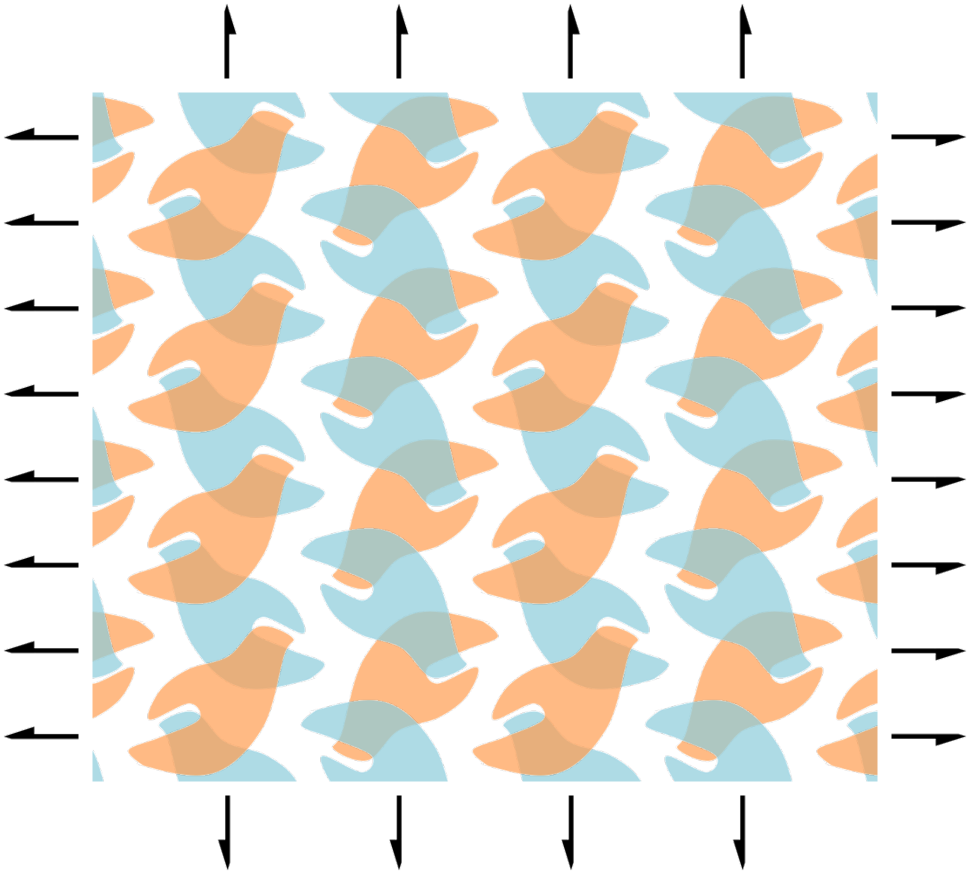


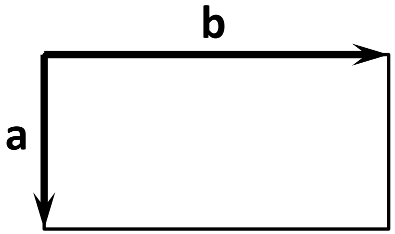



$2_1$ (plane of figure): ⟵ ⟶

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

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

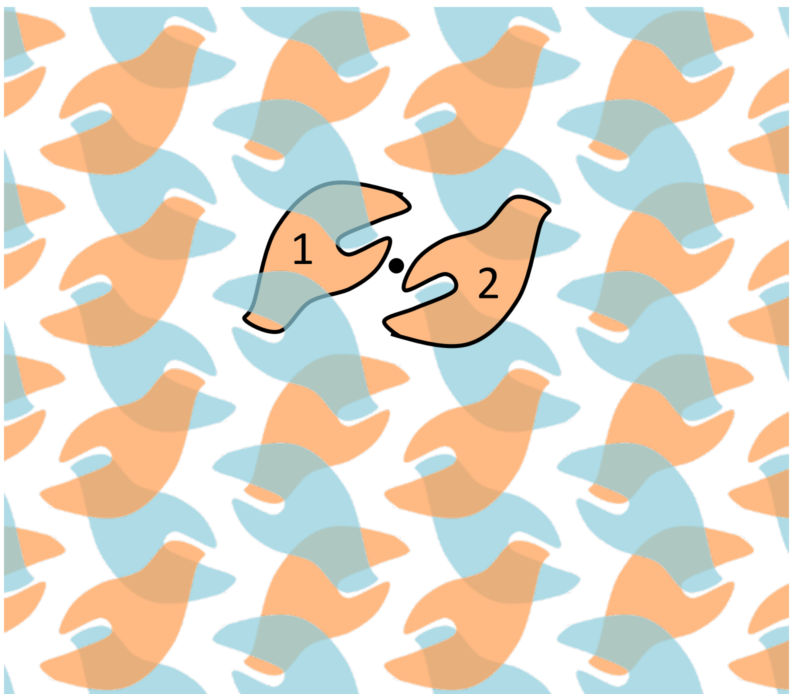


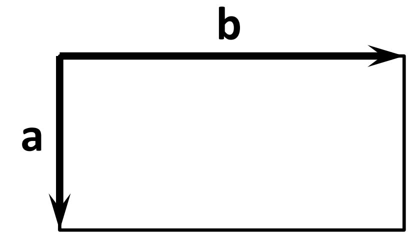


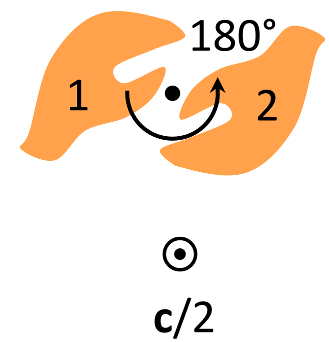

$2_1$ (plane of figure):

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

# Screw rotation 3 – into plane

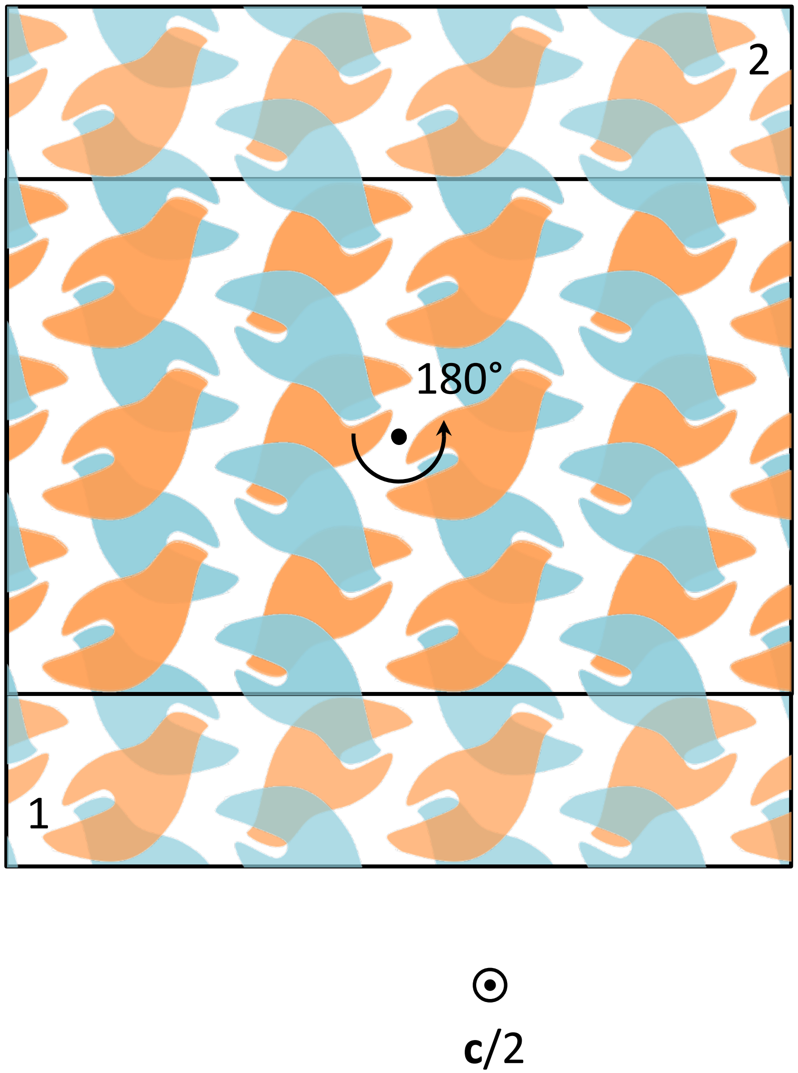


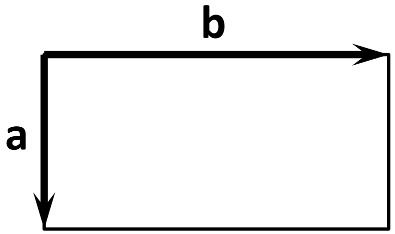




A rotation of 180º with a translation of ½ unit cell from the figure.

# Screw rotation 3 is global



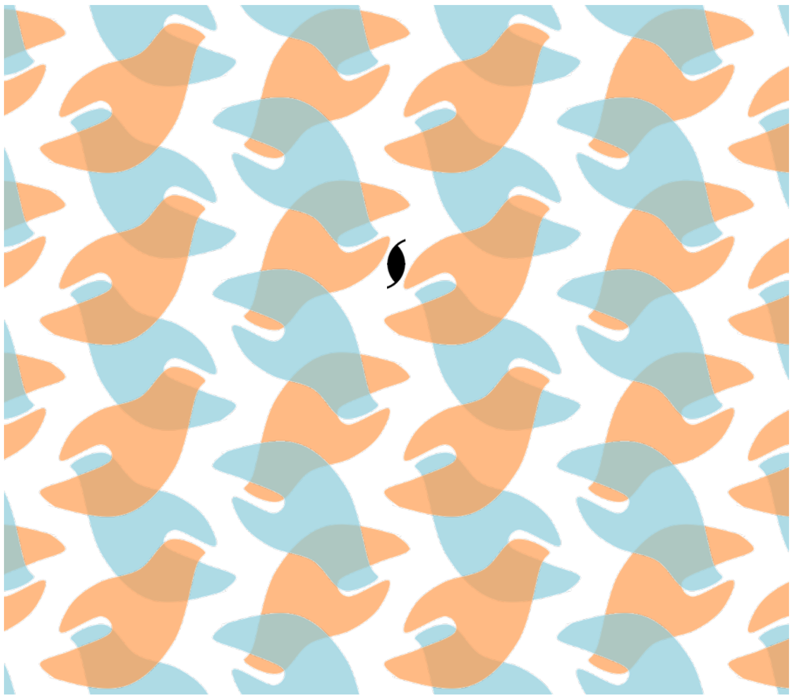

Screw rotation 3 maps the whole crystal onto itself:

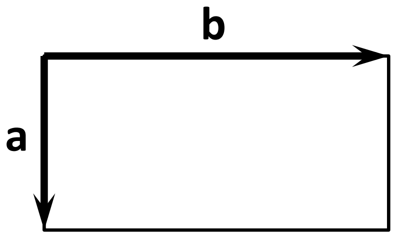
this is a crystallographic operation

The rotation axis is a crystallographic symmetry element,

it can be mapped into the structure

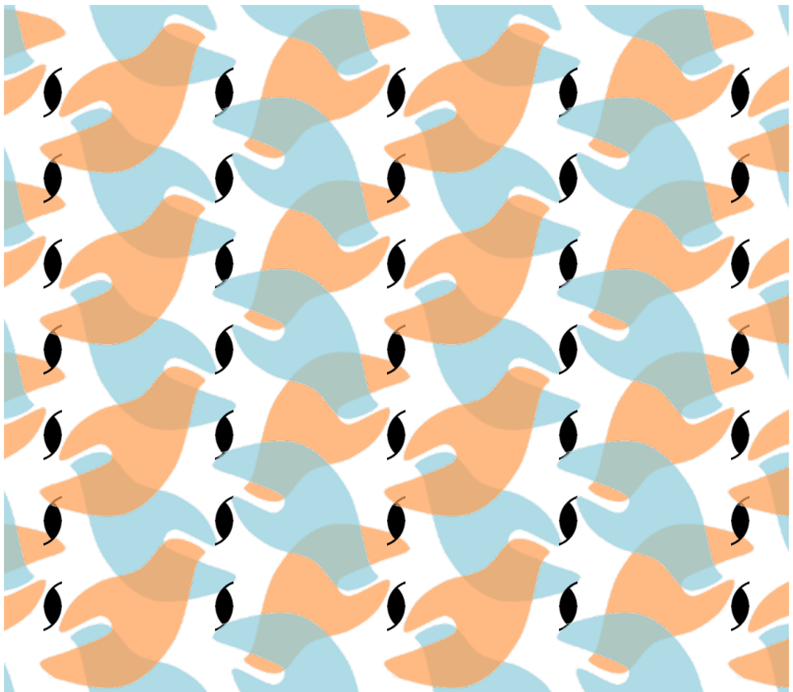
# Screw rotation 3 - symbol

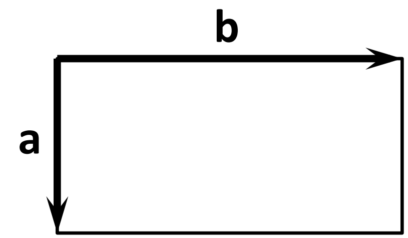





$2_1$ (along view):

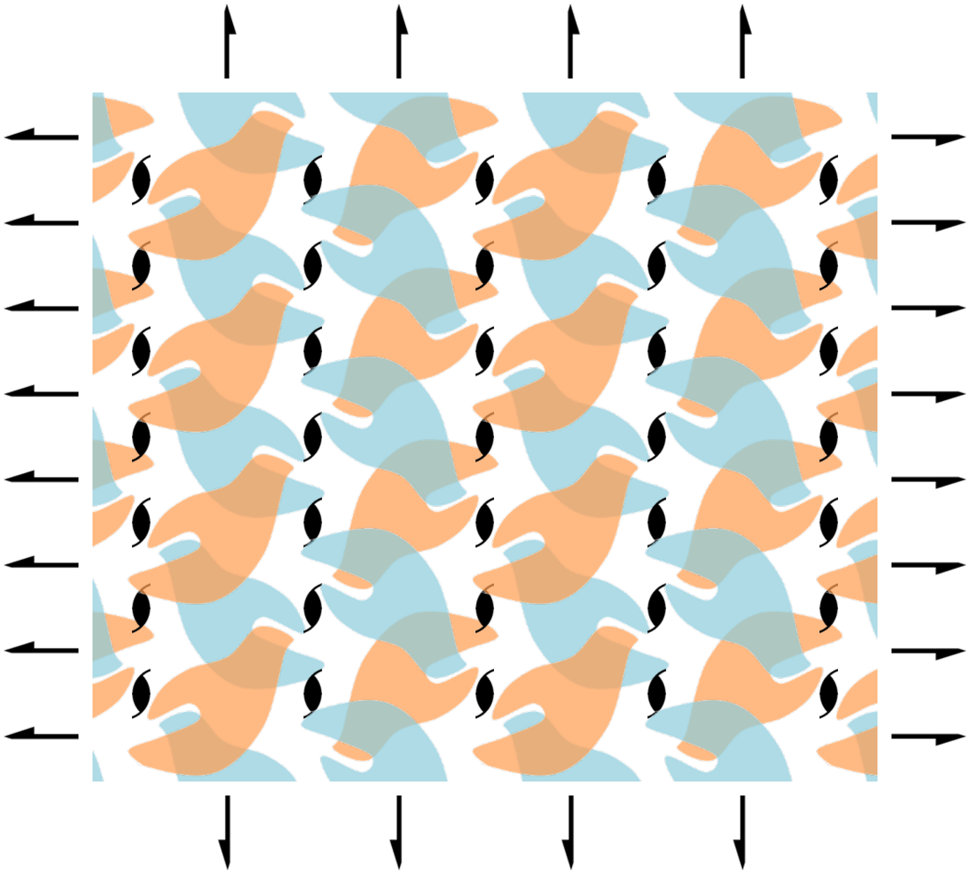
# Screw rotation 3 - repeats

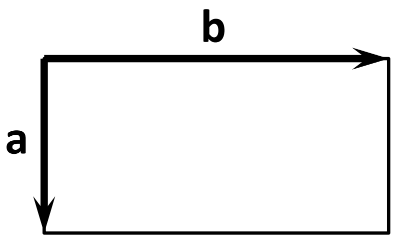





$2_1$ (along view): 

# All axes together



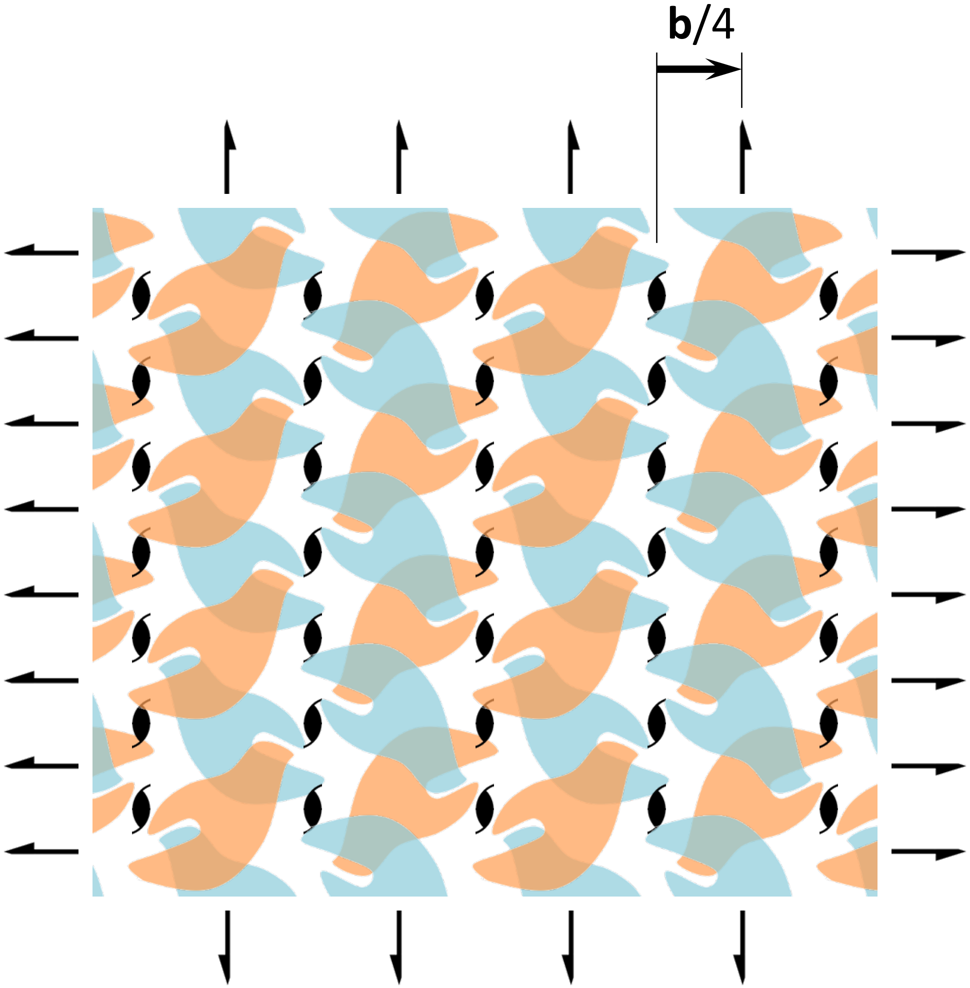


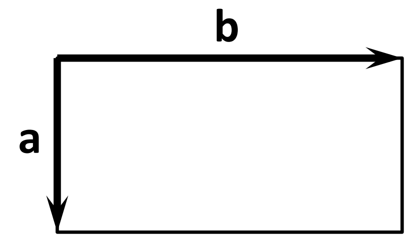

$2_1$ (plane of figure):

$2_1$ (along view):

we have built
a space group

# Relative positions of axes

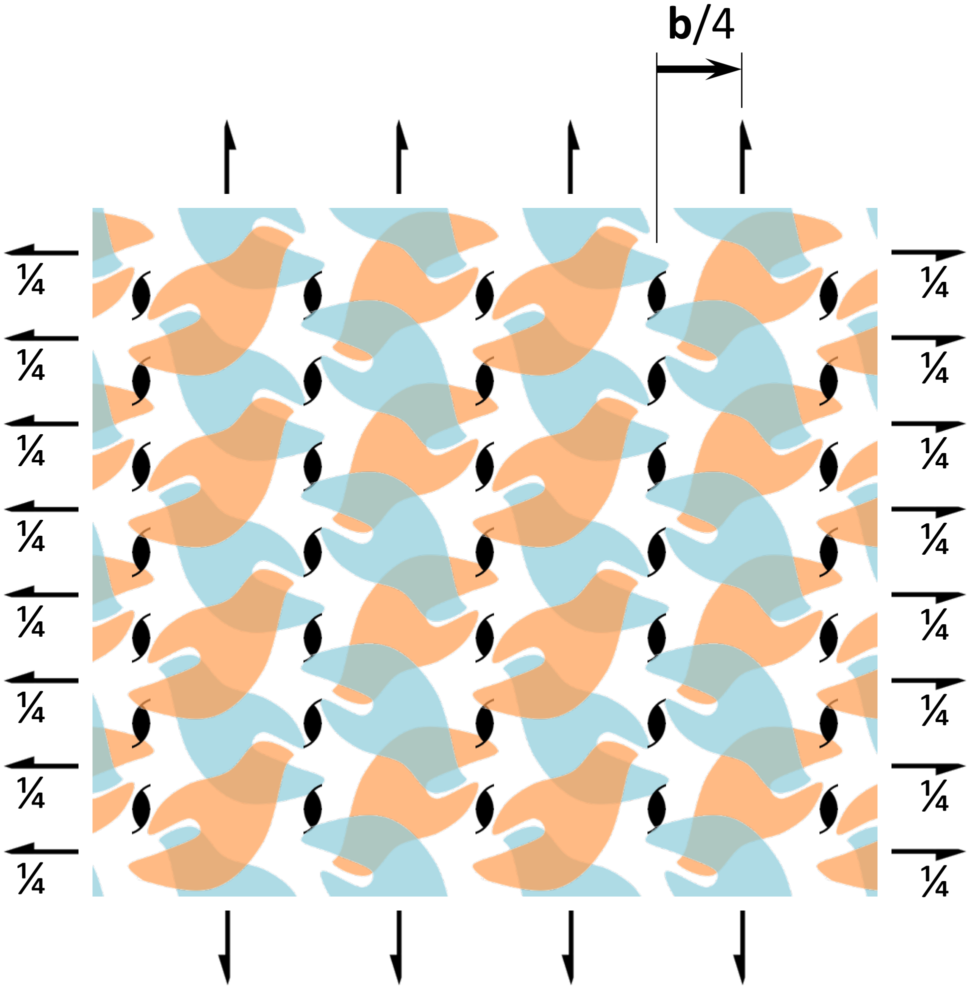


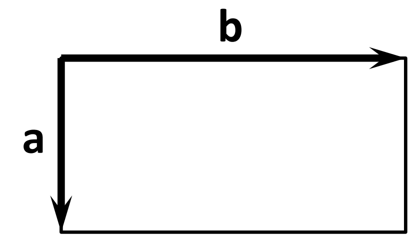




$2_1$ (plane of figure):

$2_1$ (along view):

# Relative positions of axes



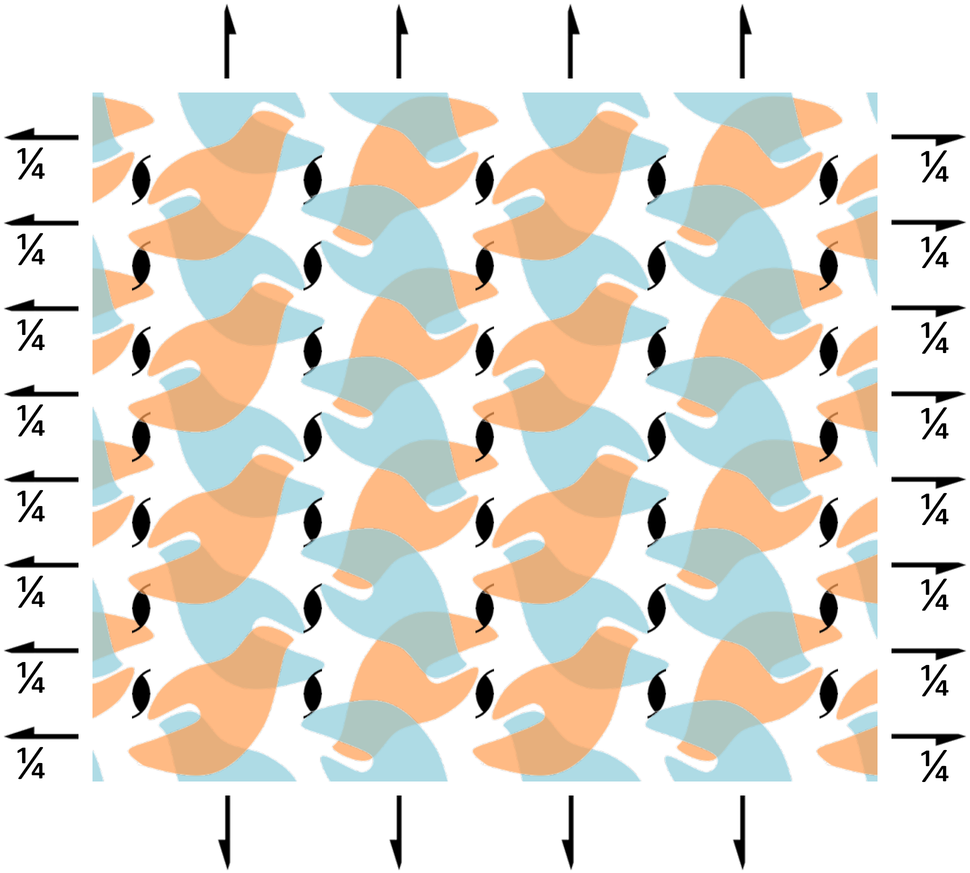

$2_1$ (plane of figure):

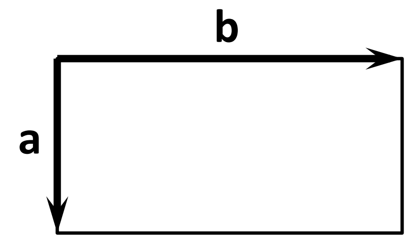
$2_1$ (along view):

The adjacent axes running in different directions are offset by ¼ unit cell edge from each other.

The horizontal ¼ indicates a offset of ¼ **c** into the figure.

# Relative positions of axes



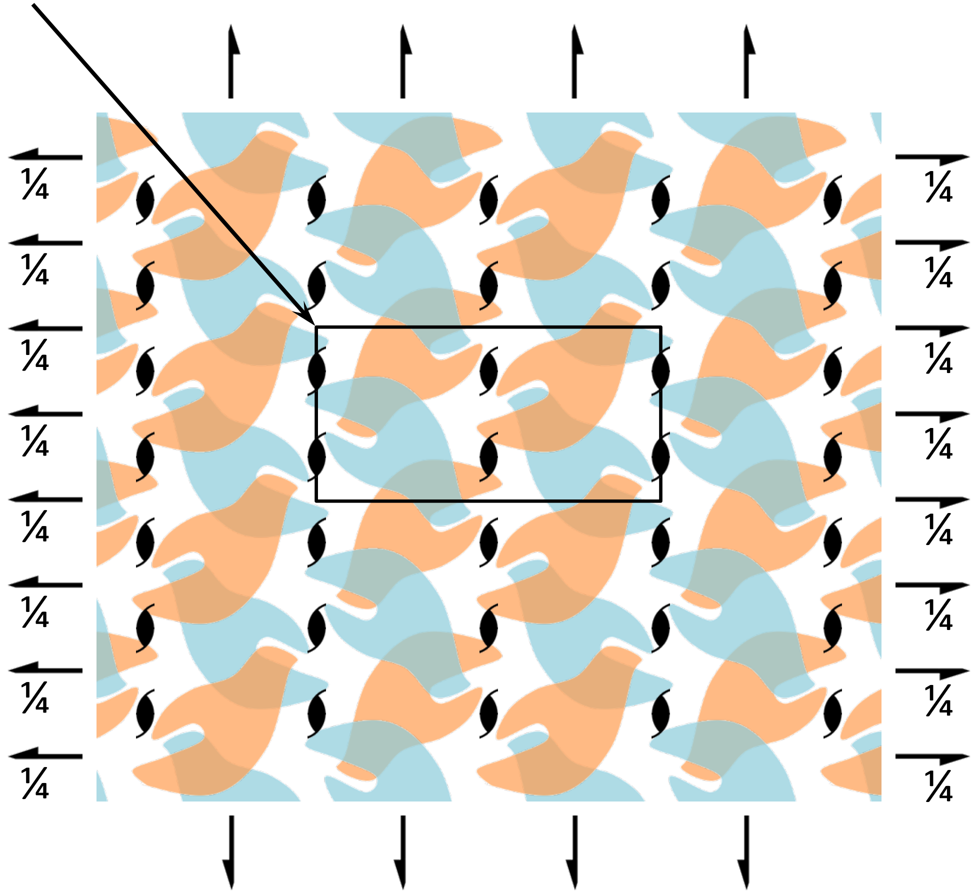



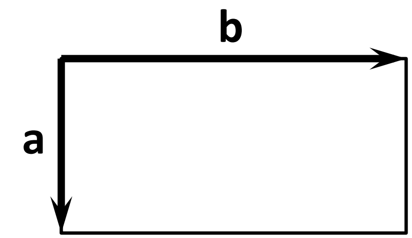

$2_1$ (plane of figure): 

$2_1$ (along view): 

# Choice of origin is a convention. Notation

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




$2_1$ (plane of figure):

$2_1$ (along view):

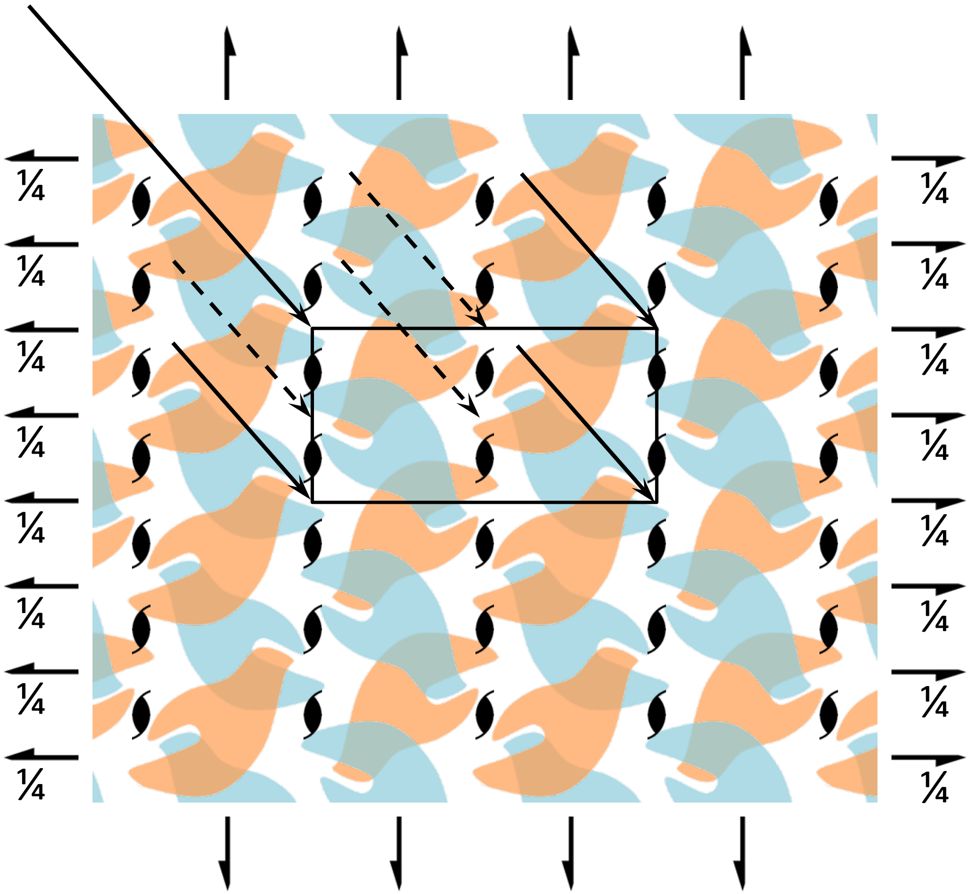
The unit cell placed on picture with symmetry elements means a choice of origin.

Such a choice is a convention.

The origin in this particular space group: is chosen to be equidistant from adjacent axes

# Equivalent and alternative origins

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




Solid arrows – origins, which are equivalent to the one chosen

Dashed arrows – alternative origins.

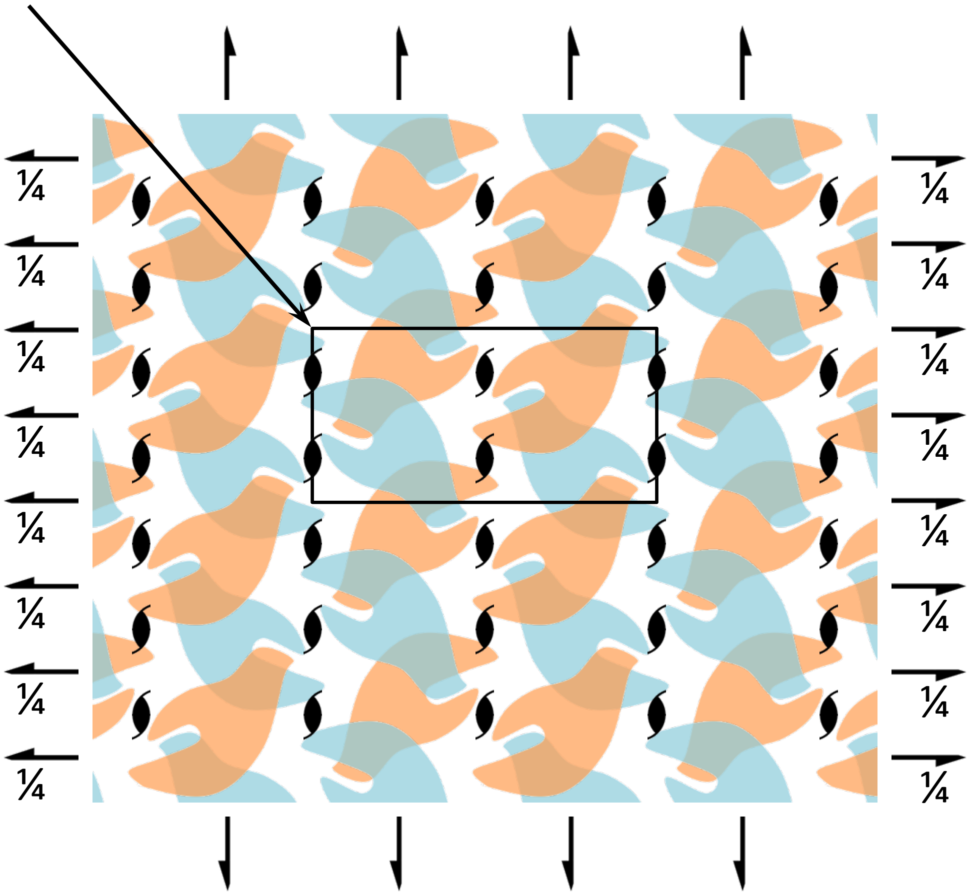
Altogether:

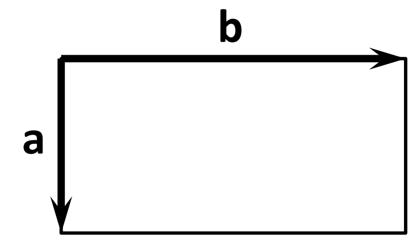
- infinite number of conventional origins
- eight types of equivalent origins in this example

The origin in this particular space group:
is chosen to be equidistant from adjacent axes

# Complete picture

The origin



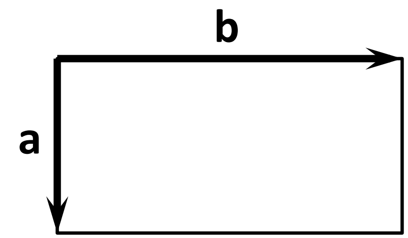

$2_1$ (plane of figure):

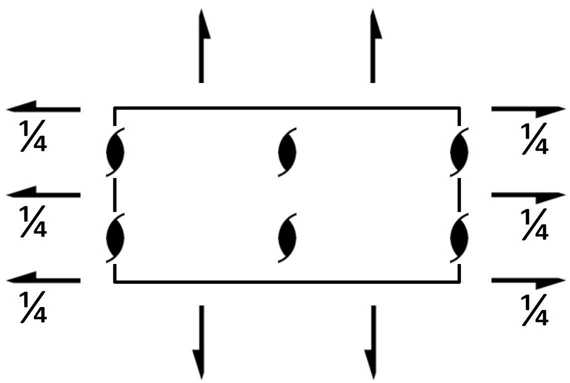
$2_1$ (along view):

# Compact representation

$P\,2_1\,2_1\,2_1$

No. 19




$2_1$ (plane of figure): 

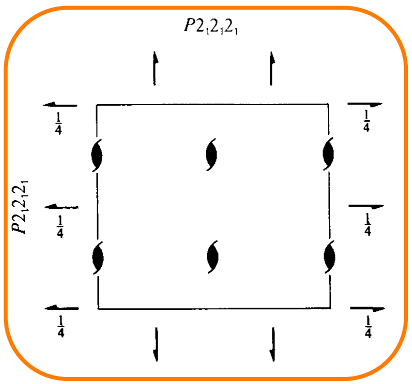
$2_1$ (along view): 

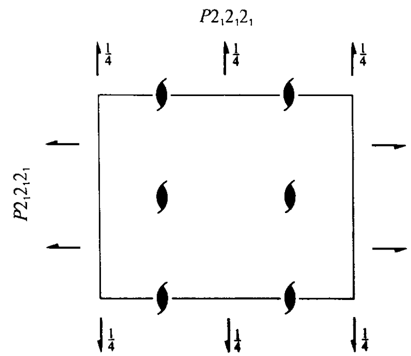
Compact representation -> space group symbol -> more info in International Tables

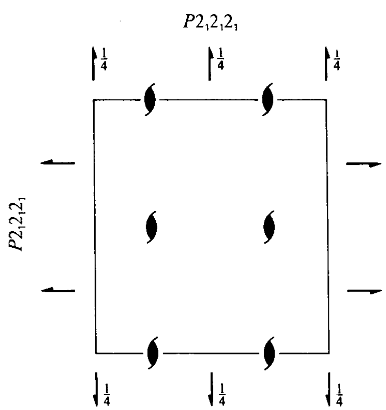
# Presentation in International Tables

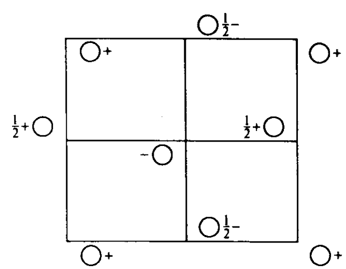
$P2_12_12_1$ | $D_2^4$ | 222 | Orthorhombic

No. 19 | $P2_12_12_1$ | Patterson symmetry $Pmmm$



# Presentation in International Tables

Short Hermann-Mauguin symbol: $P2_12_12_1$

Space group number: No. 19

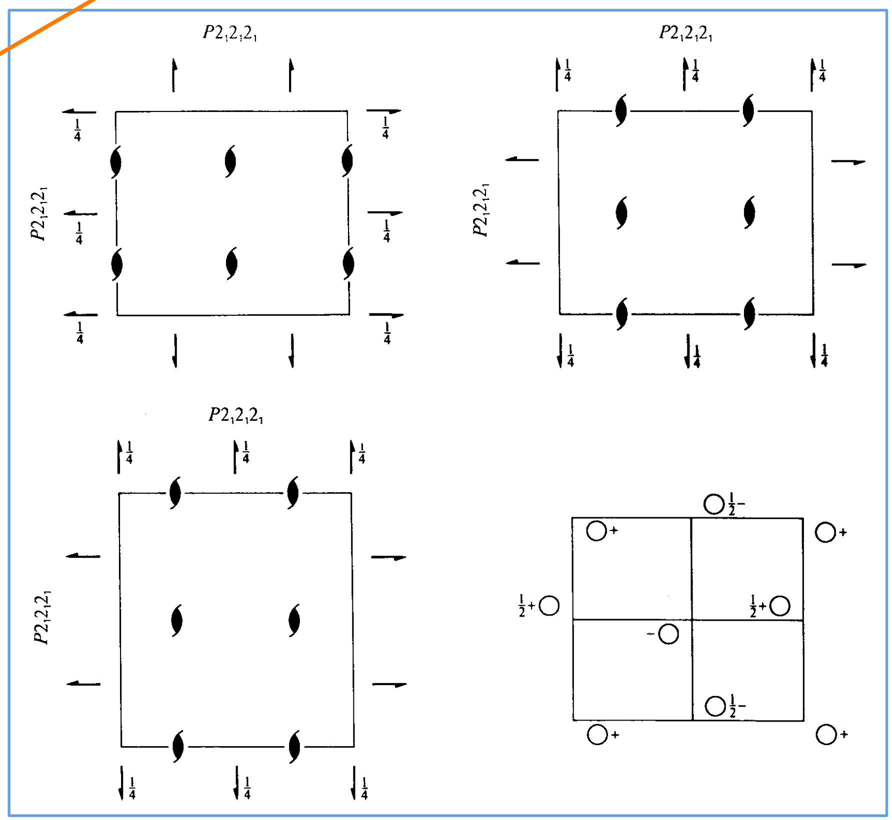
Schoenflies symbol: $D_2^4$

Hermann-Mauguin symbol: $P2_12_12_1$

Crystal Class (point group): 222

Crystal system: Orthorhombic

Patterson symmetry: Patterson symmetry $Pmmm$




Space group diagrams:

- Location of symmetry elements (one or more projections)
- Set of equivalent points in general position

# Symmetry operations and elements

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

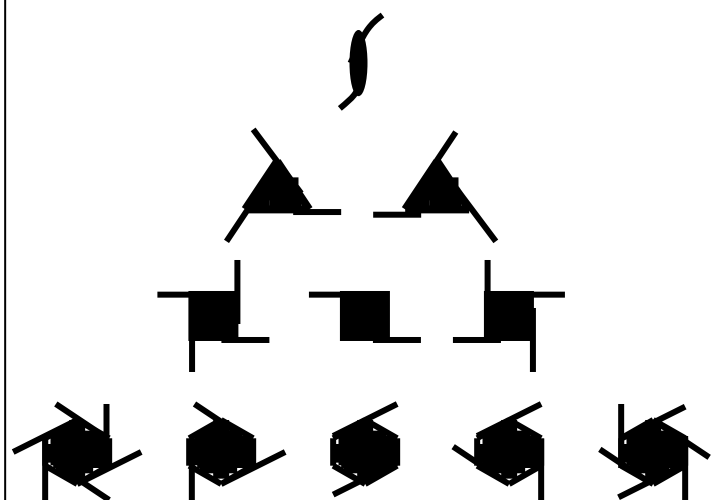
Proper rotation: Rotate by 360°/n.

Screw rotation: Rotate by 360°/n & translate by d(m/n); d= unit cell edge.

## Proper Rotations

| | Symbol | (n) |
|---|---|---|
| Two-fold | ⬮ | 2 |
| Three-fold | ▲ | 3 |
| Four-fold | ■ | 4 |
| Six-fold | ⬢ | 6 |

## Screw Rotations



| Symbol | (nm) |
|---|---|
| | $2_1$ |
| | $3_1, 3_2$ |
| | $4_1, 4_2, 4_3$ |
| | $6_1, 6_2, 6_3, 6_4, 6_5$ |

# 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 (usually ½) unit cell 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 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

* In macromolecular crystals the symmetry elements are all rotations

| **Crystal System** | **Characteristic symmetry elements** | **Convention** |
|---|---|---|
| 1. Triclinic | Translations only | |
| 2. Monoclinic | 2-fold axes, all parallel | along **b** |
| 3. Orthorhombic | 2-fold axes in three perpendicular directions | along **a**, **b** and **c** |
| 4. Tetragonal | 4-fold axes, all parallel | along **c** |
| 5. Trigonal | 3-fold axes, all parallel | along **c** |
| 6. Hexagonal | 6-fold axes, all parallel | along **c** |
| 7. Cubic | 3-fold axes in four different orientations | along body diagonals |

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| 7. Cubic | 3-fold axes in four different orientations | along body diagonals |

example

# Crystal Systems

Some SGs require use of centred **(non-primitive)** unit cells

| Crystal System | Characteristic symmetry elements | Convention |
|---|---|---|
| 1. Triclinic | Translations only | |
| 2. Monoclinic | 2-fold axes, all parallel | along **b** |
| 3. Orthorhombic | 2-fold axes in three perpendicular directions | along **a**, **b** and **c** |
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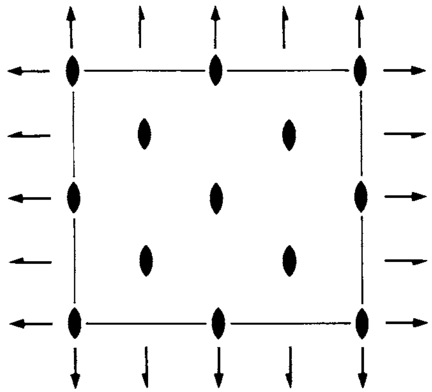
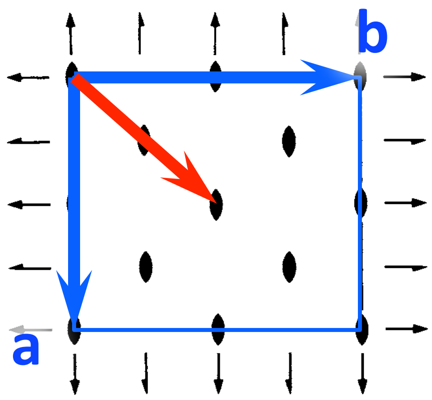
| 7. Cubic | 3-fold axes in four different orientations | along body diagonals |

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

*C*222
as presented in the
International Tables
for Crystallography

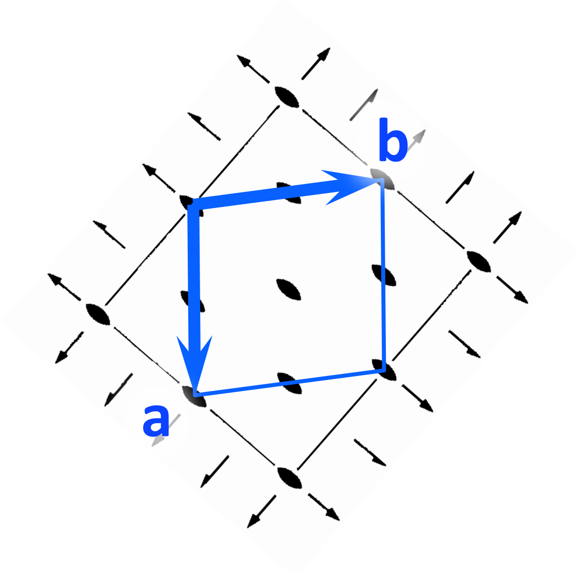


Standard unit cell;
C means additional
translation ½ (**a** + **b**)



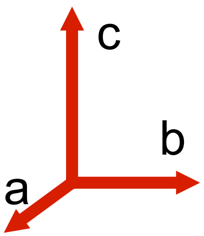

2-fold axes are
along **a**, **b** and **c**
(conventional
setting)

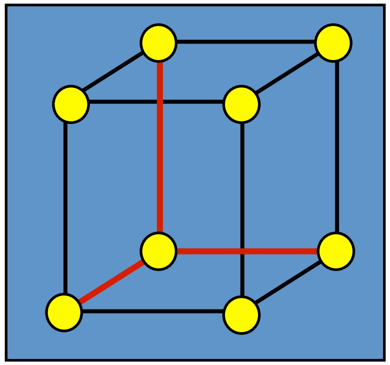
If we were using
a primitive cell



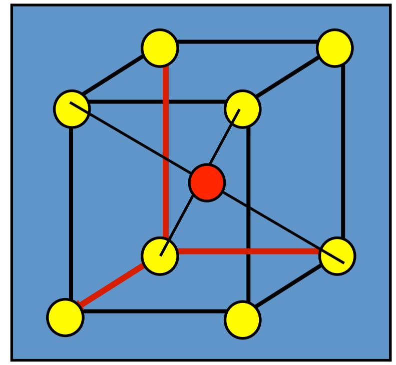

Some 2-fold axes are
along face diagonals
(non-conventional
crystal setting)

# Centred cells in pictures

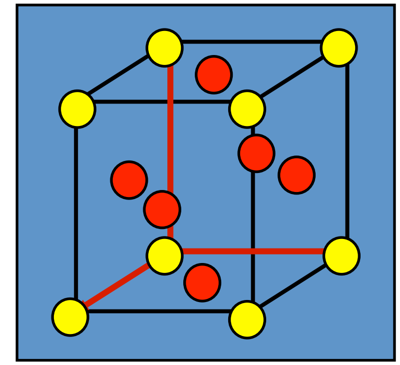


P – Primitive

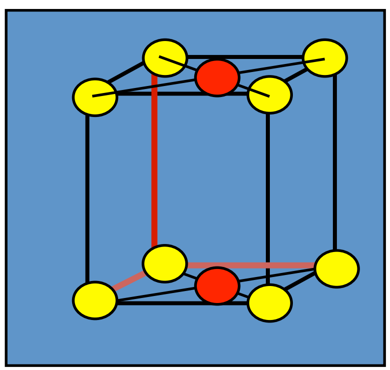


I – Body centred

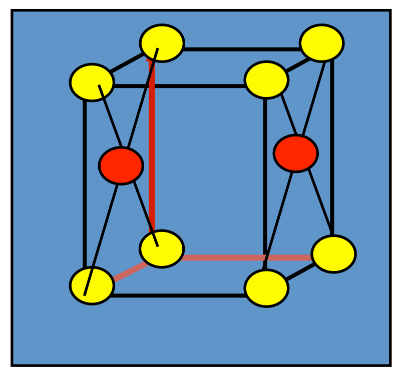


F – Face centred (all)

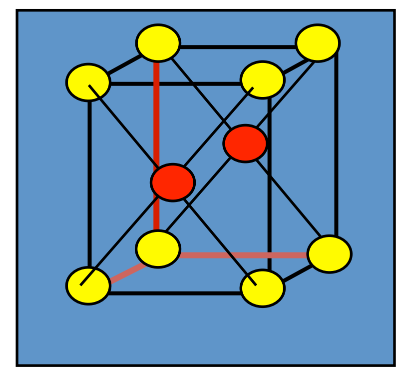
Also:
H - Hexagonal setting of rhombohedral space groups



A – Face centred (A)



B – Face centred (B)



C – Face centred (C)

# Bravais lattices

- 7 crystal systems, combined with some of the centring types (P, C, I, F or H) gives 14 Bravais lattices
  - excluded are impossible combinations (*e.g. A*4)
  - or equivalent combinations (*e.g.* C4 and *P*4)

# Bravais lattices

| **Crystal System** | **Bravais Lattices** |
|---|---|
| 1. Triclinic | 1. Primitive (*P*) |
| 2. Monoclinic | 2. Primitive (*P*)<br>3. Base-Centered (*C*) |
| 3. Orthorhombic | 4. Primitive (*P*)<br>5. Base-Centered (*C*)<br>6. Body-Centered (*I*)<br>7. Face-Centered (*F*) |
| 4. Tetragonal | 8. Primitive (*P*)<br>9. Body-Centered (*I*) |
| 5. Trigonal | 10. Primitive (*P*) |
| | 11. Rhombohedral (*R or H*) |
| 6. Hexagonal | 10. Primitive (*P*) |
| 7. Cubic | 12. Primitive (*P*)<br>13. Body-Centered (*I*)<br>14. Face-Centered (*F*) |

example ←

# Triclinic *P* 1

"*P*" means primitive lattice type

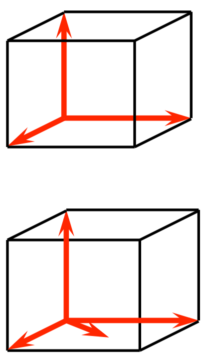
"1" means no symmetry operations except for translations

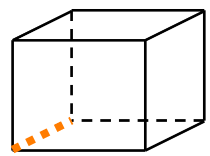
No constraints on
$a$, $b$, $c$, α, β, γ

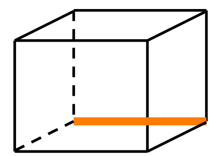
# Monoclinic

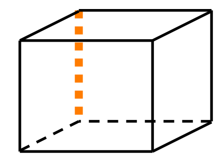
*P* 1 2 1 *P* 1 $2_1$1
*C* 1 2 1

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

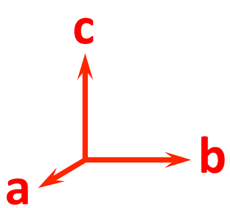








"1" means no symmetry axes in a given direction
"2" or "$2_1$" means 2-fold axes in a given direction



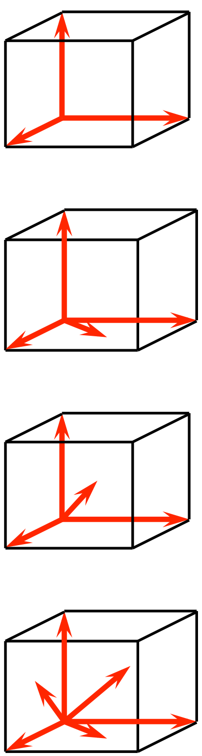

$\alpha = \gamma = 90°$

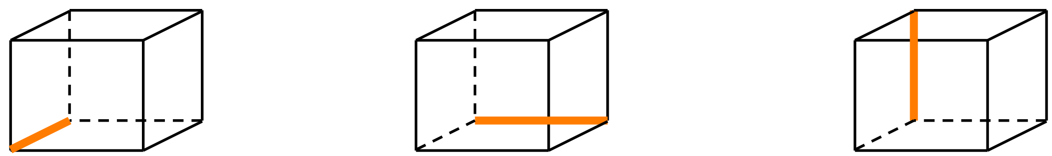
Note: by convention the 2-fold is along **b**
(other settings are sometimes used as well)

# Orthorhombic

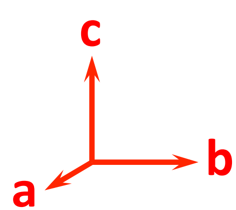
| | | | |
|---|---|---|---|
| $P\,2\,2\,2$ | $P\,2\,2\,2_1$ | $P\,2_12_12$ | $P\,2_12_12_1$ |
| $C\,2\,2\,2$ | $C\,2\,2\,2_1$ | | |
| $I\,2\,2\,2$ | | | $I\,2_12_12_1$ |
| $F\,2\,2\,2$ | | | |

*P, C, I or F* — 2 or $2_1$ — 2 or $2_1$ — 2 or $2_1$





"2" or "$2_1$" means 2-fold axes in a given direction




$\alpha = \beta = \gamma = 90°$

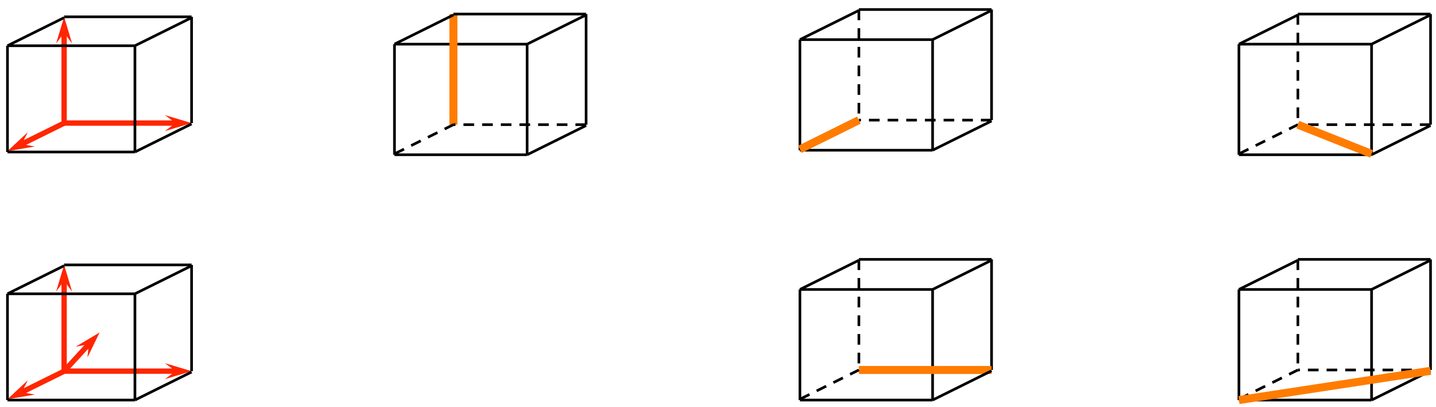
# Tetragonal

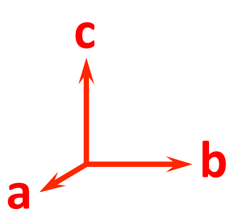
$P\,4\,2_12$ $P\,4_12_12$ $P\,4_22_12$ $P\,4_32_12$ $P4$ $P4_1$ $P4_2$ $P4_3$

$P\,4\,2\,2$ $P\,4_12\,2$ $P\,4_22\,2$ $P\,4_3\,2\,2$

$I\,4\,2\,2$ $I\,4_12\,2$ $I\,4$ $I\,4_1$

*P* or *I* | $4_N$ | 2, $2_1$ or None | 2 or None





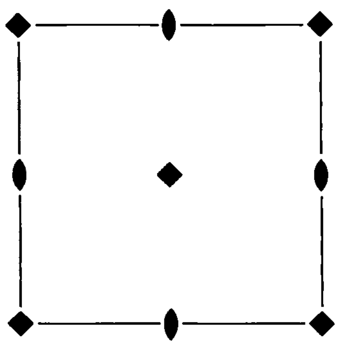

$\alpha = \beta = \gamma = 90°$
$a = b$

a ≡ b due to the 4-fold relating them

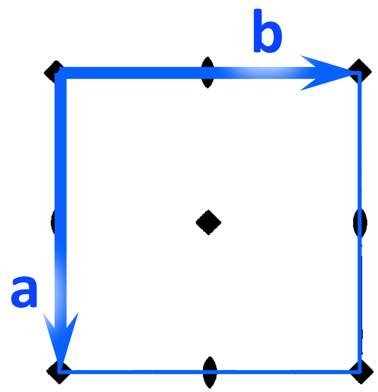
All 2-fold axes are also related via 4-fold rotations and either
- all of them are present or
- none of them are present

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

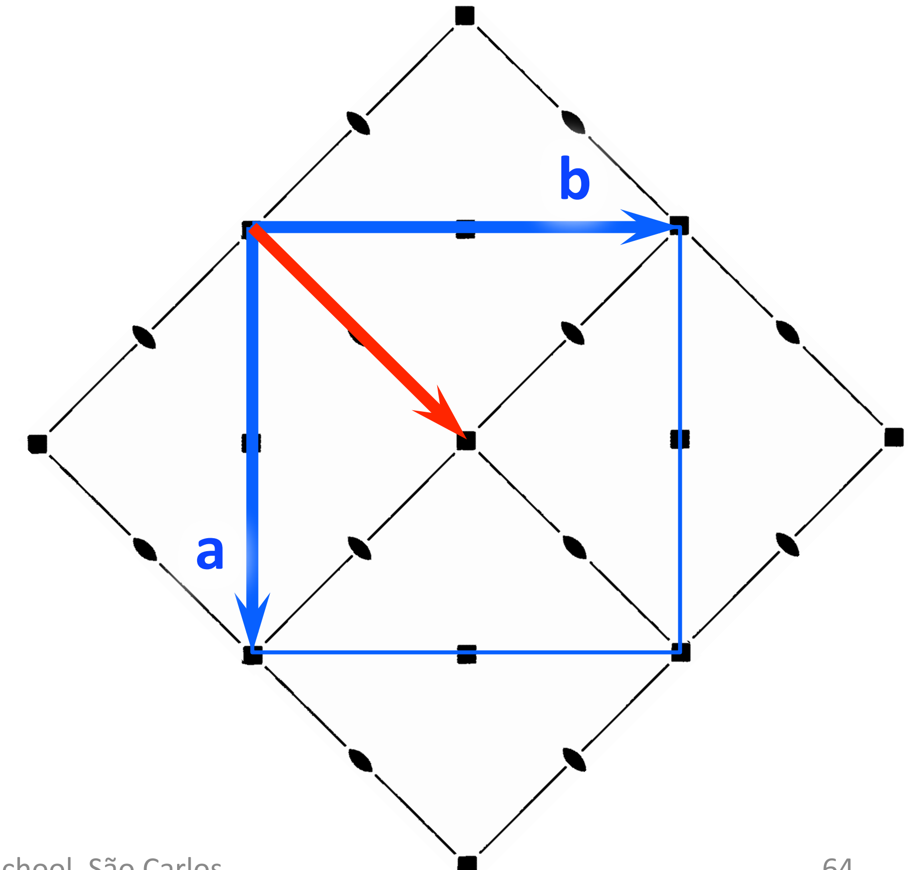
*P*4
as presented in the International Tables for Crystallography



and with base vectors shown




*C*4
This is a valid, but redundant spacegroup as it is obtained from P4
- by rotation 45° and
- redefining base vectors
- additional translation (**a** + **b**)/ 2



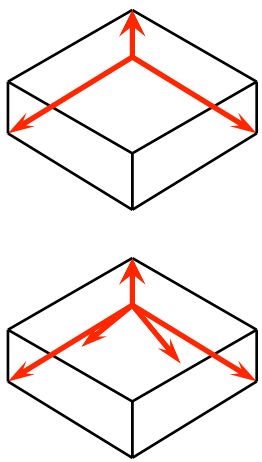
# Trigonal

$P\,3\,2\,1$ $P\,3_1 2\,1$ $P\,3_2 2\,1$ $P3$ $P3_1$ $P3_2$

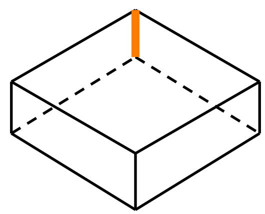
$P\,3_1 1\,2$ $P\,3_2 1\,2$

$H\,3\,2$ $H3$

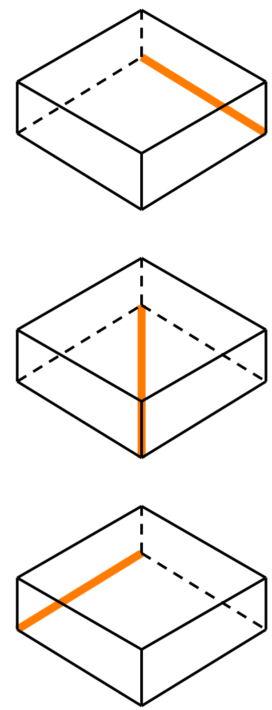
*P* or *H*(*)



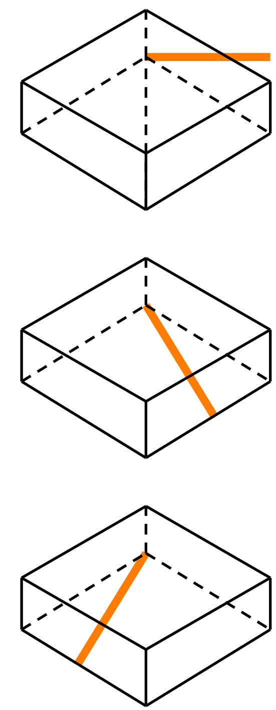
$3_N$

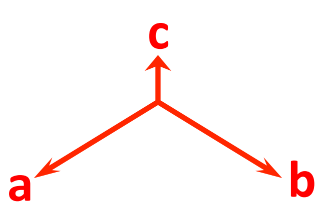


2 or None



2 or None





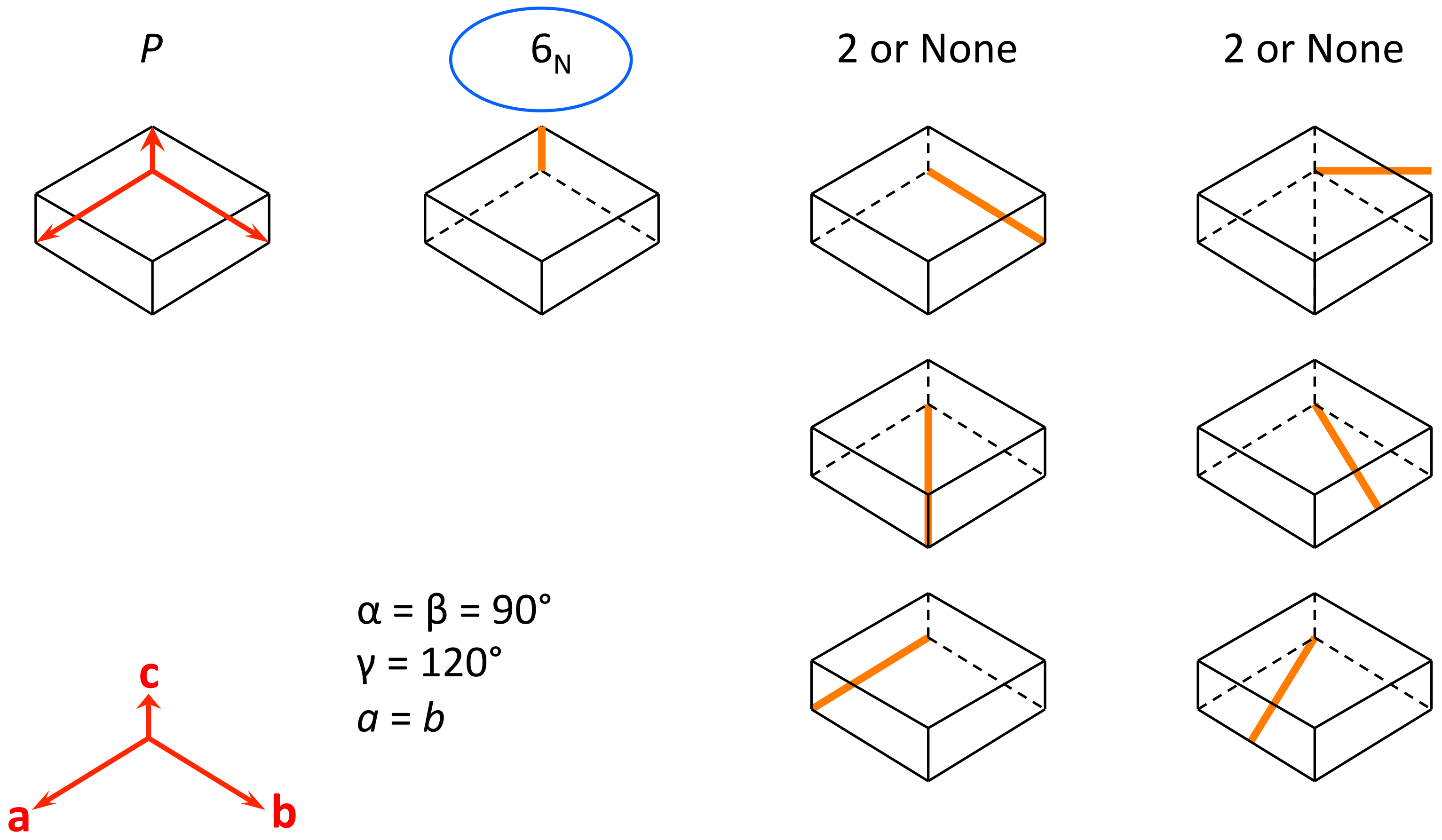

$\alpha = \beta = 90°$
$\gamma = 120°$
$a = b$

(*) an alternative rhombohedral (*R*) is also used

# Hexagonal

$P\,6\,2\,2$ $\quad P\,6_1 2\,2$ $\quad P\,6_2 2\,2$ $\quad P\,6_3 2\,2$ $\quad P6$ $\quad P6_1$ $\quad P6_2$ $\quad P6_3$

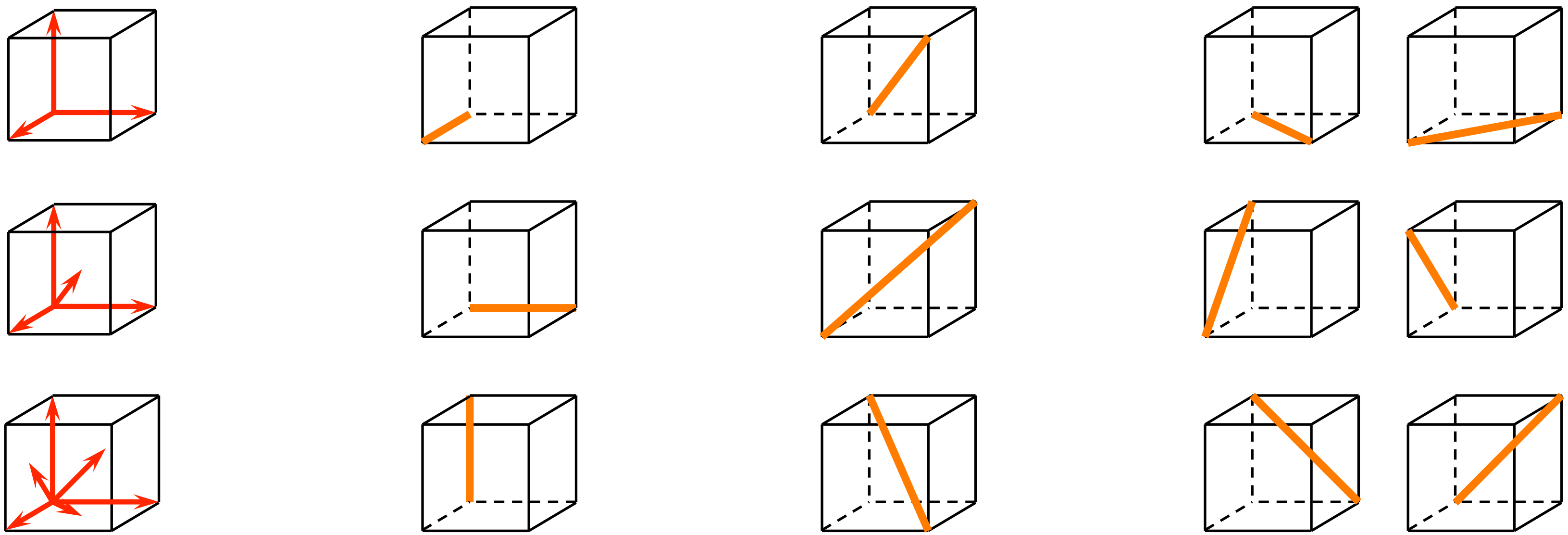
$P\,6_5 2\,2$ $\quad P\,6_4 2\,2$ $\quad P6_5$ $\quad P6_4$

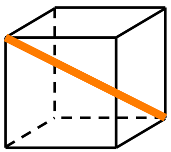


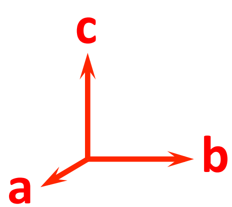
# Cubic

| | | | | | |
|---|---|---|---|---|---|
| *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 | |

*P, I or F* | $4_N$ or $2_N$ | 3 | 2 or None








$\alpha = \beta = \gamma = 90°$

$a = b = c$

# Monoclinic (lattice based setting)

$\alpha = \gamma = 90°$

additional condition:
$\beta < 120°$

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

*C* 1 2 1

*I* 1 2 1

In orange frame:
- the same space group
- different crystal setting

# Orthorhombic (lattice based setting)

$\alpha = \beta = \gamma = 90°$

additional condition:
$a < b < c$

| | | | |
|---|---|---|---|
| $P\,2\,2\,2$ | $P\,2\,2\,2_1$ | $P\,2_12_12$ | $P\,2_12_12_1$ |
| | $P\,2\,2_12$ | $P\,2_12\,2_1$ | |
| | $P\,2_12\,2$ | $P\,2\,2_12_1$ | |
| $C\,2\,2\,2$ | $C\,2\,2\,2_1$ | | |
| $I\,2\,2\,2$ | | | $I\,2_12_12_1$ |
| $F\,2\,2\,2$ | | | |

In orange frames:
- the same space group
- different crystal setting

# Rules in a Table

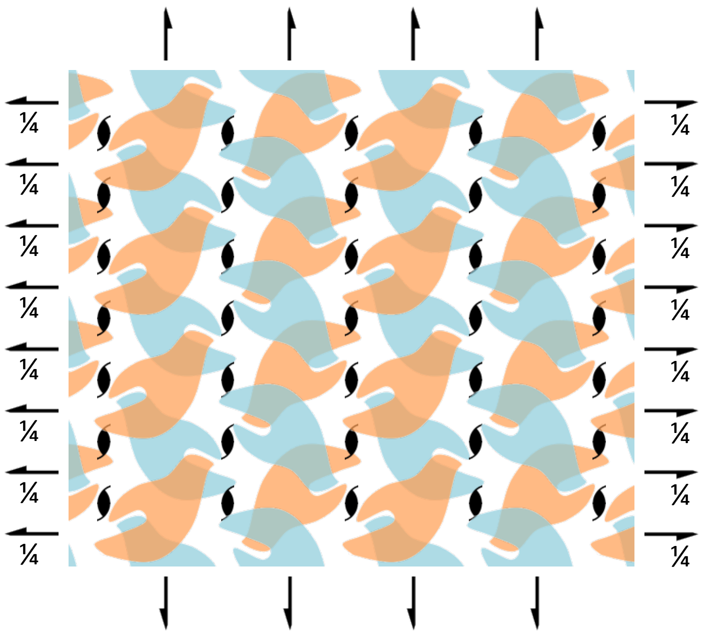
| **Crystal System** | **Characteristic symmetry elements** | **Bravais Lattices** | **Unit Cell Geometry** |
|---|---|---|---|
| 1. Triclinic | None | 1. Primitive (*P*) | $a \neq b \neq c$;<br>$\alpha \neq \beta \neq \gamma$ |
| 2. Monoclinic | 2-fold axes, all parallel | 2. Primitive (*P*)<br>3. Base-Centered (*C*) | $a \neq b \neq c$;<br>$\alpha = \gamma = 90° \neq \beta$ |
| 3. Orthorhombic | 2-fold axes in three perpendicular directions | 4. Primitive (*P*)<br>5. Base-Centered (*C*)<br>6. Body-Centered (*I*)<br>7. Face-Centered (*F*) | $a \neq b \neq c$;<br>$\alpha = \beta = \gamma = 90°$ |
| 4. Tetragonal | 4-fold axes, all parallel | 8. Primitive (*P*)<br>9. Body-Centered (*I*) | $a = b \neq c$;<br>$\alpha = \beta = \gamma = 90°$ |
| 5. Trigonal | 3-fold axes, all parallel | 10. Primitive (*P*)<br>11. Rhombohedral (*H* - setting) | $a = b \neq c$;<br>$\alpha = \beta = 90°, \gamma = 120°$ |
| 6. Hexagonal | 6-fold axes, all parallel | 10. Primitive (*P*) | $a = b \neq c$;<br>$\alpha = \beta = 90°, \gamma = 120°$ |
| 7. Cubic | 3-fold axes in four different orientations | 12. Primitive (*P*)<br>13. Body-Centered (*I*)<br>14. Face-Centered (*F*) | $a = b = c$;<br>$\alpha = \beta = \gamma = 90°$ |

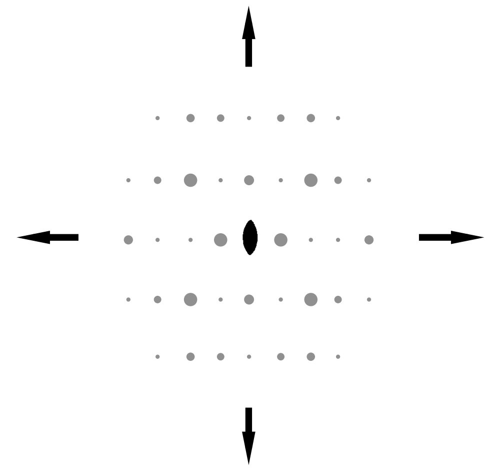
# Symmetry of intensities

The concept of reciprocal lattice is based on angular relation 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



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

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

# Space group and point group

*Crystal space group*

*International Tables for Crystallography* (2006). Vol. A,

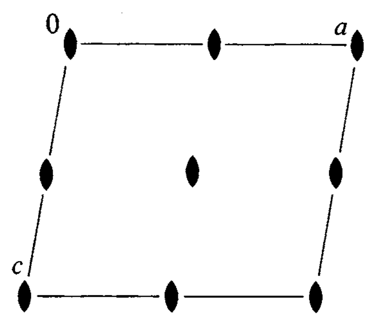
$P2$

No. 3

$C_2^1$

$P121$

UNIQUE AXIS $b$

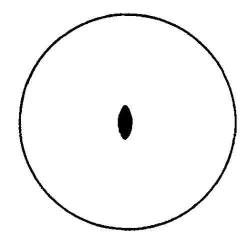



*Arithmetic crystal class*

$2P$

*Crystal point group*

2



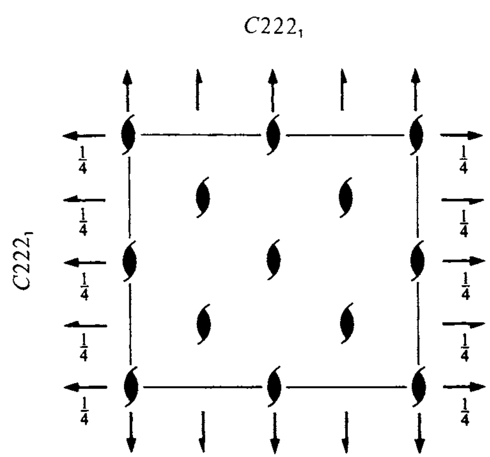
# Space group and point group

*Crystal space group*

**International Tables for Crystallography (2006). Vol. A,**

$C222_1$ $\quad D_2^5$

No. 20 $\quad C222_1$

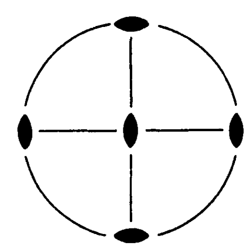



*Arithmetic crystal class*

222*C*

*Crystal point group*

222



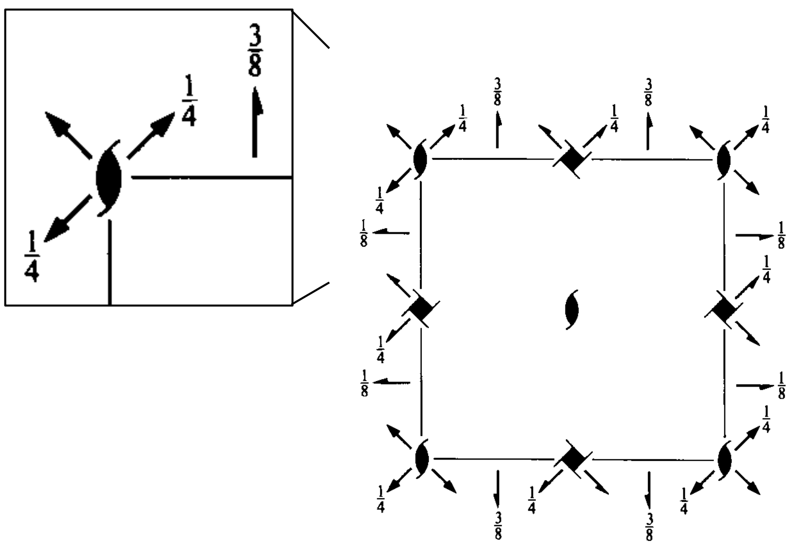
# Space group and point group

<u>*Crystal space group*</u>

*International Tables for Crystallography* (2006). Vol. A,

$P4_12_12$ $D_4^4$

No. 92 $P4_12_12$

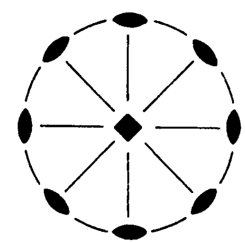



<u>*Arithmetic crystal class*</u>

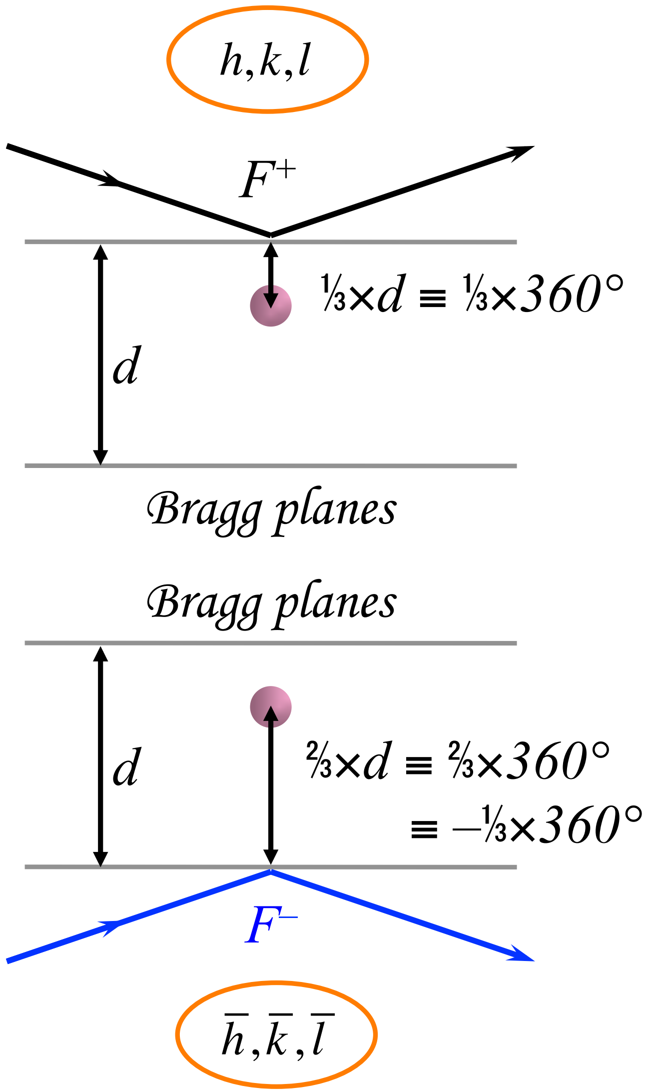
422*P*

<u>*Crystal point group*</u>

422



# Friedel's law




- Bragg planes
  - define reference phase
- Probe atom:

$$\Delta\varphi\left(\bar{h},\bar{k},\bar{l}\right) = -\Delta\varphi\left(h,k,l\right)$$

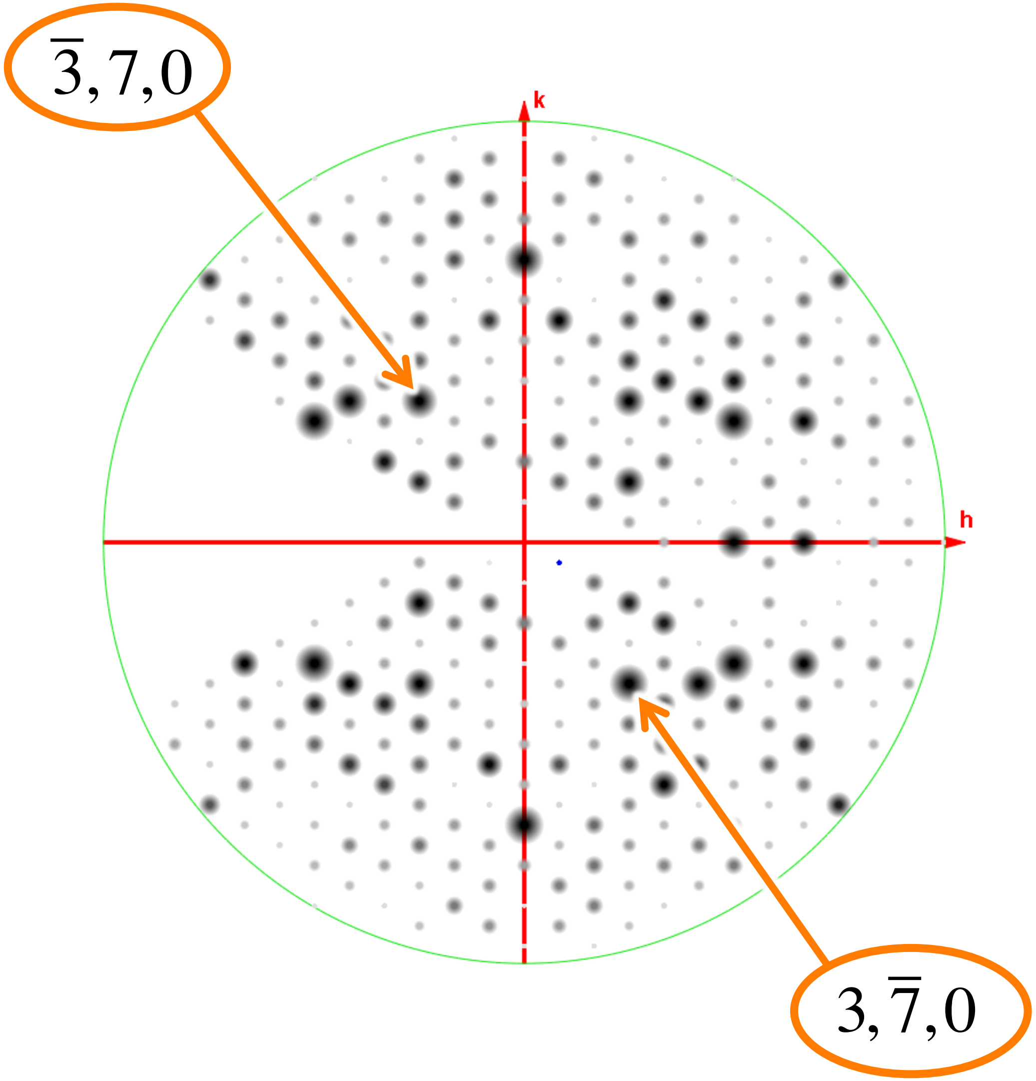
$$\Delta F\left(\bar{h},\bar{k},\bar{l}\right) = \Delta F^{*}\left(h,k,l\right)$$

- Total:

$$F\left(\bar{h},\bar{k},\bar{l}\right) = F^{*}\left(h,k,l\right)$$

$$I\left(\bar{h},\bar{k},\bar{l}\right) = I\left(h,k,l\right)$$

# Friedel's law




$$I(\bar{3},7,0) = I(3,\bar{7},0)$$

# Point group and Laue group

+ inversion =

*Arithmetic crystal class*

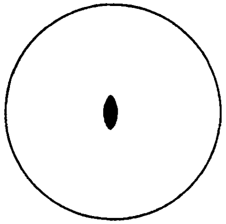
2*P*

*Patterson space group*

*P* 1 2/m 1

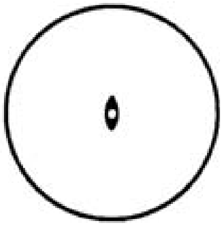
*Crystal point group*

2



*Laue point group*

2/m



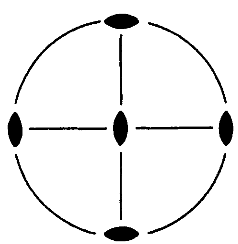
# Point group and Laue group

+ inversion =

*Arithmetic crystal class*

222*C*

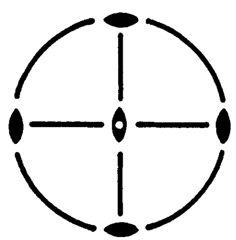
*Crystal point group*

222 

*Patterson space group*

*C* m m m

*Laue point group*

m m m 

# Point group and Laue group

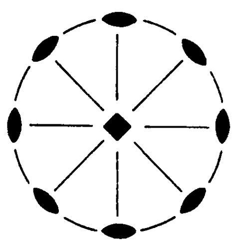
+ inversion =

*Arithmetic crystal class*

422*P*

*Crystal point group*

422

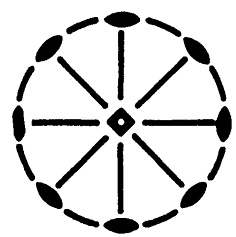


*Patterson space group*

*P* 4/m m m

*Laue point group*

4/m m m

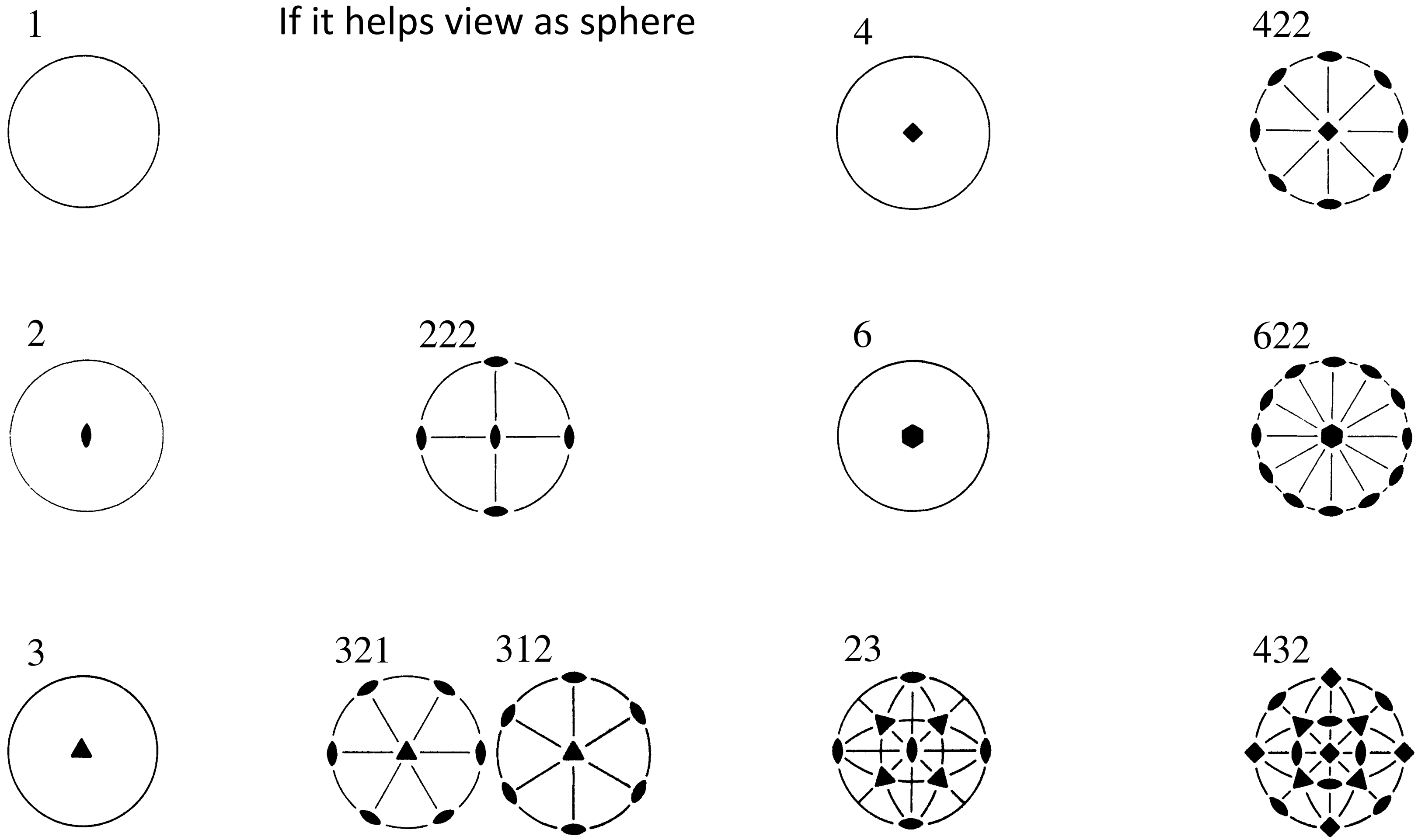


# The eleven point groups or crystal classes

| Crystal system | Laue point group | Non-centrosymmetric point groups belonging to the Laue point group | | |
|---|---|---|---|---|
| Cubic | *m*3*m* | 432 | $\bar{4}3m$ | |
| | *m*3 | 23 | | |
| Tetragonal | 4/*mmm* | 422 | 4*mm* | $\bar{4}2m$ |
| | 4/*m* | 4 | $\bar{4}$ | |
| Orthorhombic | *mmm* | 222 | *mm*2 | |
| Trigonal | 3*m* | 32 | 3*m* | |
| | 3 | 3 | | |
| Hexagonal | 6/*mmm* | 622 | 6*mm* | $\bar{6}m2$ |
| | 6/*m* | 6 | $\bar{6}$ | |
| Monoclinic | 2/*m* | 2 | *m* | |
| Triclinic | $\bar{1}$ | 1 | | |

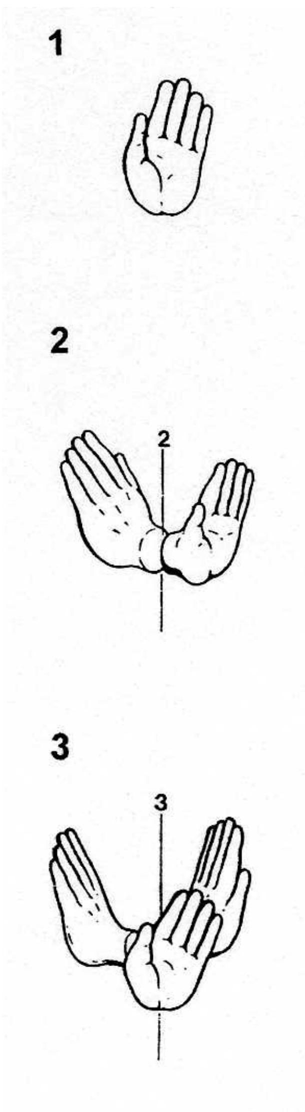
# The point groups that can exist in protein crystals

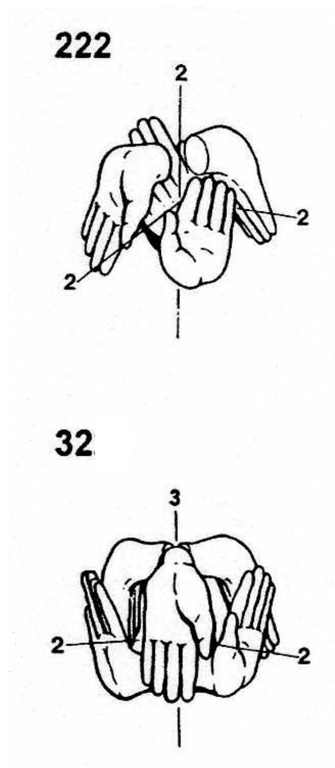
If it helps view as sphere

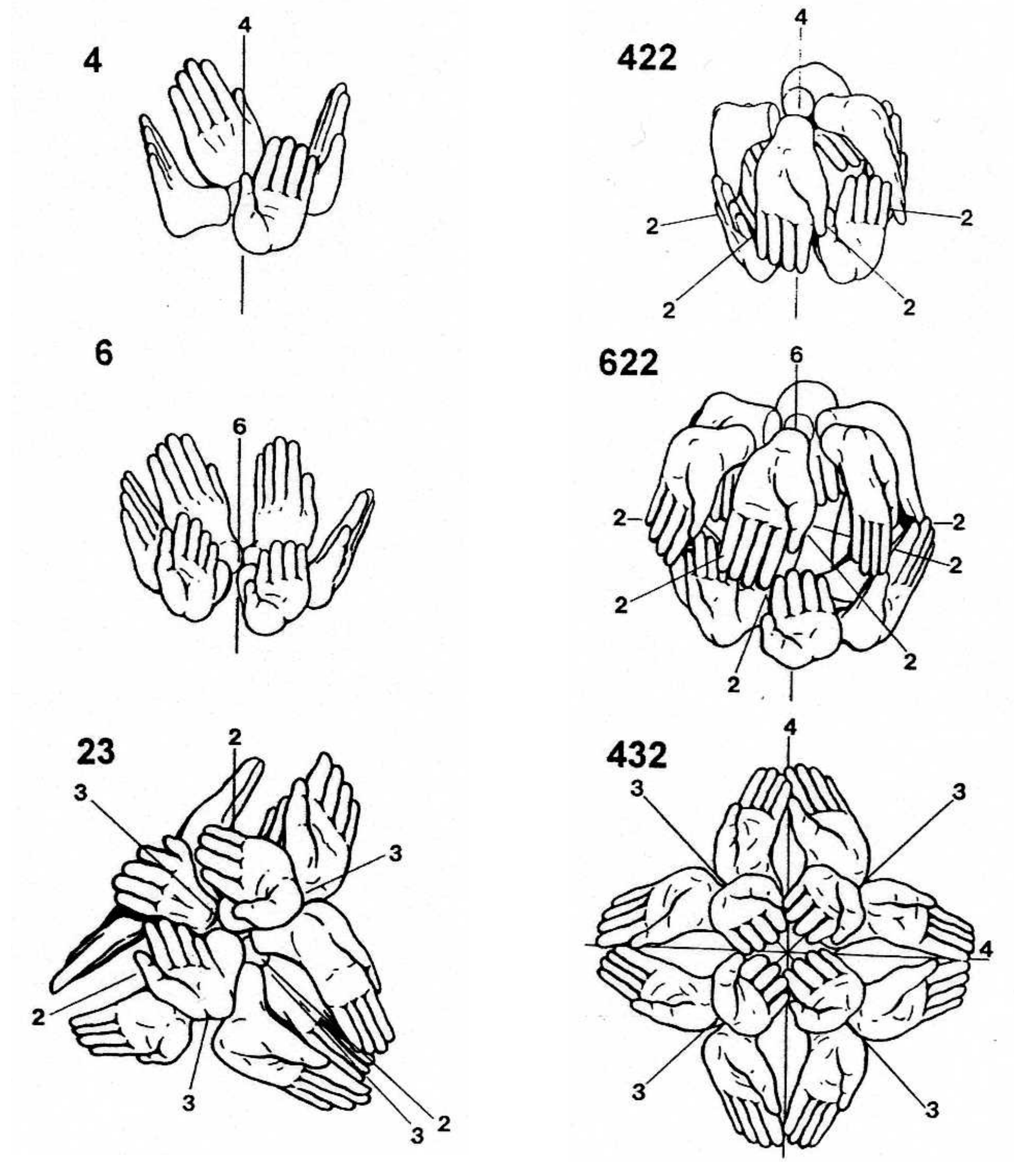


# The point groups that can exist in protein crystals

maybe an easier representation



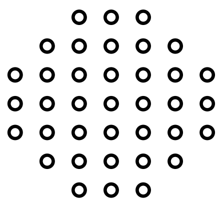



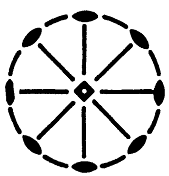
# How do we deduce the Space Group in practice?

- We start in reciprocal space (point group)
- We go all way back from symmetry in reciprocal space to crystal space group
  - Data processing gives values of the unit cell parameters
  - Lattice symmetry is derived from the unit cell parameters
  - Comparison of related intensities gives crystal point group
  - Systematic absences allow to reduce the number of possible space groups.
  - Space group is only a hypothesis until structure is complete

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

Reciprocal space lattice (positions of reflections)

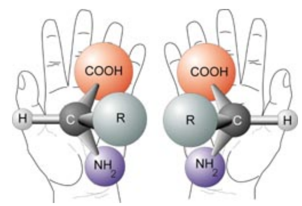


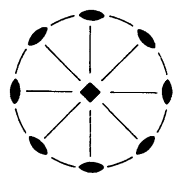


$4/mmm$

(Approximate) lattice point group

Mirror symmetry is <u>not</u> allowed in biological macromolecules

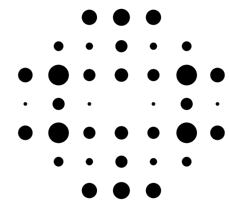


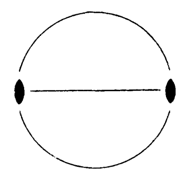



422

Highest possible crystal point group

Intensities of reflections

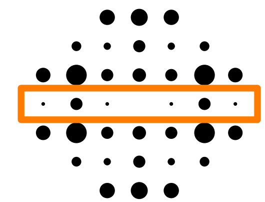


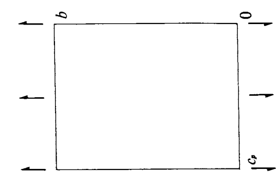


2

Probable crystal point group

Intensities of axial reflections





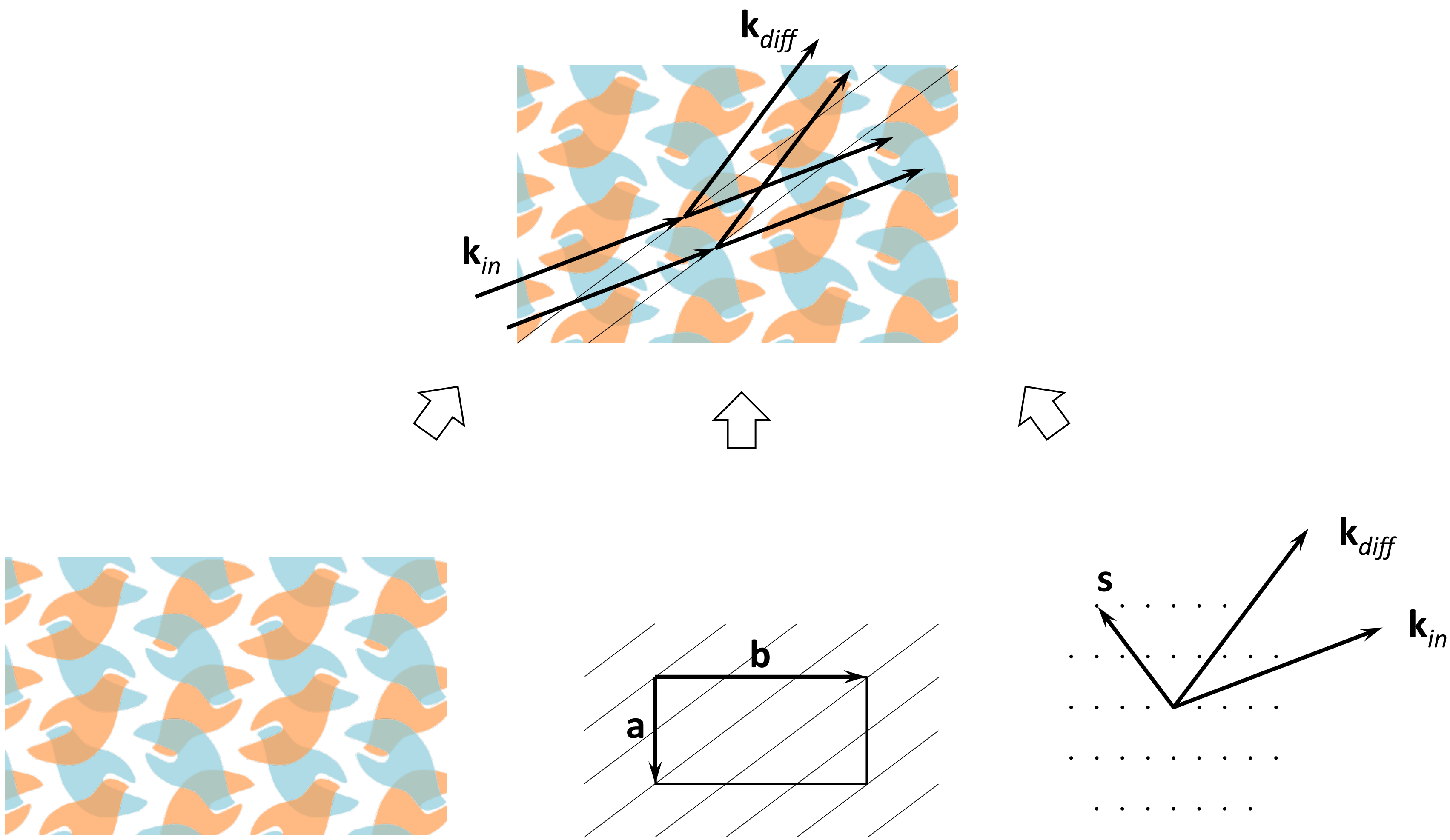
$P2_1$

Probable crystal space group

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

# End

# Conventional diffraction scheme

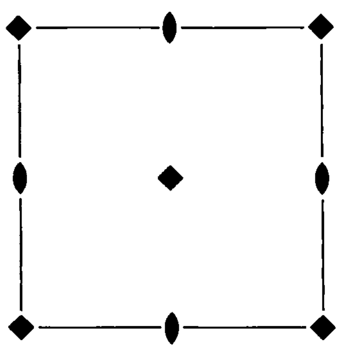



real space

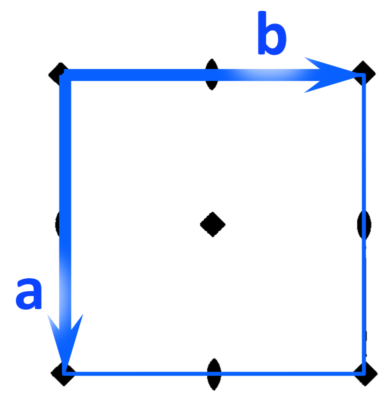
reciprocal space

# *C4*: an example of a redundant space group

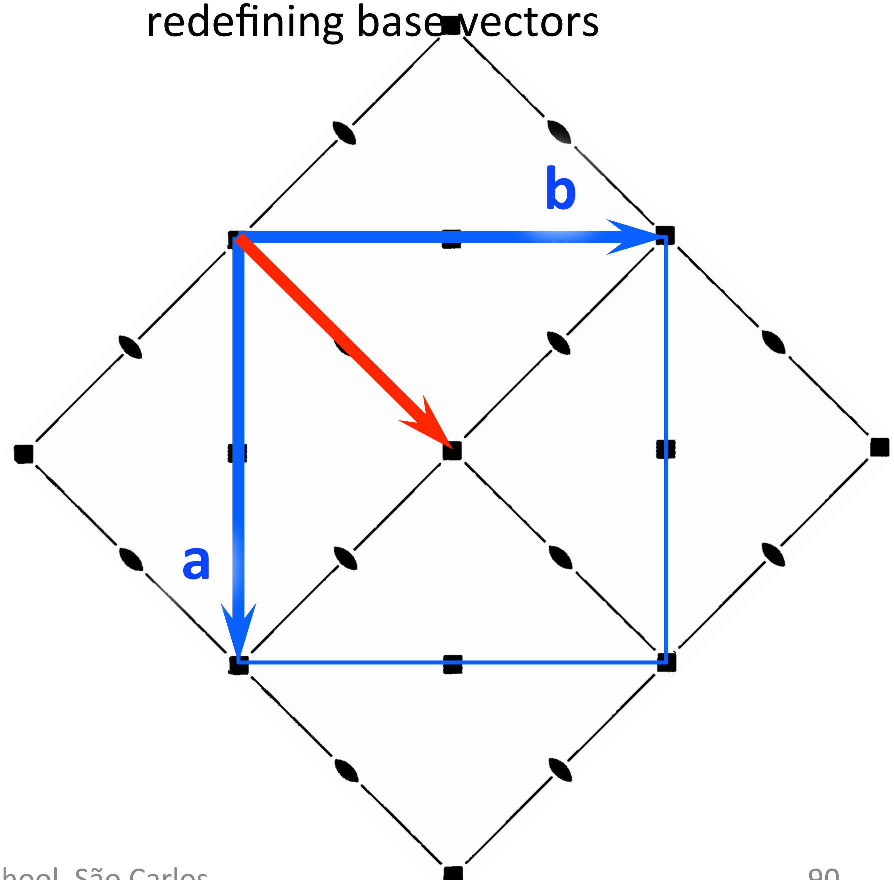
*P4*
as presented in the International Tables for Crystallography



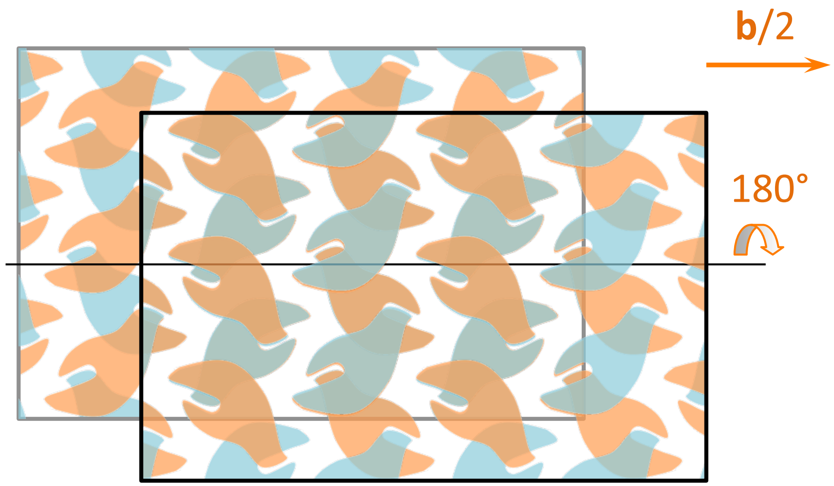
Standard unit cell;
C means additional translation **a** + **b**

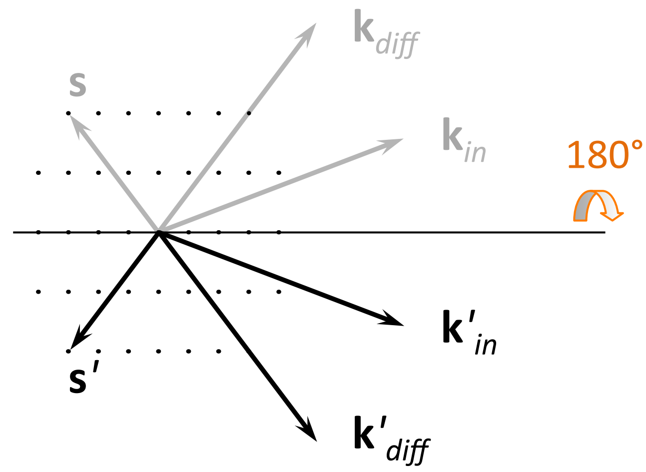



*C4*
This is a valid, but redundant spacegroup as it is obtained from P4 by
rotation 45° and
redefining base vectors

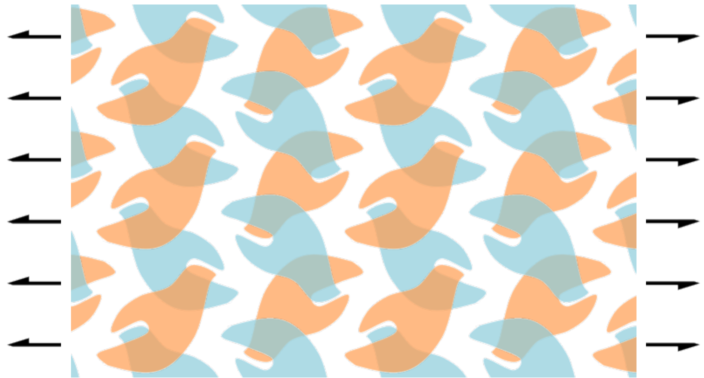


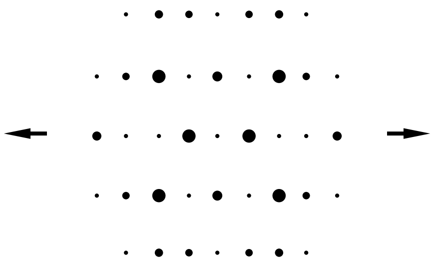

**A new slide; it needs a bit of thinking and some reforamtting + one more slide on impossible combination of crystal class and centring type**




$I(\mathbf{s}') = I(\mathbf{s})$





# Monoclinic
## (lattice based setting)

$P\,1\,2\,1$ $P\,1\,2_1 1$

$C\,1\,2\,1$

$I\,1\,2\,1$

α = γ = 90°

additional condition:
β < 120°

In orange frame:
- the same space group
- different crystal setting

# Orthorhombic
## (lattice based setting)

$\alpha = \beta = \gamma = 90°$

additional condition:
$a < b < c$

$P\,2\,2\,2$

$P\,2\,2\,2_1$
$P\,2\,2_1 2$
$P\,2_1 2\,2$

$P\,2_1 2_1 2$
$P\,2_1 2\,2_1$
$P\,2\,2_1 2_1$

$P\,2_1 2_1 2_1$

In orange frames:
- the same space group
- different crystal setting

# Orthorhombic (lattice based setting)

$\alpha = \beta = \gamma = 90°$

additional condition:
$a < b < c$

| | | | |
|---|---|---|---|
| $P\,2\,2\,2$ | $P\,2\,2\,2_1$ | $P\,2_12_12$ | $P\,2_12_12_1$ |
| | $P\,2\,2_12$ | $P\,2_12\,2_1$ | |
| | $P\,2_12\,2$ | $P\,2\,2_12_1$ | |

In orange frames:
- the same space group
- different crystal setting

# Centred (non-primitive) unit cells

Highlighted in orange

- *Triclinic*: P1, $P\bar{1}$
- *Monoclinic*: P2, $P2_1$, **C**2, ...
- *Orthorhombic*: P222, $P222_1$, $P2_12_12$, $P2_12_12_1$, **C**222, **C**$222_1$, **F**222, **I**222, **I**$2_12_12_1$, ...
- ...