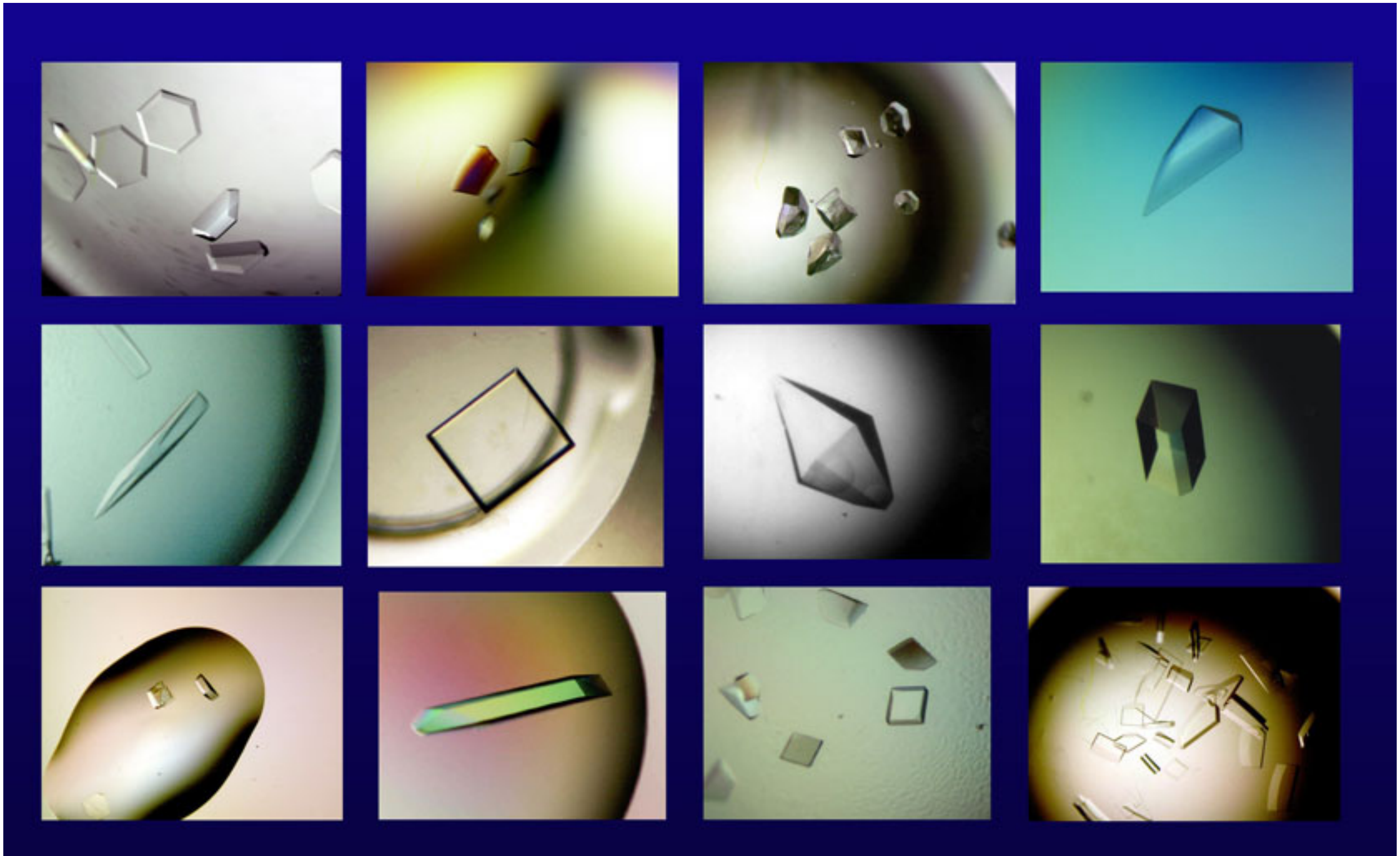
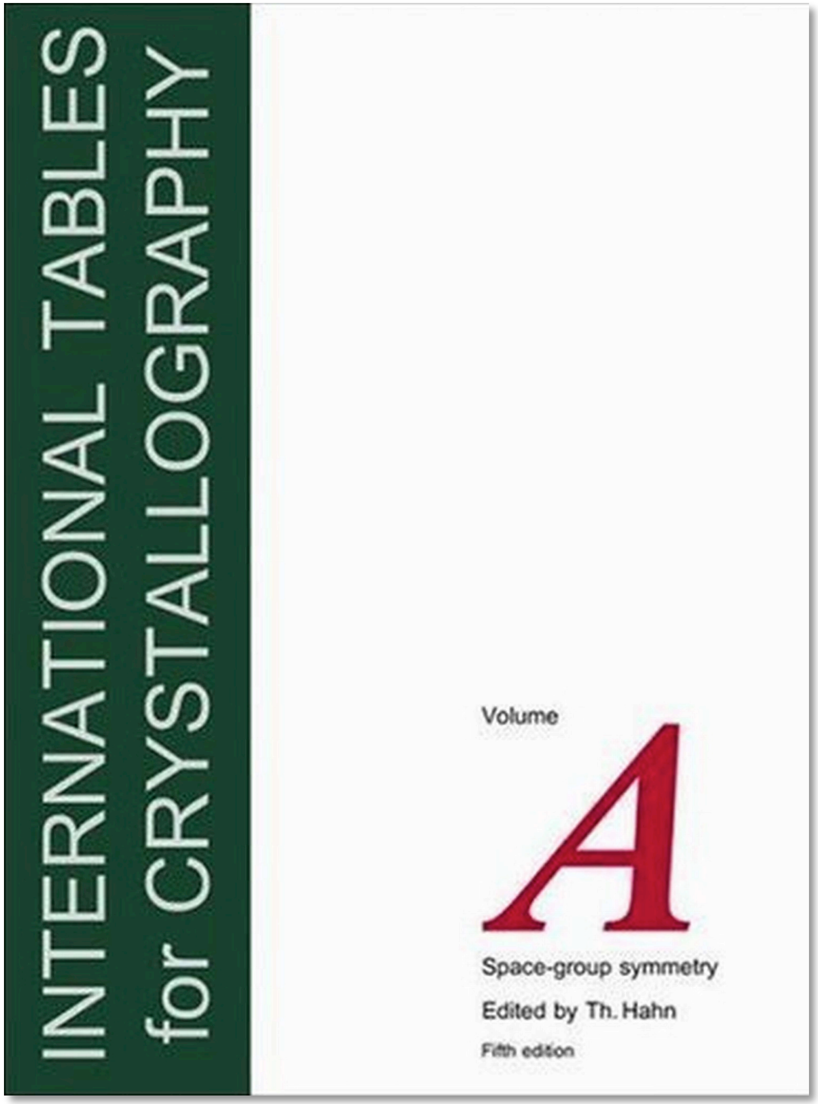
Introduction to symmetry

Andrey Lebedev, CCP4

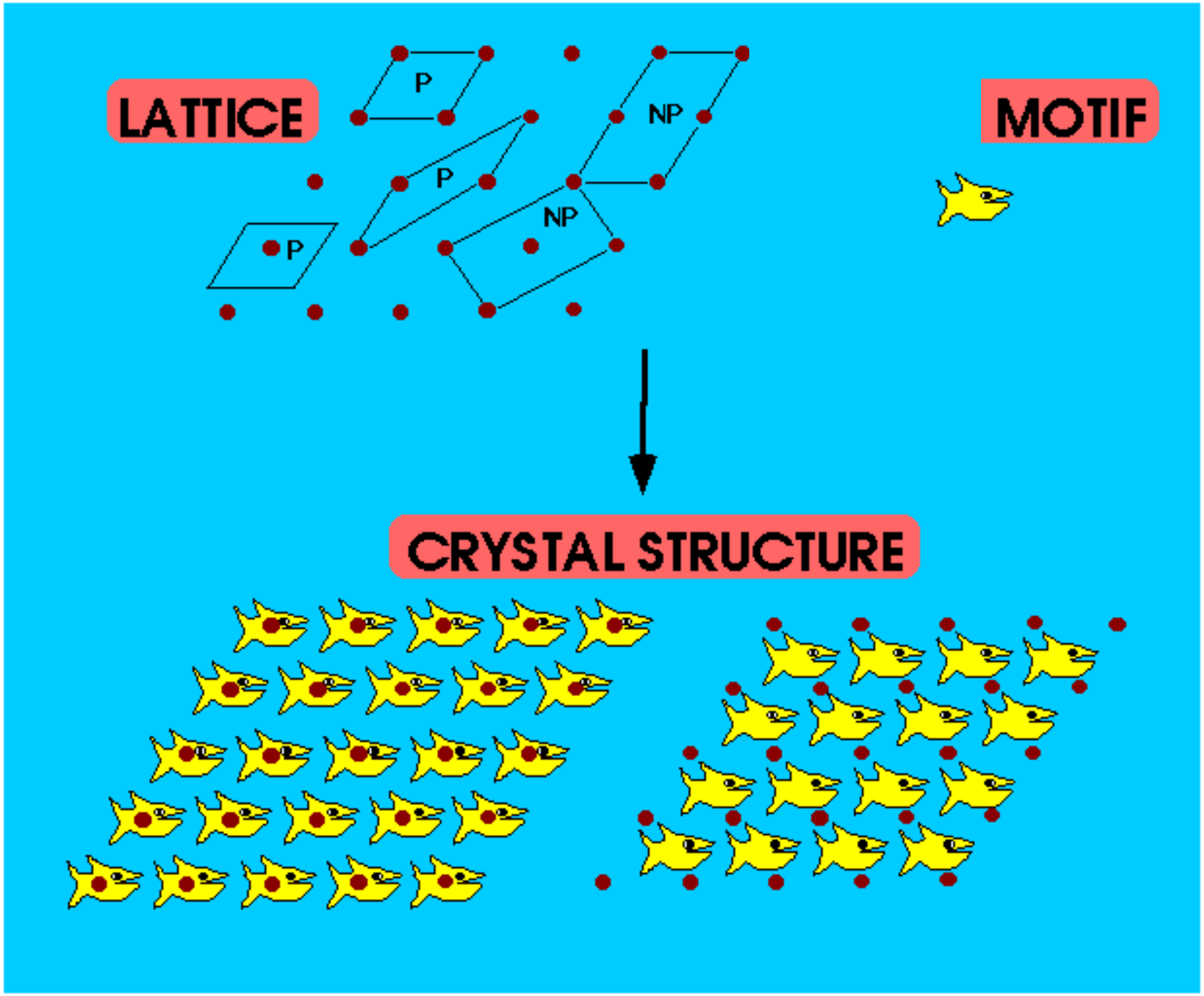


The Reference



Crystal: repeated structural motif

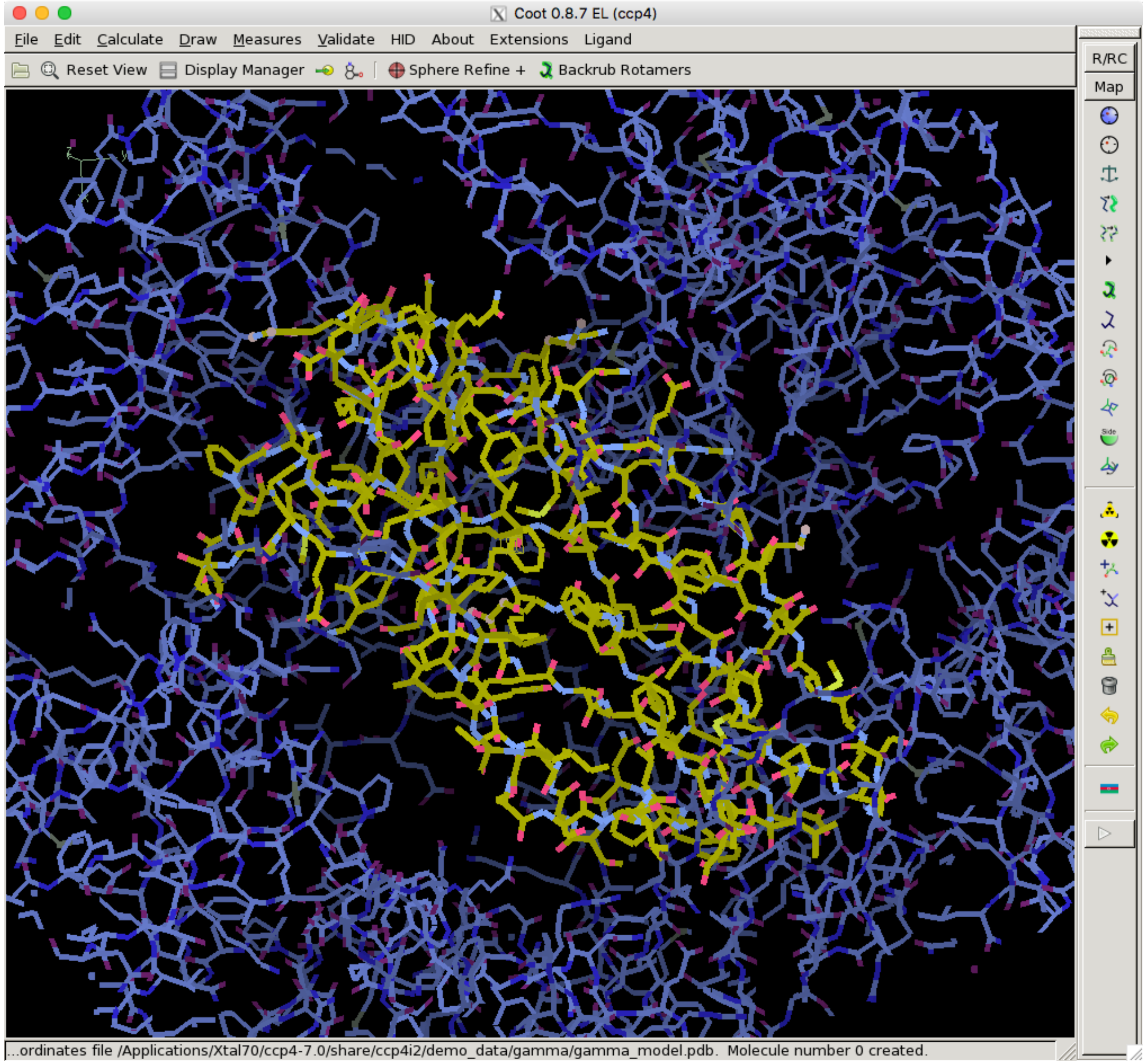
Conventional (constructive) definition of crystal structure.



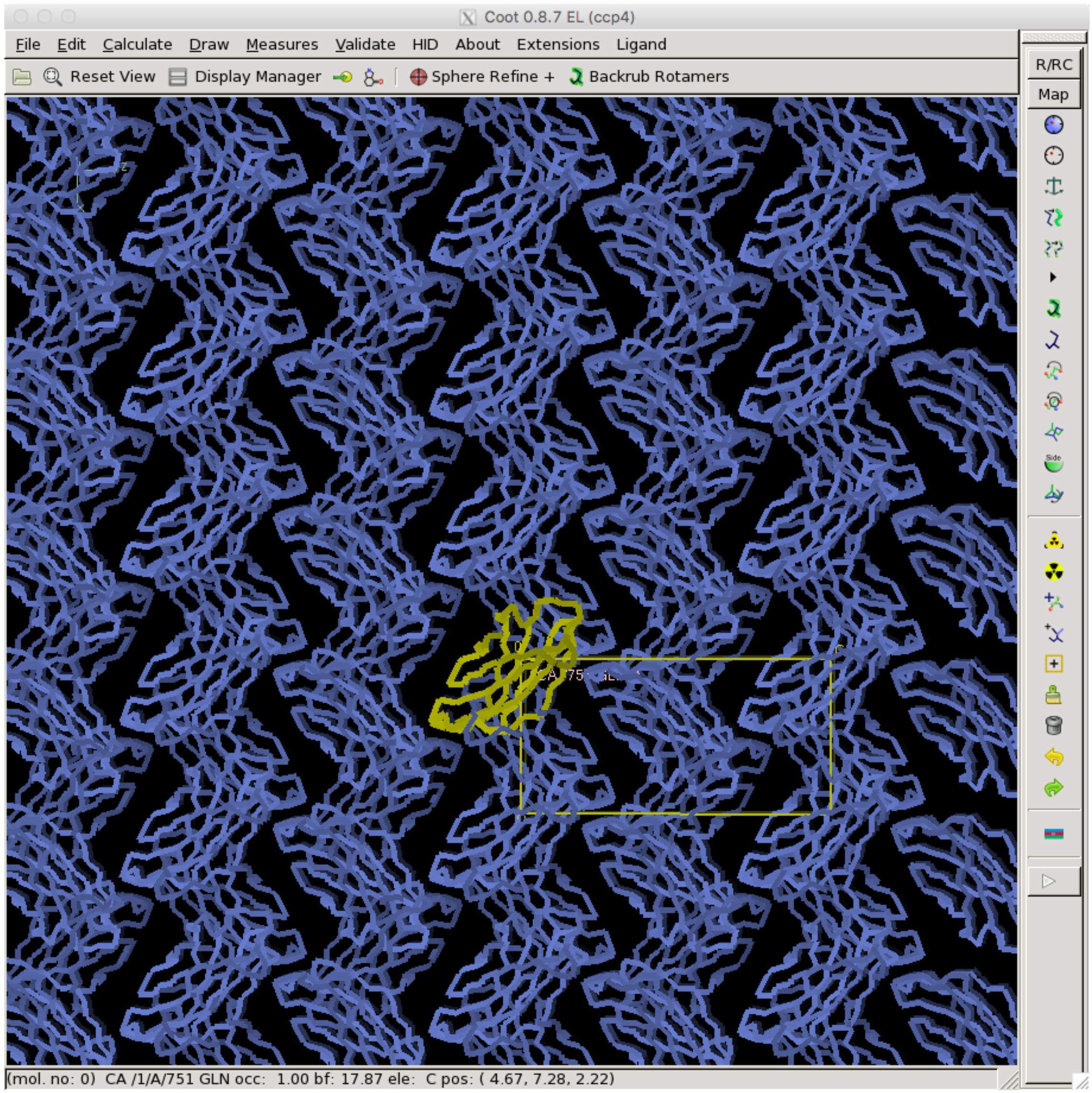
- Example structure (using Coot)
  - examine symmetry operations
  - construct space group
  - assign crystallographic origin
  - identify space group
- Classification of space groups
- Space group symbols
- Symmetry of diffraction pattern
  - point groups
- SG determination in structure solution process

- Example structure (using Coot)
  - examine symmetry operations
  - construct space group
  - assign crystallographic origin
  - identify space group
- Classification of space groups
- Space group symbols
- Symmetry of diffraction pattern
  - point groups
- SG determination in structure solution process

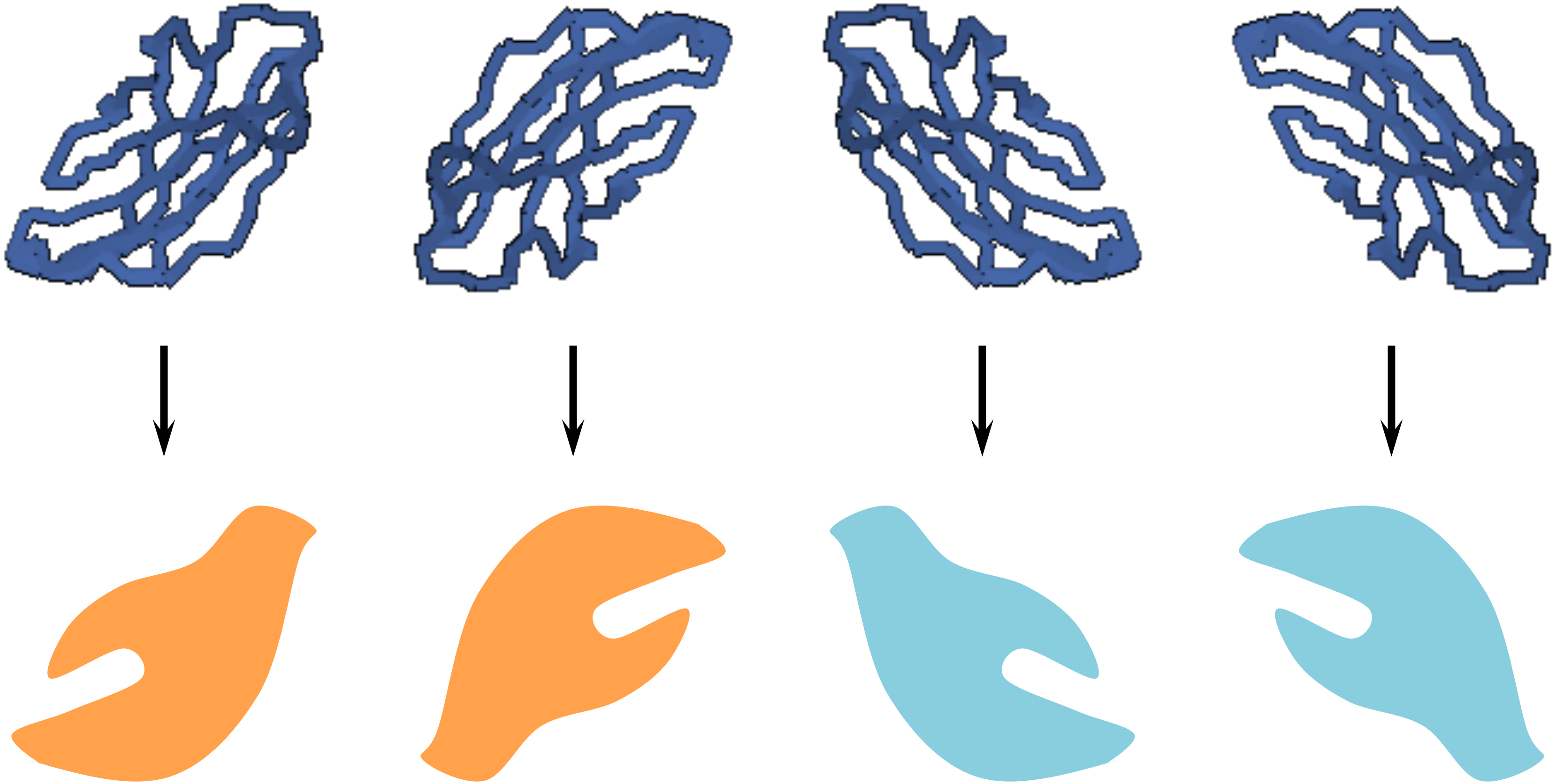
Examine structure in Coot



Symmetry view in Coot

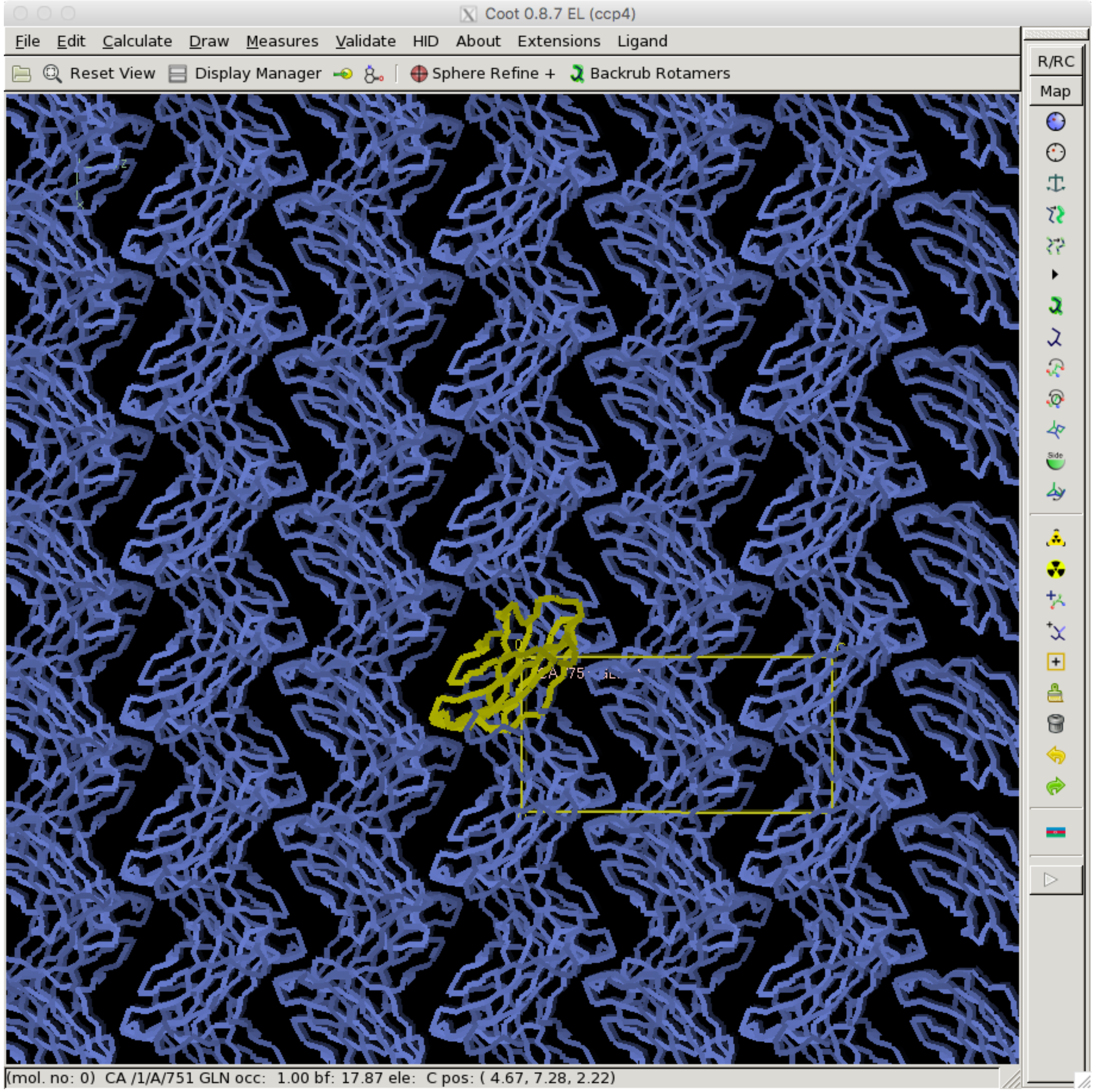


Simplified representation

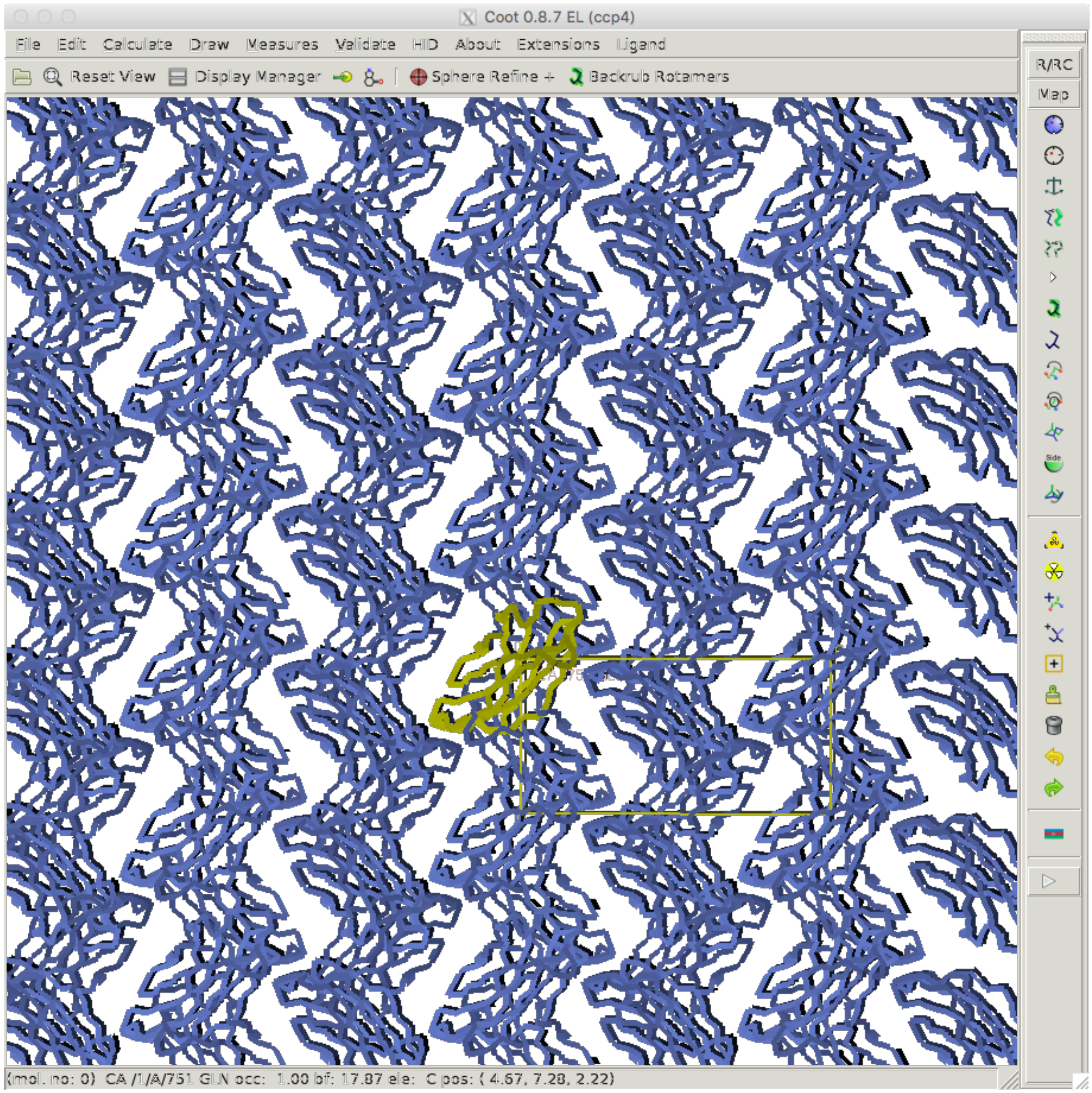


Opposite sides of molecules a denoted with different colours

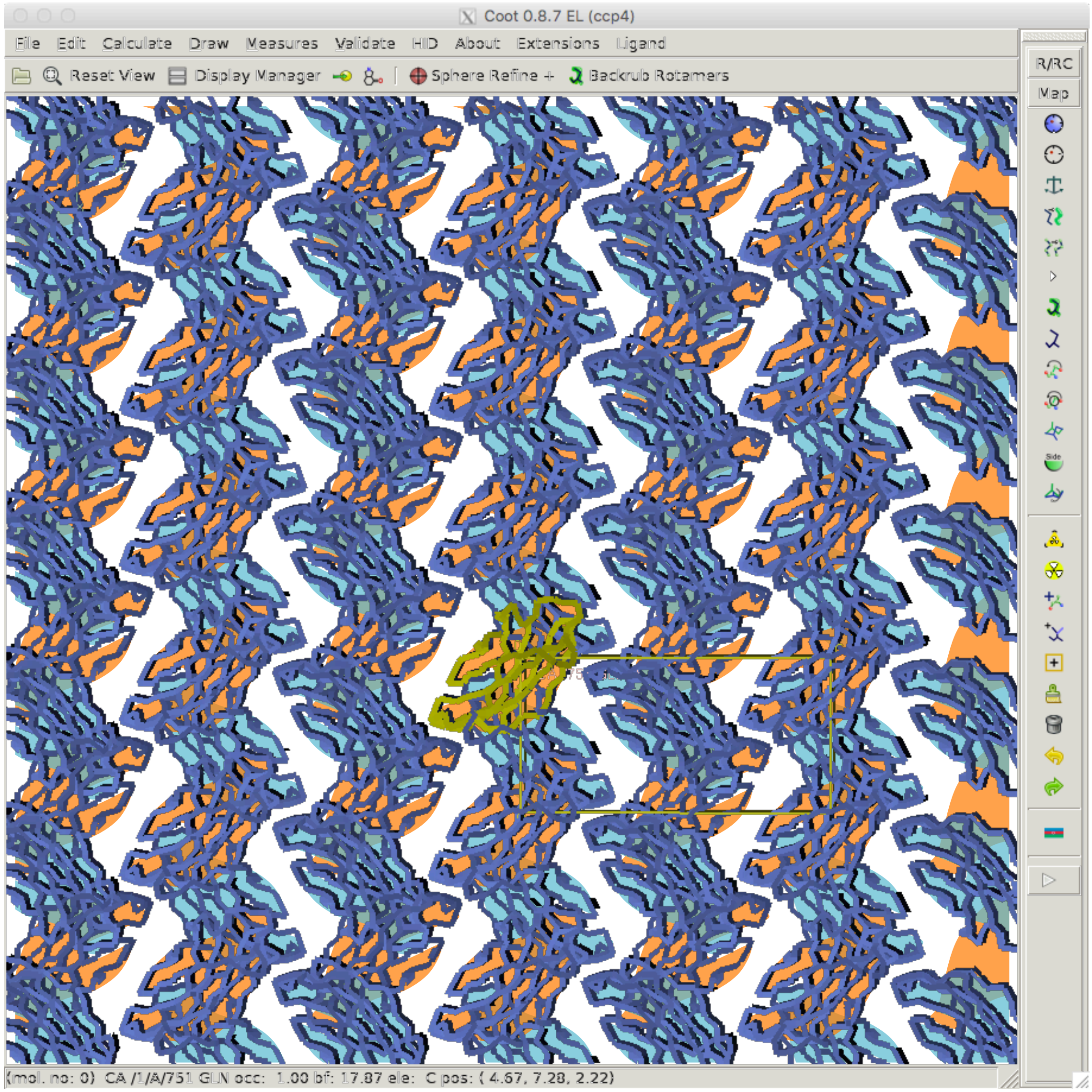
Simplified representation



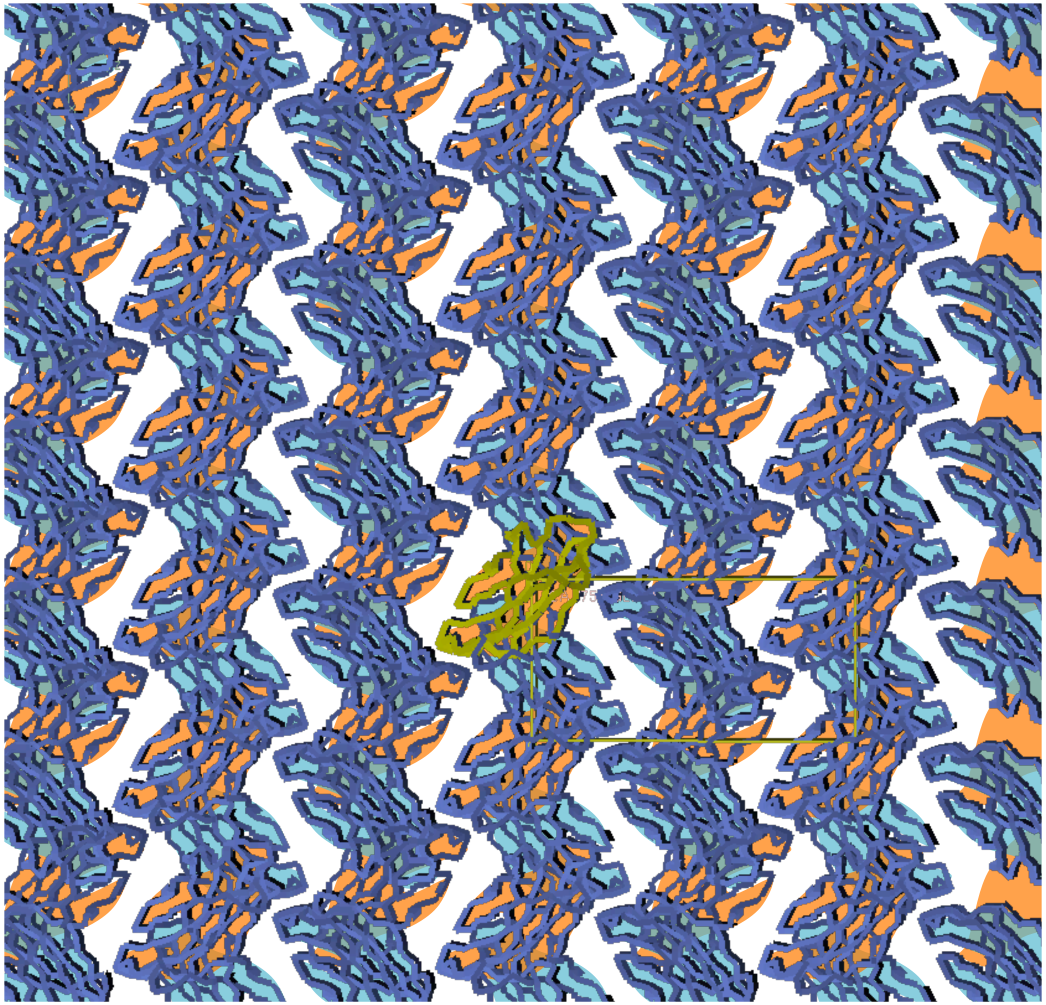
Simplified representation



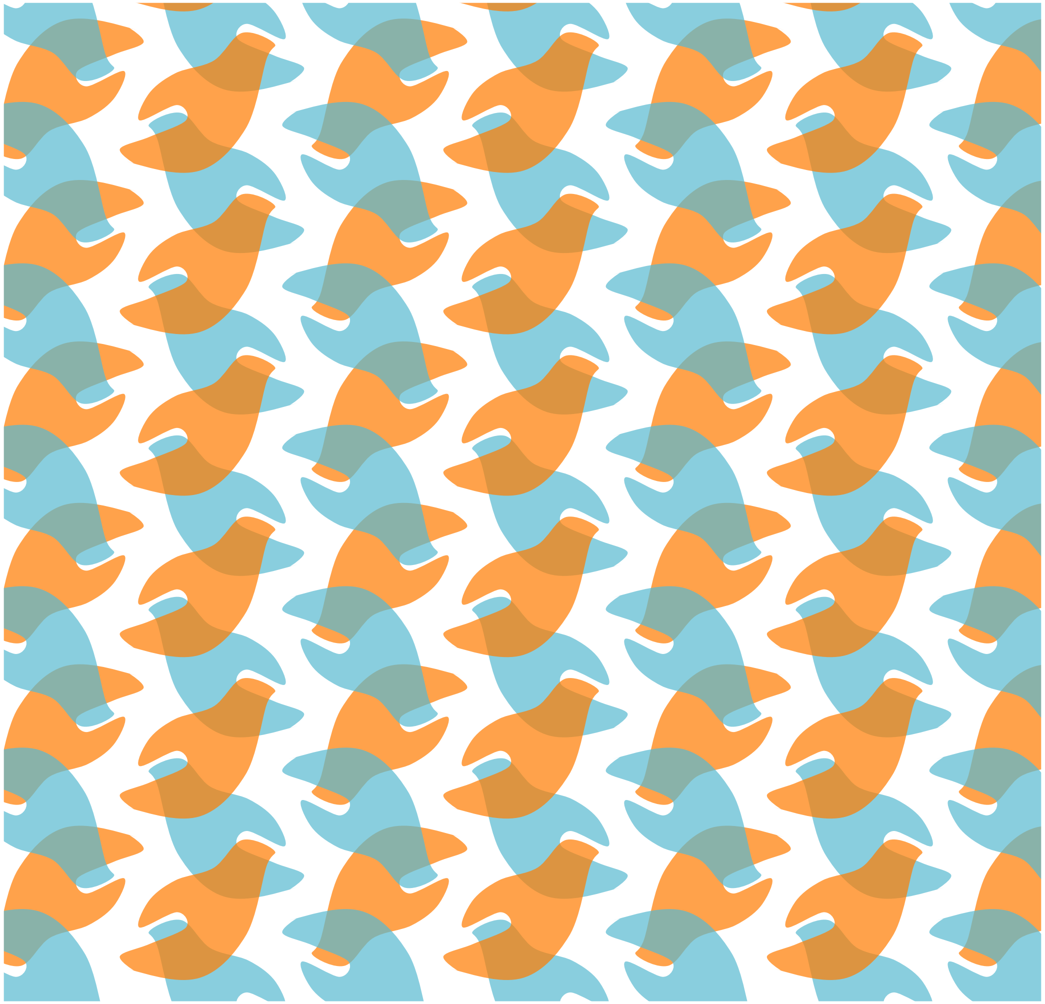
Simplified representation



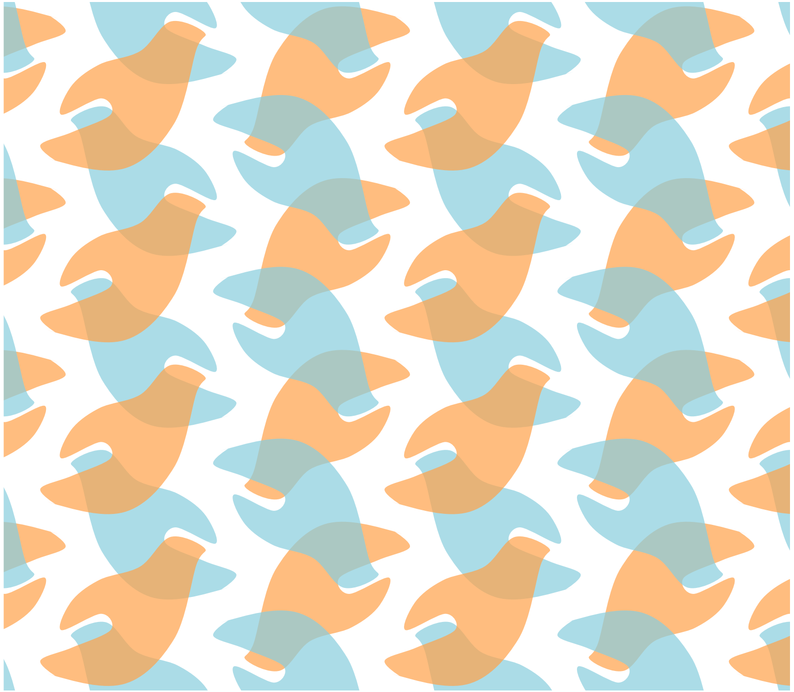
Simplified representation



Simplified representation

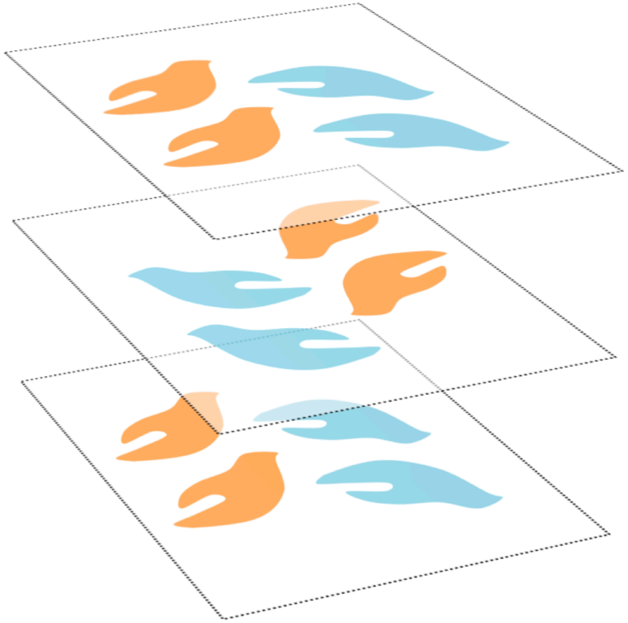


Simplified representation

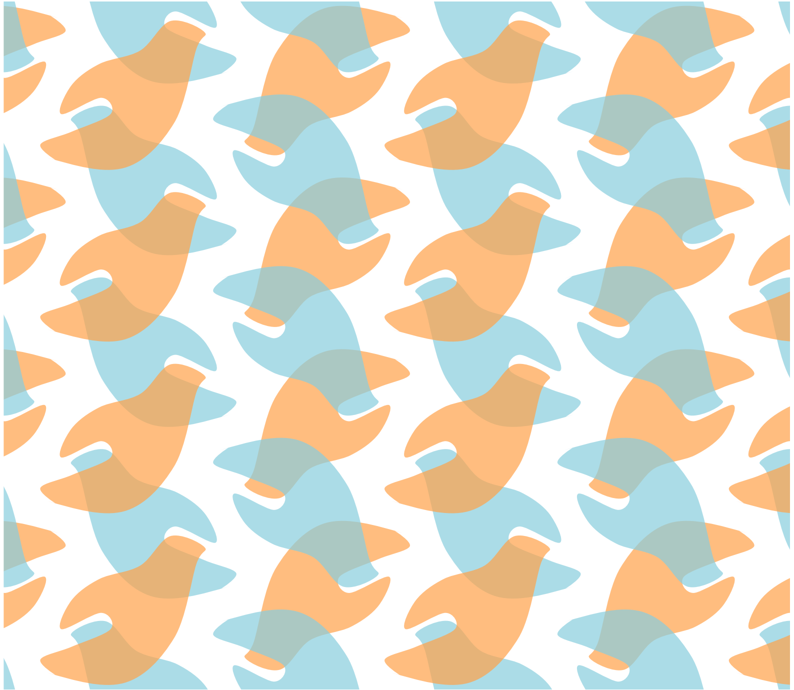


View from the top

There is a third dimension.



Simplified representation



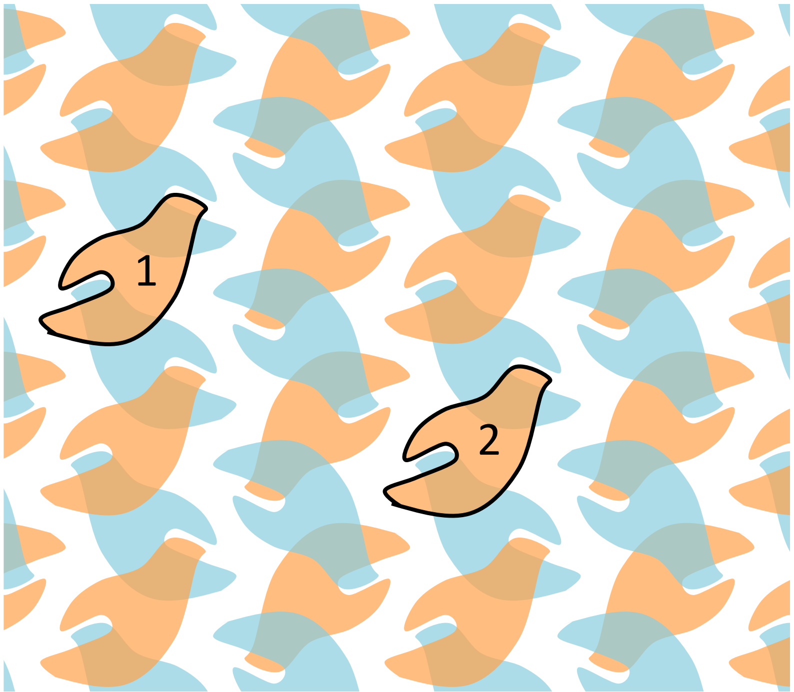
1 2 3 4

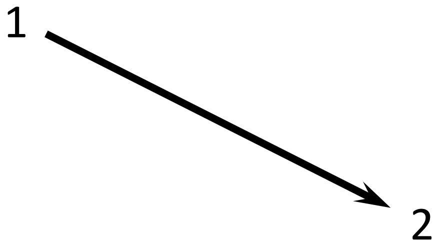
Orange and blue represent opposite sides of molecules

A slice is shown, where

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

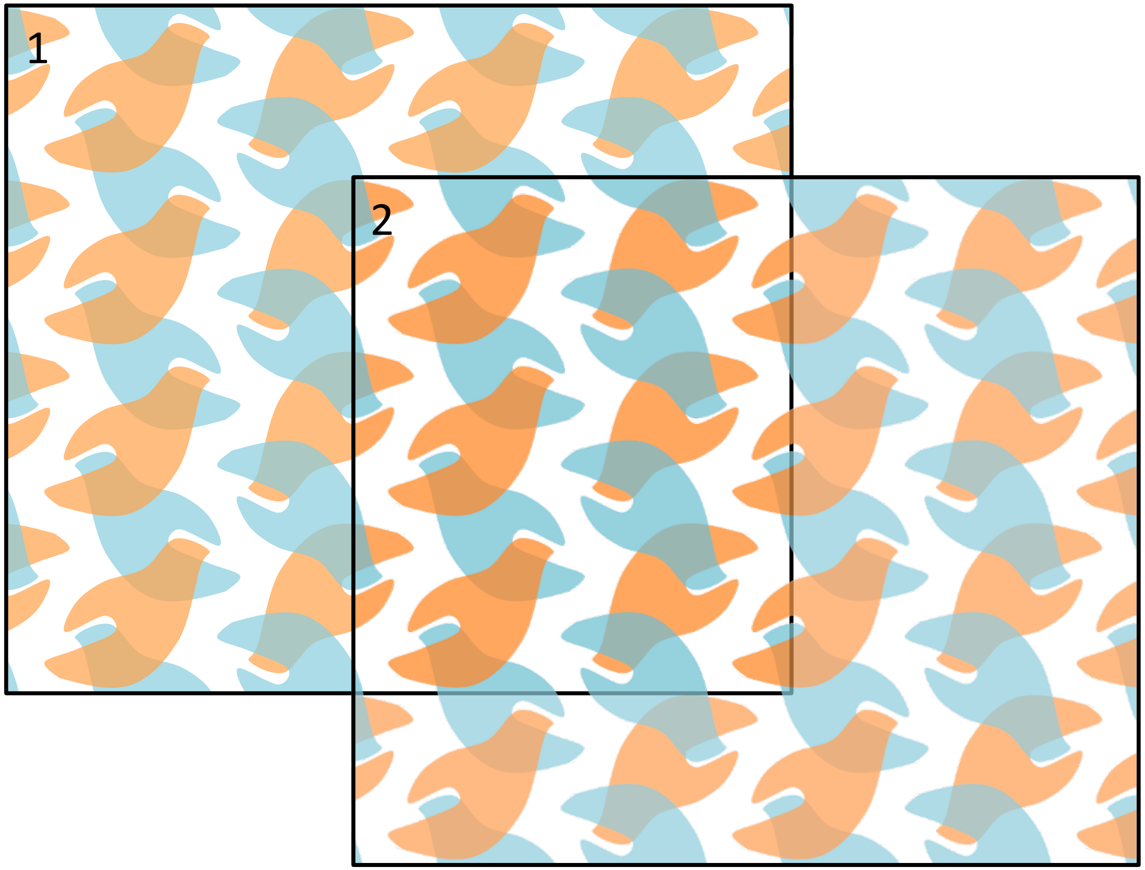
Translation 1

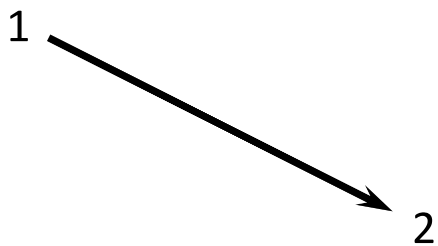




Vector maps 1 -> 2

Translation 1 is global





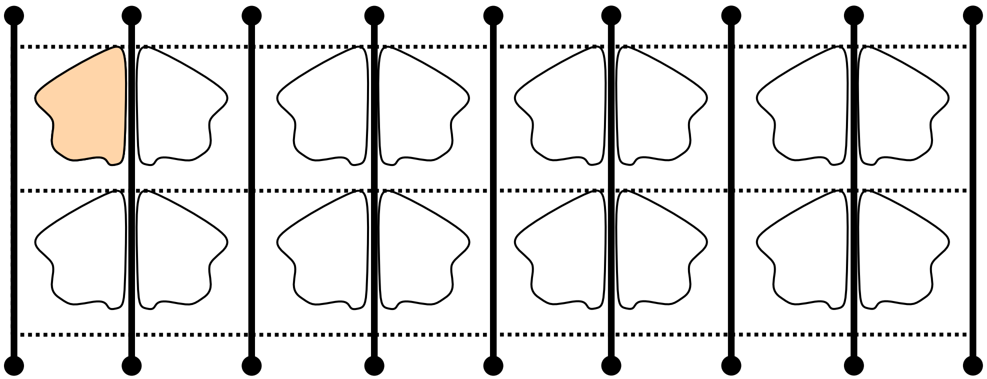
Vector 1->2 maps the whole crystal onto itself:

it defines a crystallographic operation

Crystallographic Translation and Pseudo-translation

Crystallographic translation

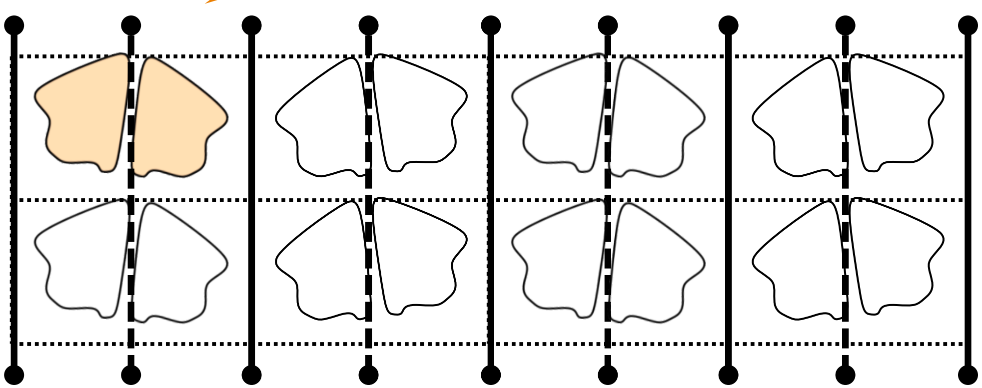
(symmetry is global and exact)



Crystallographic translation

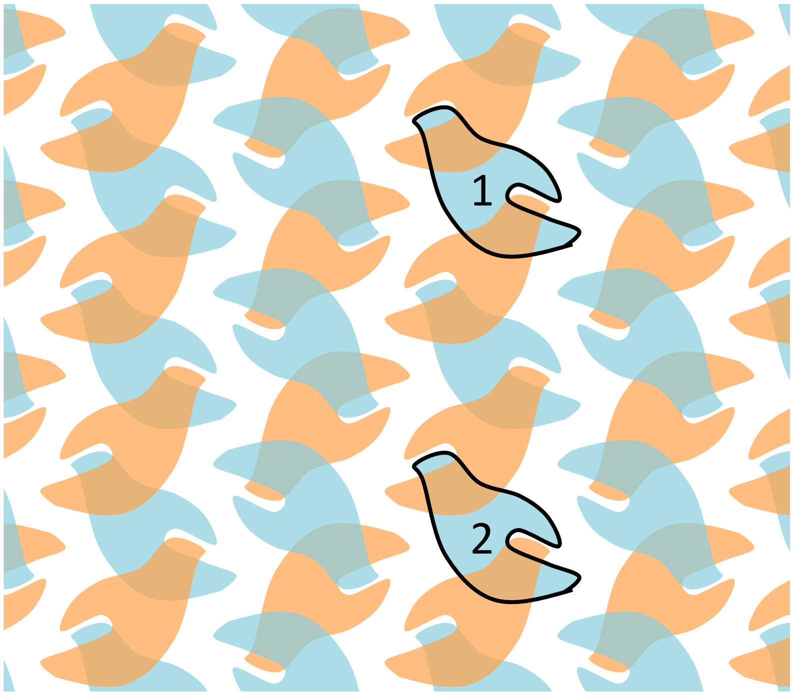
Pseudo-translation

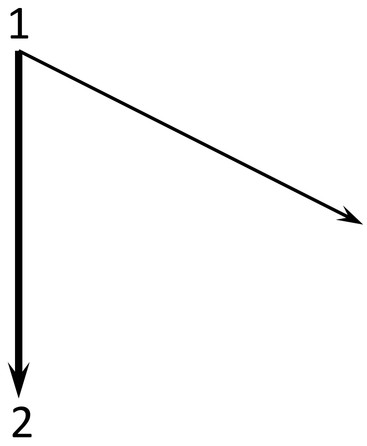
(symmetry is global but approximate)



This is a special case of translational Non-Crystallographic Symmetry (tNCS)

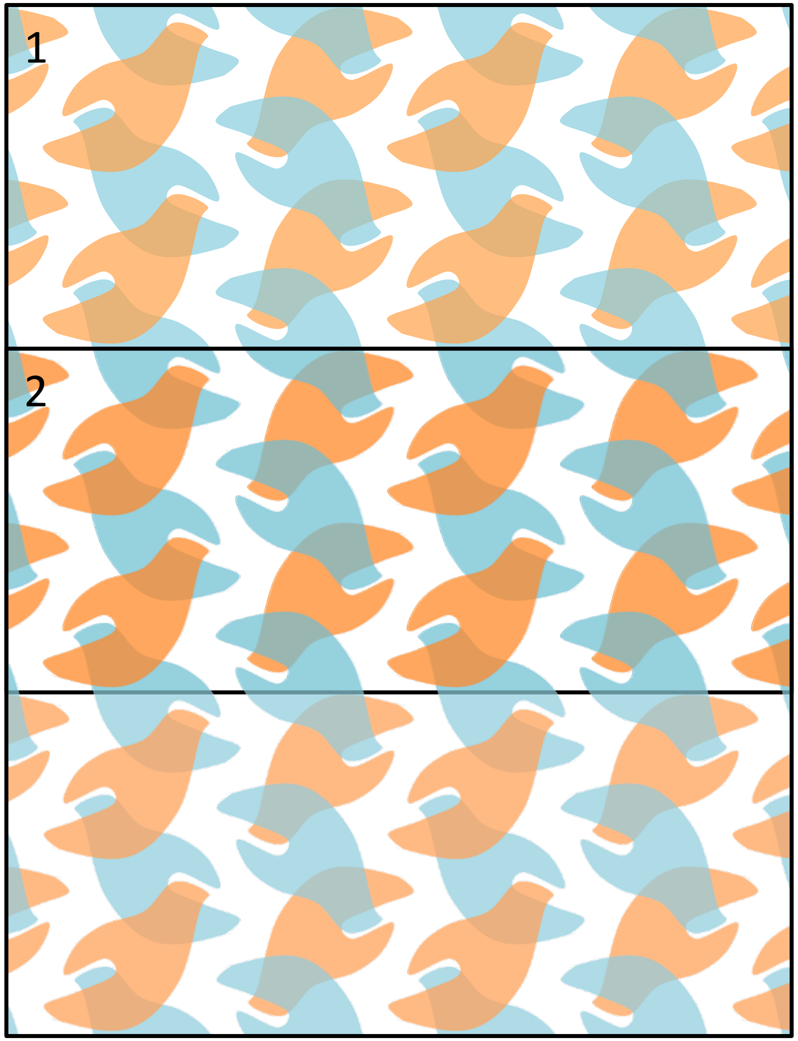
Translation 2

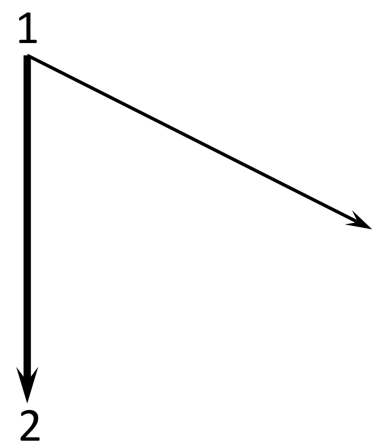




Highlighted vector maps 1 -> 2

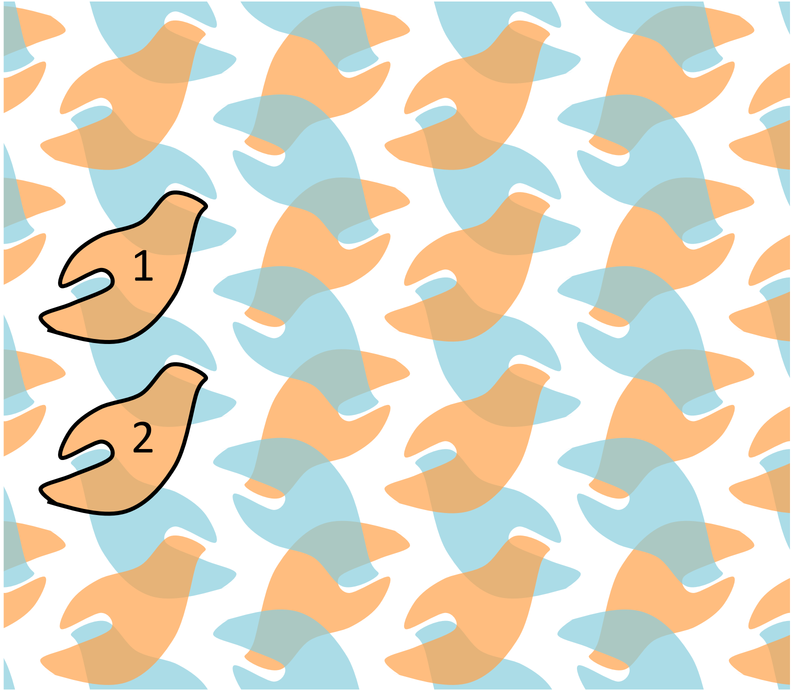
Translation 2 is global

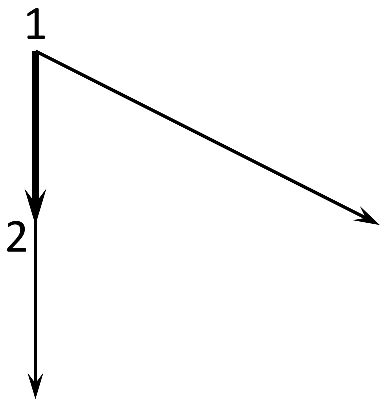




Highlighted vector maps the whole crystal onto itself

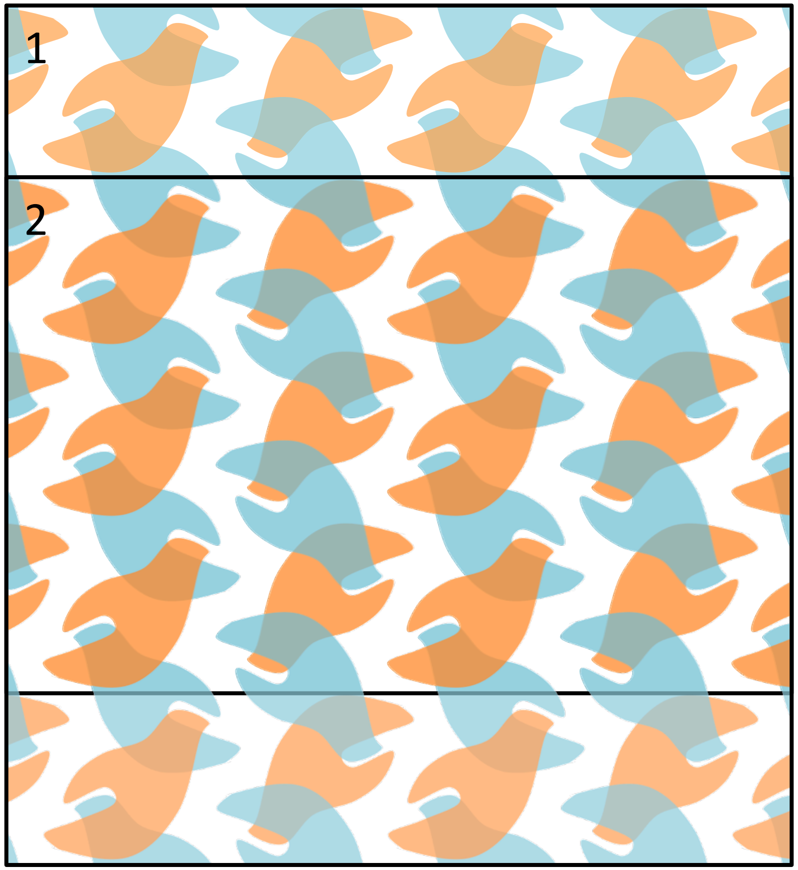
Translation 3

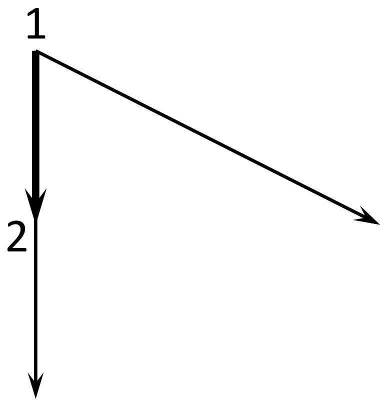




Highlighted vector maps 1 -> 2

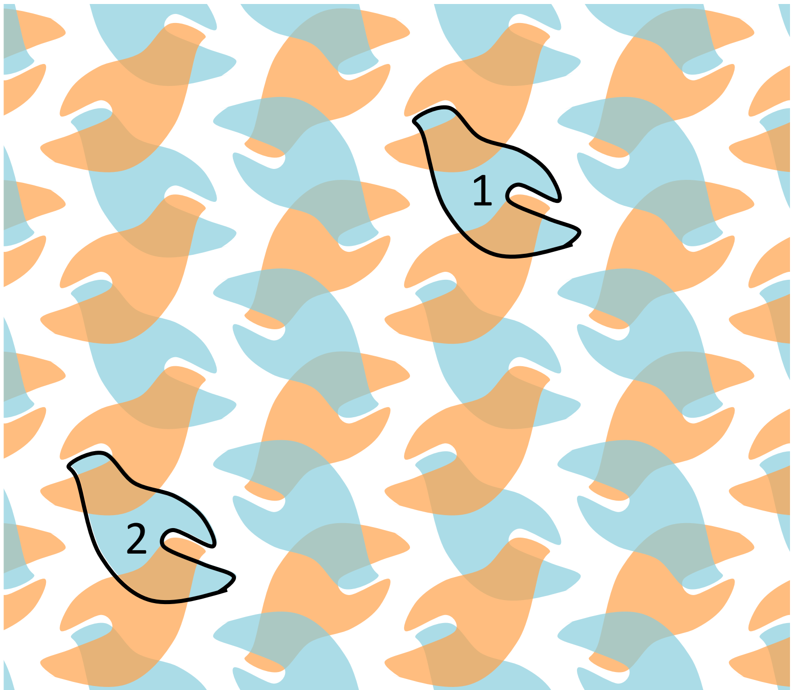
Translation 3 is global

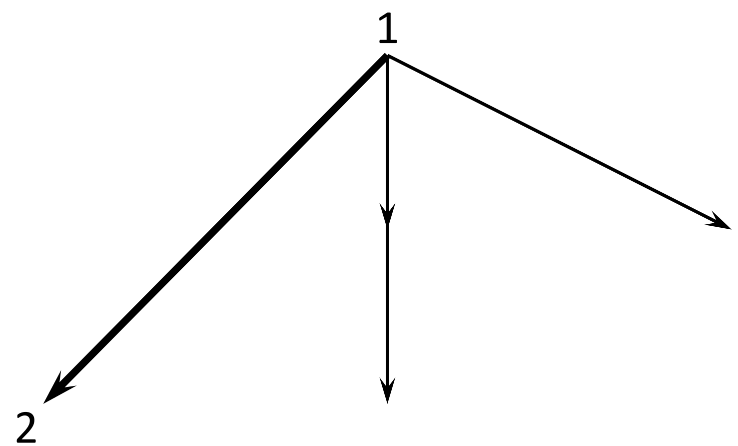




Highlighted vector maps the whole crystal onto itself

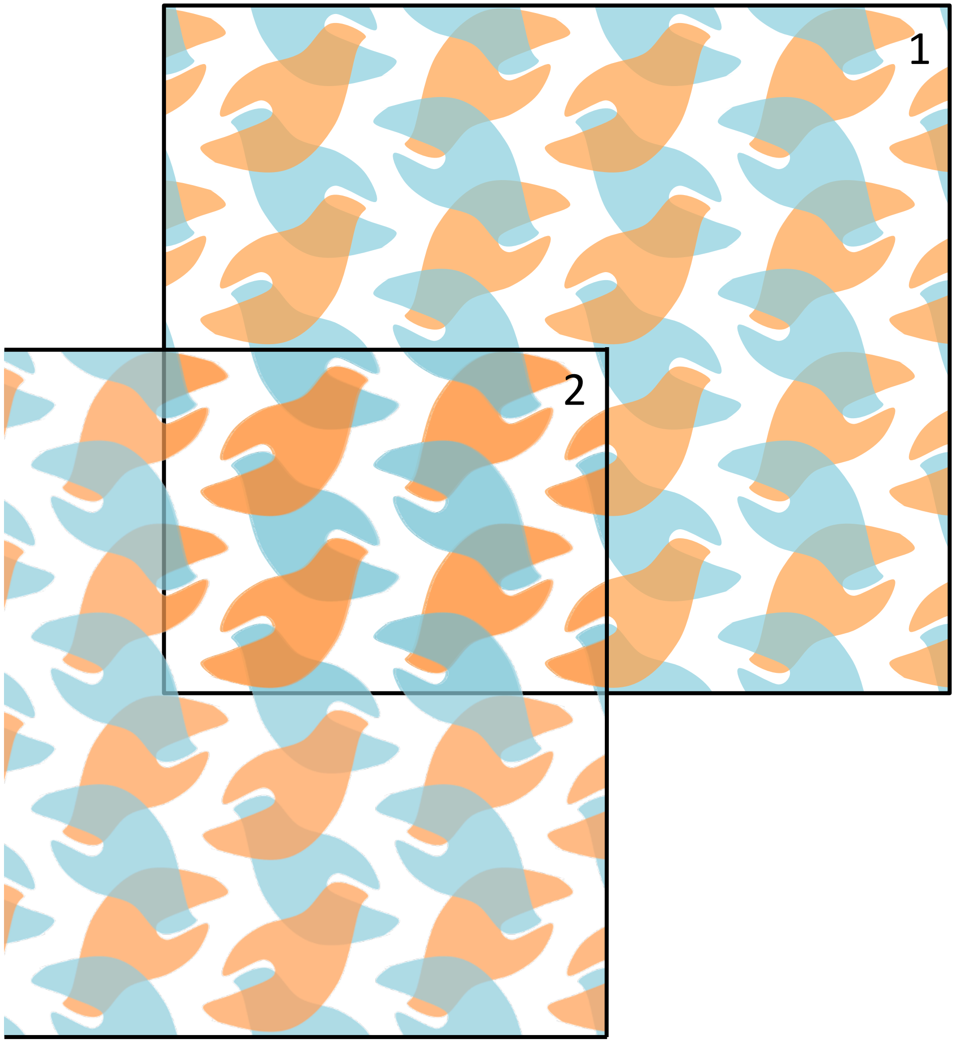
Translation 4

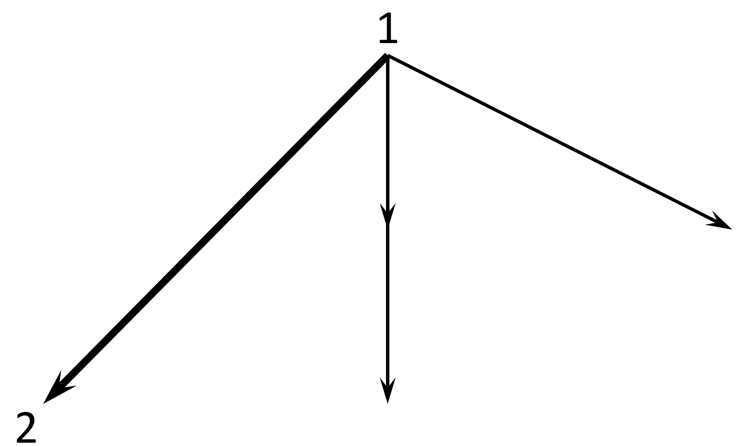




Highlighted vector maps 1 -> 2

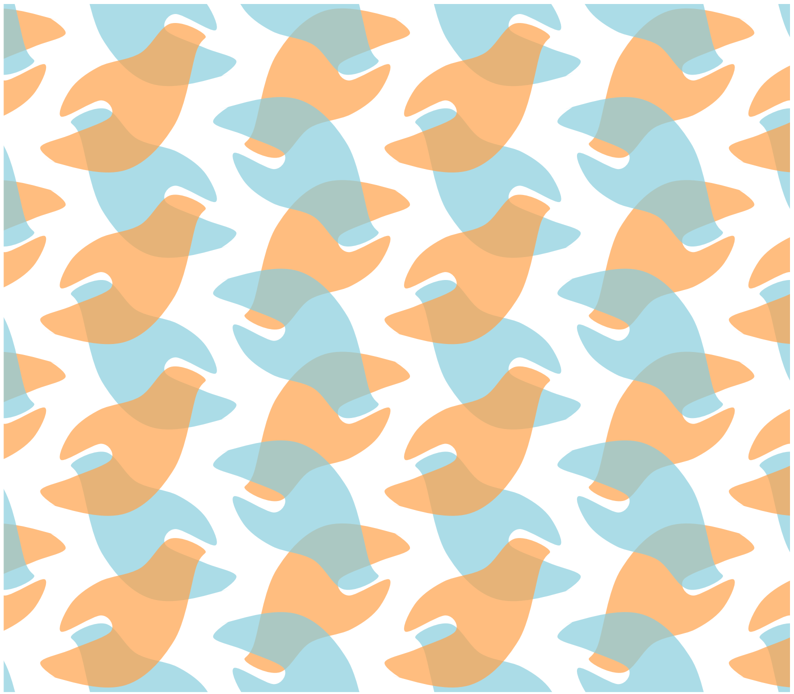
Translation 4 is global

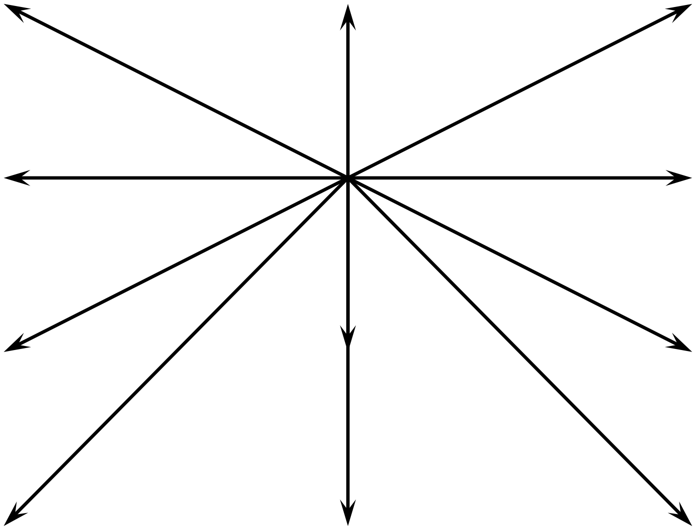




Highlighted vector maps the whole crystal onto itself

All translations form an infinite group

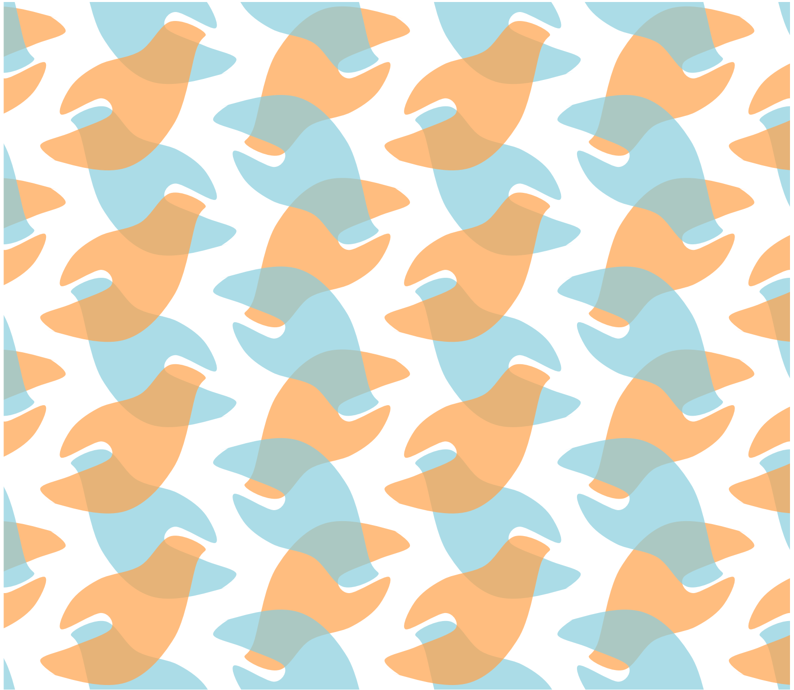


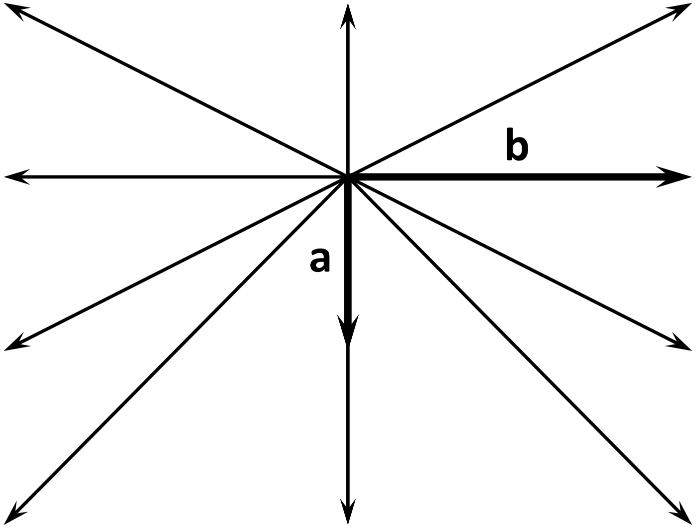


An infinite group (over vector sum):

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

Basis set

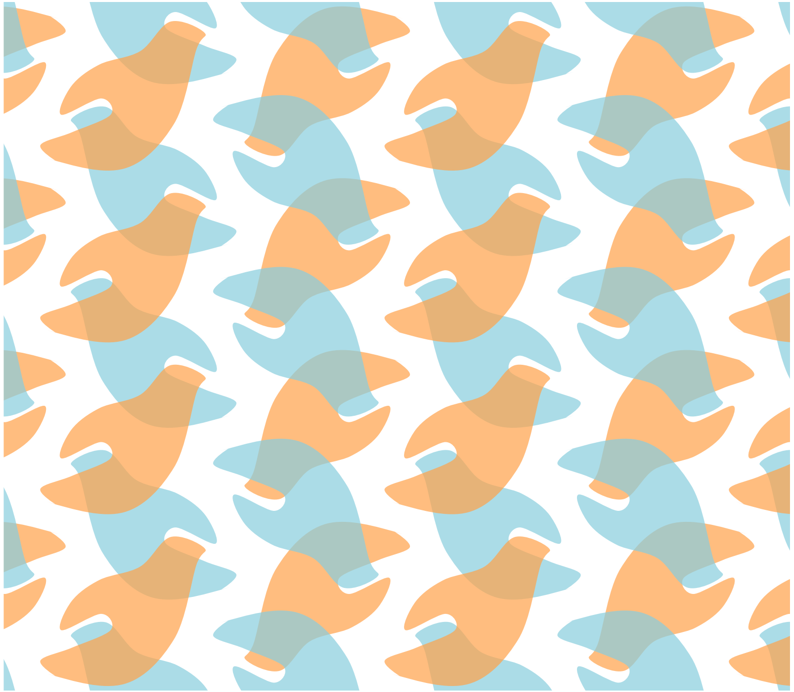


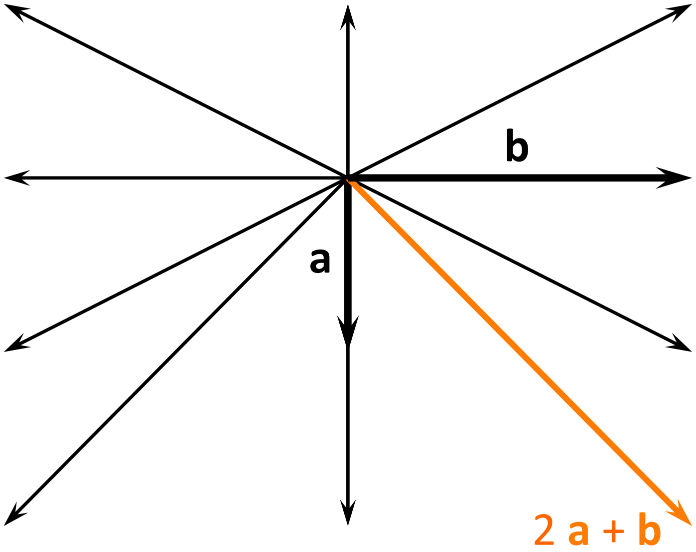


All the translations that map the crystal onto itself can be produced from a basis set: **a**, **b**, **c**

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

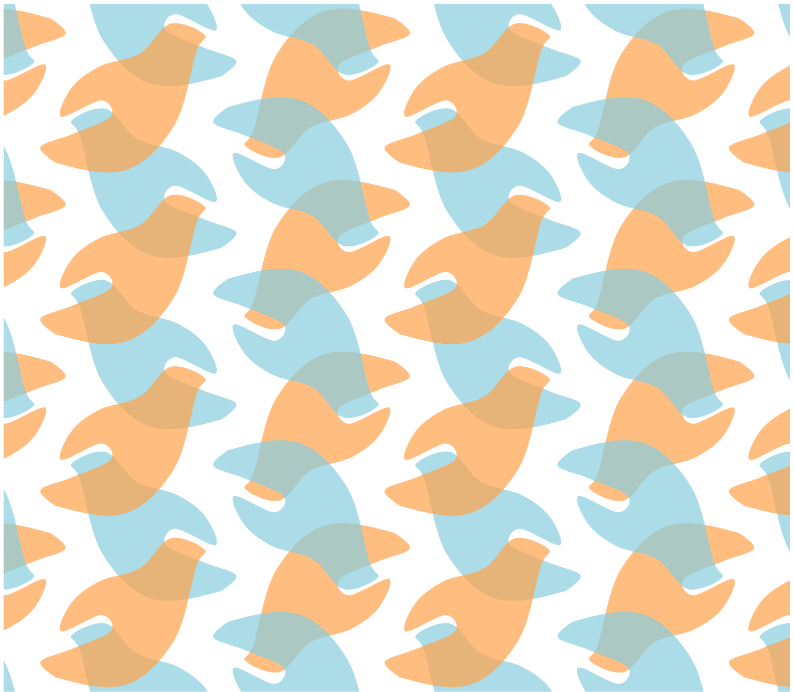
Basis set

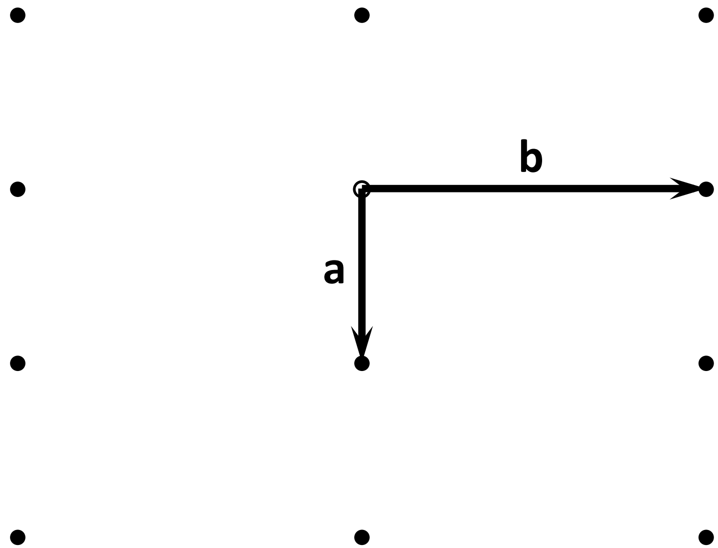




For example, the highlighted vector is expressed as 2 **a** + **b**.

Lattice

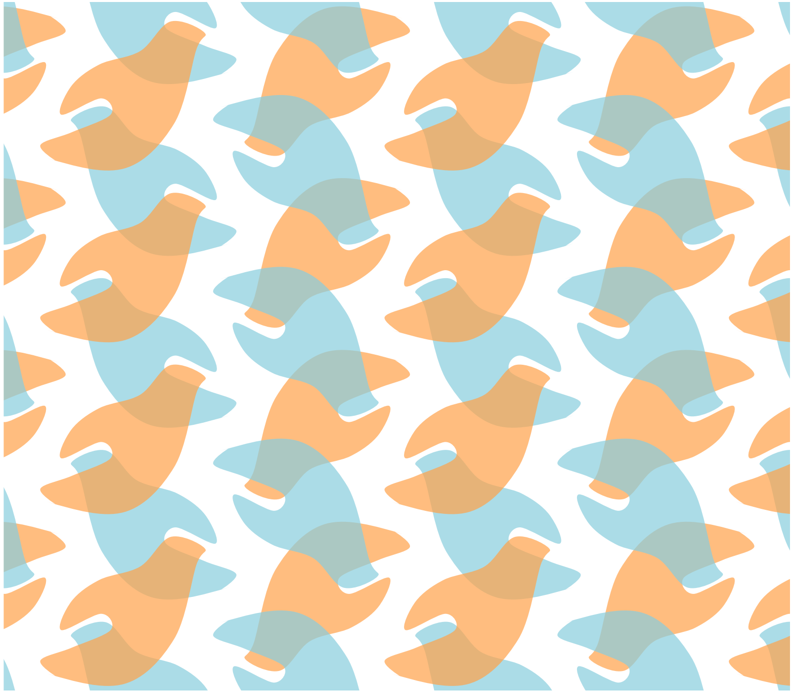


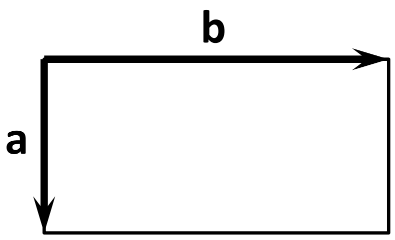


All the crystallographic translations can be represented as a lattice.

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

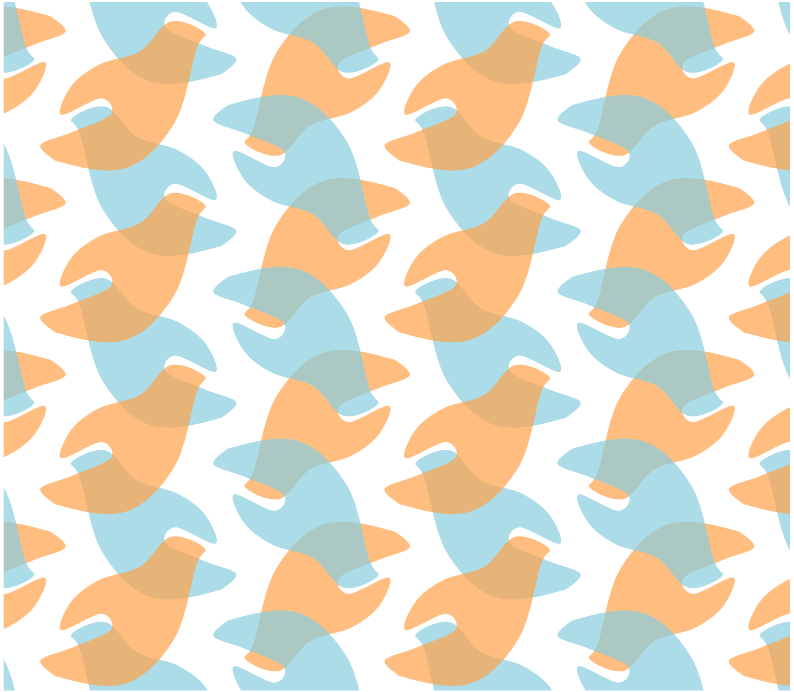
Unit cell

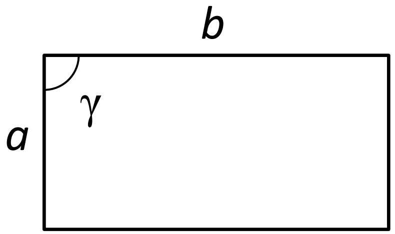




A compact representation of translational symmetry and base vectors.

Unit cell

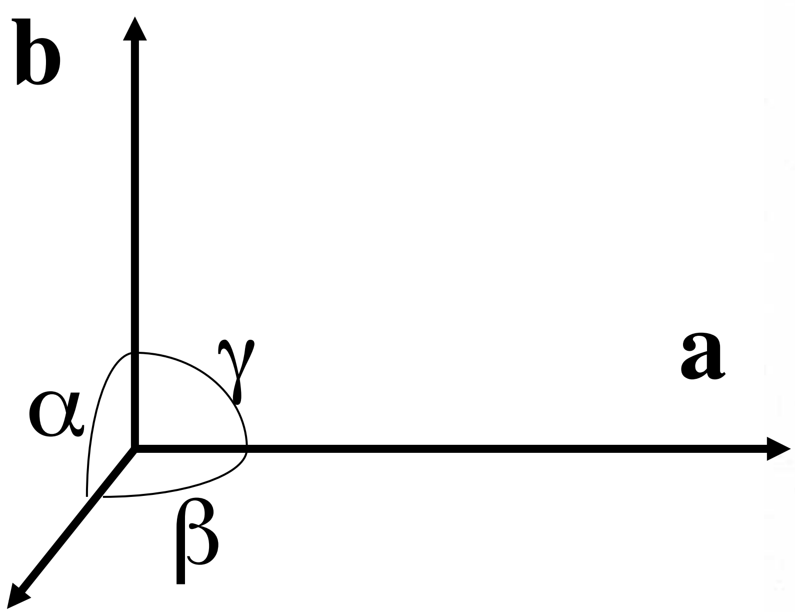


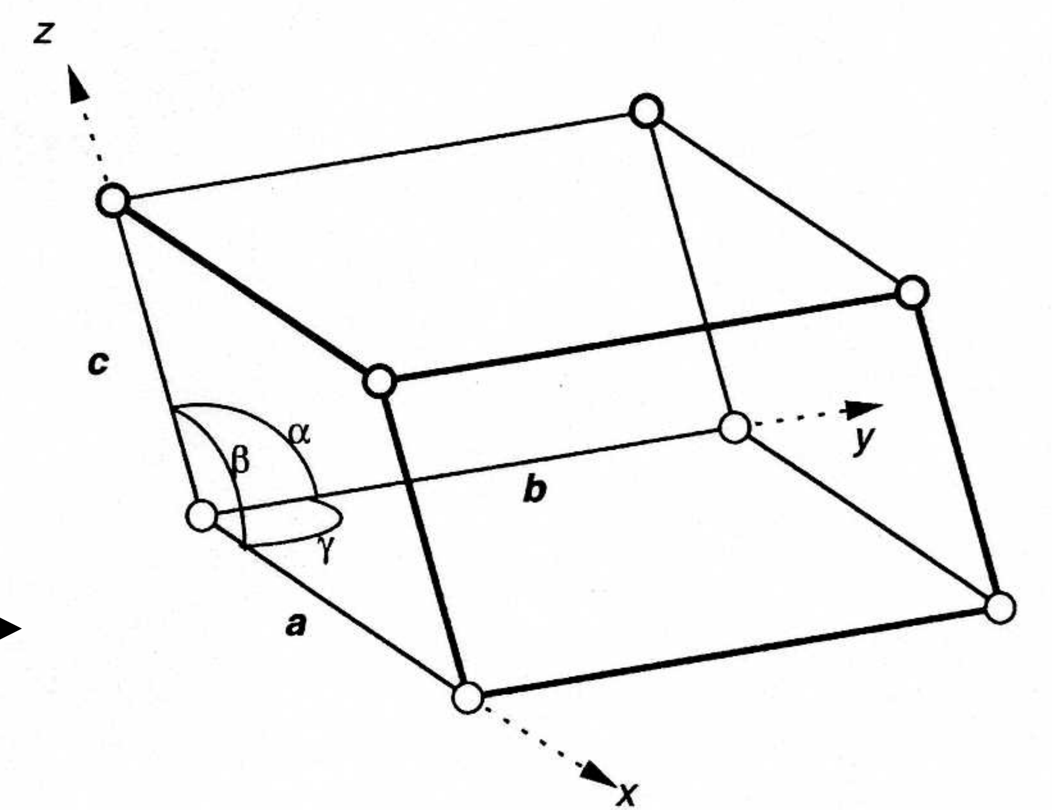


Can be fully characterised by six numbers
(the third dimension is not shown here)

Unit cell parameters (3D view)

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

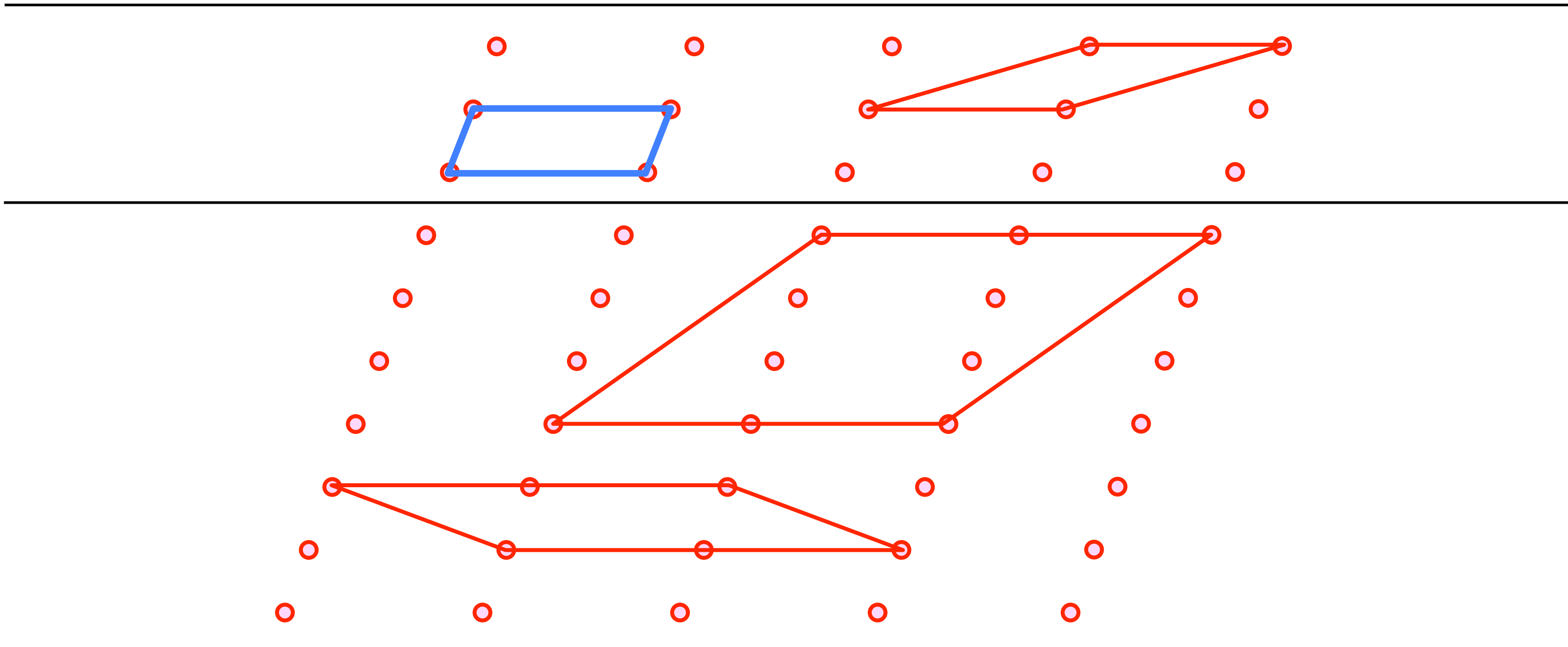




Unit cells are usually defined in terms of the *lengths* of these vectors and angles between them. For example,

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

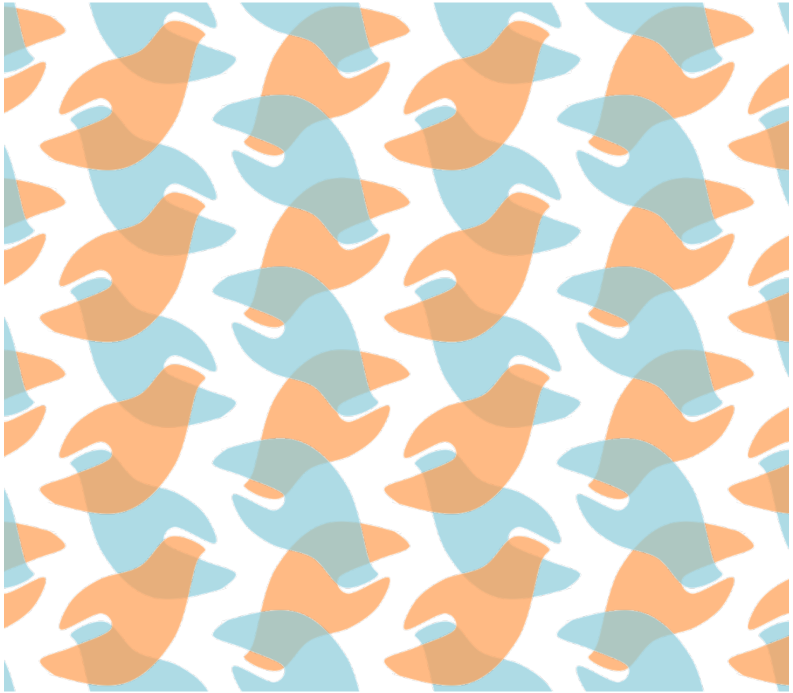
`Choice of unit cell

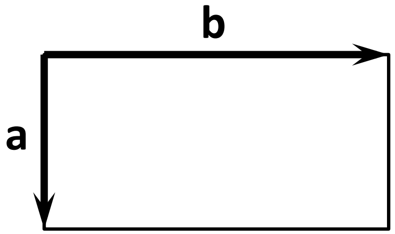


The top two do define all translations = primitive unit cells
The bottom two do NOT define all translations = non-primitive unit cells

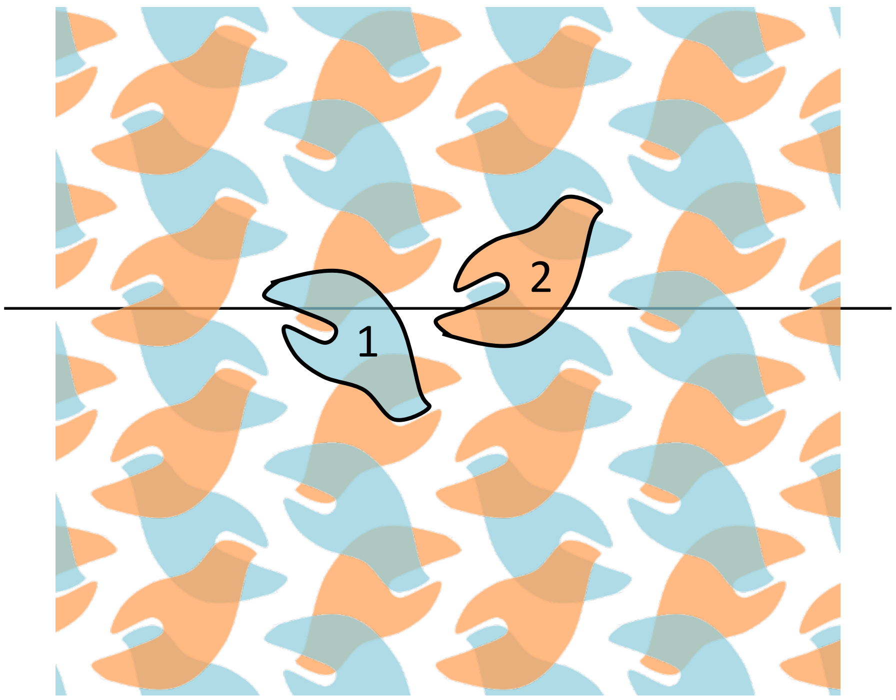
The top left: primitive reduced – the standard for <u>some</u> space groups

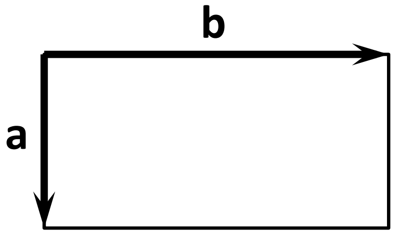
Back to example

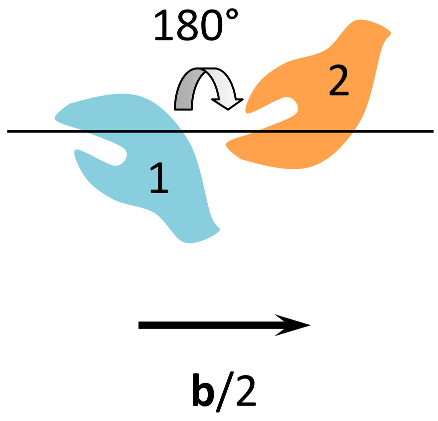




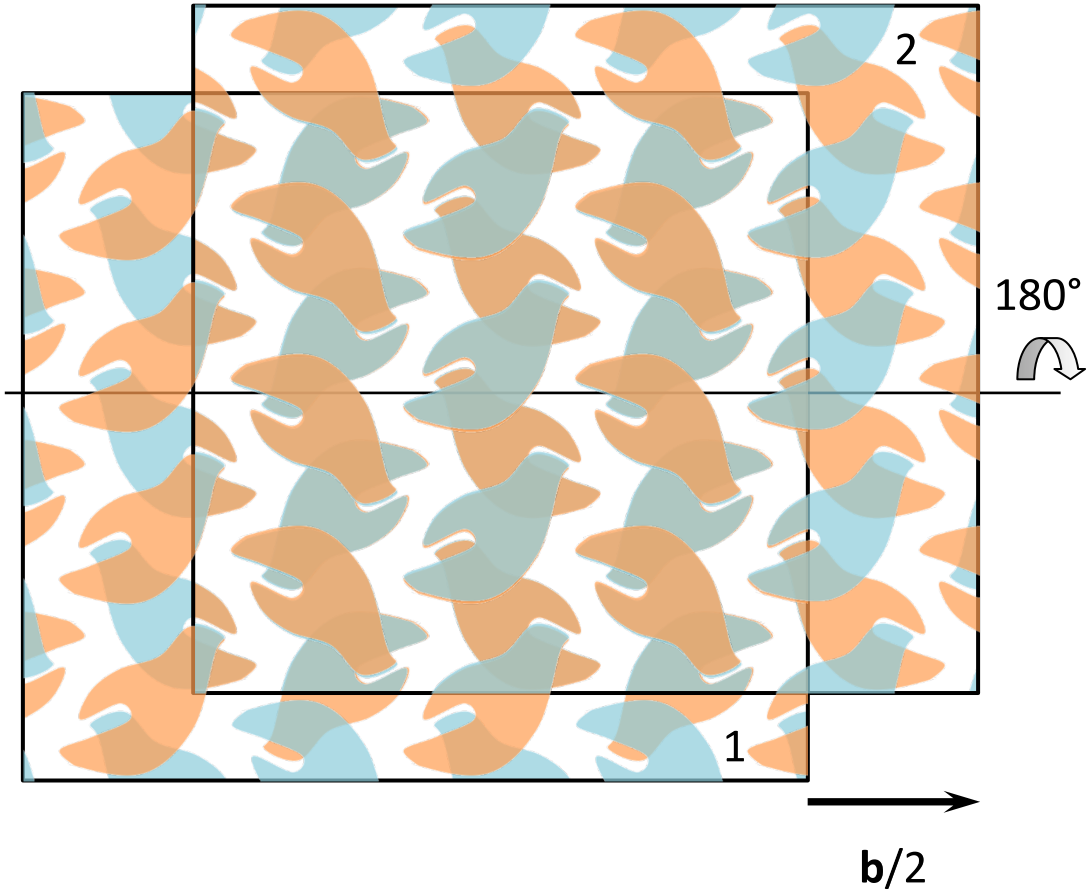
Screw rotation 1

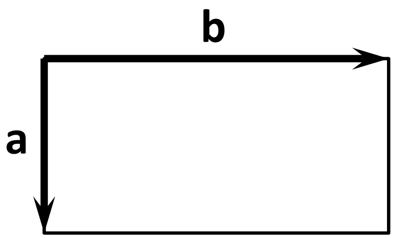






Screw rotation axis





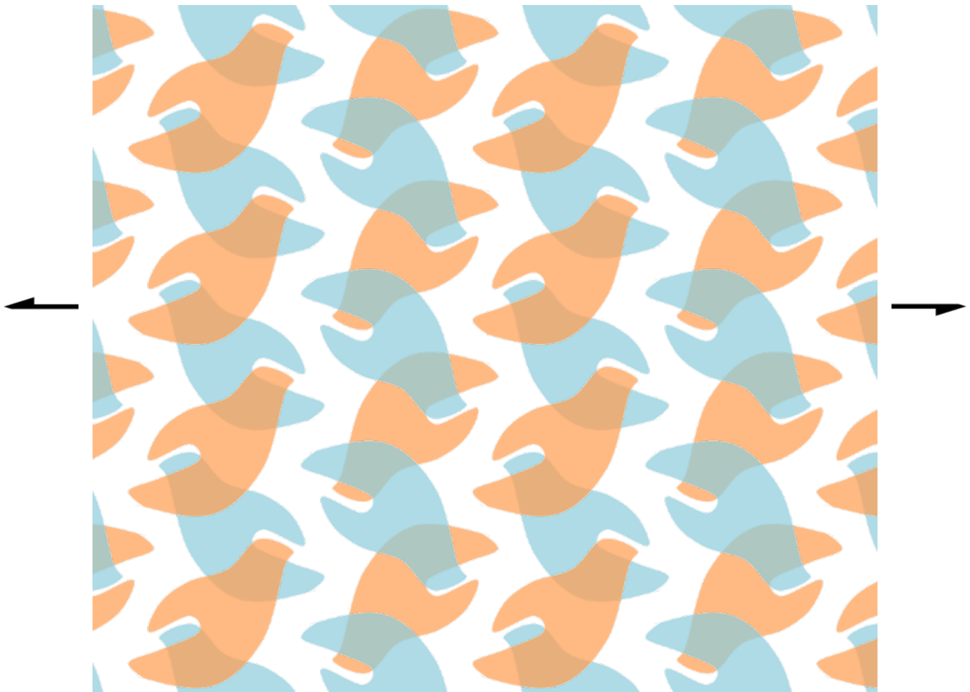
Operation 1->2
maps the whole crystal onto itself:

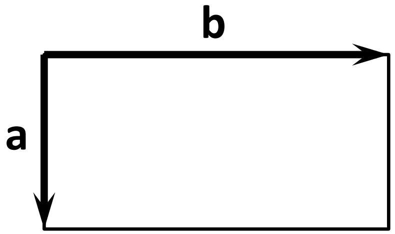
this is a crystallographic operation

The axis is a crystallographic symmetry element,

it can be mapped into the structure

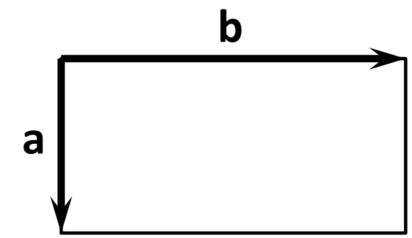
Screw rotation 1 - symbol

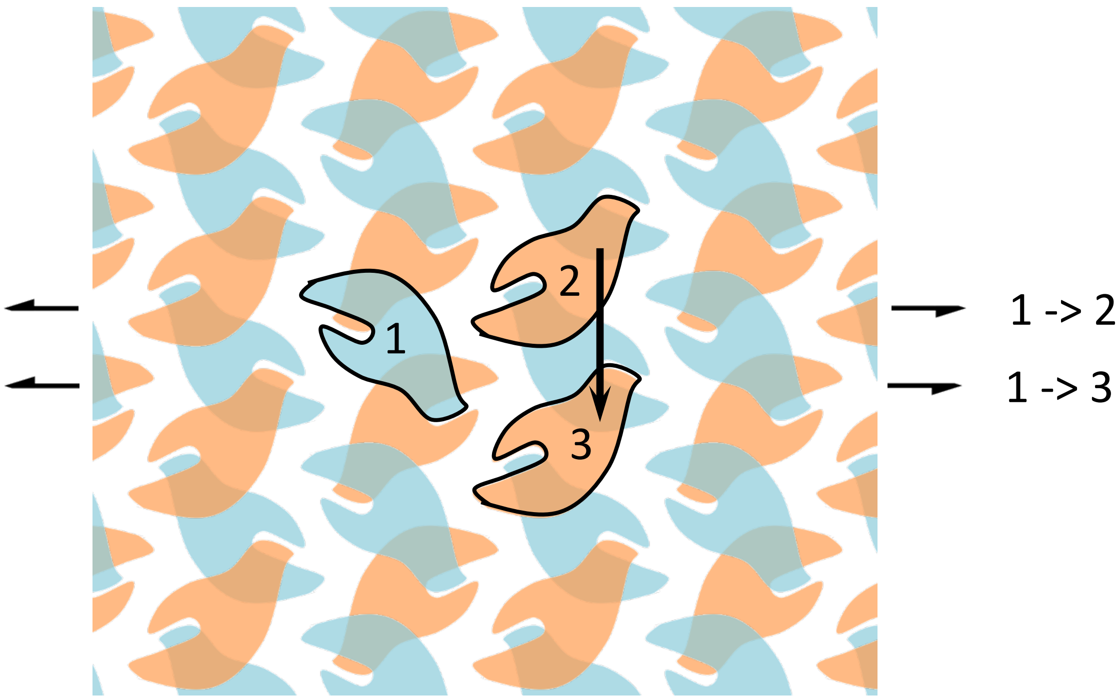




2_1 (plane of figure):

Screw rotation 1 - repeats



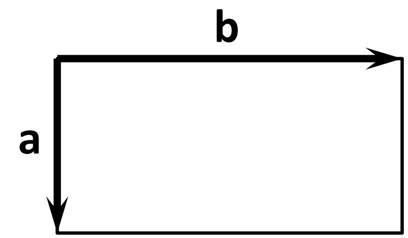


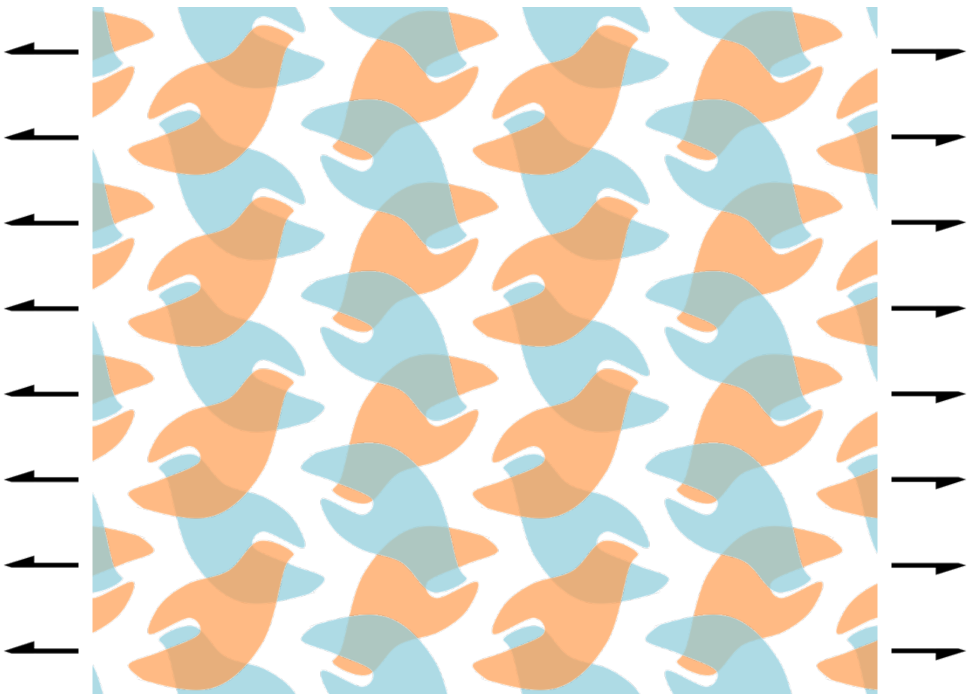
action of top axis
$\times$
translation **a**
=
action of bottom axis

(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

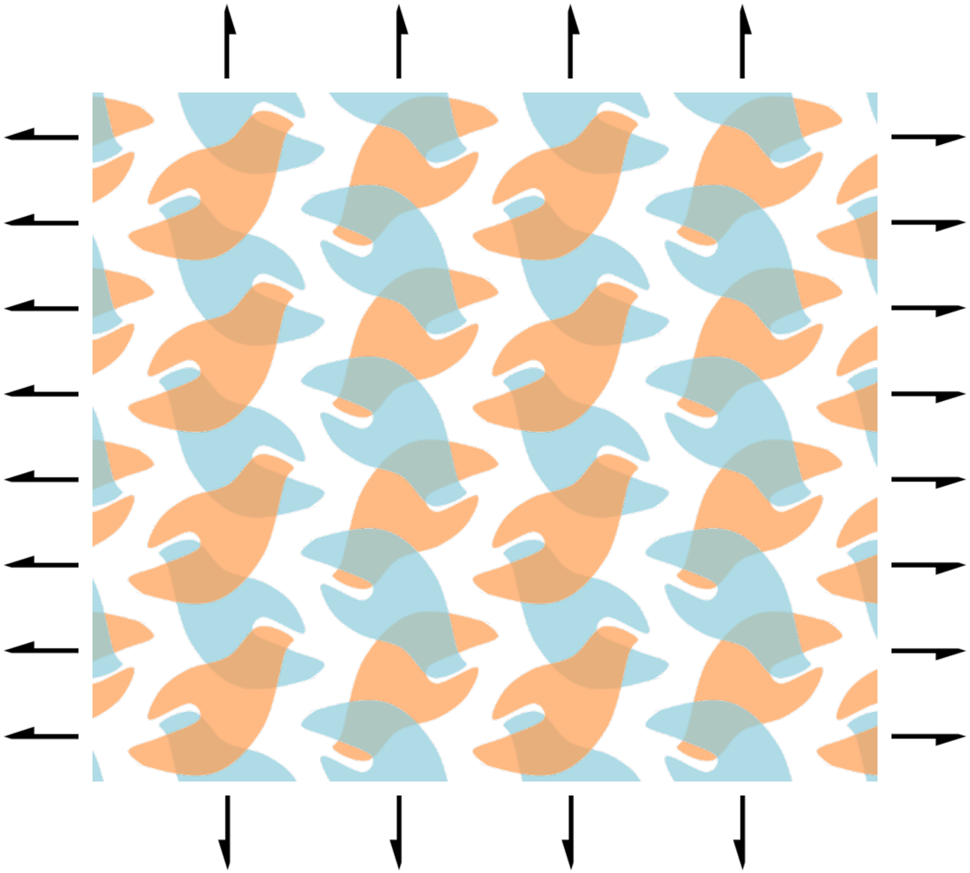


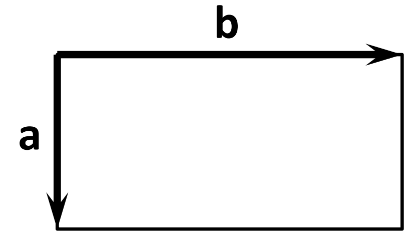


2_1 (plane of figure): 

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

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

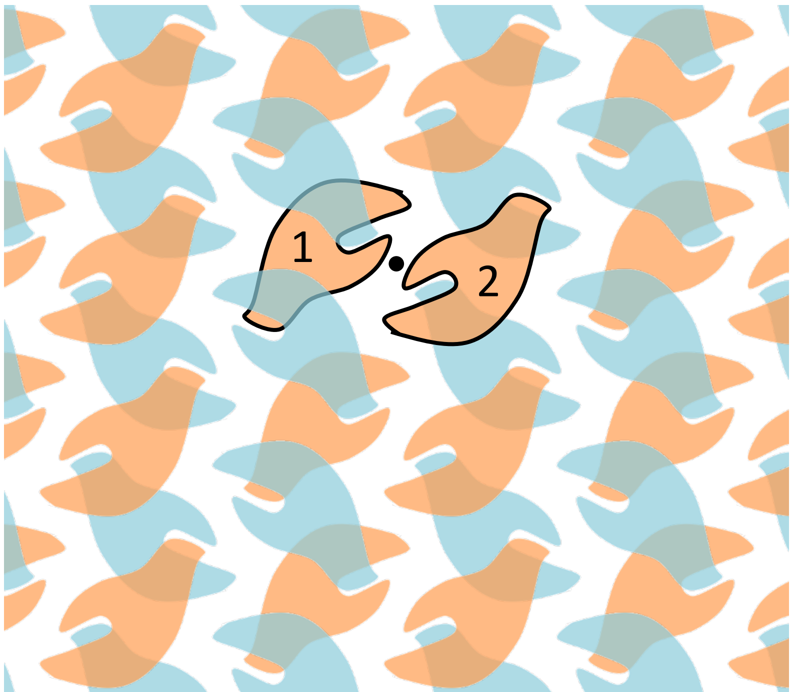


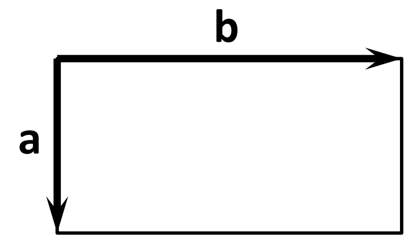


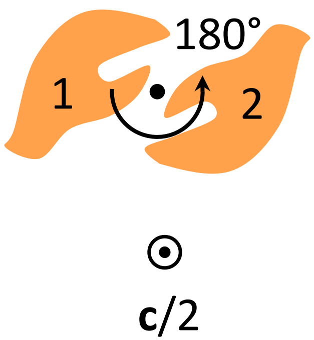
2_1 (plane of figure):

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

Screw rotation 3 – into plane

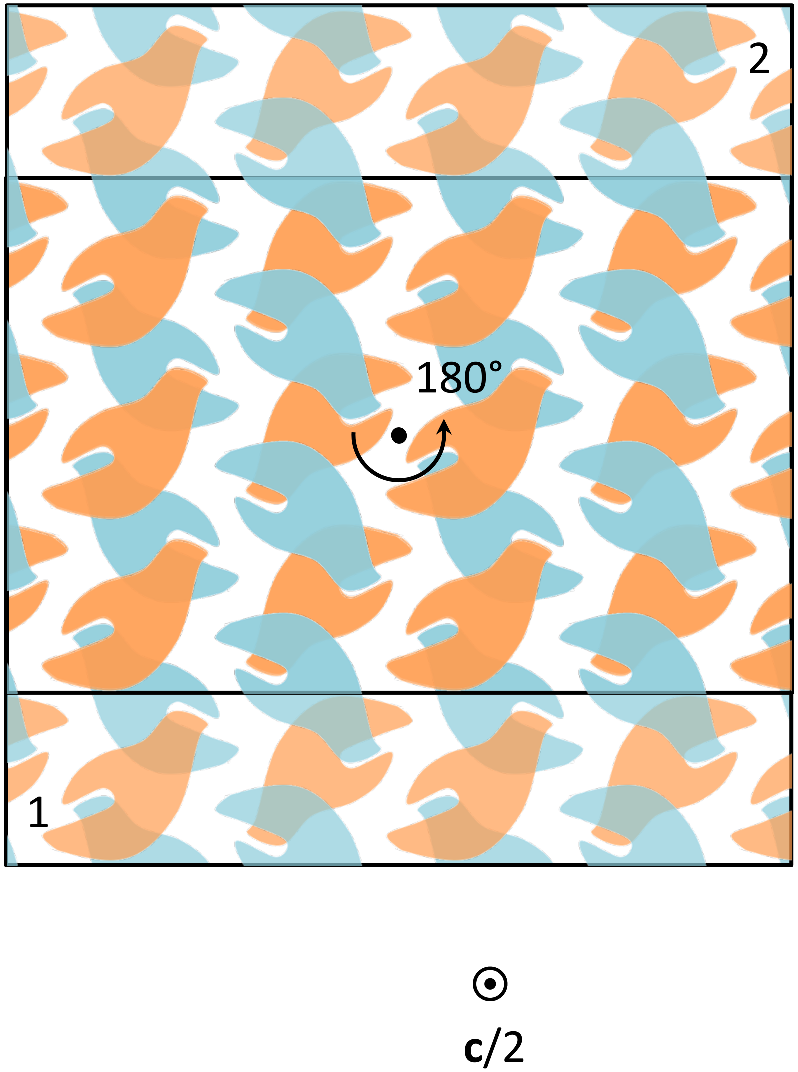


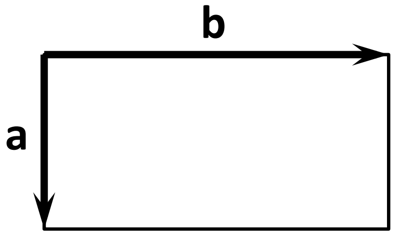




A rotation of 180º with a translation of ½ unit cell from the figure.

Screw rotation 3 is global





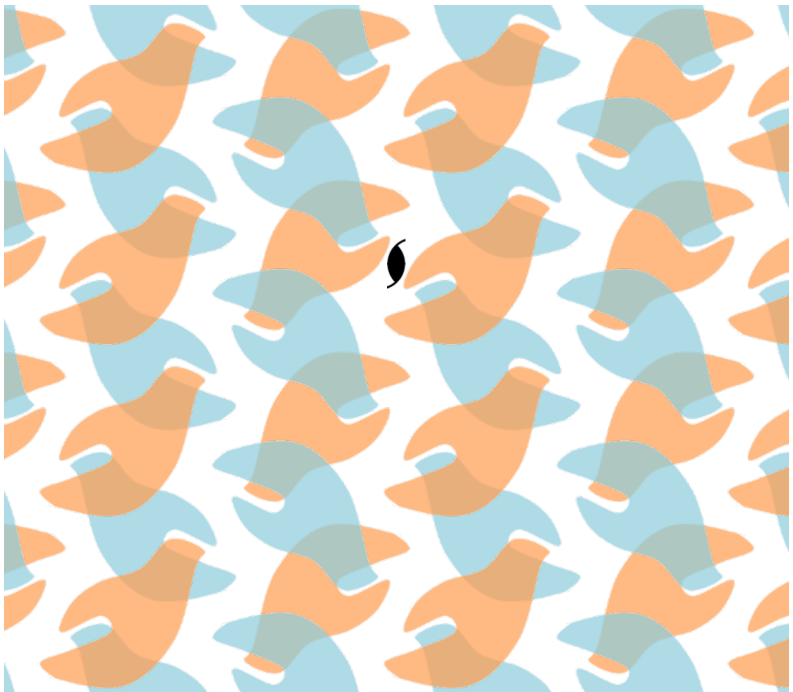
Screw rotation 3 maps the whole crystal onto itself:

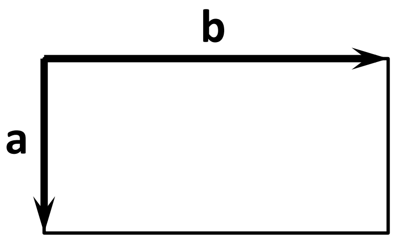
this is a crystallographic operation

The rotation axis is a crystallographic symmetry element,

it can be mapped into the structure

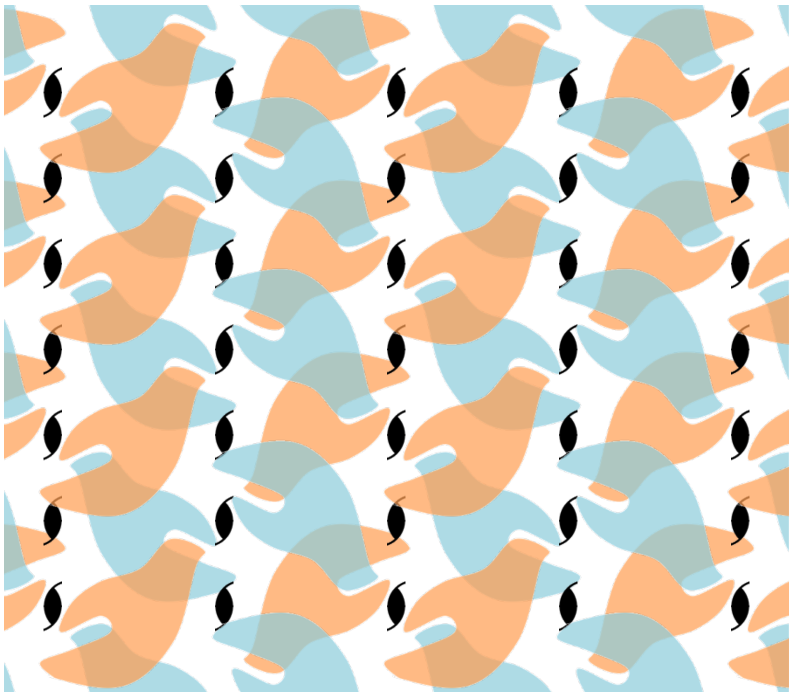
Screw rotation 3 - symbol

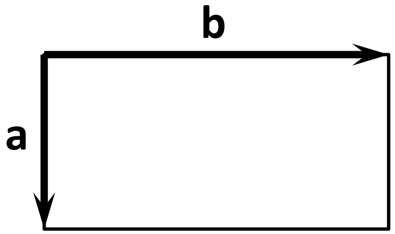




2_1 (along view):

Screw rotation 3 - repeats

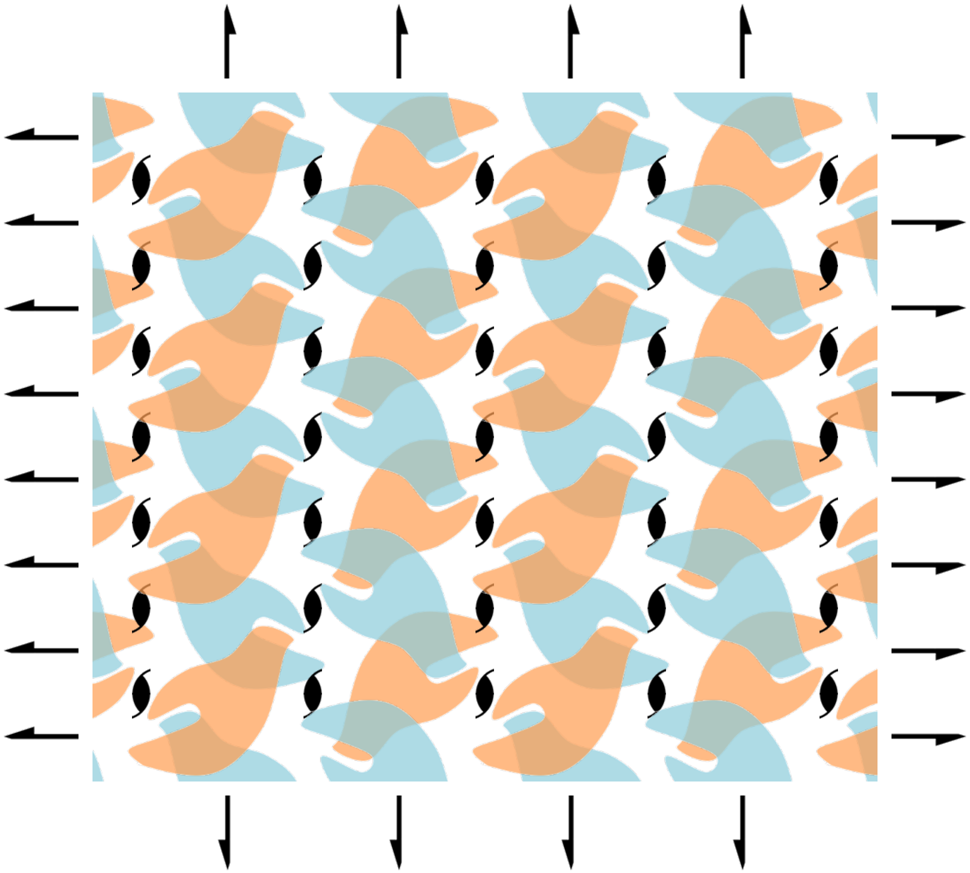


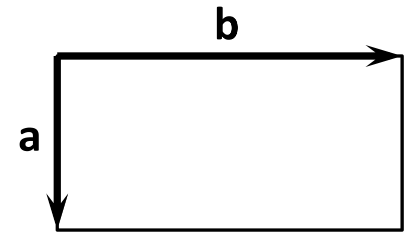


2_1 (along view):

As for the in-plane axes, there are repeated axes into the plane that leave the crystal unchanged.

All axes together



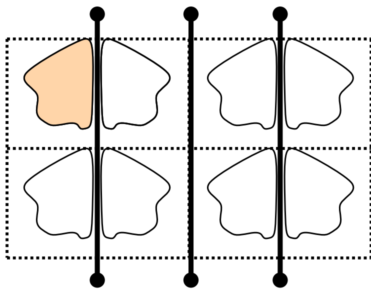


2_1 (plane of figure):

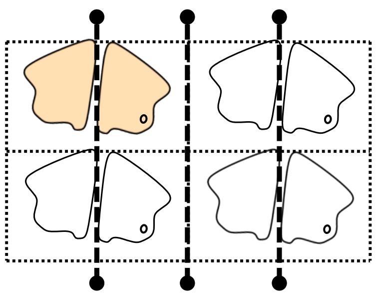
2_1 (along view):

we have built
a space group

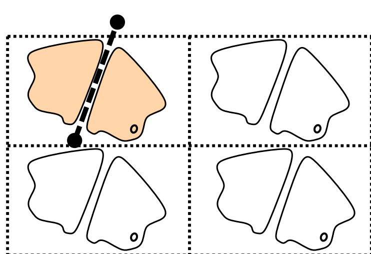
Crystallographic Symmetry, Pseudosymmetry and Non-Crystallographic Symmetry (NCS)



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

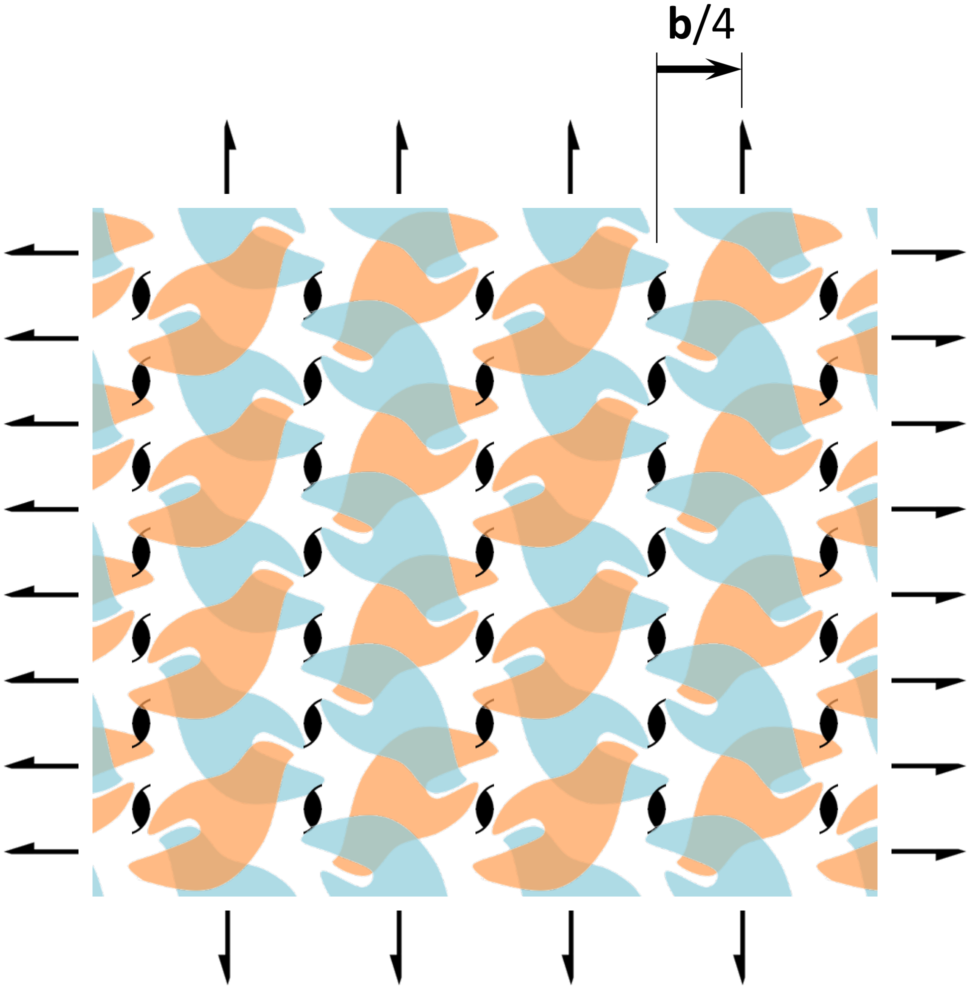


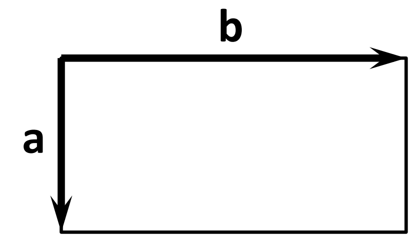
Pseudosymmetry (a limiting case of NCS)
- symmetry is **global** and **approximate**



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

Relative positions of axes

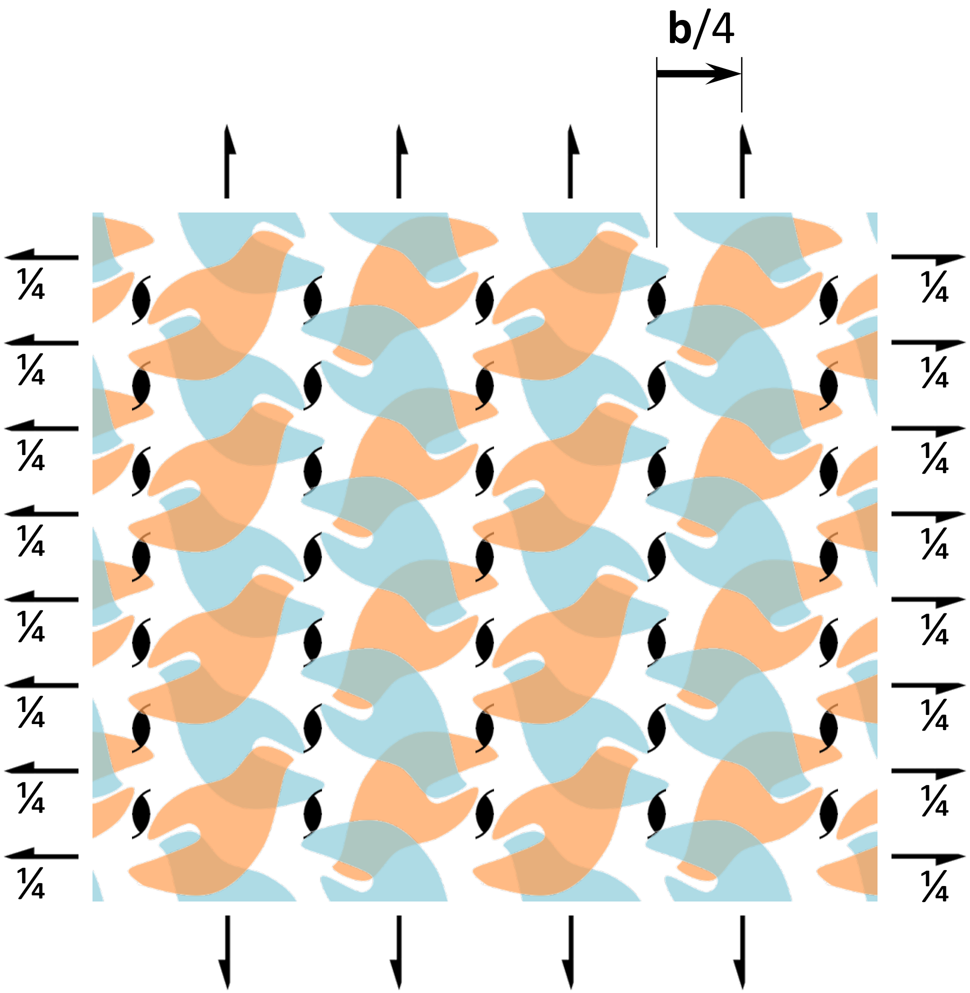


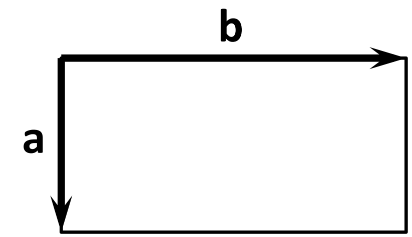


2_1 (plane of figure):

2_1 (along view):

Relative positions of axes





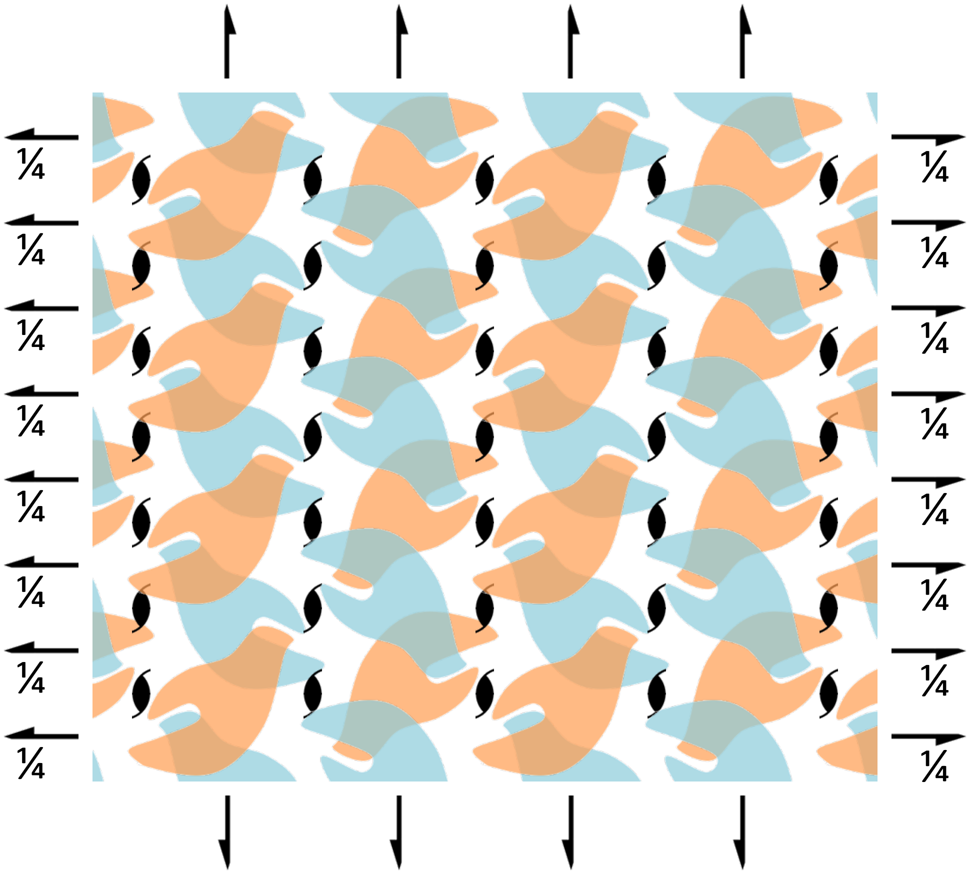
2_1 (plane of figure):

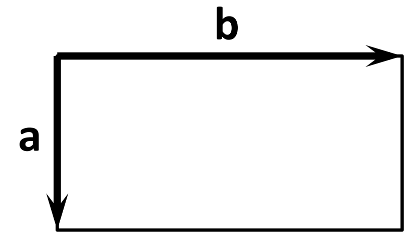
2_1 (along view):

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

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

Relative positions of axes



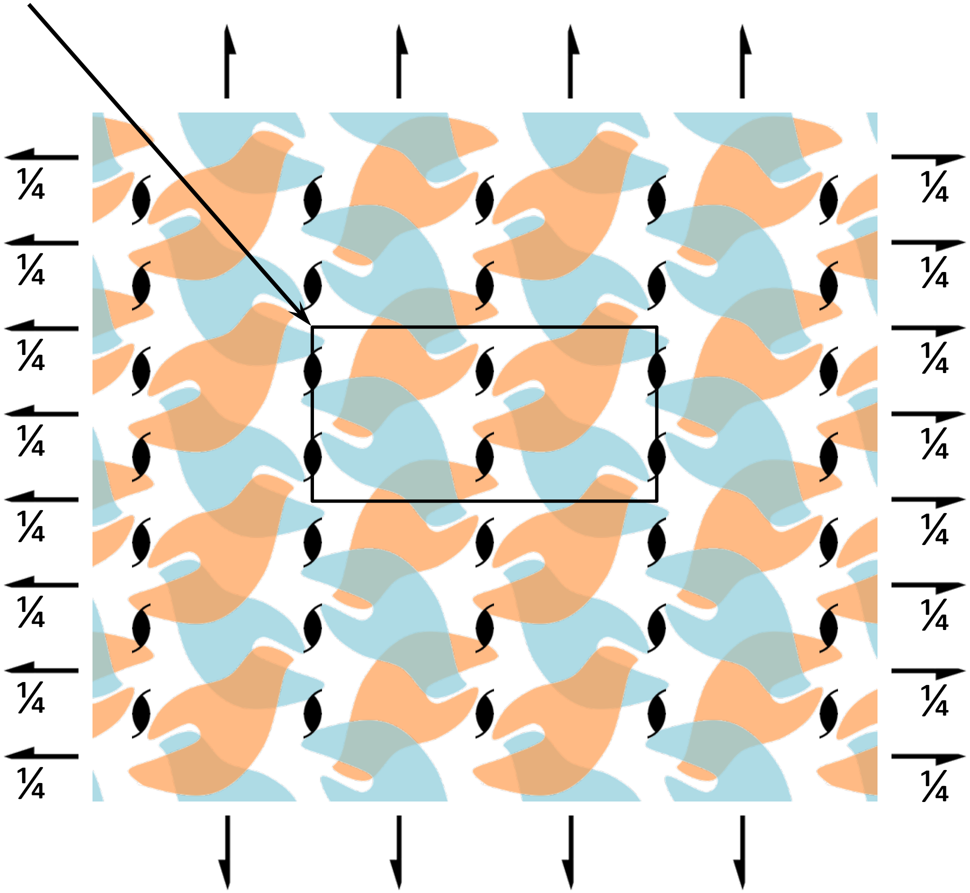


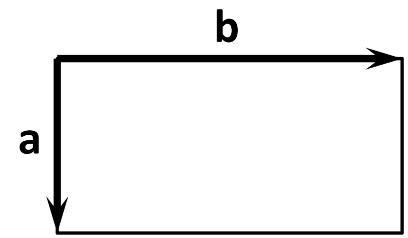
2_1 (plane of figure):

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):

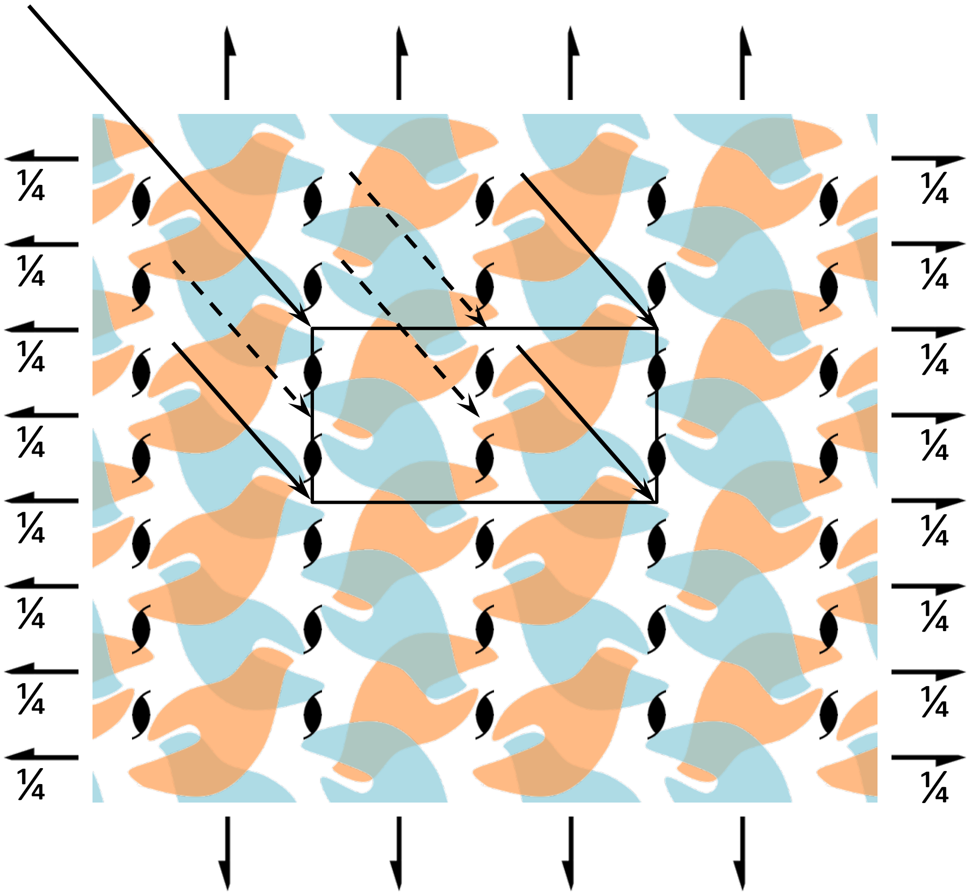
The unit cell placed on picture with symmetry elements means a choice of origin.

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.

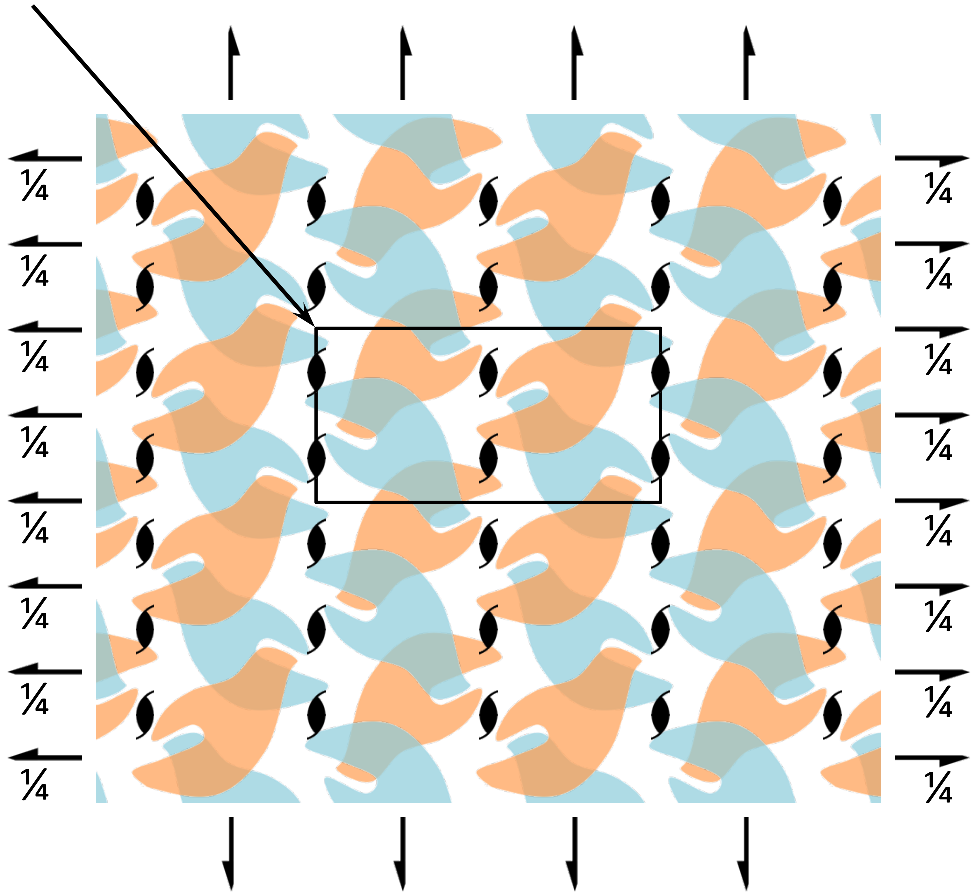
Altogether:

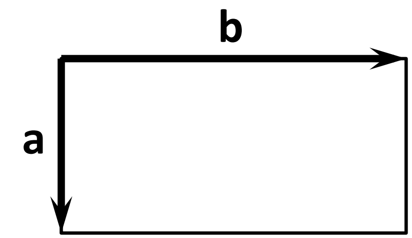
- infinite number of conventional origins
- eight types of equivalent origins in this example

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

Complete picture

The origin





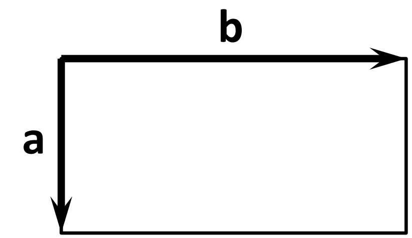
2_1 (plane of figure):

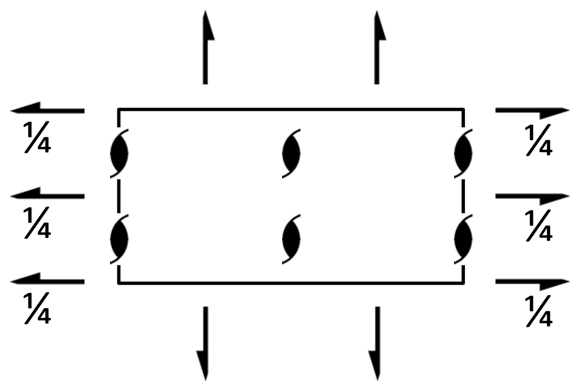
2_1 (along view):

Compact representation

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

No. 19





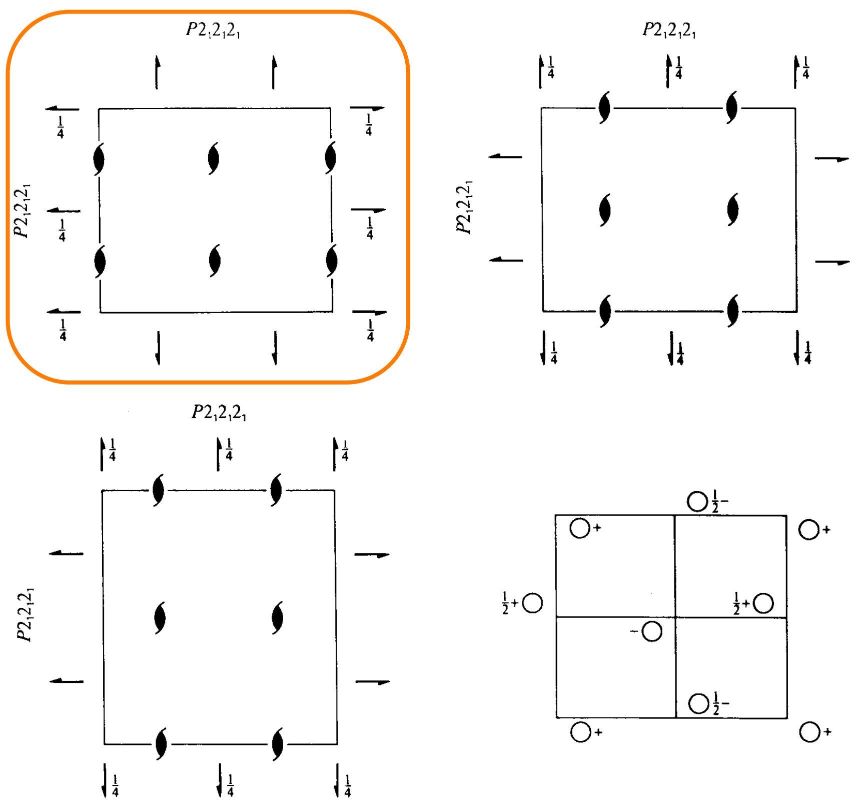
2_1 (plane of figure):

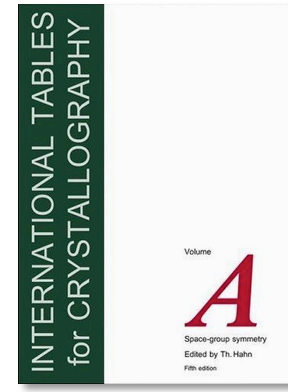
2_1 (along view):

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

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

$P2_12_12_1$

No. 19

Space group number

Schoenflies symbol

D_2^4

$P2_12_12_1$

Hermann-Mauguin symbol

Crystal Class (point group)

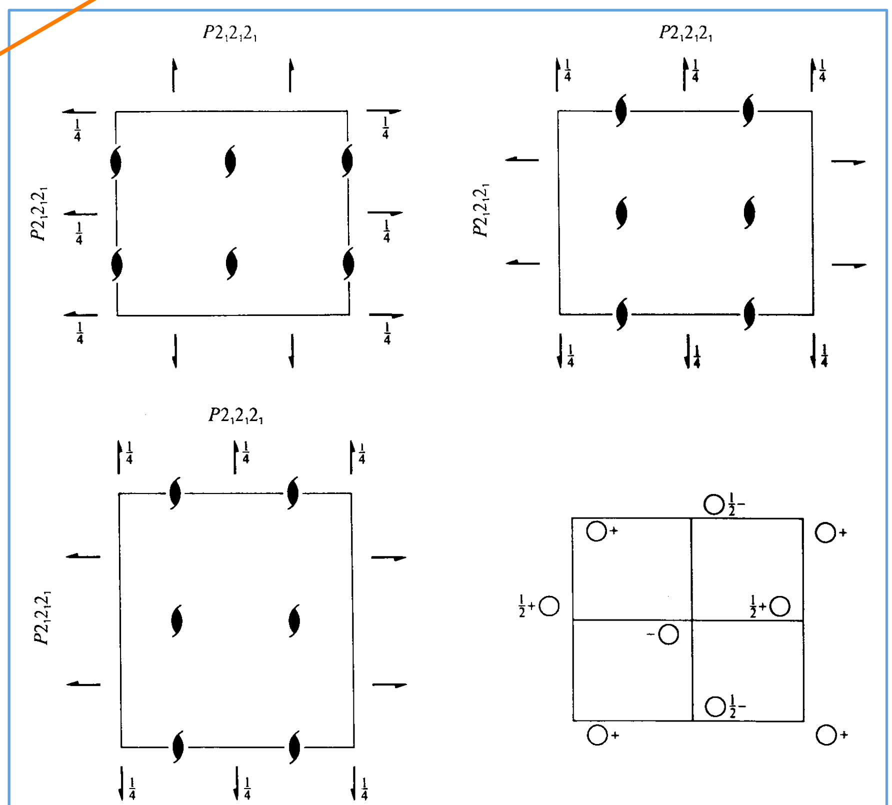
222

Crystal system

Orthorhombic

Patterson symmetry $Pmmm$

Patterson symmetry



Space group diagrams:

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

Discussed later in this talk

Crystal Class (point group)

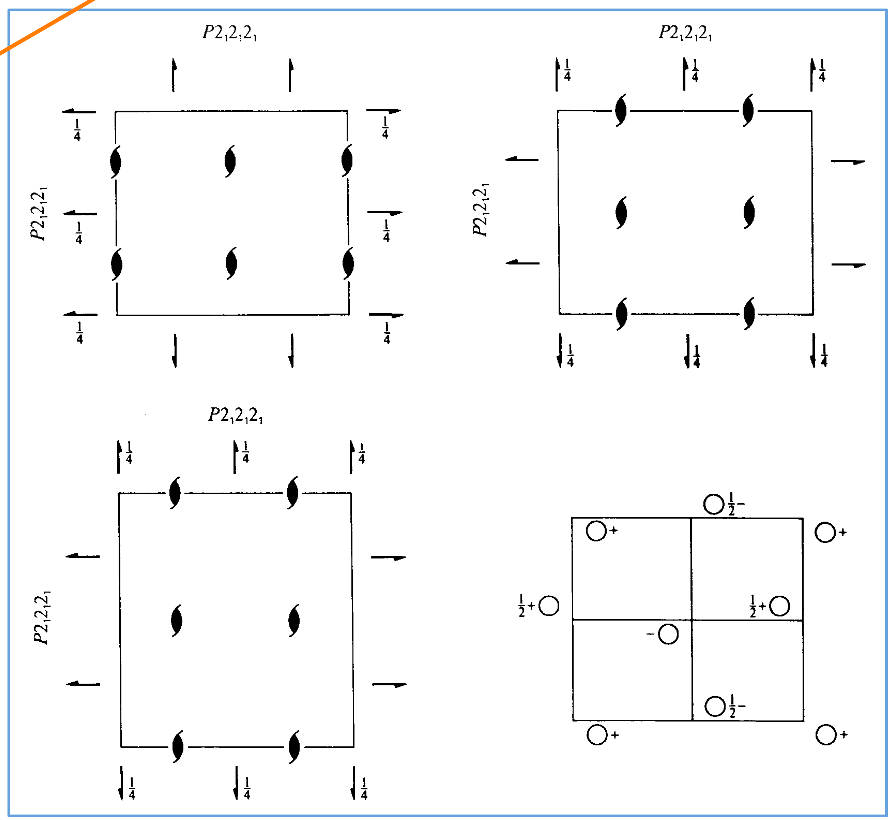
Crystal system

$P\,2_1\,2_1\,2_1$ $\quad D_2^4$ $\quad$ $\boxed{222}$ $\quad$ $\boxed{\text{Orthorhombic}}$

No. 19 $\quad \boxed{P\,2_1\,2_1\,2_1}$ $\quad$ Patterson symmetry $\boxed{Pmmm}$

Patterson symmetry

Hermann-Mauguin symbol



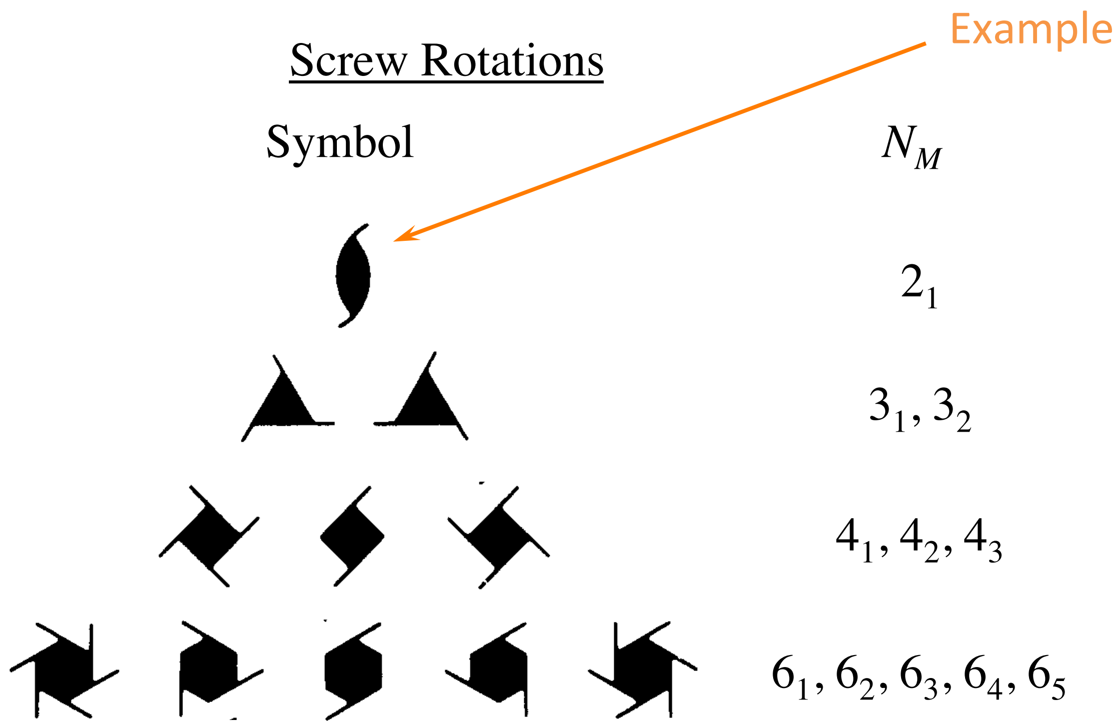
- Example structure (using Coot)
  - examine symmetry operations
  - construct space group
  - assign crystallographic origin
  - identify space group
- Classification of space groups
- Space group symbols
- Symmetry of diffraction pattern
  - point groups
- SG determination in structure solution process

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* and translate by (**t** *M* / *N*) where **t** is the shortest crystallographic translation along the rotation axis



	Proper Rotations		Screw Rotations	
	Symbol	N	Symbol	N_M
Two-fold		2		2_1
Three-fold		3		$3_1, 3_2$
Four-fold		4		$4_1, 4_2, 4_3$
Six-fold		6		$6_1, 6_2, 6_3, 6_4, 6_5$

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 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

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

example

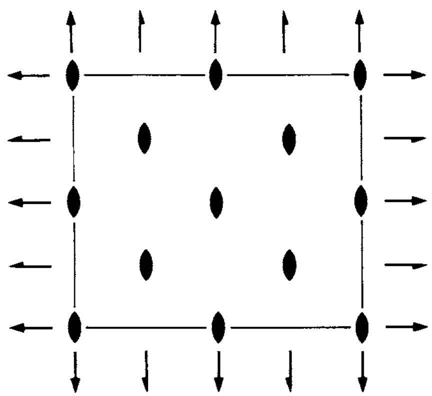
Crystal Systems

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

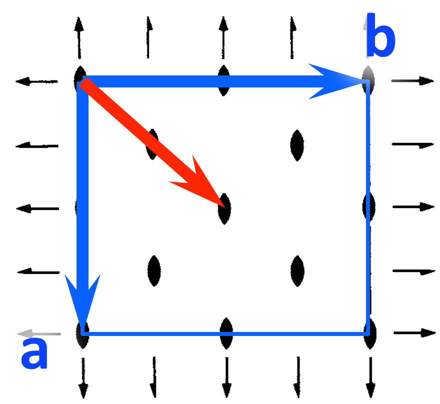
Crystal System	**Characteristic symmetry elements**	**Convention**
1. Triclinic	Translations only	
2. Monoclinic	2-fold axes, all parallel	along **b**
3. Orthorhombic	2-fold axes in three perpendicular directions	along **a**, **b** and **c**
4. Tetragonal	4-fold axes, all parallel	along **c**
5. Trigonal	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

*C*222: an example of a centred cell

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

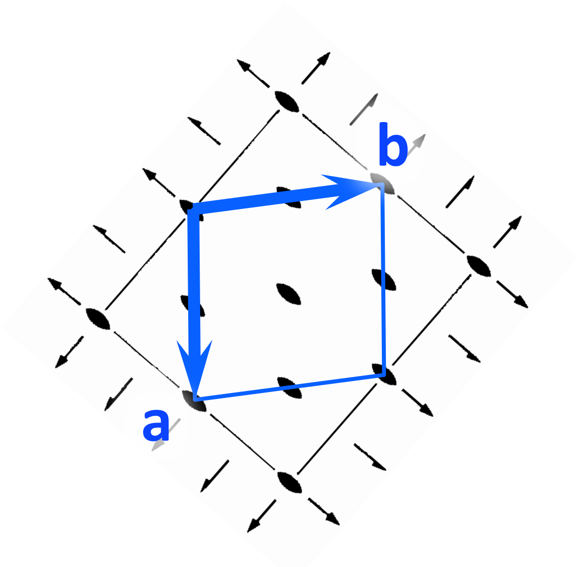


<u>Standard</u> setting;
C means additional translation ½ (**a** + **b**)



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

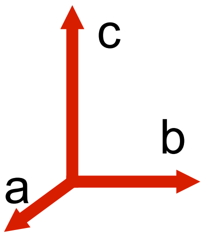
If we were using a primitive cell

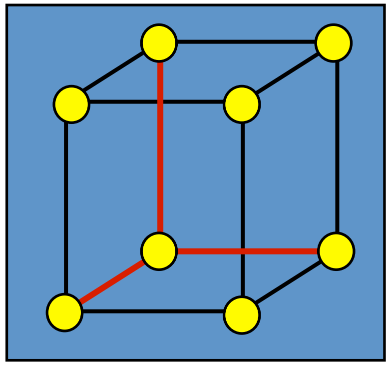


2-fold axes are along face diagonals (non-conventional crystal setting)

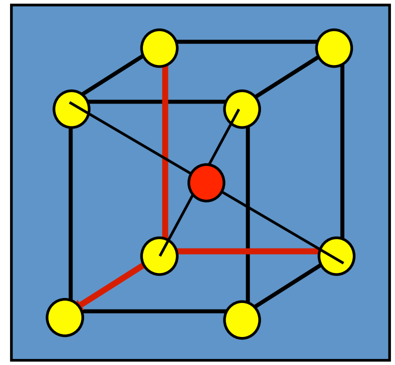
Centred cells in pictures

Not a natural phenomenon, but just a notion required by convention on direction of axes

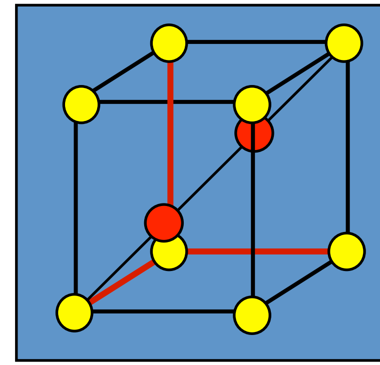




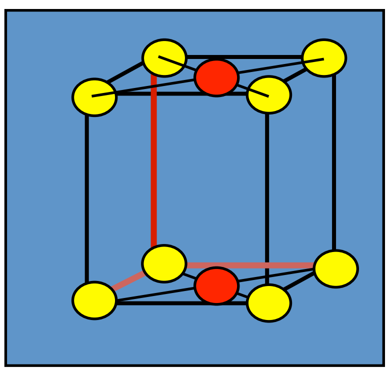
P – Primitive



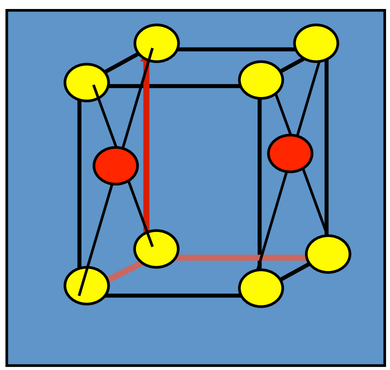
I – Body centred



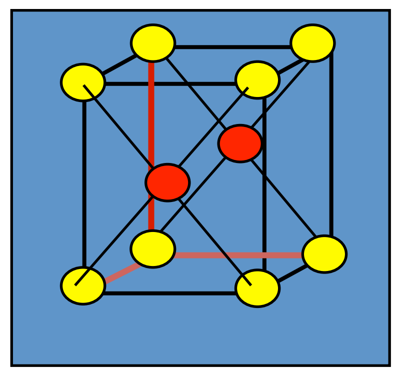
H – Hexagonal



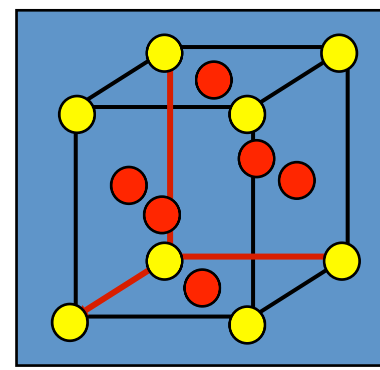
A – Face centred (A)



B – Face centred (B)



C – Face centred (C)



F – Face centred (all)

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 one of equivalent combinations (*e.g.* C4 and *P*4)

Bravais lattices

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

example

- Example structure (using Coot)
  - examine symmetry operations
  - construct space group
  - assign crystallographic origin
  - identify space group
- Classification of space groups
- **Space group symbols**
- Symmetry of diffraction pattern
  - point groups
- SG determination in structure solution process

Triclinic P 1

"*P*" means primitive lattice type

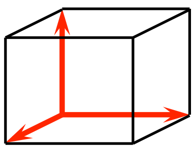
"1" means no symmetry operations except for translations

No constraints on
a, b, c, α, β, γ

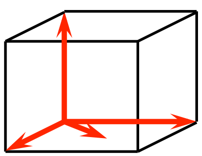
Monoclinic

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

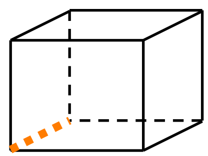
P or C



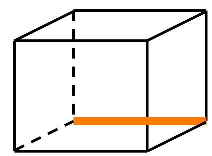
or



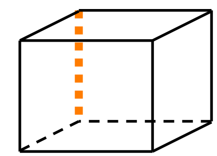
1



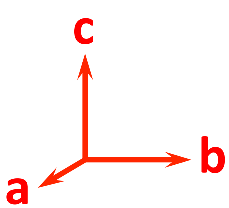
2 or 2_1



1



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



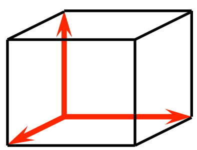
$\alpha = \gamma = 90°$

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

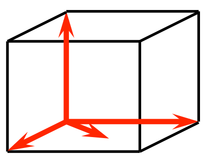
Orthorhombic

$P\,2\,2\,2$	$P\,2\,2\,2_1$	$P\,2_12_12$	$P\,2_12_12_1$
$C\,2\,2\,2$	$C\,2\,2\,2_1$		
$I\;\,2\,2\,2$			$I\;\,2_12_12_1$
$F\,2\,2\,2$			

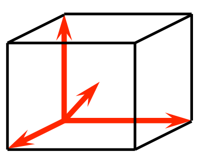
P, C, I or F



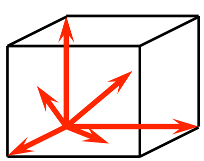
or



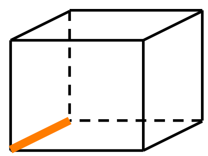
or



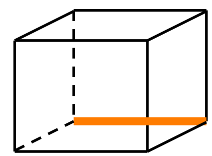
or



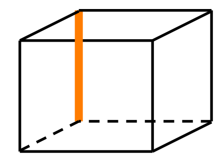
2 or 2_1



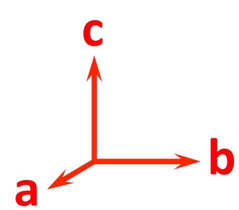
2 or 2_1



2 or 2_1



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



$\alpha = \beta = \gamma = 90°$

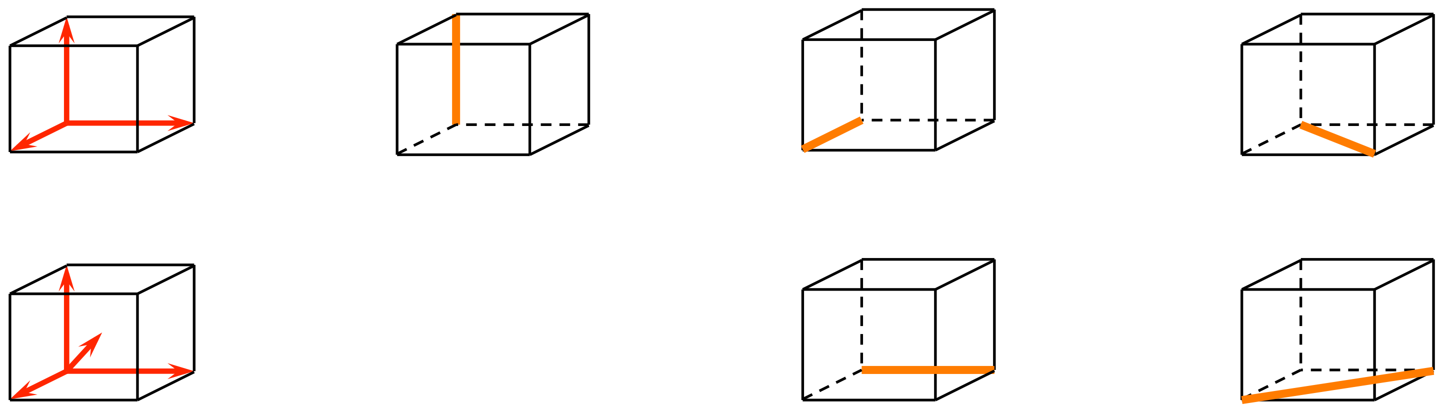
Tetragonal

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

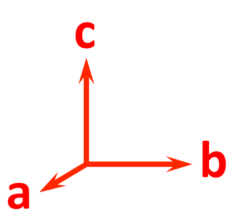
$P\,4\,2\,2$ $P\,4_12\,2$ $P\,4_22\,2$ $P\,4_3\,2\,2$

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

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



or



$\alpha = \beta = \gamma = 90°$

$a = b$

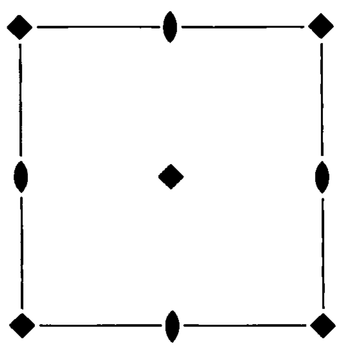
a ≡ b due to the 4-fold relating them

All 2-fold axes are also related via 4-fold rotations and either

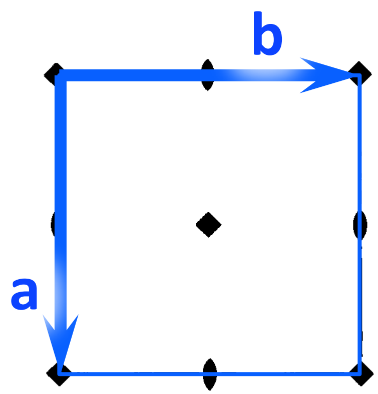
- all of them are present or
- none of them are present

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

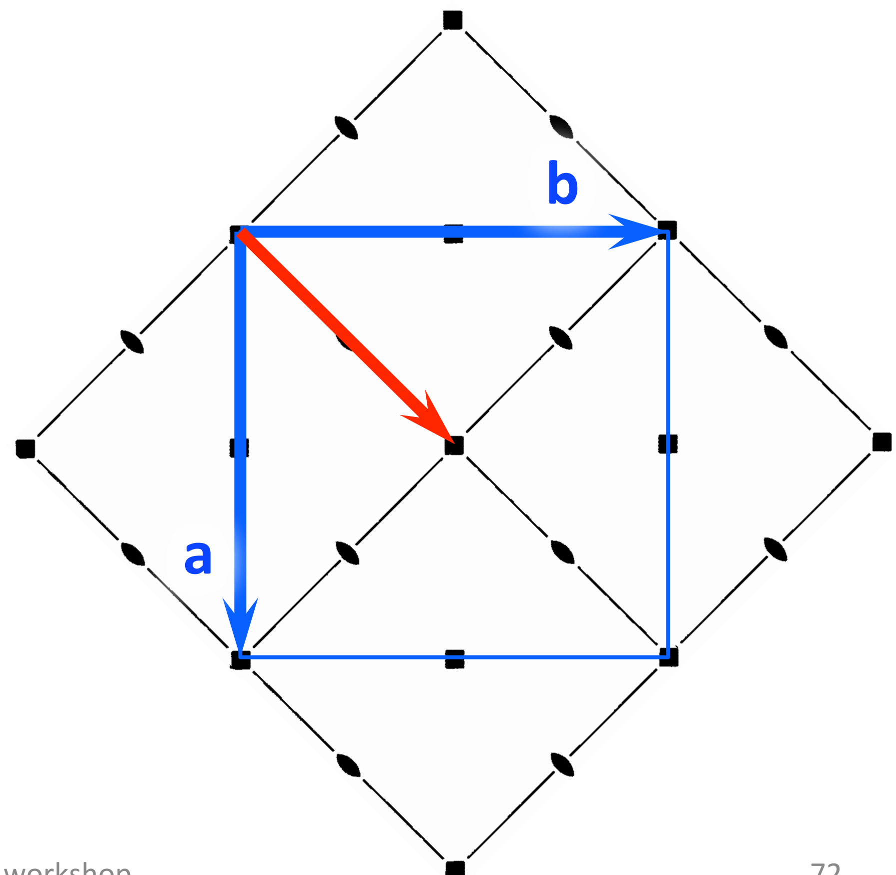
*P*4
as presented in the International Tables for Crystallography



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



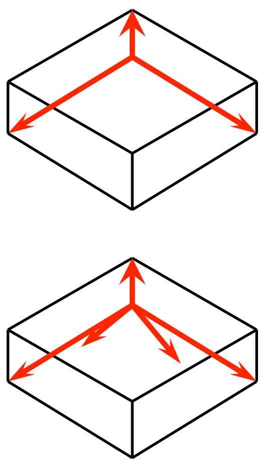
Trigonal

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

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

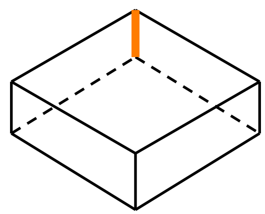
$H\,3\,2$ $H3$

P or *H*(*)

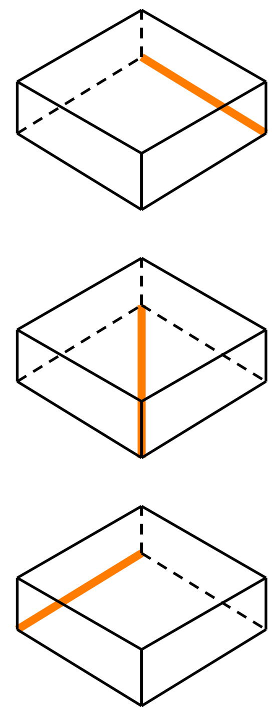


or

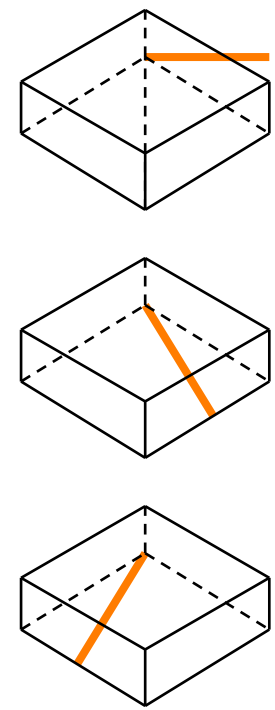
3_N

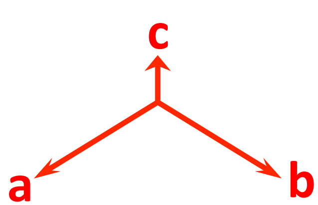


2, 1 or None



2, 1 or None





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

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

Ones

P 1	~~*P* 1 1 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~~

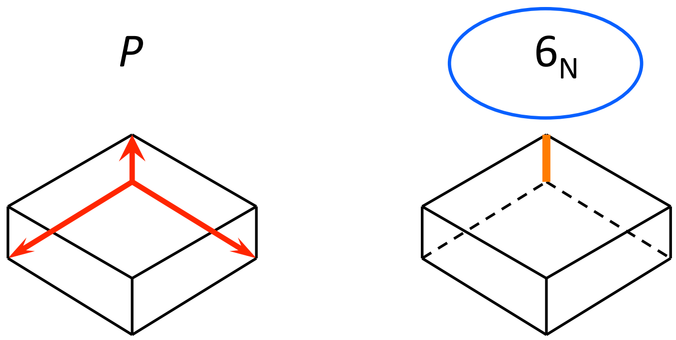
Subscripts

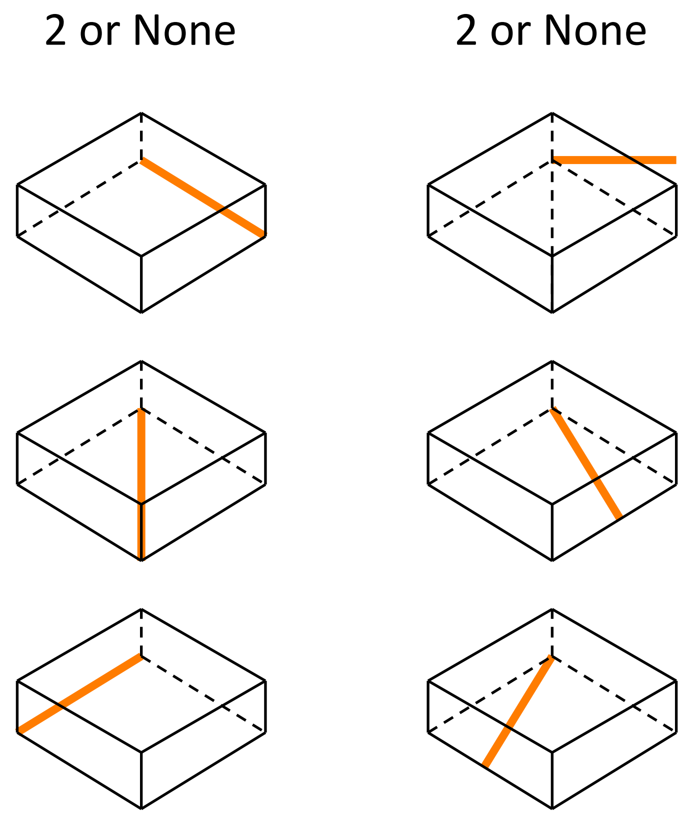
P43212 P 43 21 2 P 4(3) 2(1) 2 P 4_3 2_1 2

Hexagonal

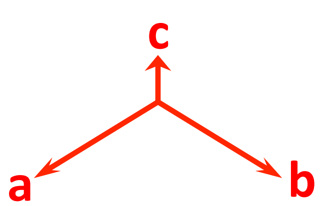
$P\,6\,2\,2$ $P\,6_1 2\,2$ $P\,6_2 2\,2$ $P\,6_3 2\,2$ $P6$ $P6_1$ $P6_2$ $P6_3$

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





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



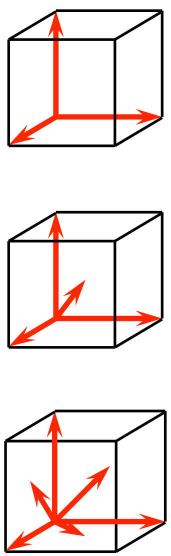
Cubic

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

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

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

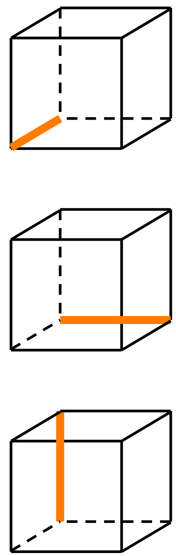
P, I or F



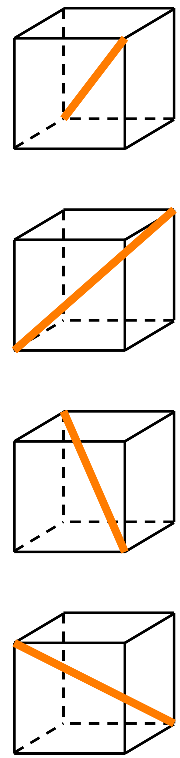
or

or

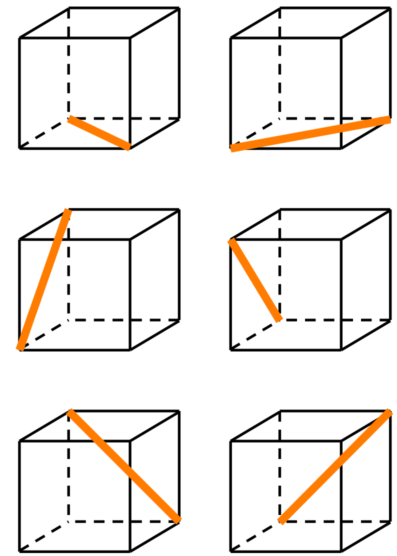
4_N or 2_N

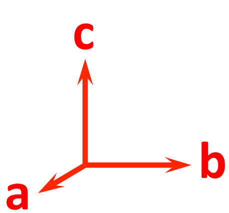


3



2 or None





$\alpha = \beta = \gamma = 90°$

$a = b = c$

Monoclinic (lattice based setting)

$\alpha = \gamma = 90°$

additional condition:
$\beta < 120°$

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

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

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

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

Orthorhombic (lattice based setting)

$\alpha = \beta = \gamma = 90°$

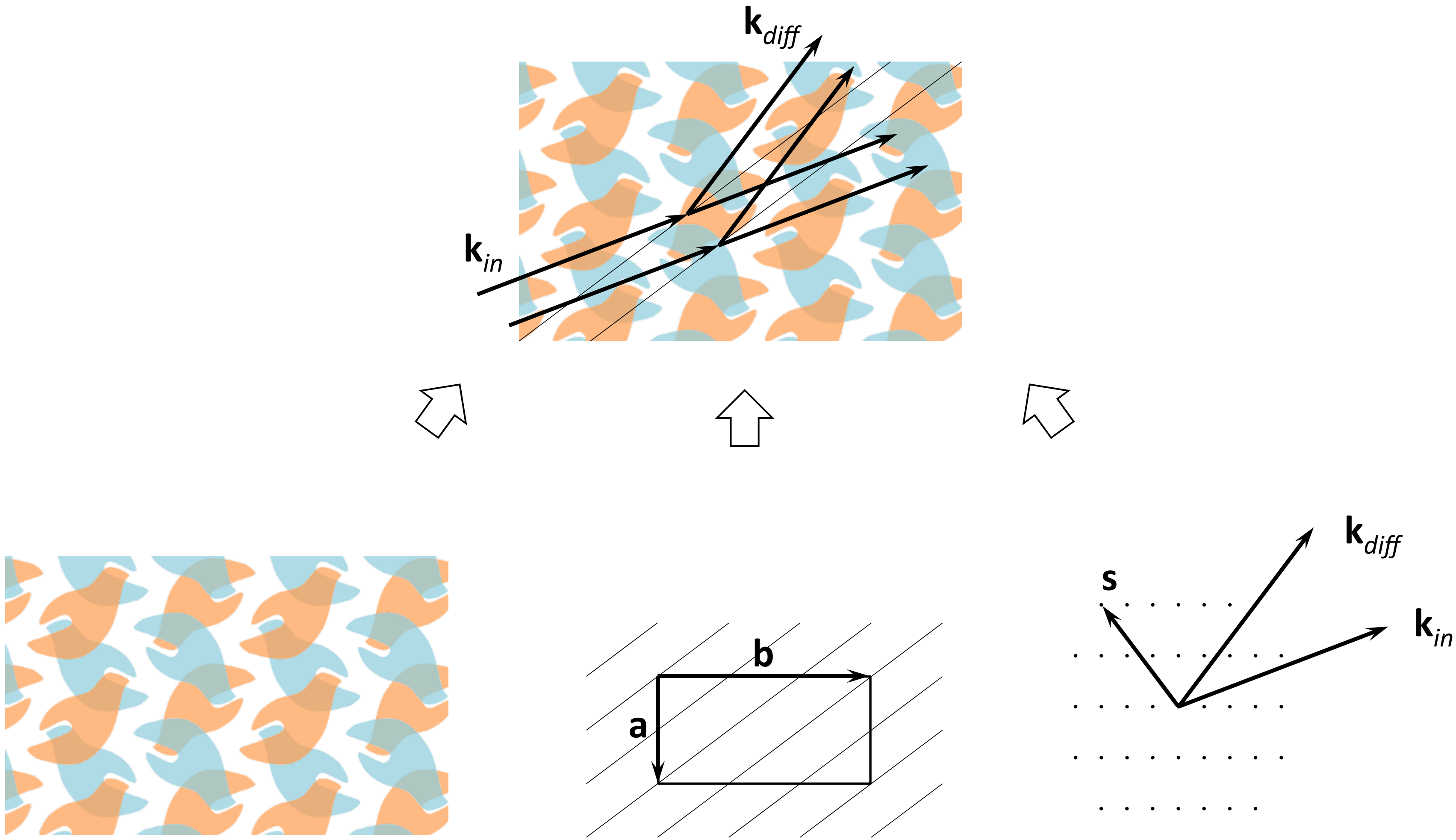
additional condition:
$a < b < c$

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

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

- Example structure (using Coot)
  - examine symmetry operations
  - construct space group
  - assign crystallographic origin
  - identify space group
- Classification of space groups
- Space group symbols
- Symmetry of diffraction pattern
  - point groups
- SG determination in structure solution process

Conventional diffraction scheme



real space

Bragg planes

reciprocal space

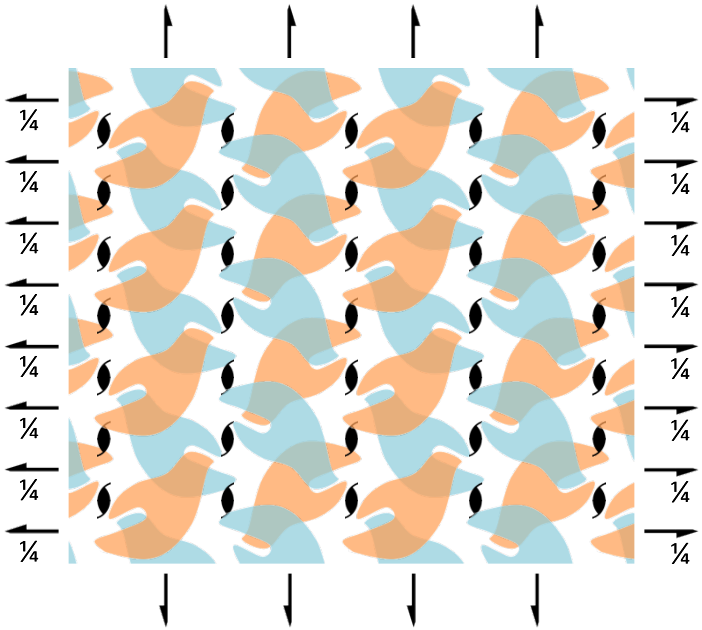
Symmetry of intensities

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

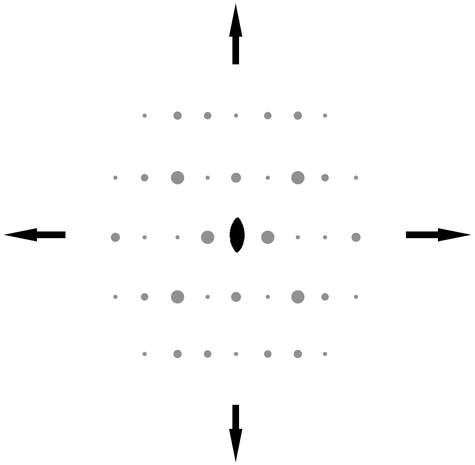
- Reciprocal lattice rotates together with crystal
- However, reciprocal lattice is not translated together with crystal

Symmetry of intensities

real space



reciprocal space



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

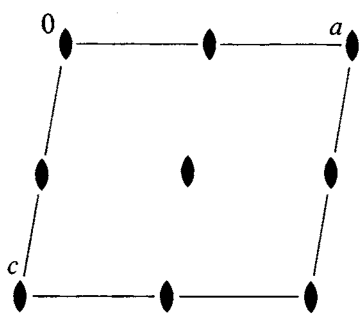
Crystal space group

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

$P2$ $\quad$ C_2^1

No. 3 $\quad$ $P121$

UNIQUE AXIS b

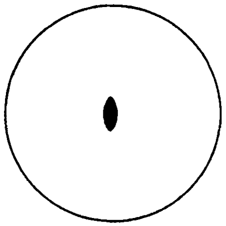


Arithmetic crystal class

$2P$

Crystal point group

2



Space group and point group

Crystal space group

Arithmetic crystal class

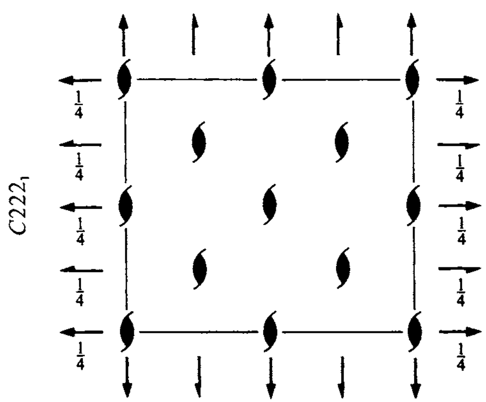
International Tables for Crystallography **(2006). Vol. A,**

$C222_1$ $\quad$ D_2^5

No. 20 $\quad$ $C222_1$

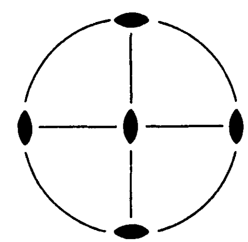
222*C*

$C222_1$



Crystal point group

222



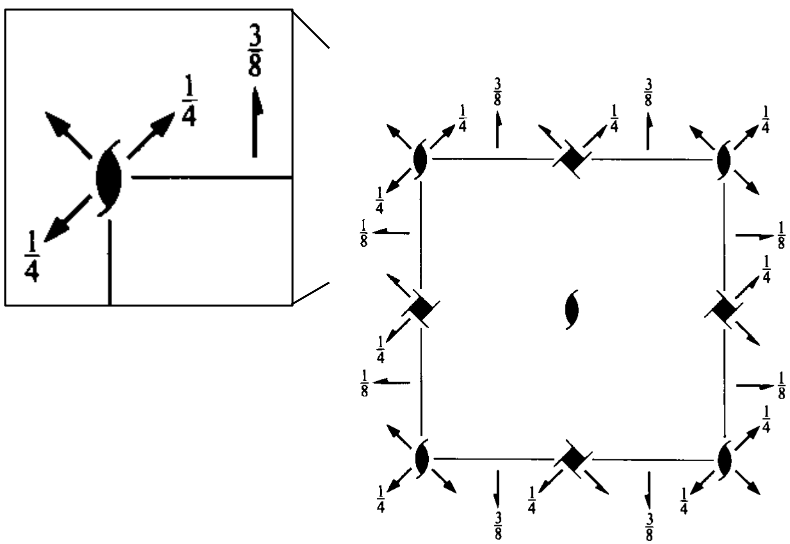
Space group and point group

Crystal space group

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

$P4_12_12$ $\qquad$ D_4^4

No. 92 $\qquad$ $P4_12_12$

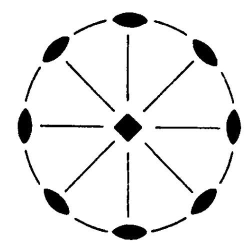


Arithmetic crystal class

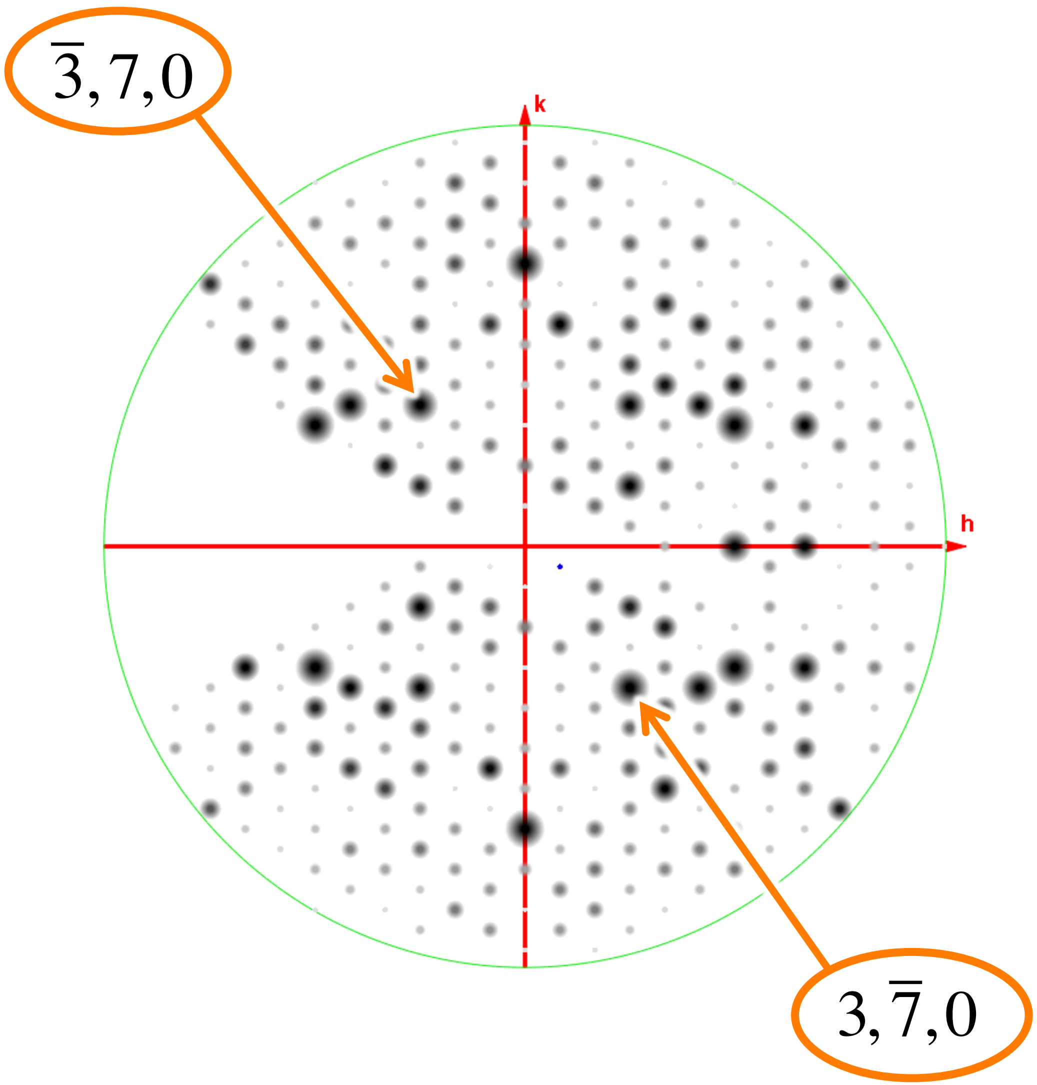
$422P$

Crystal point group

422



Friedel's law



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

Point group and Laue group

+ inversion =

Arithmetic crystal class

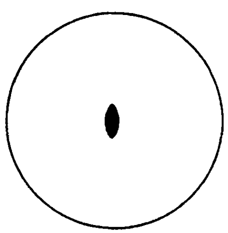
2*P*

Patterson space group

P 1 2/m 1

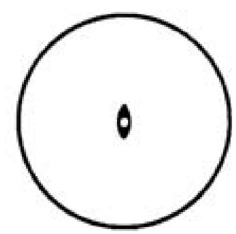
Crystal point group

2



Laue point group

2/m



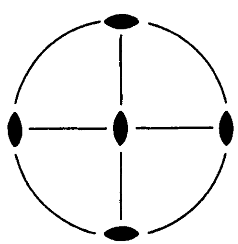
Point group and Laue group

+ inversion =

Arithmetic crystal class

222*C*

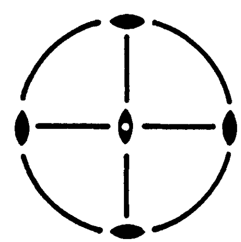
Crystal point group

222 

Patterson space group

C m m m

Laue point group

m m m 

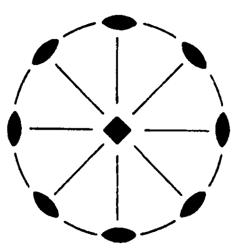
Point group and Laue group

+ inversion =

Arithmetic crystal class

422*P*

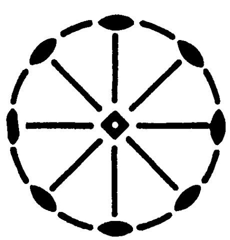
Crystal point group

422 

Patterson space group

P 4/m m m

Laue point group

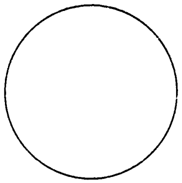
4/m m m 

The eleven Laue point groups or crystal classes

Crystal system	Laue point group	Non-centrosymmetric point groups belonging to the Laue point group
Cubic	$m3m$	$432 \quad \bar{4}3m$
	$m3$	23
Tetragonal	$4/mmm$	$422 \quad 4mm \quad \bar{4}2m$
	$4/m$	$4 \quad \bar{4}$
Orthorhombic	mmm	$222 \quad mm2$
Trigonal	$3m$	$32 \quad 3m$
	3	3
Hexagonal	$6/mmm$	$622 \quad 6mm \quad \bar{6}m2$
	$6/m$	$6 \quad \bar{6}$
Monoclinic	$2/m$	$2 \quad m$
Triclinic	$\bar{1}$	1

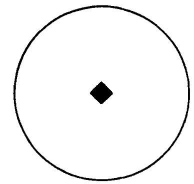
The point groups that can exist in protein crystals

1

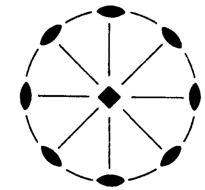


If it helps view as sphere

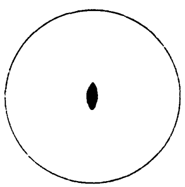
4



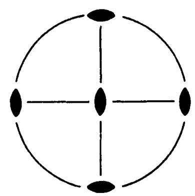
422



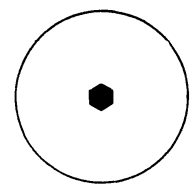
2



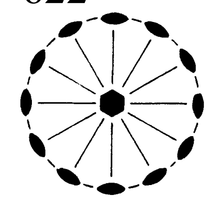
222



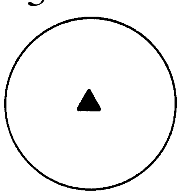
6



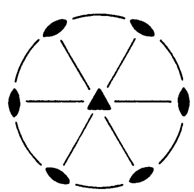
622



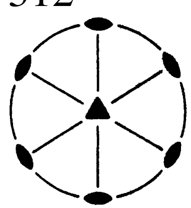
3



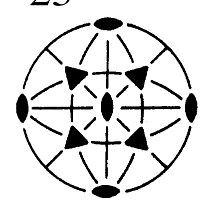
321



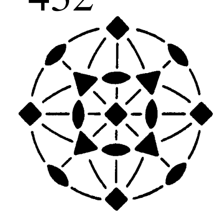
312



23

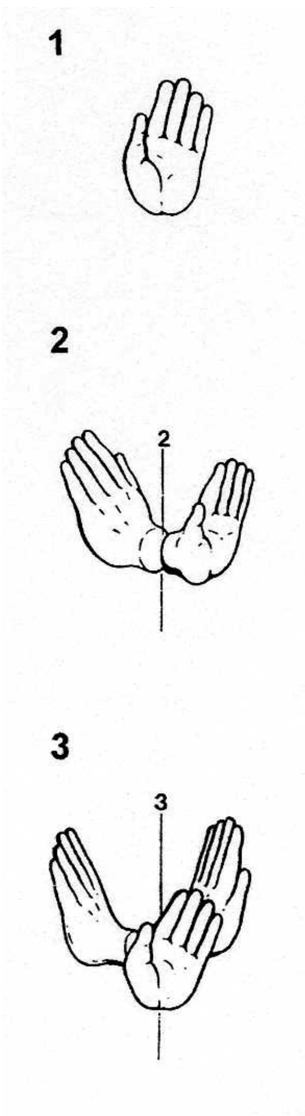


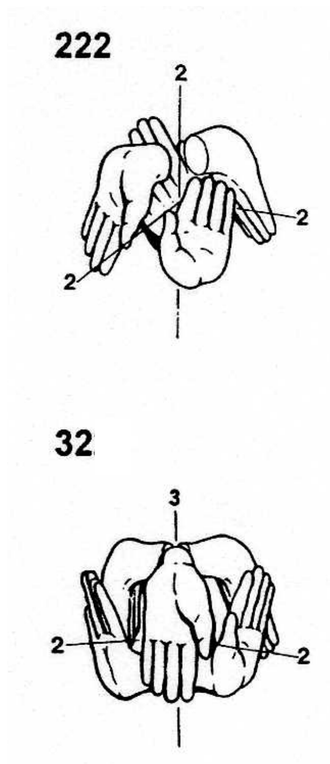
432

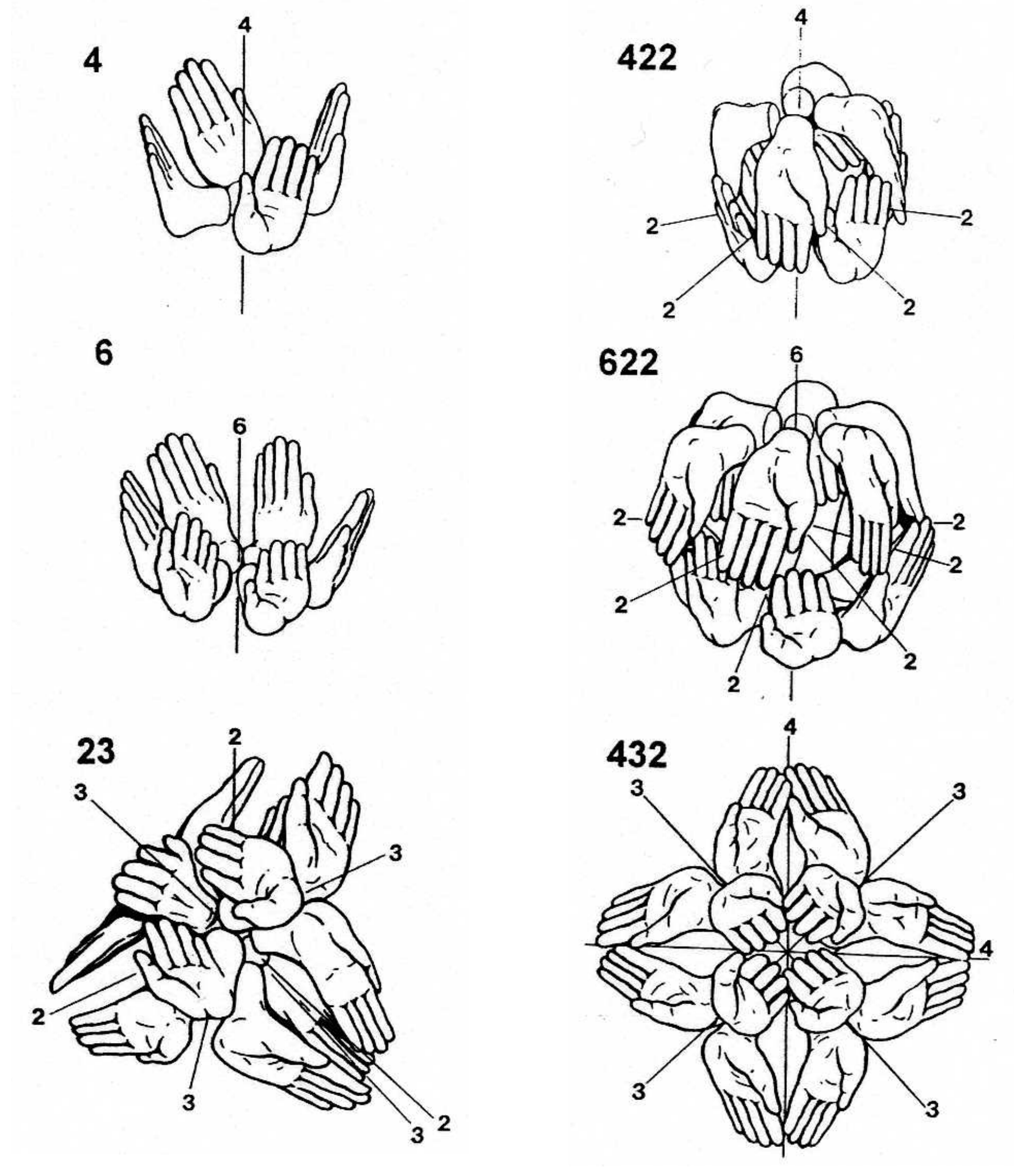


The point groups that can exist in protein crystals

maybe an easier representation







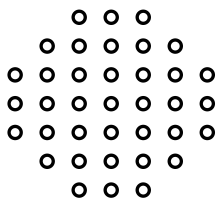
- Example structure (using Coot)
  - examine symmetry operations
  - construct space group
  - assign crystallographic origin
  - identify space group
- Classification of space groups
- Space group symbols
- Symmetry of diffraction pattern
  - point groups
- SG determination in structure solution process

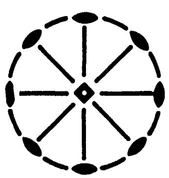
How do we deduce the Space Group in practice?

- 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)

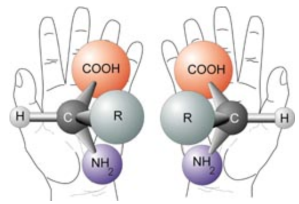


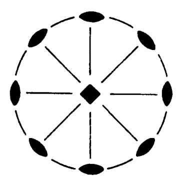


$4/mmm$

(Approximate) lattice point group

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

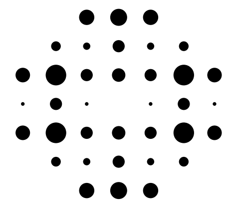


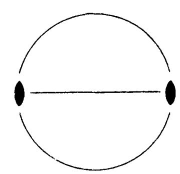


422

Highest possible crystal point group

Intensities of reflections

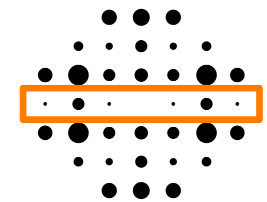


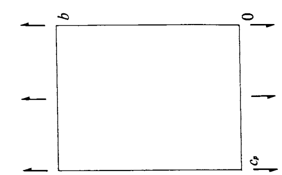


2

Probable crystal point group

Intensities of axial reflections





$P2_1$

Probable crystal space group

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

End