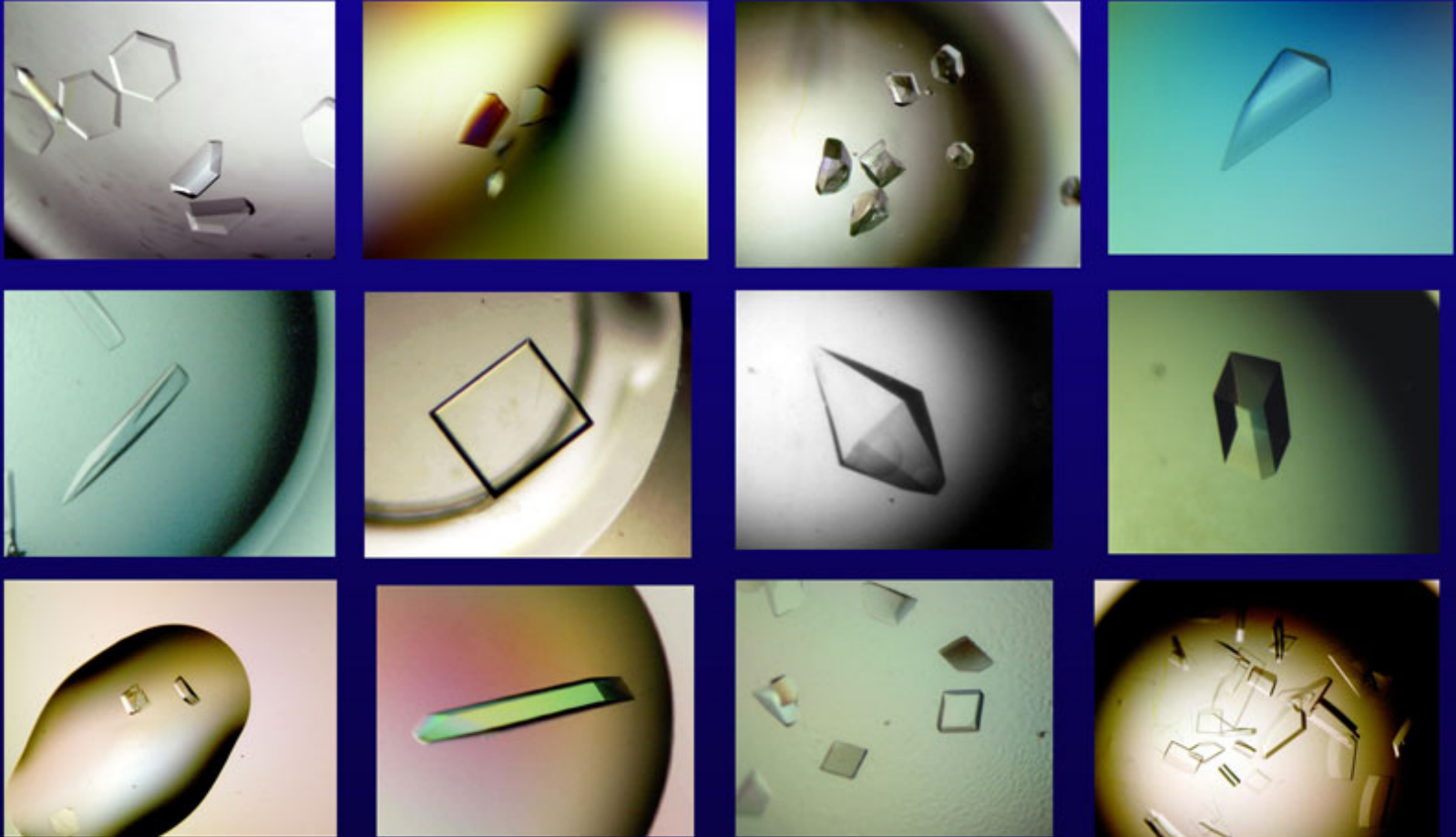
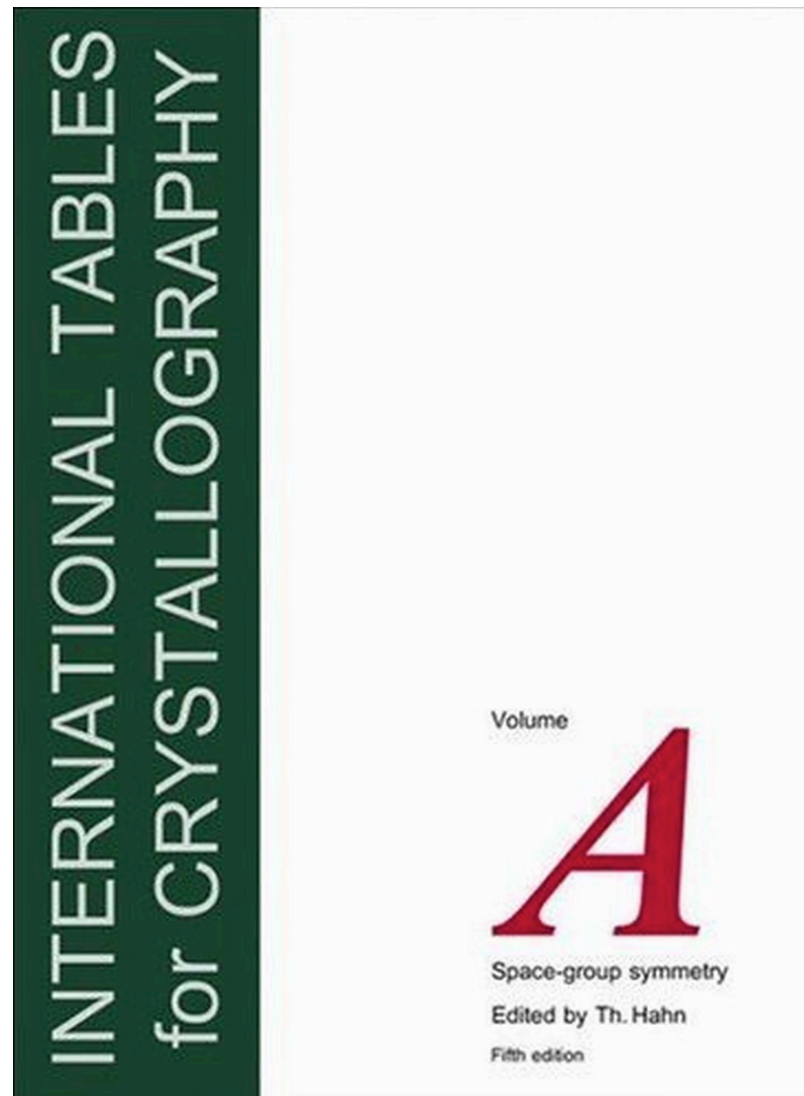


Introduction to symmetry

Andrey Lebedev, CCP4

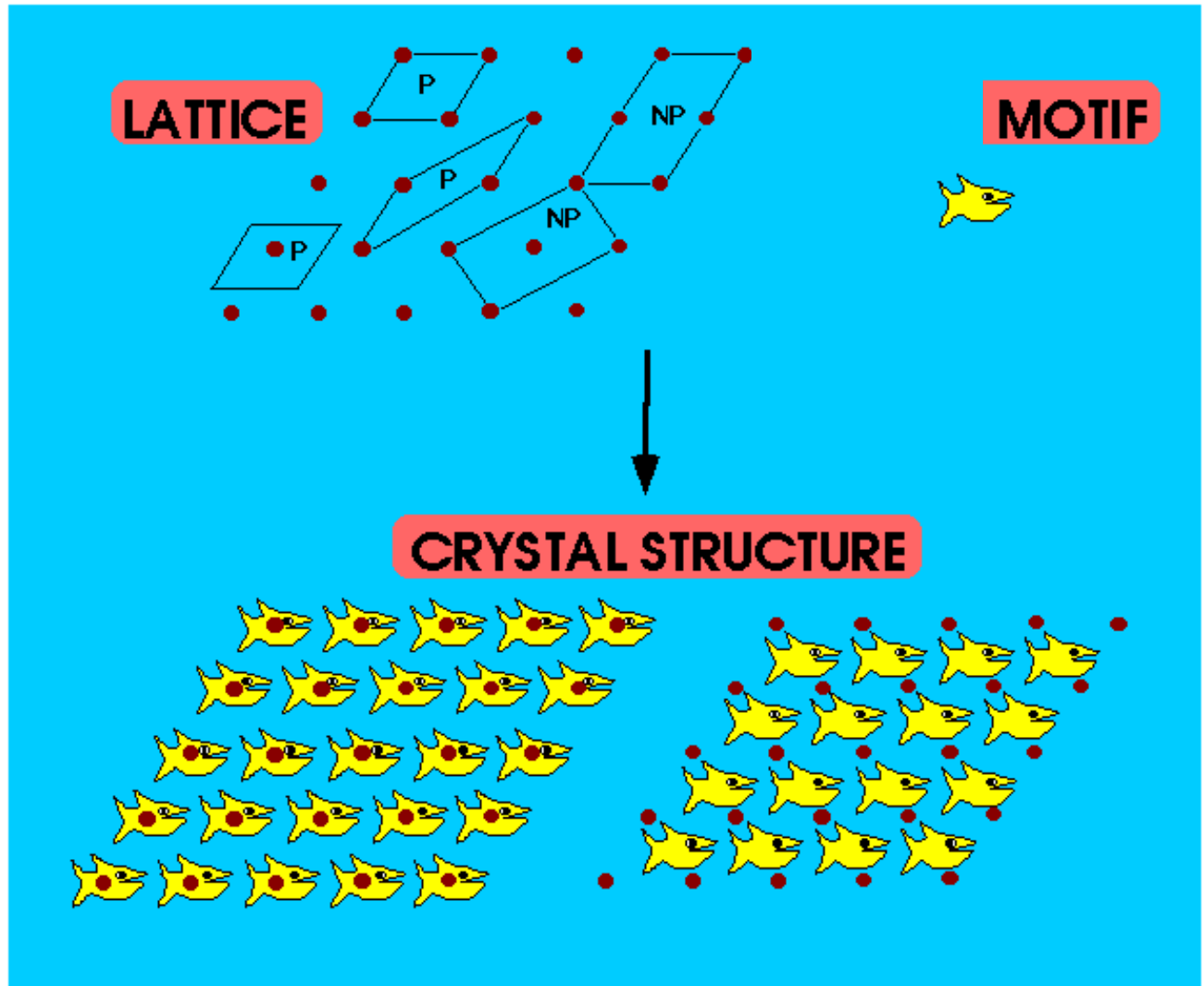


The Reference



Crystal: repeated structural motif

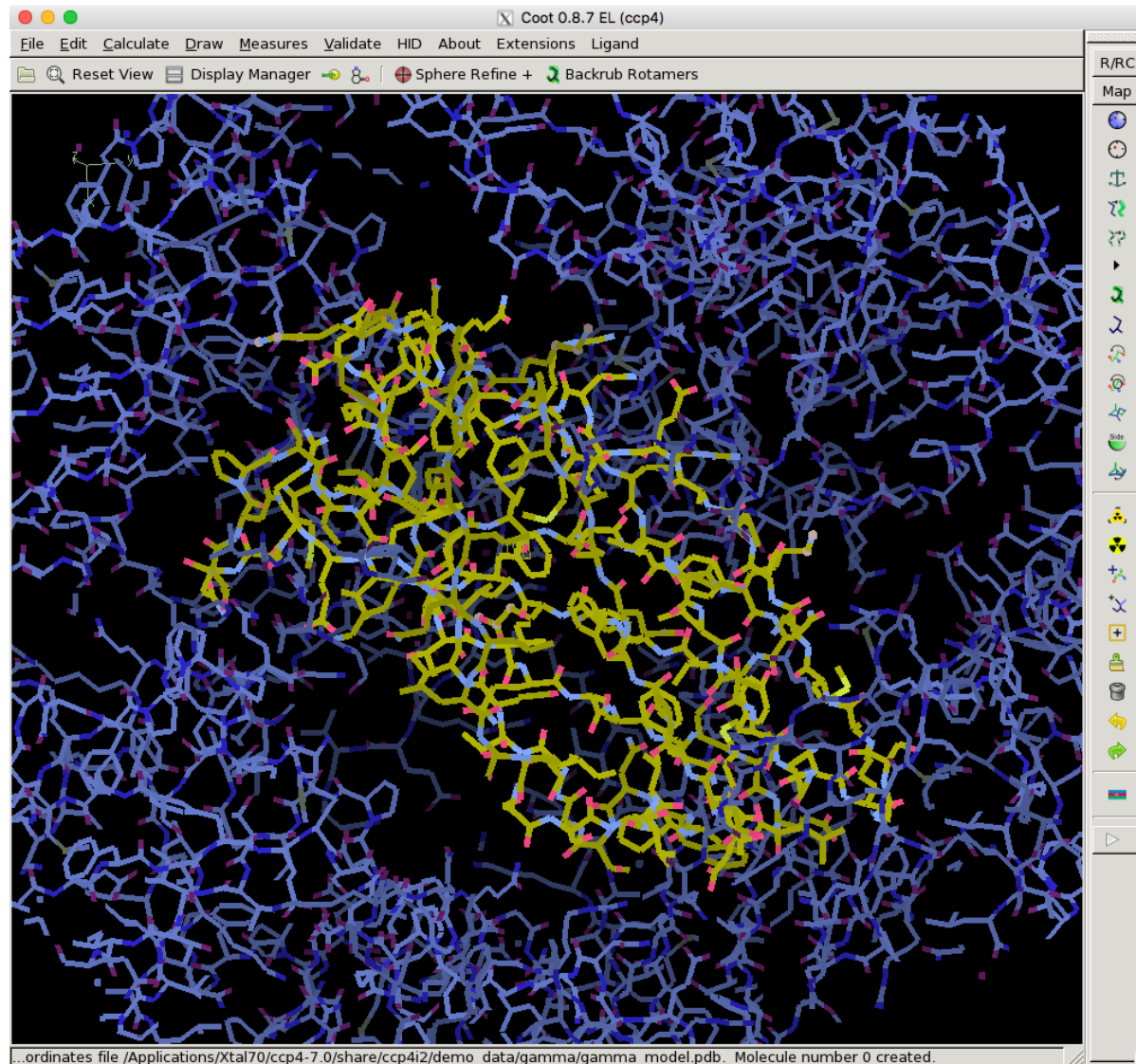
Conventional
(constructive)
definition
of crystal
structure.



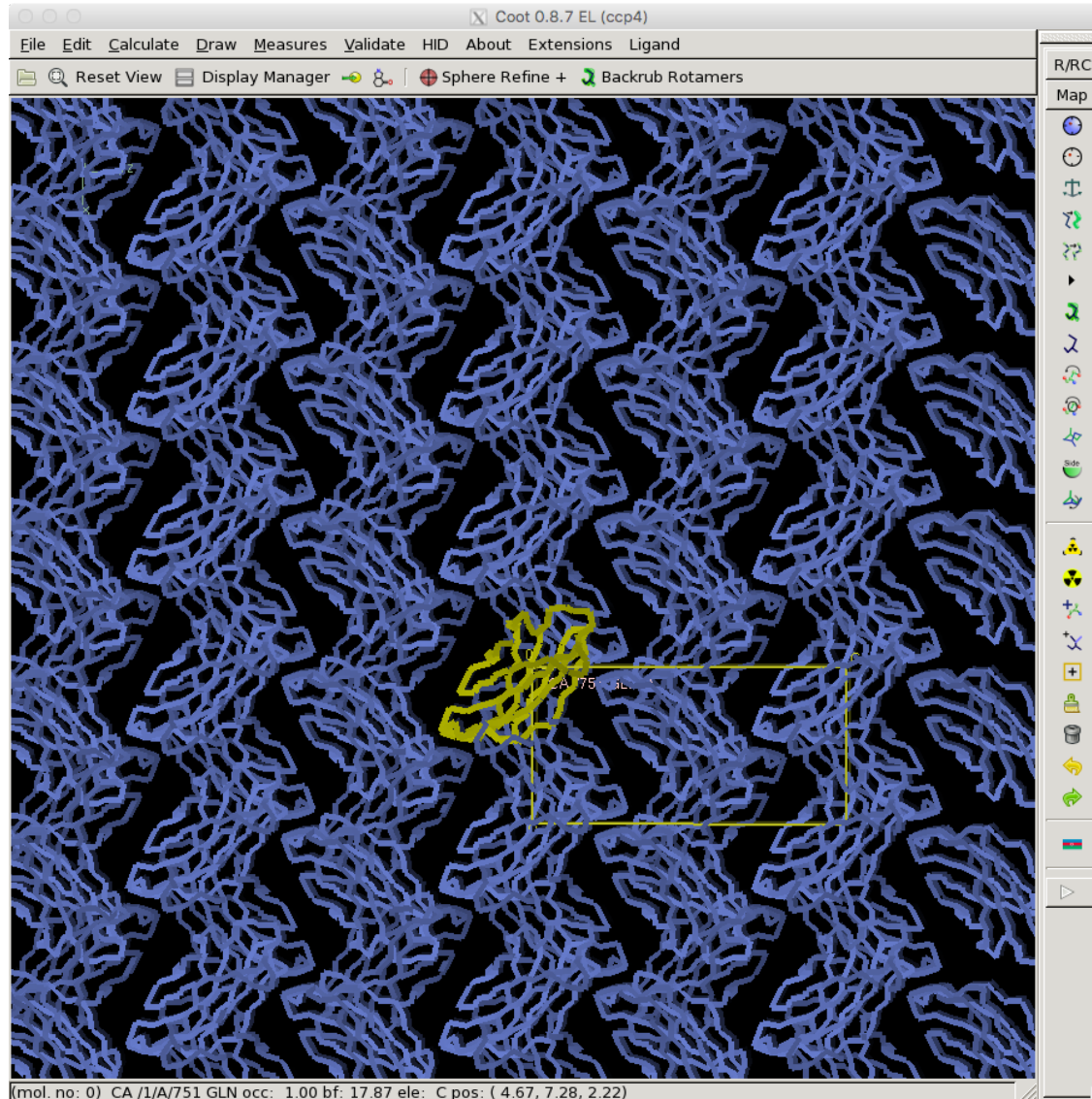
- Example structure (using Coot)
 - examine symmetry operations
 - construct space group
 - assign crystallographic origin
- Classification of space groups
- Space group symbols
 - identify space group of the example structure
- Space groups in the International Tables
- Symmetry of diffraction pattern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

- Example structure (using Coot)
 - examine symmetry operations
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- Space groups in the International Tables
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 - point groups
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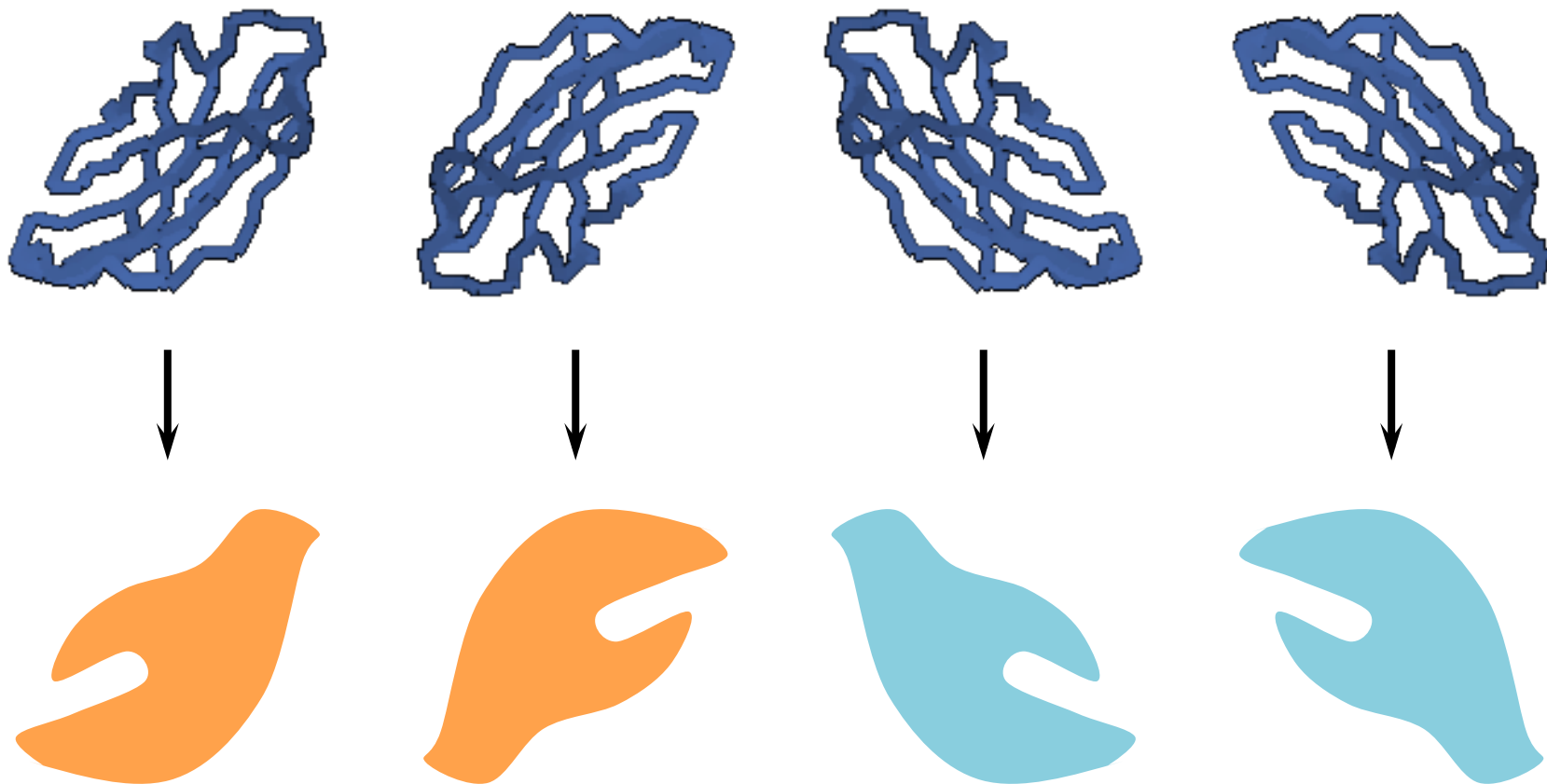
Examine structure in Coot



Symmetry view in Coot

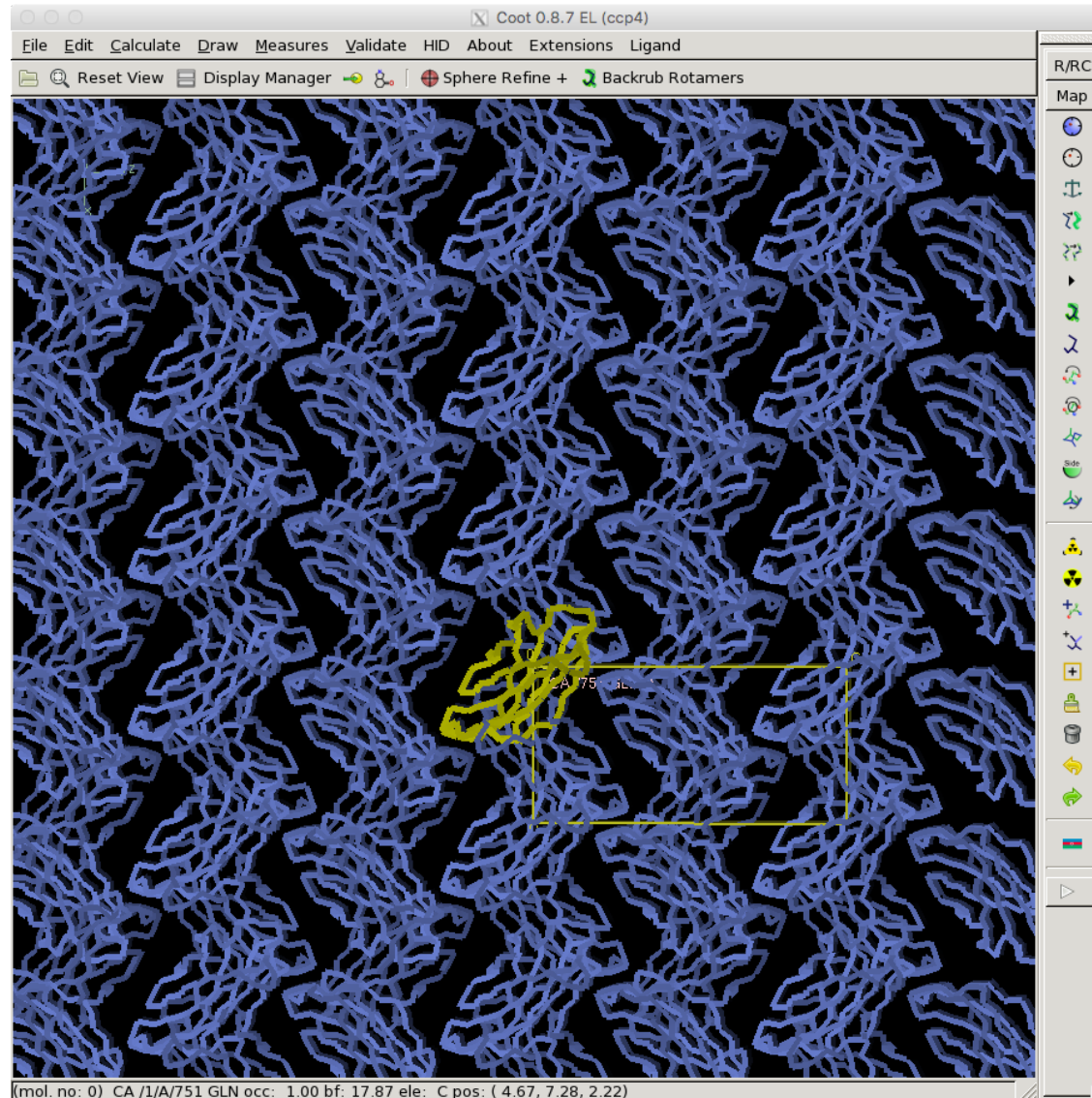


Simplified representation

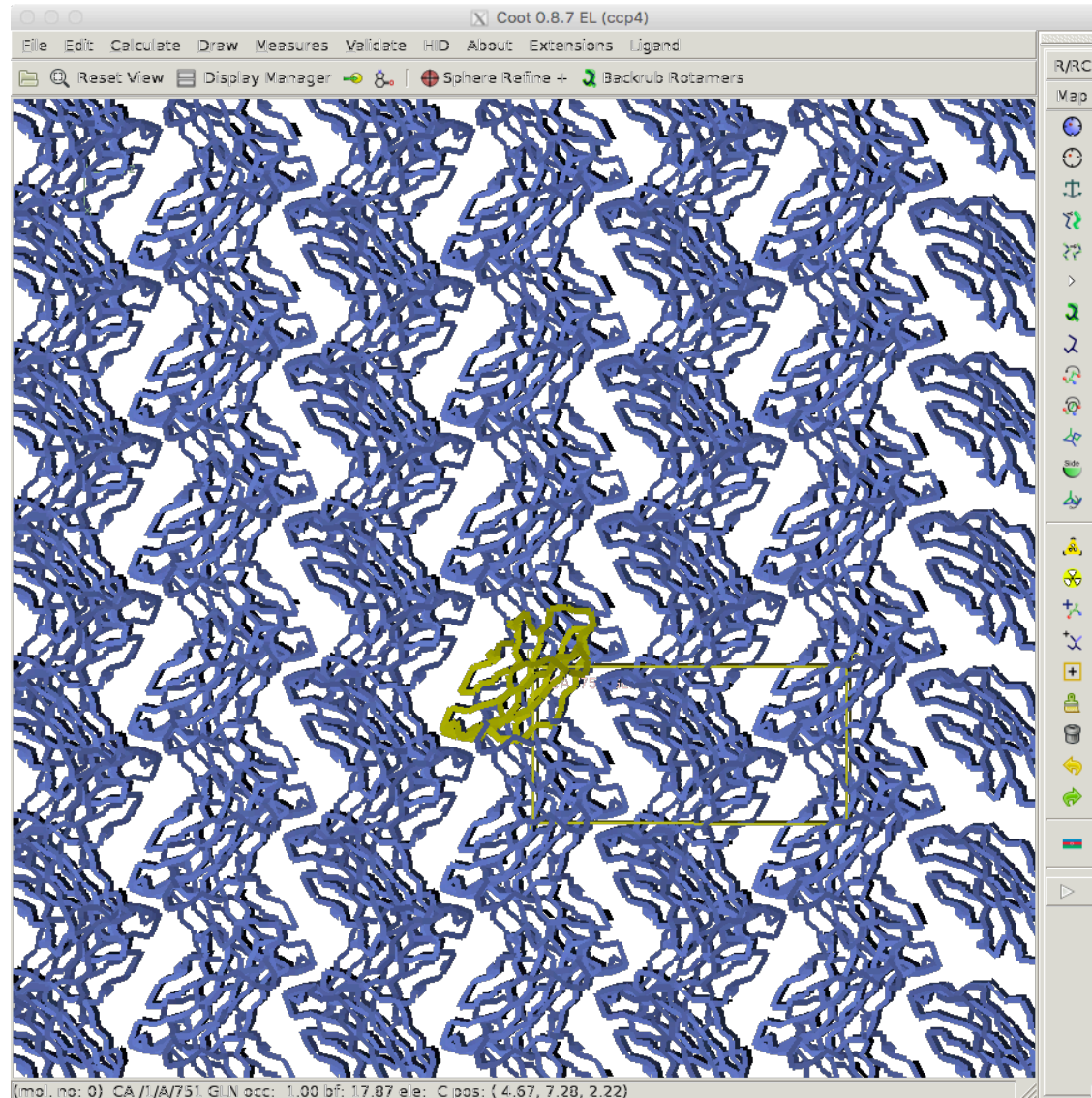


Opposite sides of molecules are denoted with different colours

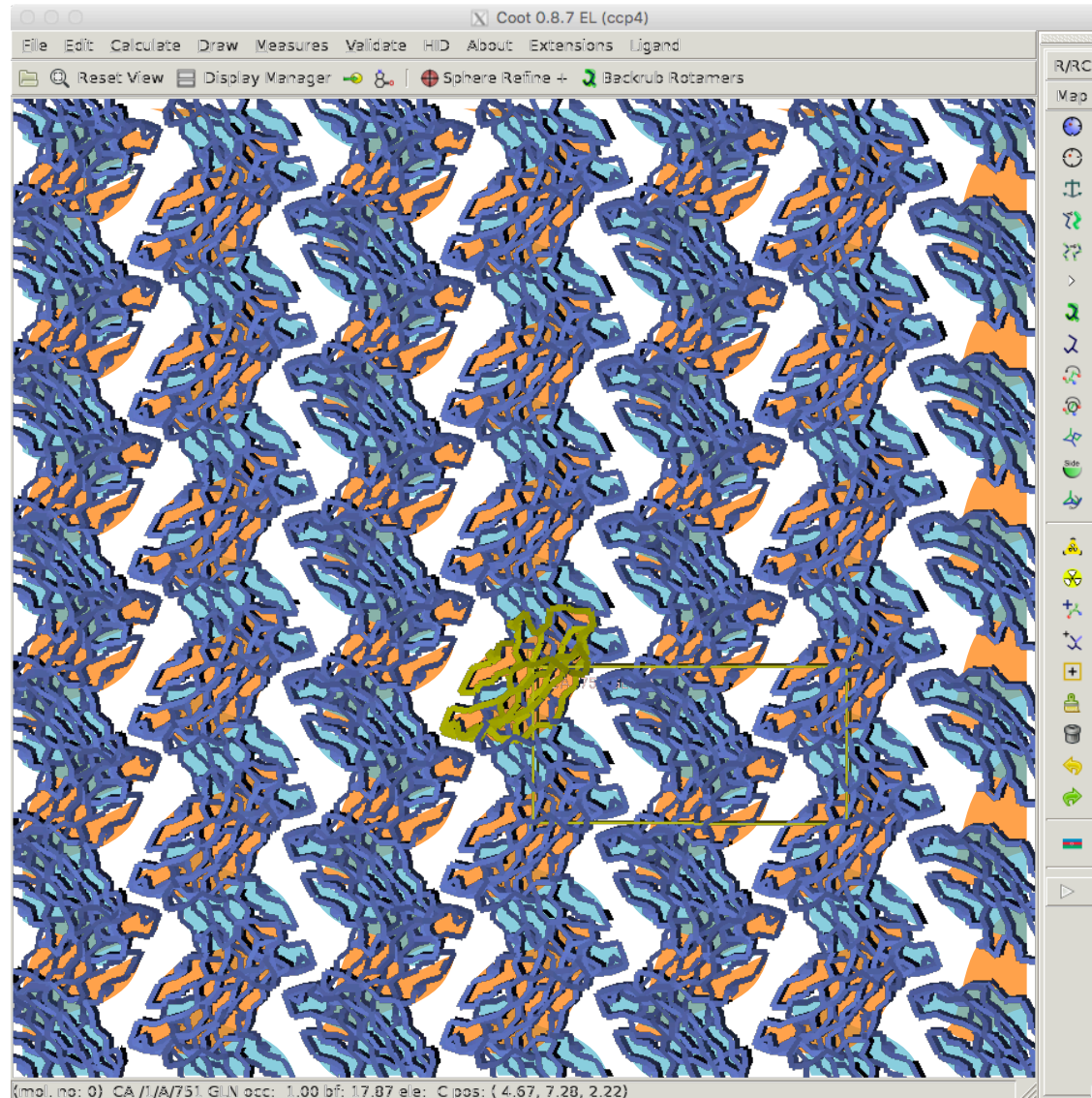
Simplified representation



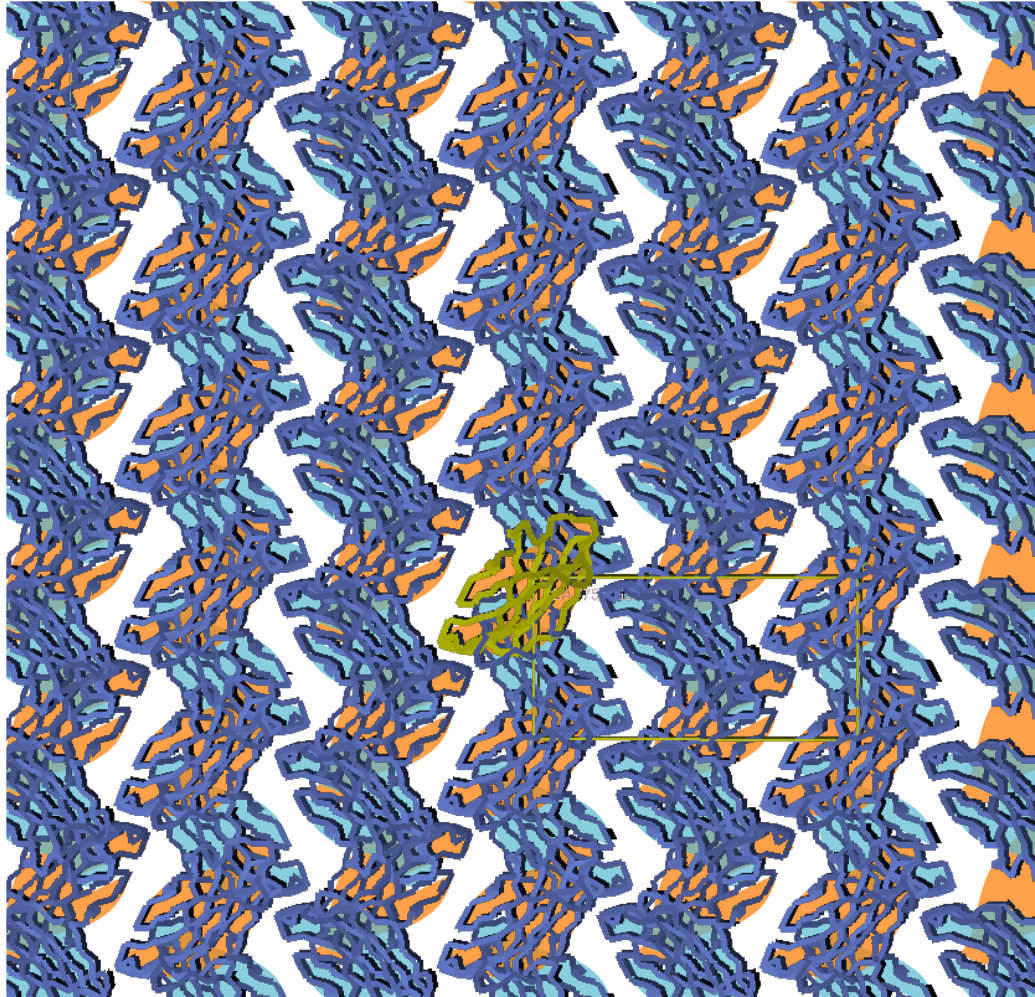
Simplified representation



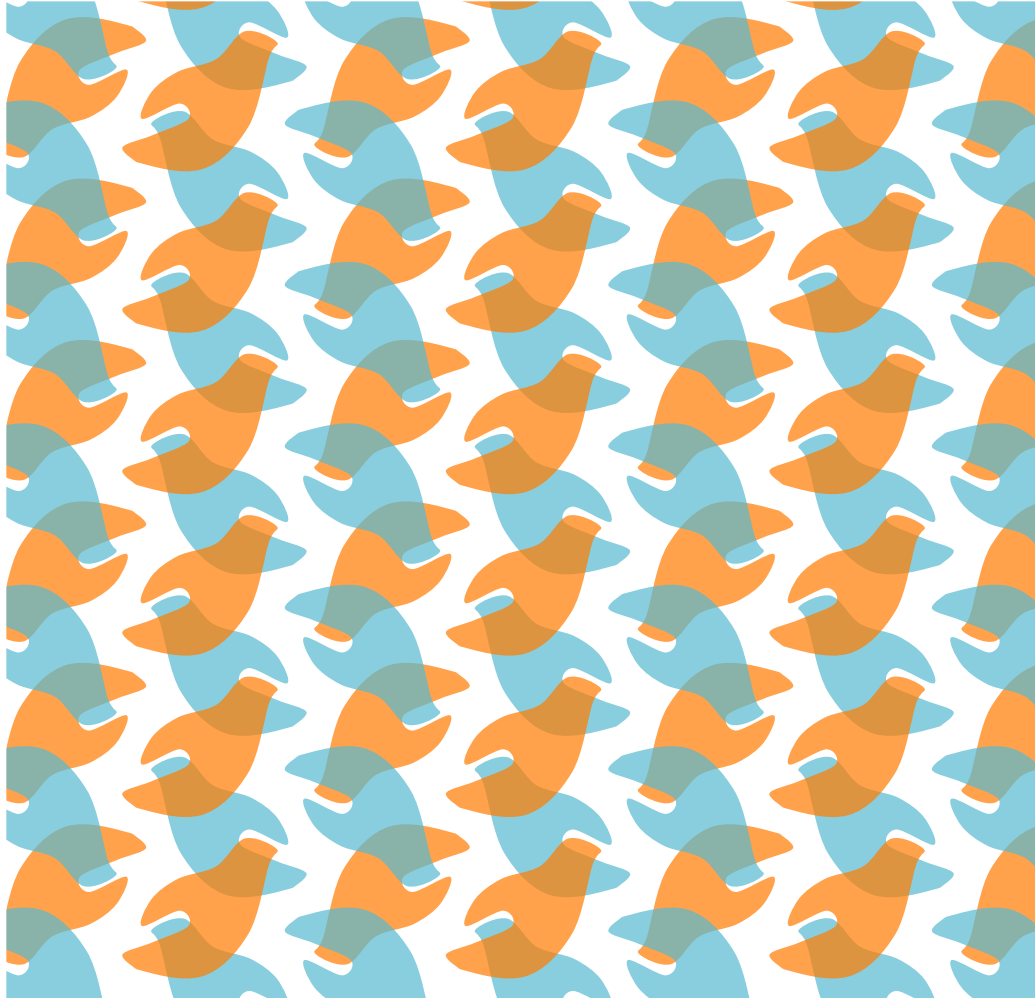
Simplified representation



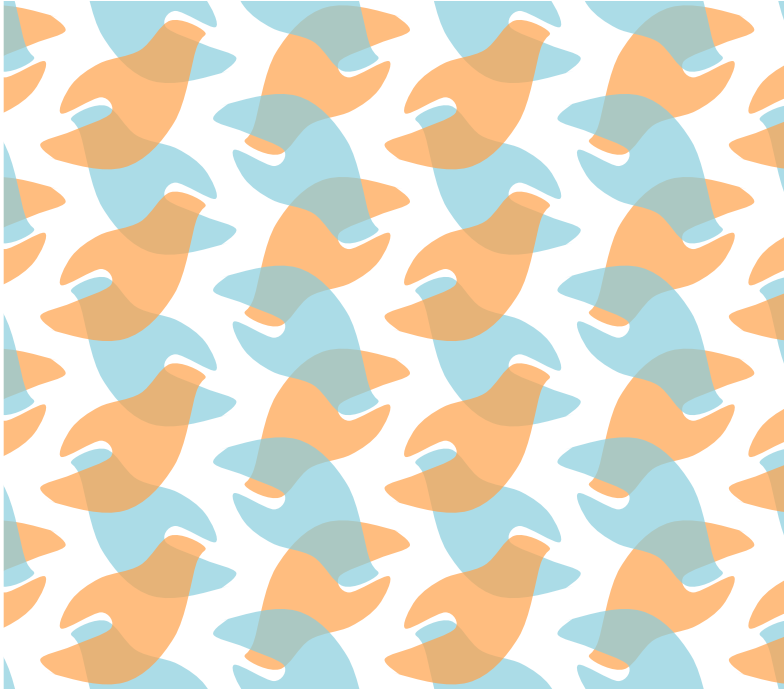
Simplified representation



Simplified representation

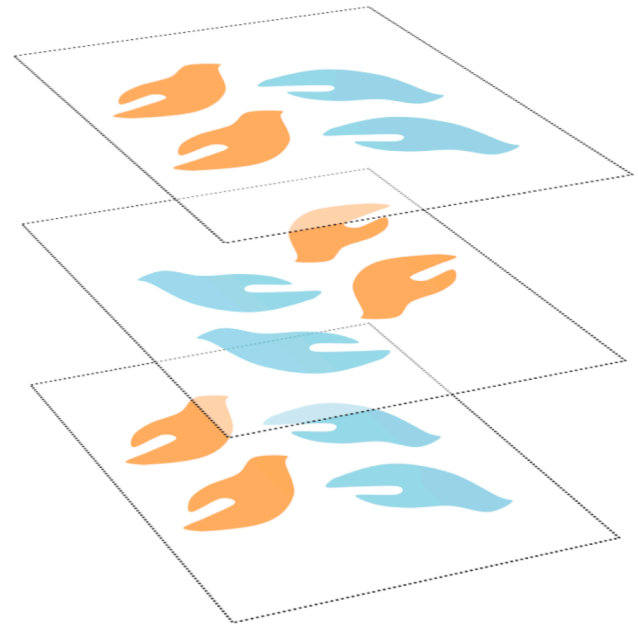


Simplified representation

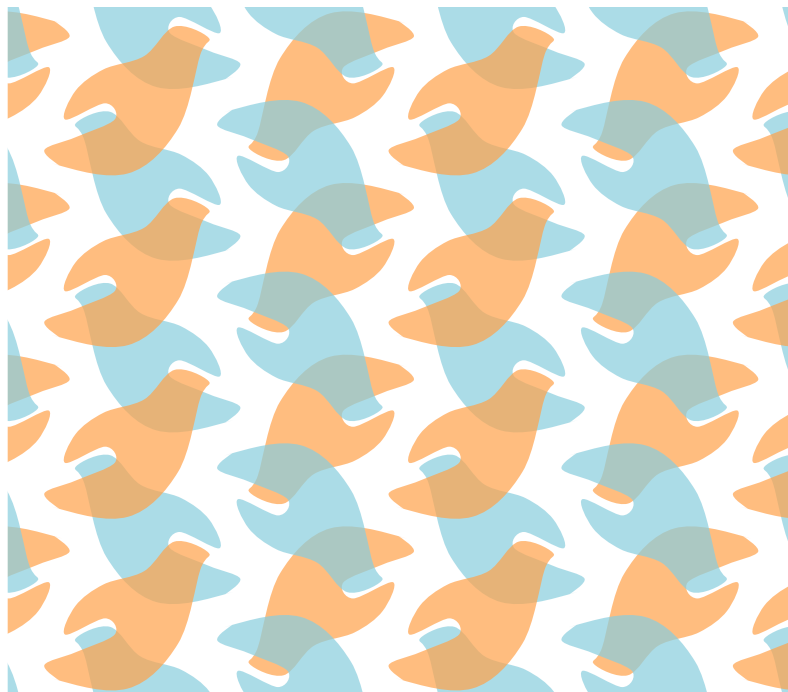


View from the top

There is a third dimension.



Simplified representation



1

2

3

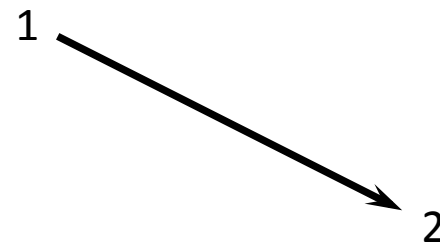
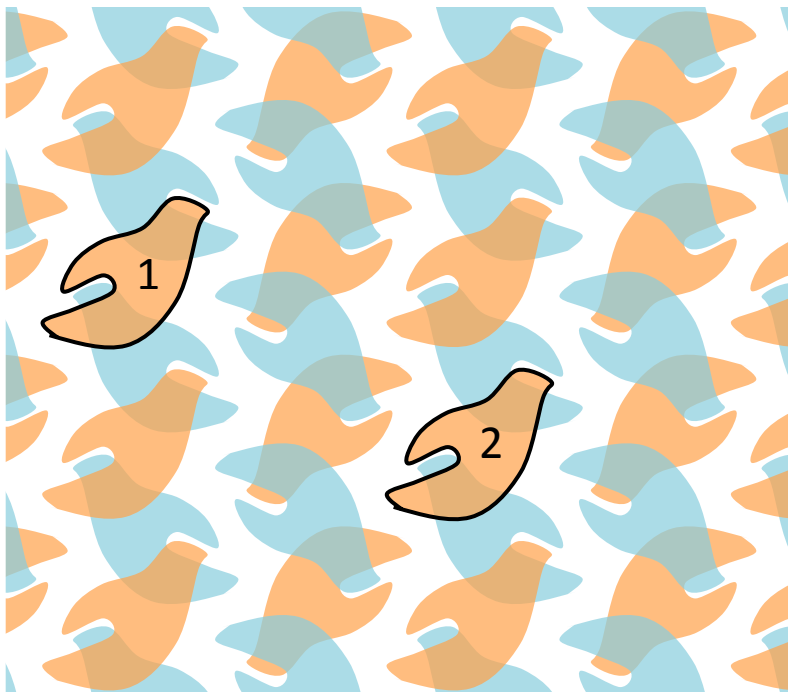
4

Orange and blue represent opposite sides of molecules

A slice is shown, where

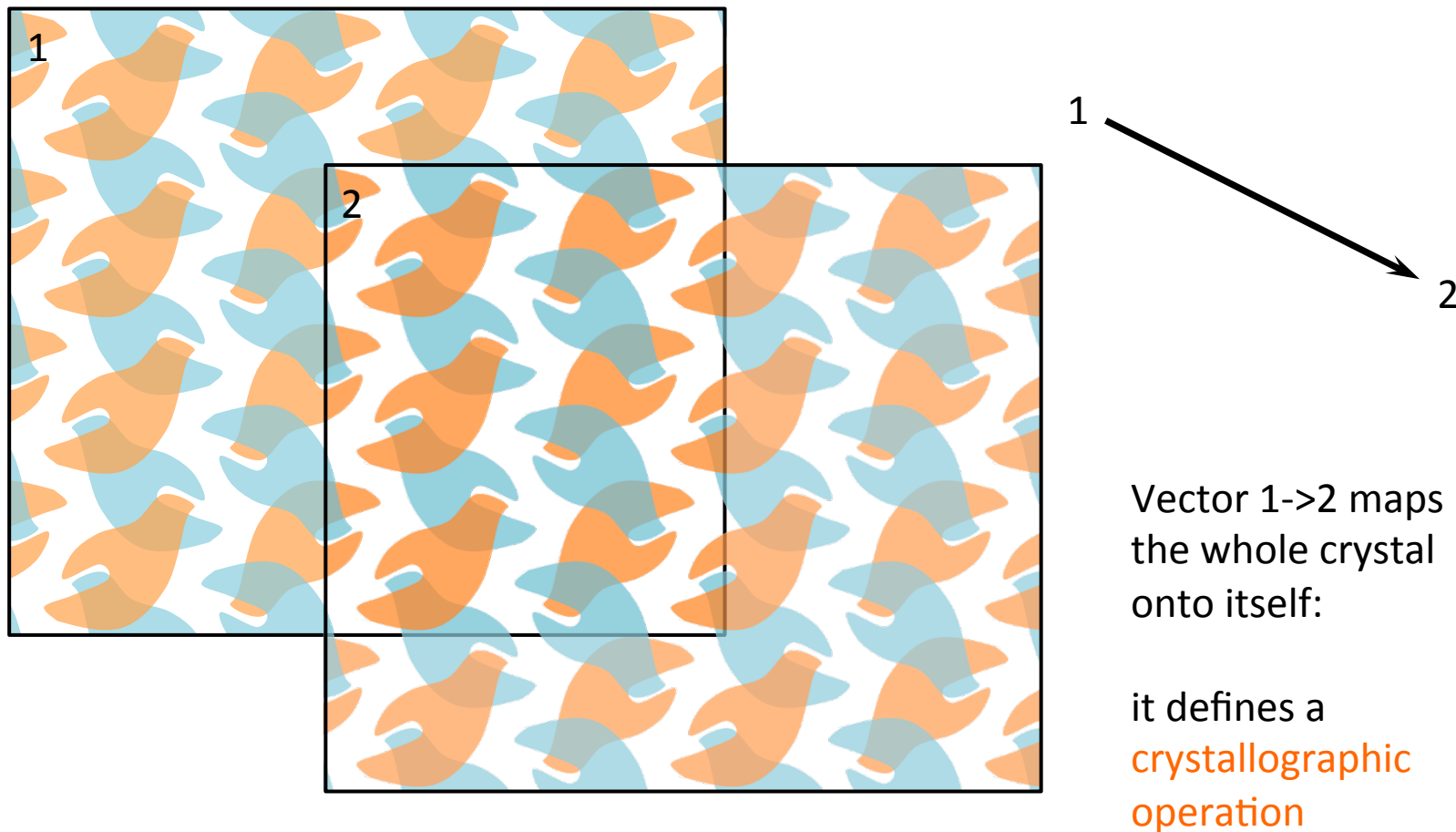
- column 1, 3 : orange-sided molecules on top
- column 2, 4: blue-sided molecules on top
- etc.

Translation 1



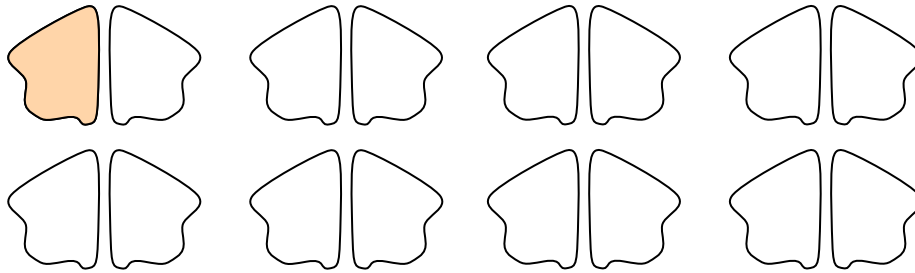
Vector maps 1 -> 2

Translation 1 is global



Crystallographic Translation and Pseudo-translation

Crystallographic translation

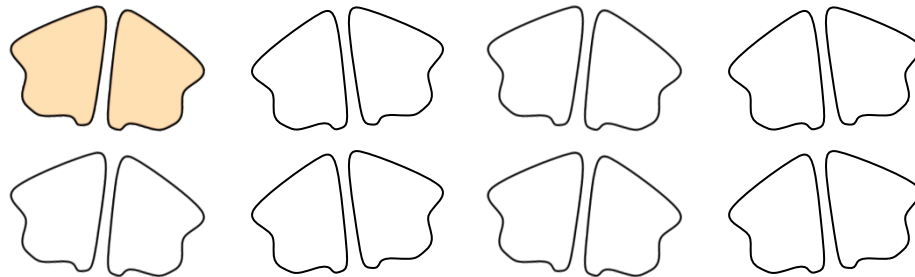


(symmetry is **global** and **exact**)

Crystallographic translation



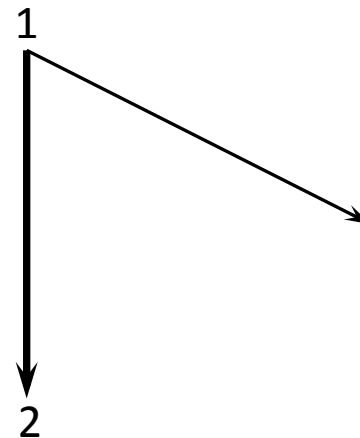
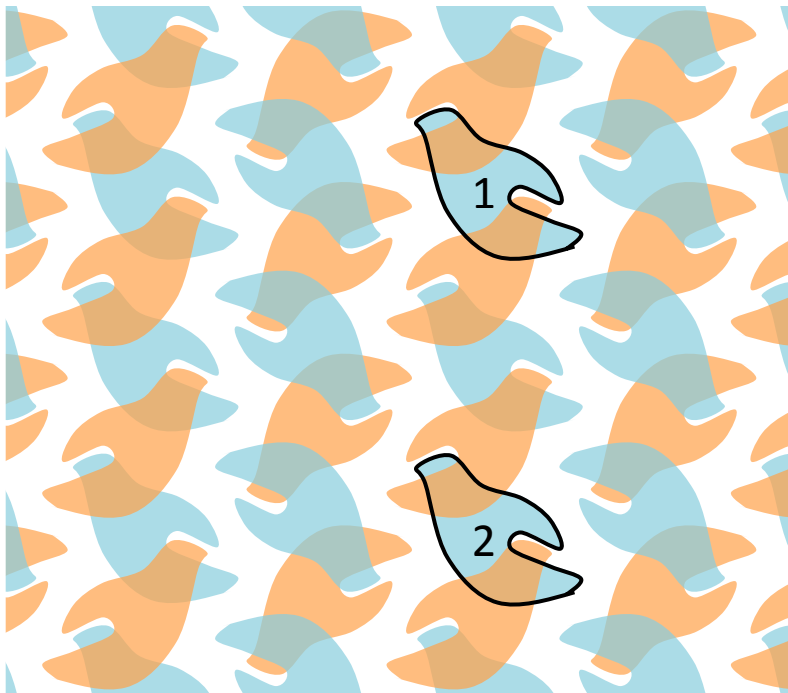
Pseudo-translation



(symmetry is **global** but **approximate**)

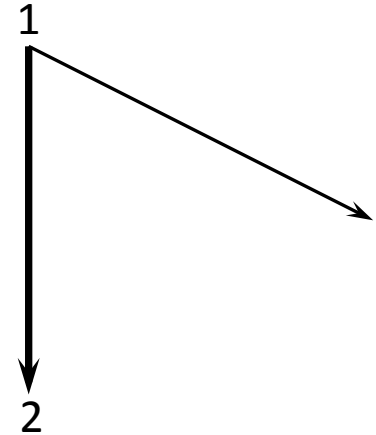
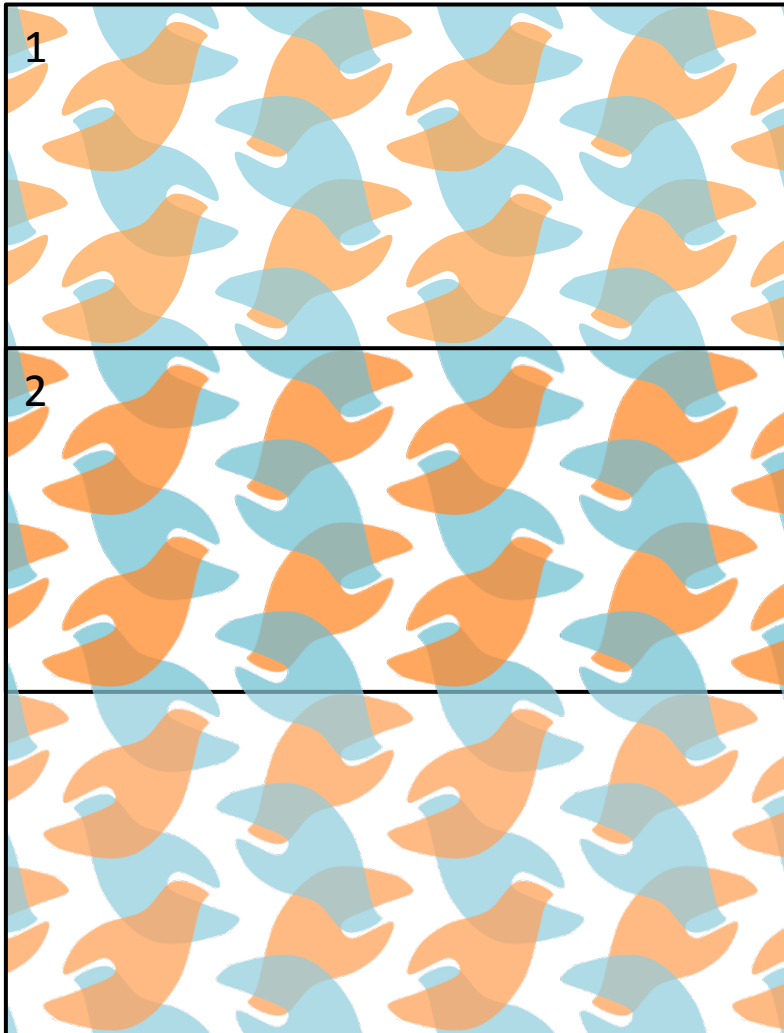
This is a special case of translational
Non-Crystallographic Symmetry (tNCS)

Translation 2



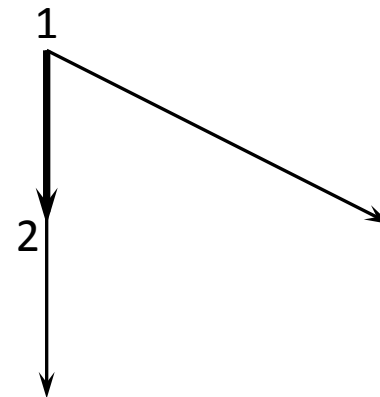
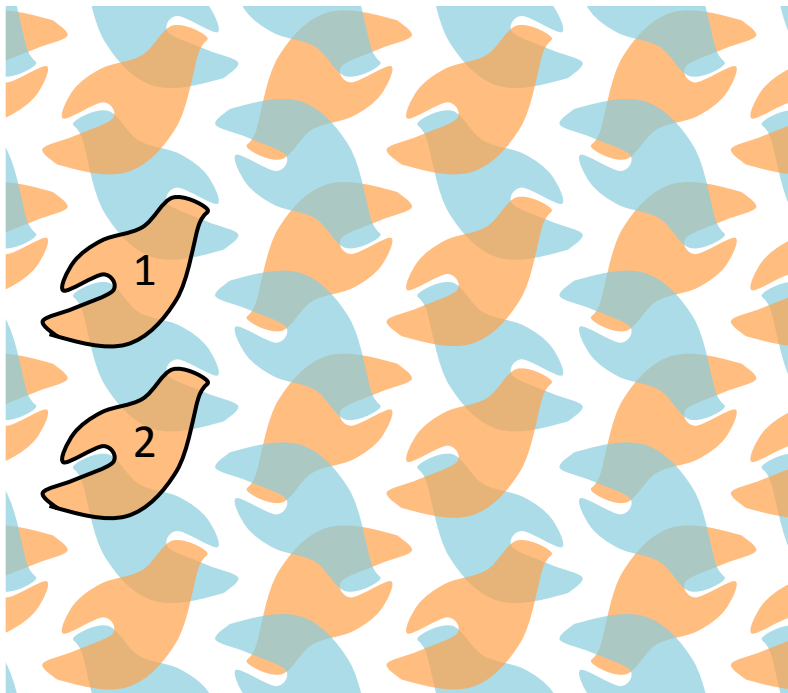
Highlighted vector
maps 1 -> 2

Translation 2 is global



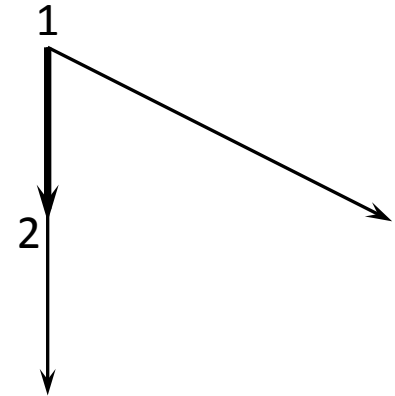
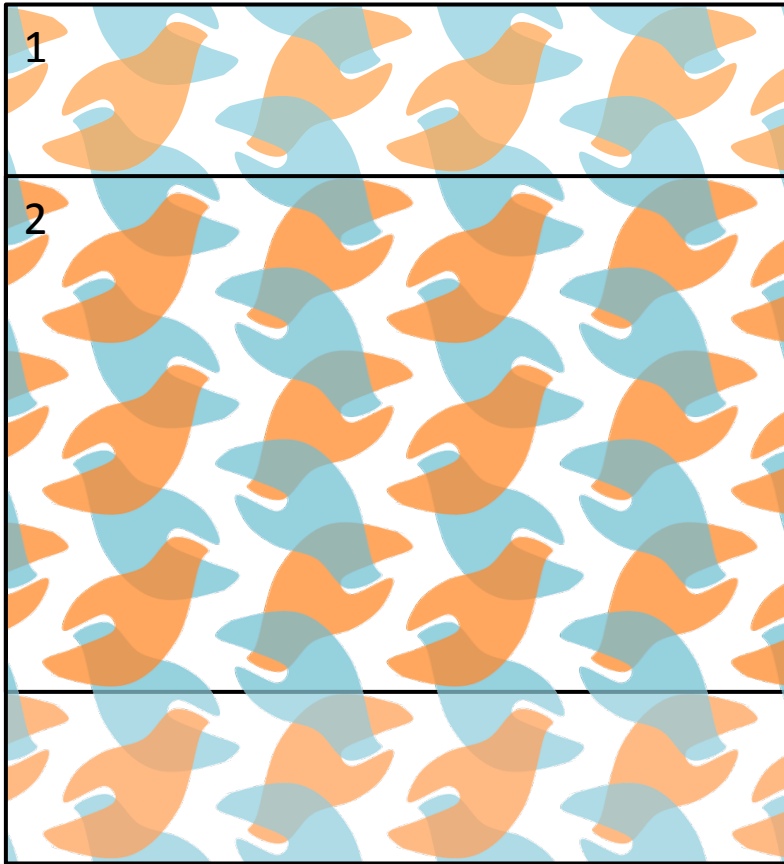
Highlighted vector
maps the whole
crystal onto itself

Translation 3



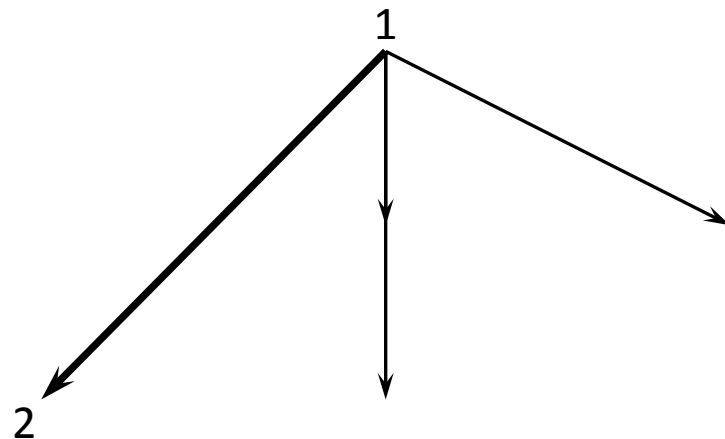
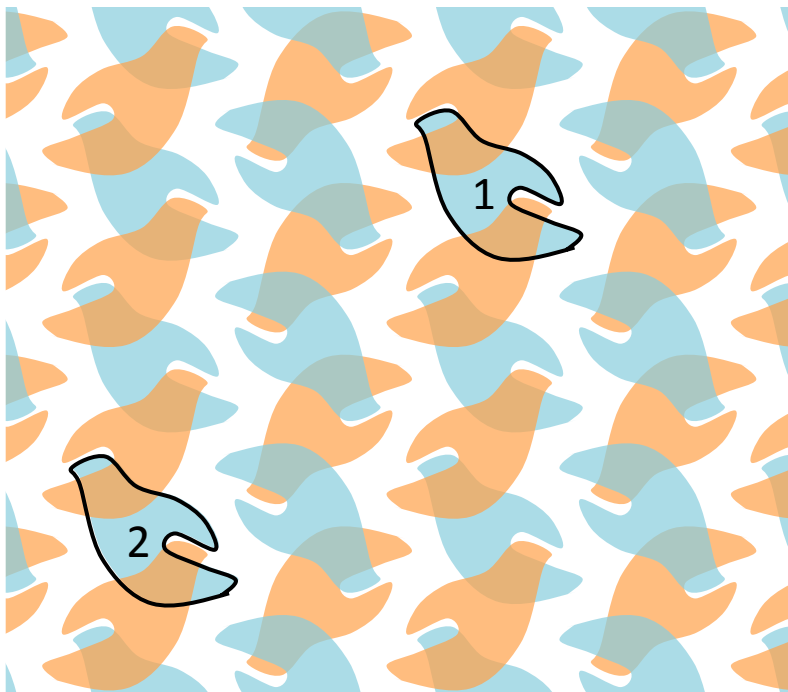
Highlighted vector
maps 1 -> 2

Translation 3 is global



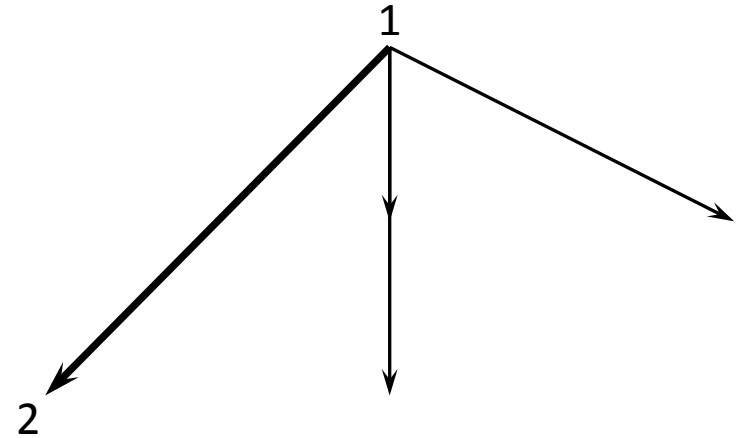
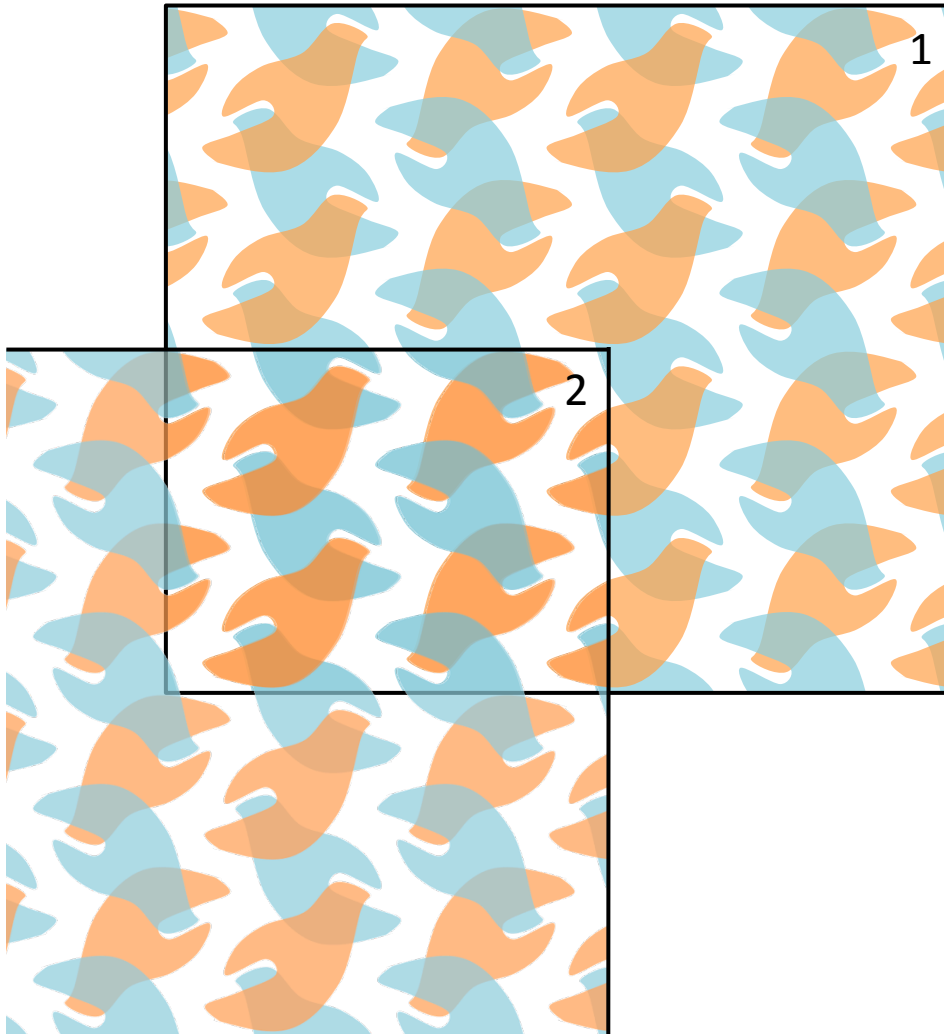
Highlighted vector
maps the whole
crystal onto itself

Translation 4



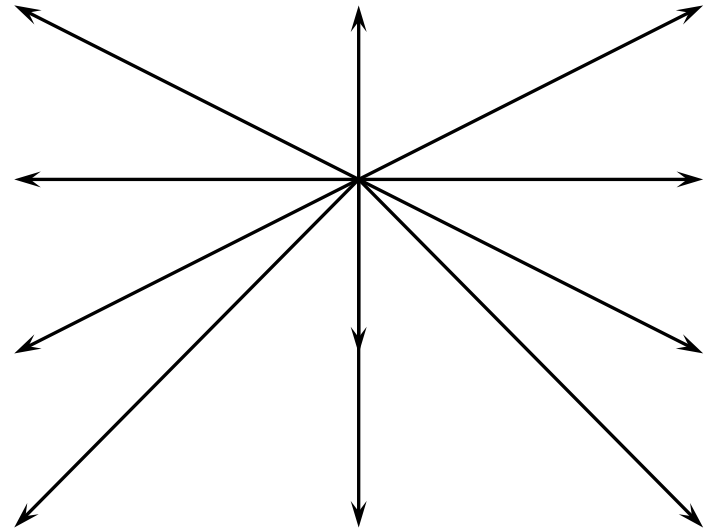
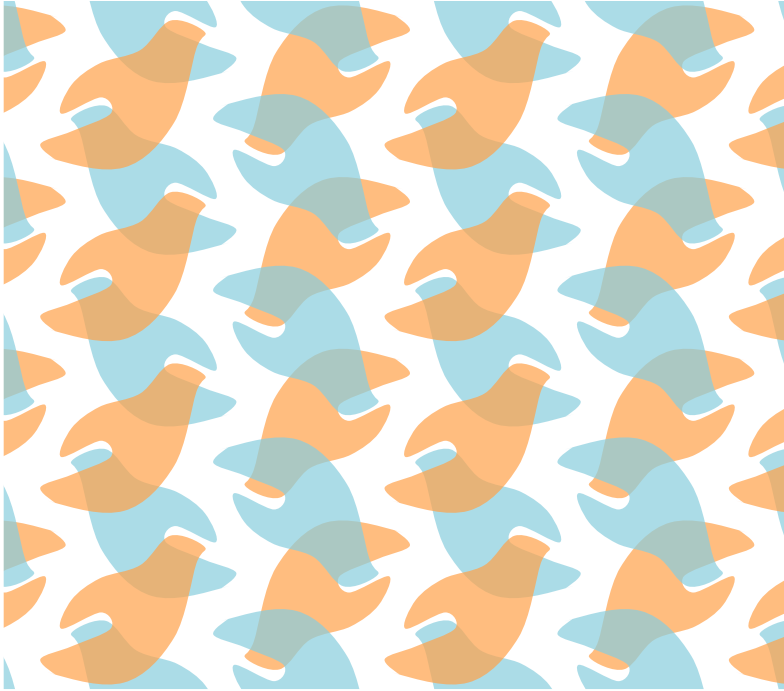
Highlighted vector
maps 1 -> 2

Translation 4 is global



Highlighted vector
maps the whole
crystal onto itself

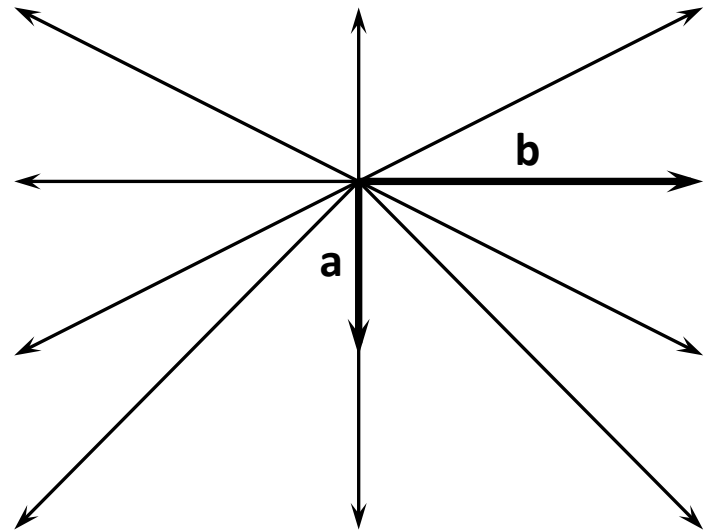
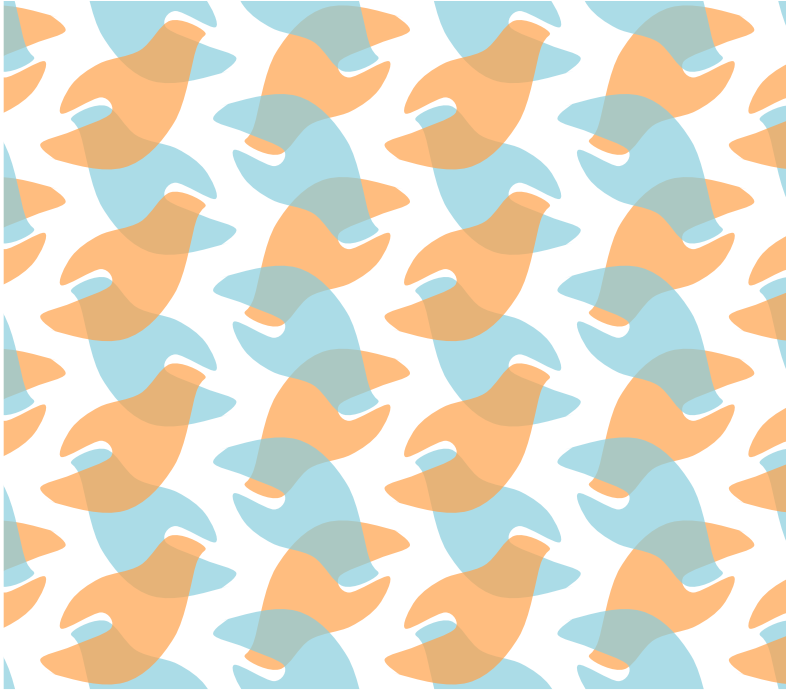
All translations form an infinite group



An infinite group (over vector sum):

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

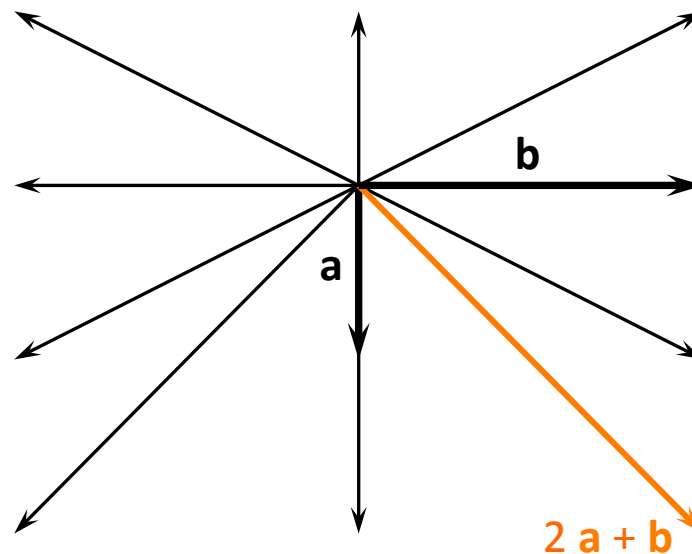
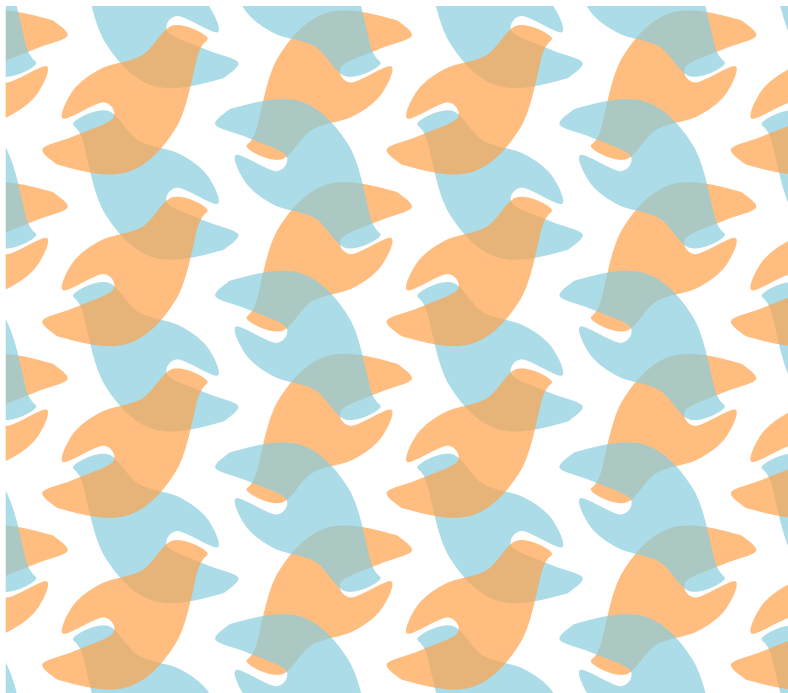
Basis set



All the translations that map the crystal onto itself can be produced from a basis set: $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$

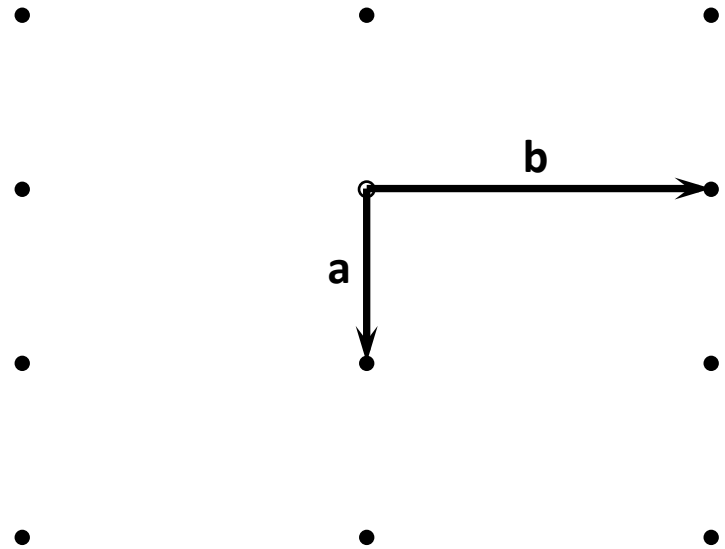
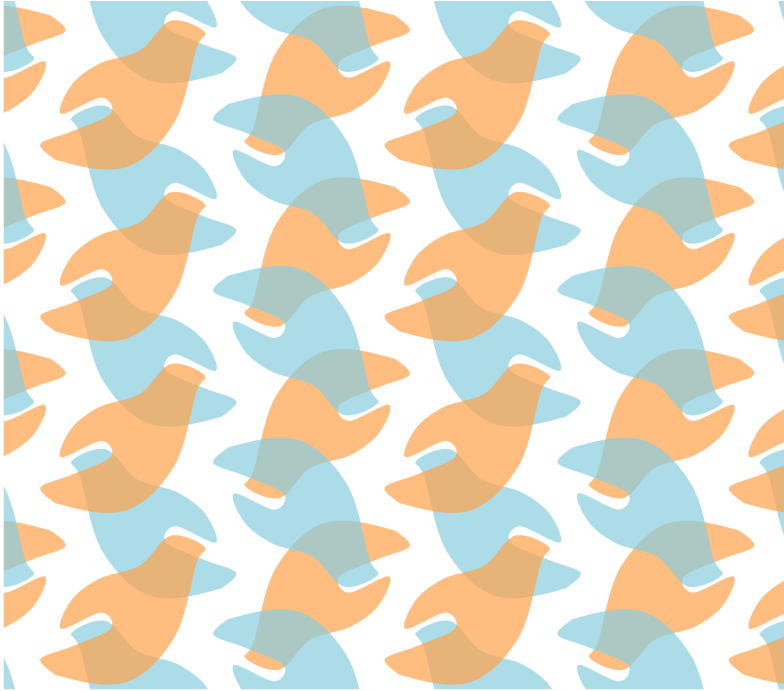
($\mathbf{c}$ is perpendicular to the plane)

Basis set



For example, the highlighted vector is expressed as $2\mathbf{a} + \mathbf{b}$.

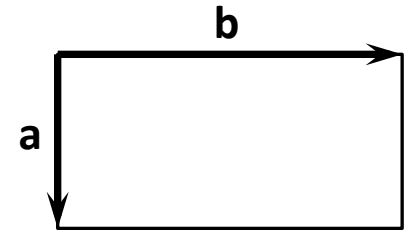
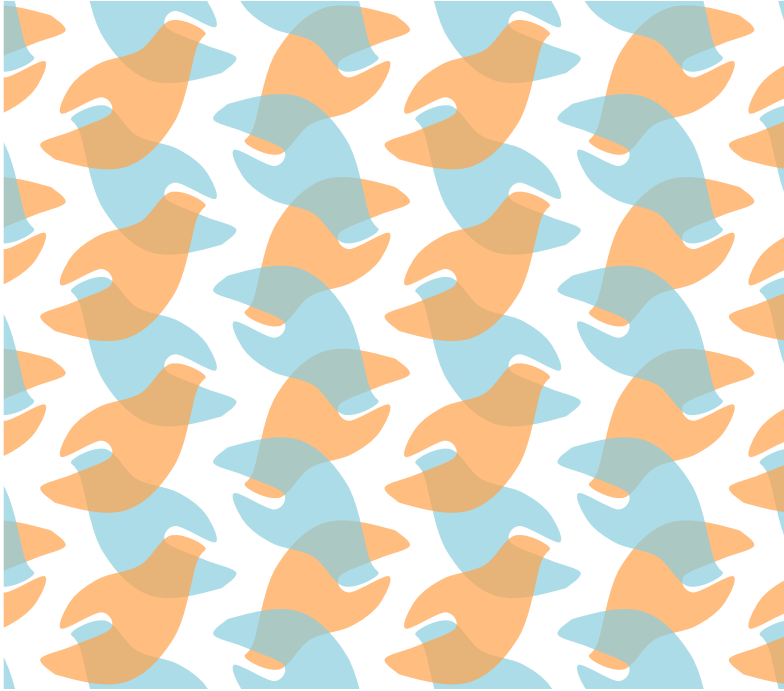
Lattice



All the crystallographic translations can be represented as a lattice.

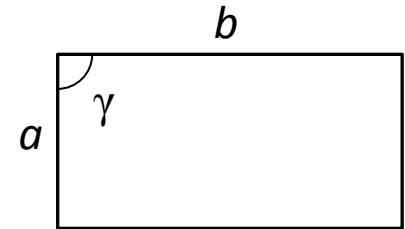
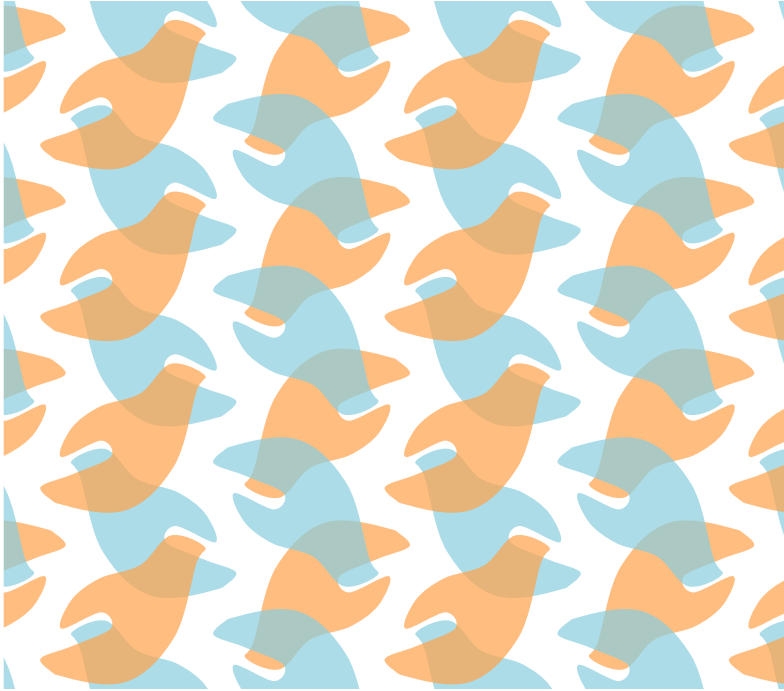
Translations live in a separate space, not connected to crystal (for now)

Unit cell



A compact representation of translational symmetry and base vectors.

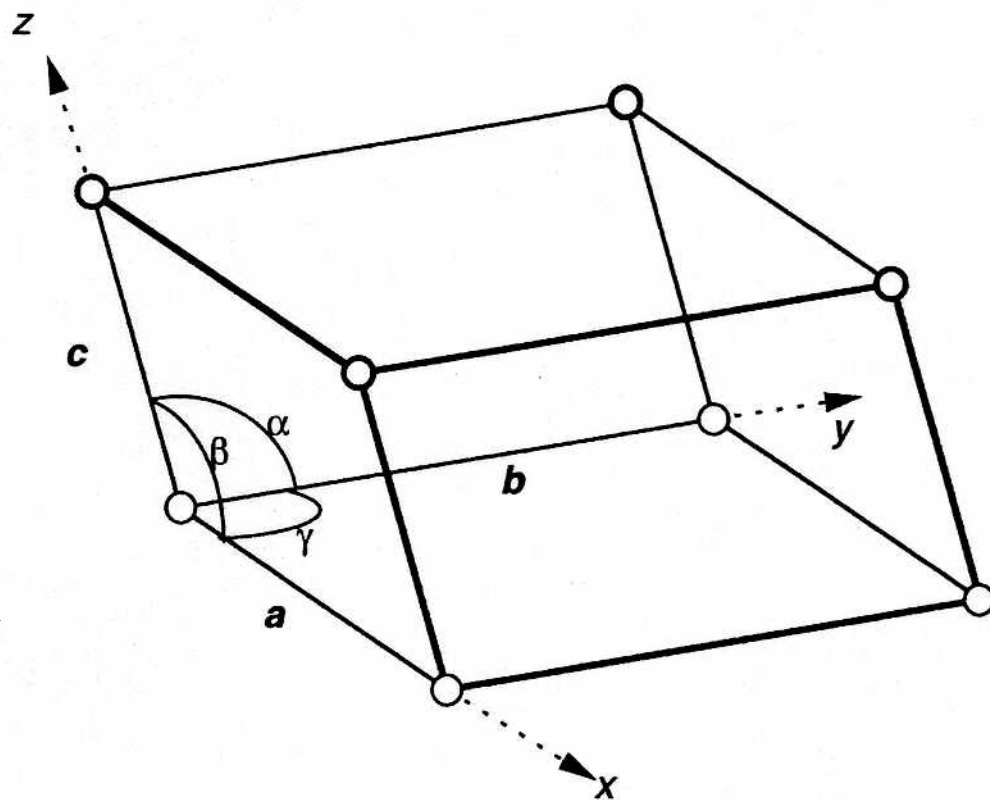
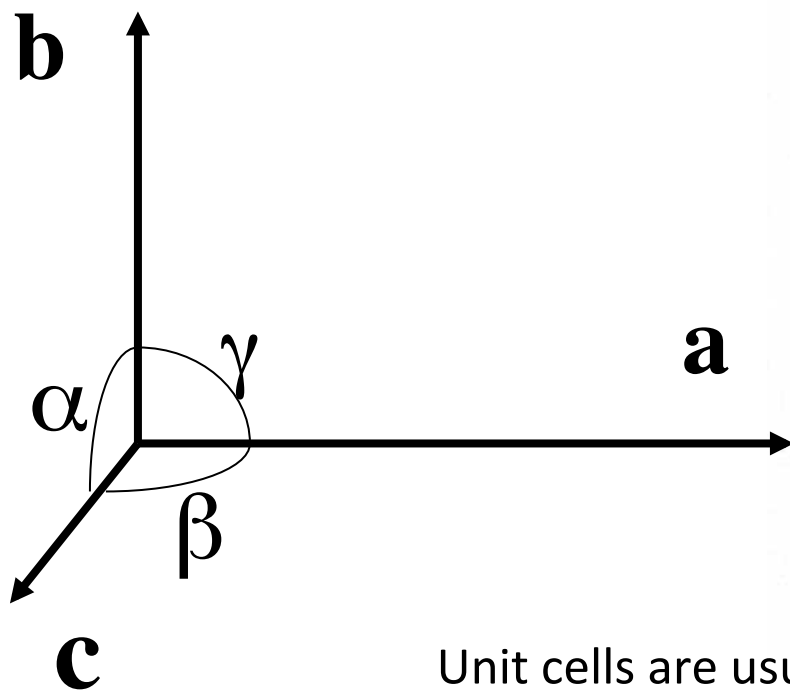
Unit cell



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

Unit cell parameters (3D view)

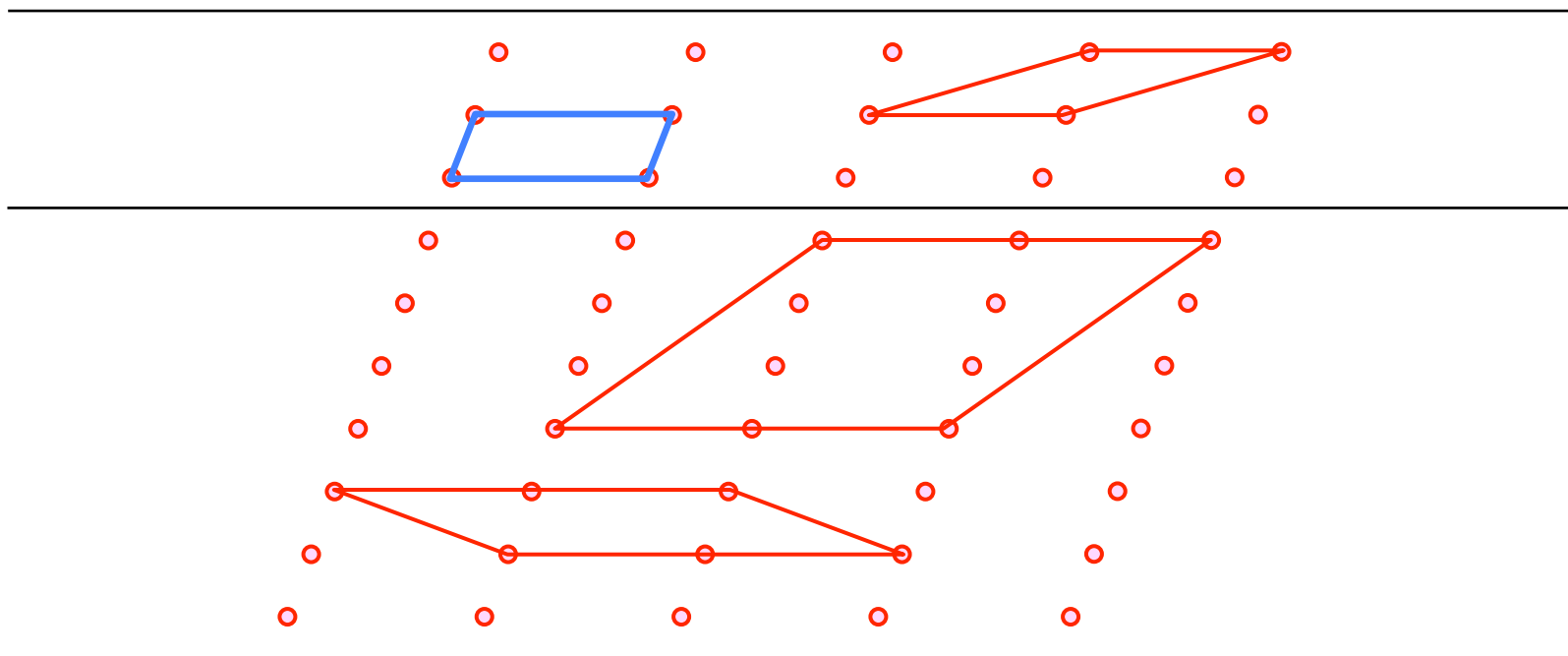
Translation symmetry is defined by three base vectors **a**, **b**, and **c**.



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

$$a=94.2\text{\AA}, b=72.6\text{\AA}, c=30.1\text{\AA}, \alpha=90^\circ, \beta=102.1^\circ, \gamma=90^\circ.$$

'Choice of unit cell

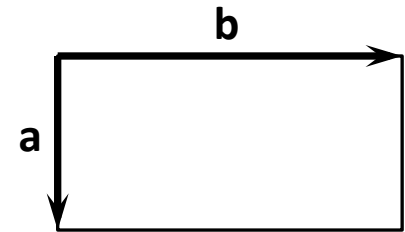
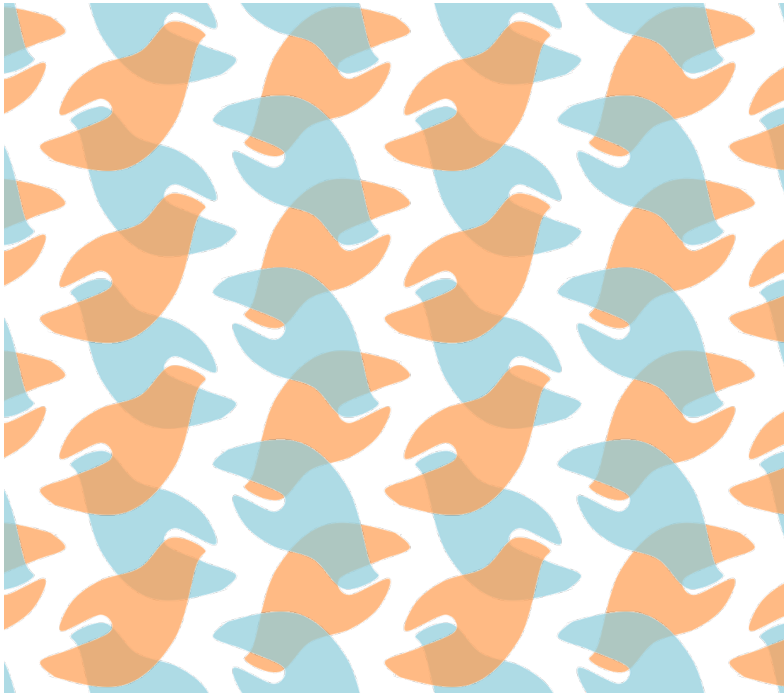


The top two do define all translations = these are unit cells
The bottom two do NOT define all translations = these are NOT unit cells

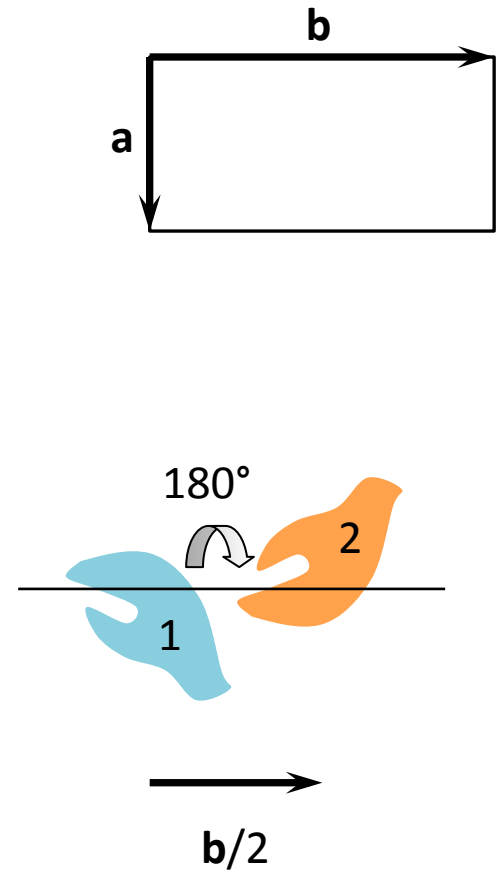
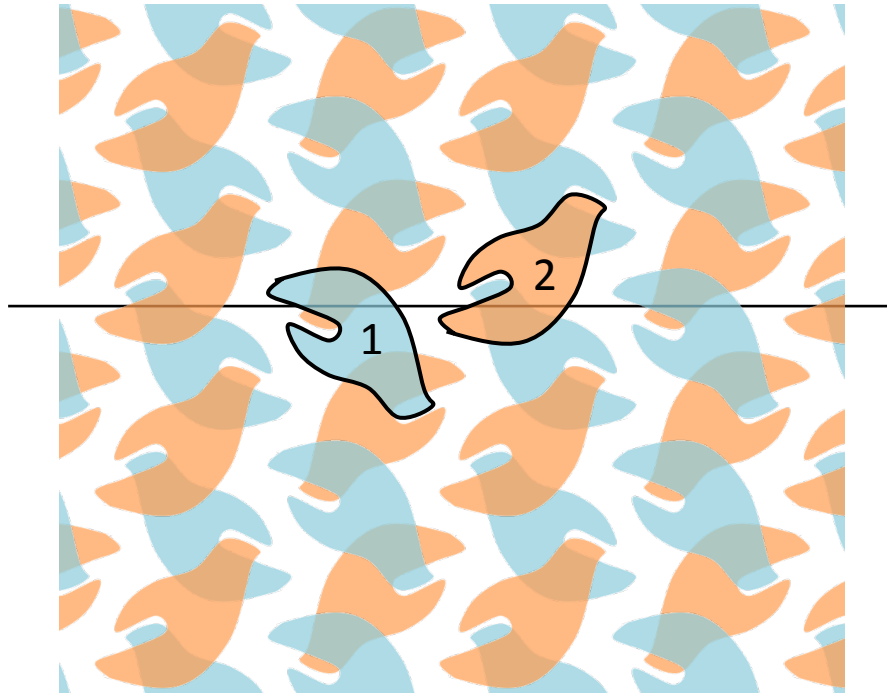
The top left: primitive reduced – the standard for some space groups

Non-primitive unit cells (which, strictly speaking are not unit cells) are discussed later

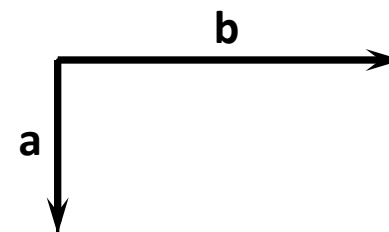
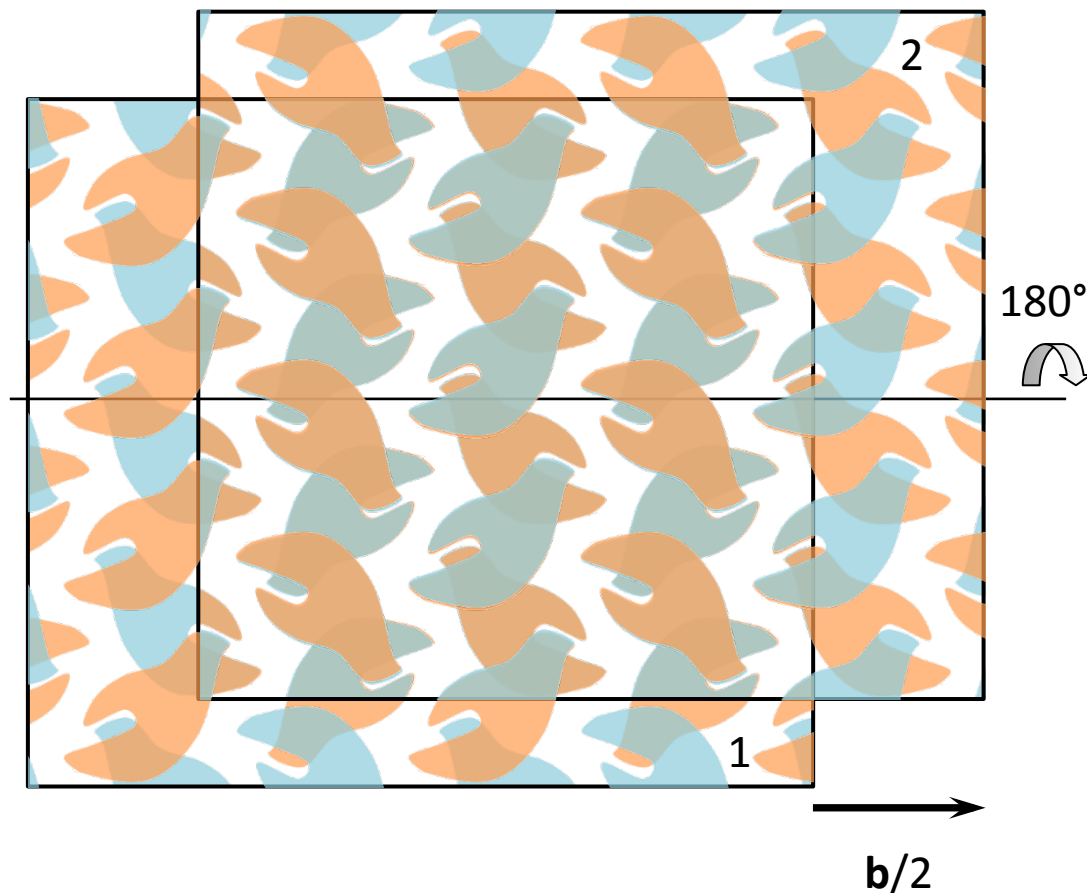
Back to example



Screw rotation 1



Screw rotation axis



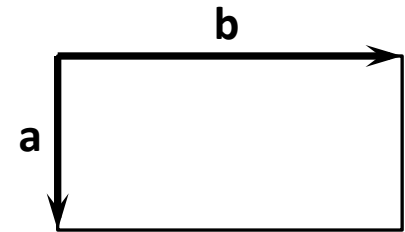
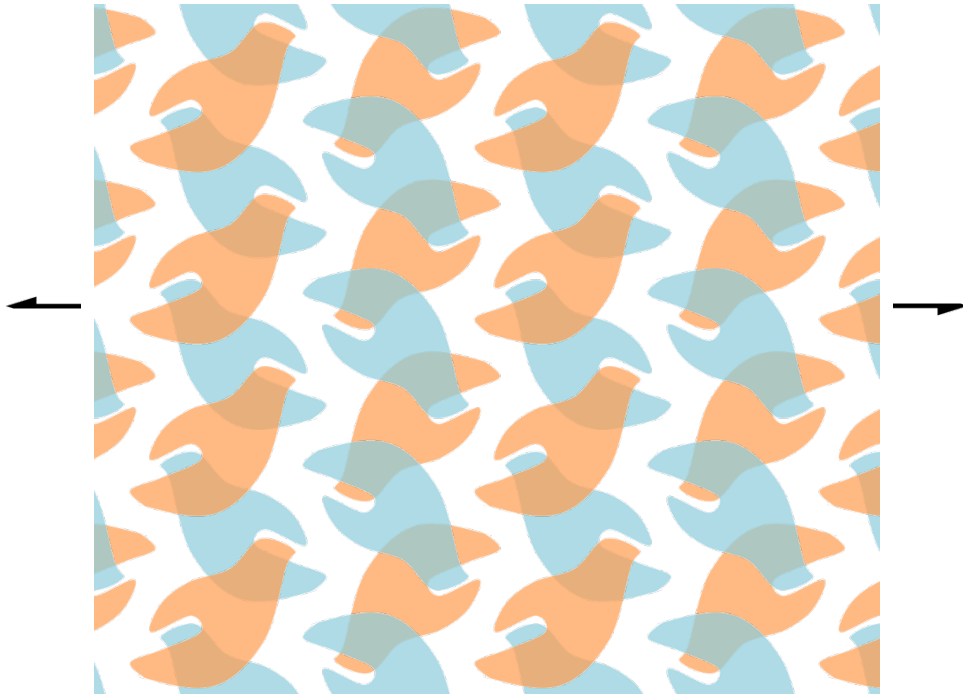
Operation 1→2
maps the whole crystal
onto itself:

this is a **crystallographic
operation**

The axis is a
crystallographic
symmetry element,

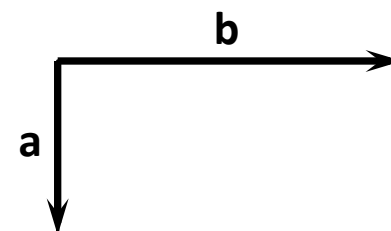
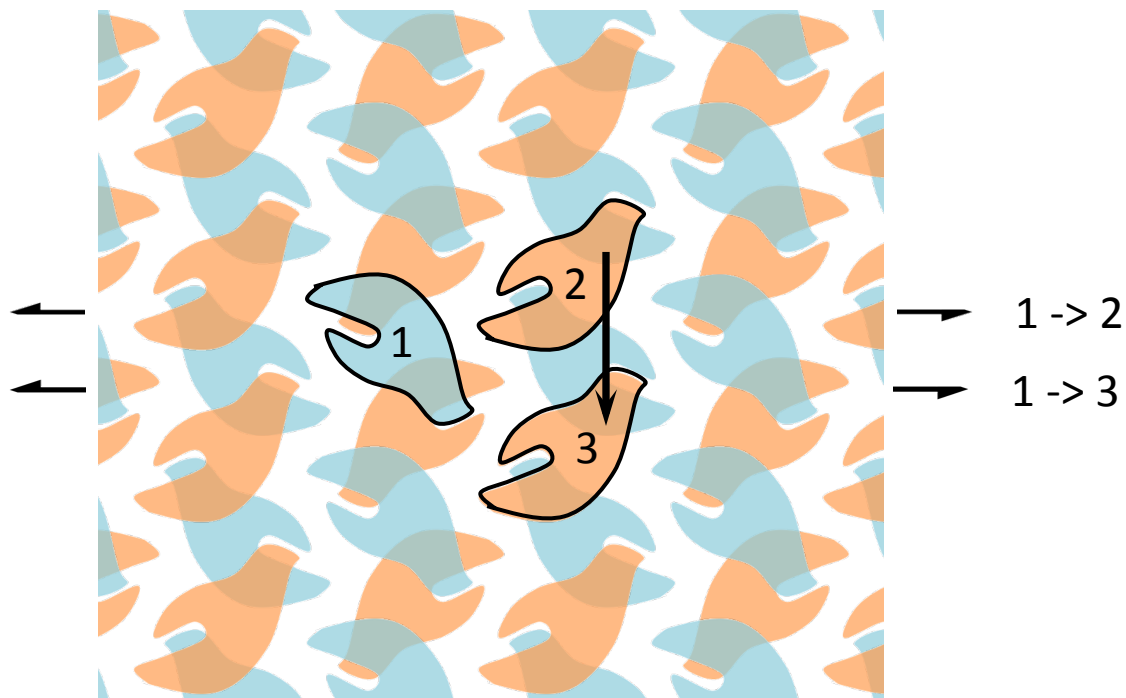
it can be **mapped into
the structure**

Screw rotation 1 - symbol



2_1 (plane of figure): $\longleftrightarrow$

Screw rotation 1 - repeats

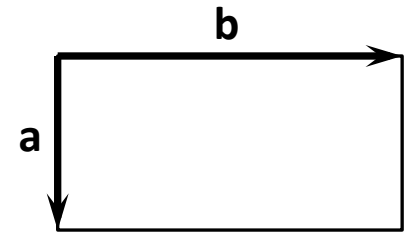
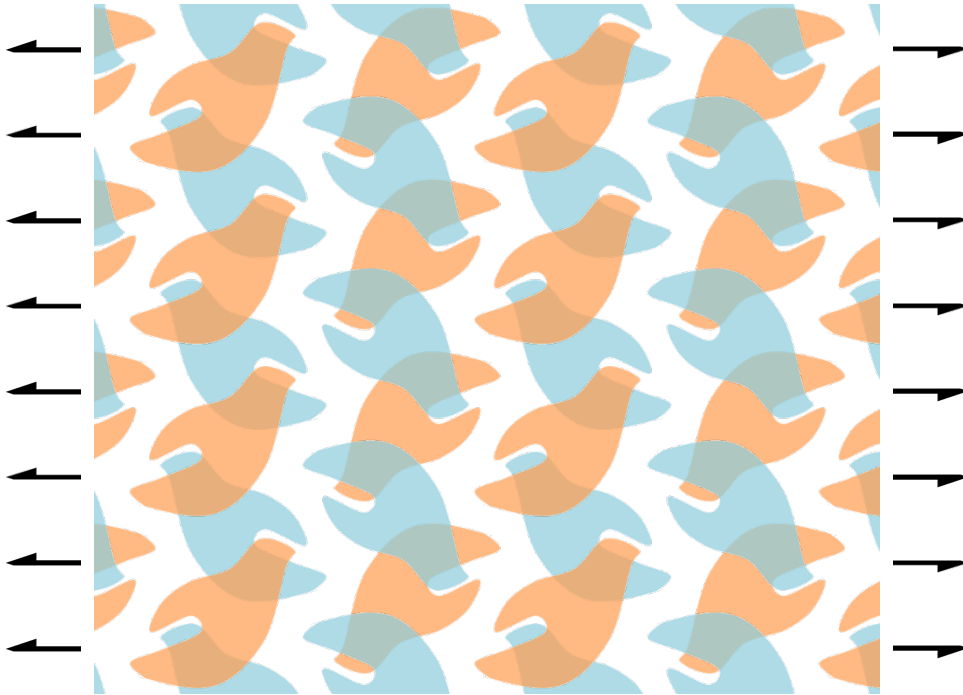


action of top axis
 $\times$
translation **a**
 $=$
action of bottom axis

(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 $\frac{1}{2} \mathbf{a}$ is also available.

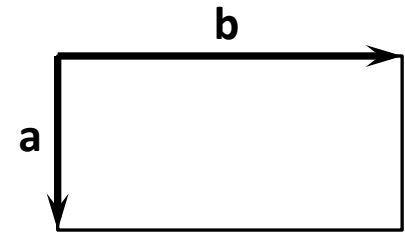
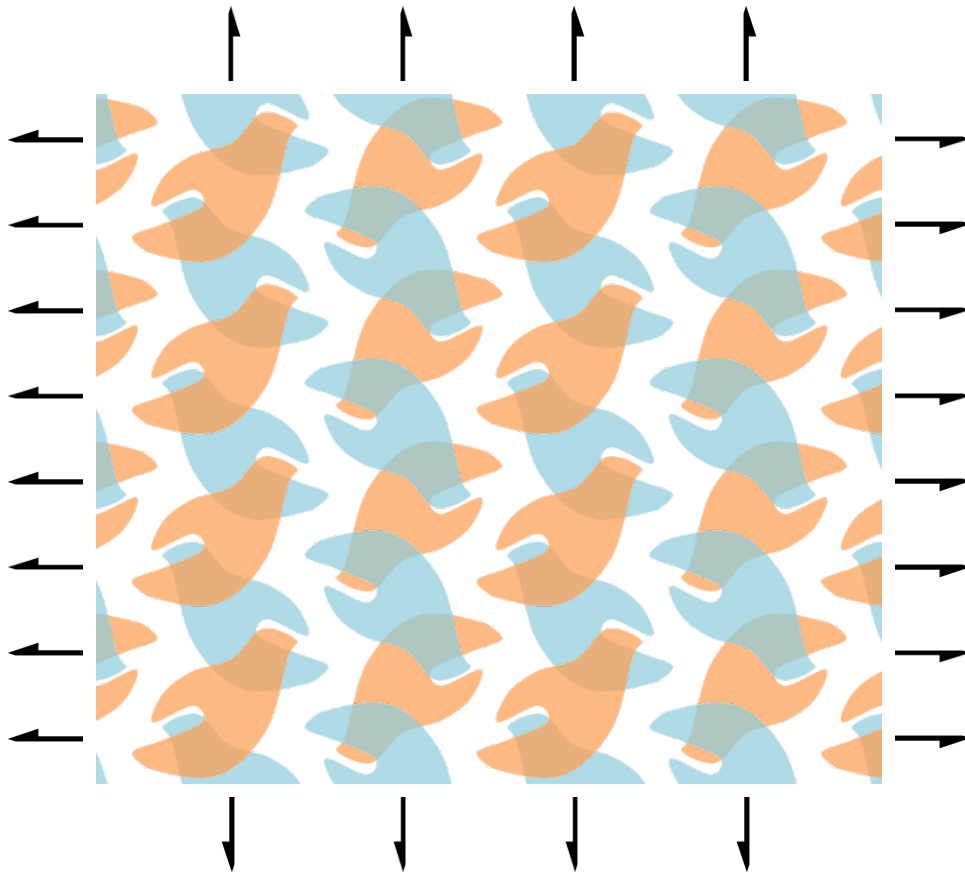
Screw rotation 1 - repeats



2_1 (plane of figure): $\leftarrow \rightarrow$

Also repeated in 3d dimension
with offset of $\frac{1}{2} c$

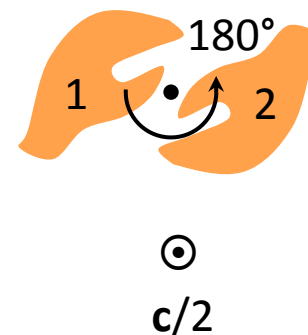
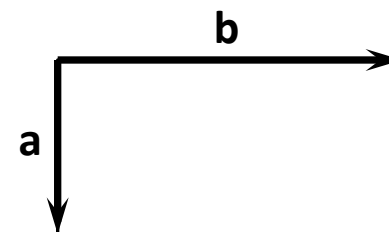
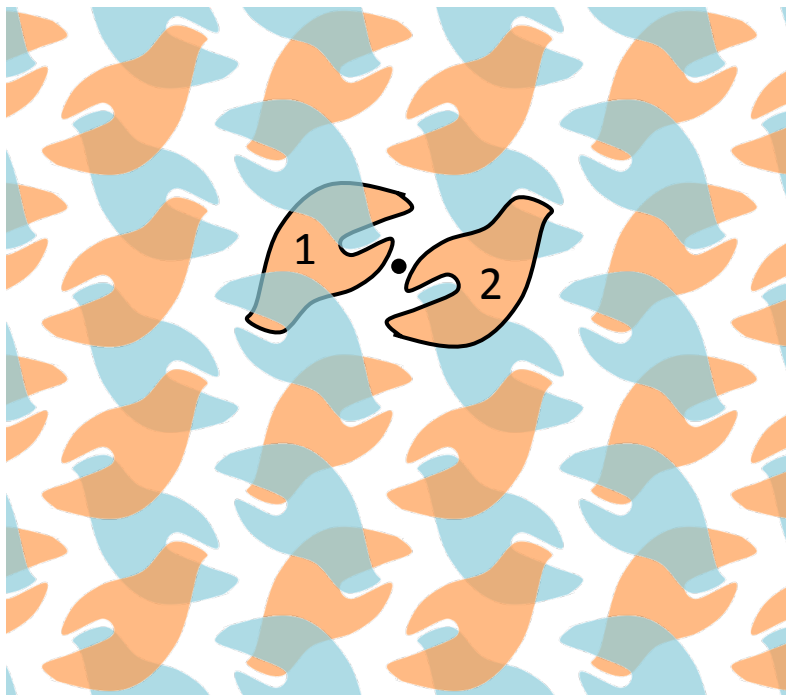
Screw rotations parallel to **a** and **b**



2_1 (plane of figure): $\leftarrow \rightarrow$

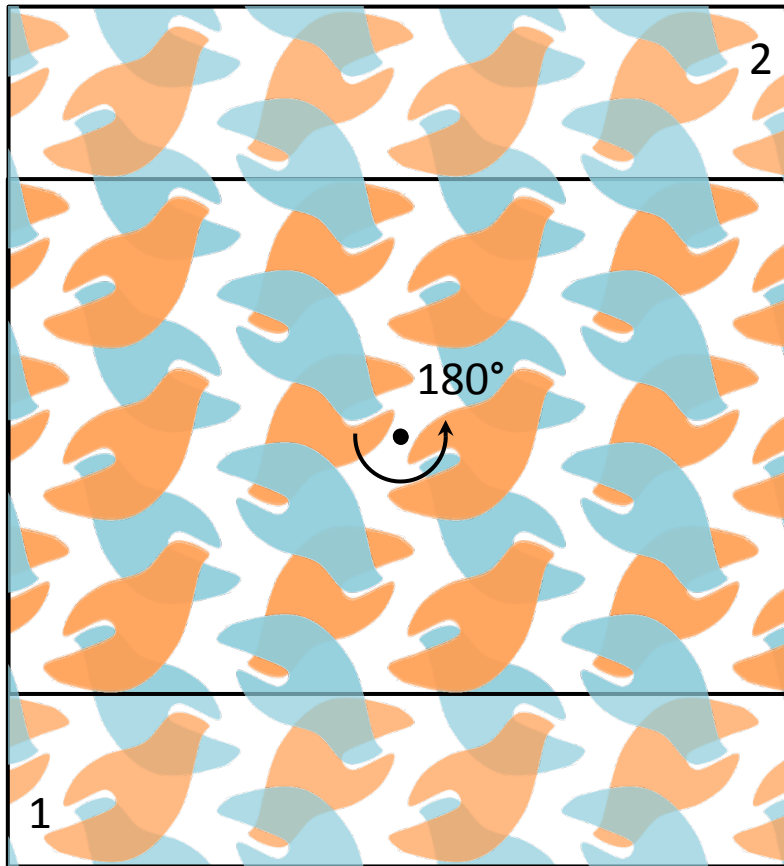
Series of 2_1 axes offset by $\frac{1}{2}$ unit cell from each other.

Screw rotation 3 – into plane

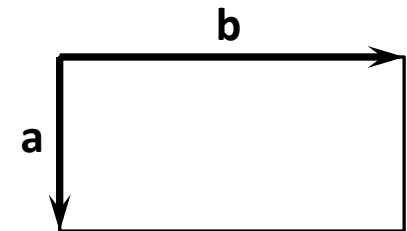


A rotation of 180° with a translation of $\frac{1}{2}$ unit cell from the figure.

Screw rotation 3 is global



⊙
 $c/2$



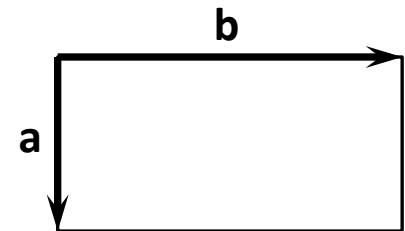
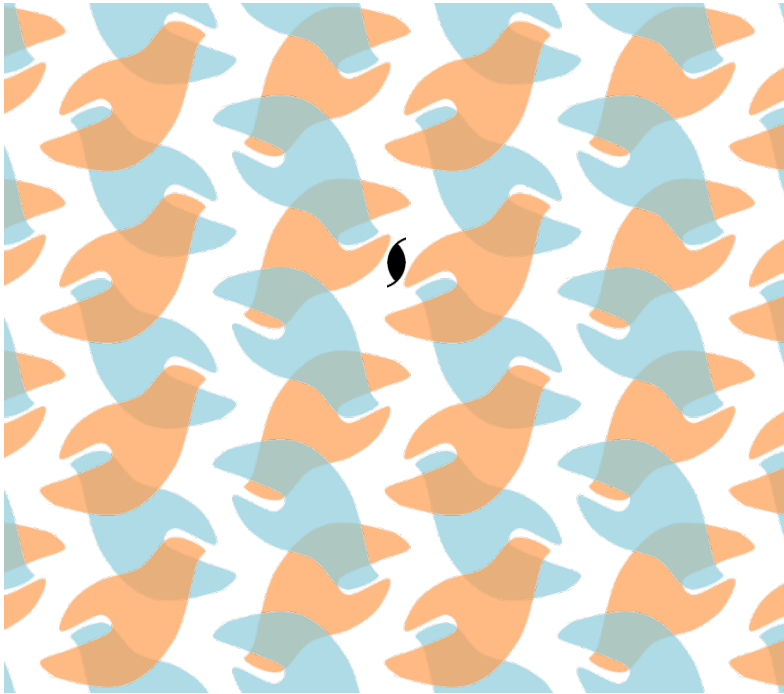
Screw rotation 3
maps the whole crystal
onto itself:

this is a **crystallographic
operation**

The rotation axis is a
crystallographic
symmetry element,

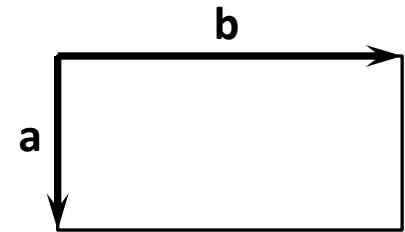
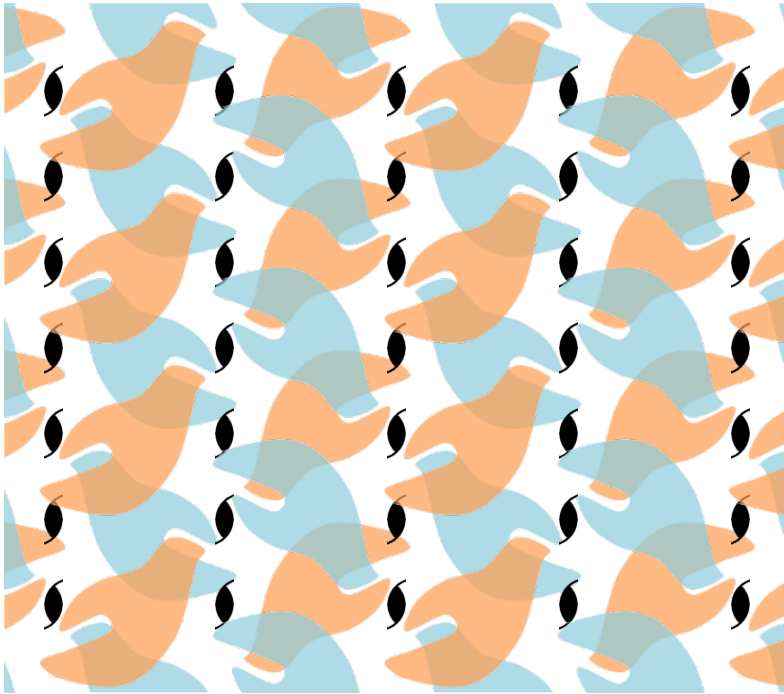
it can be **mapped into
the structure**

Screw rotation 3 - symbol



2_1 (along view):

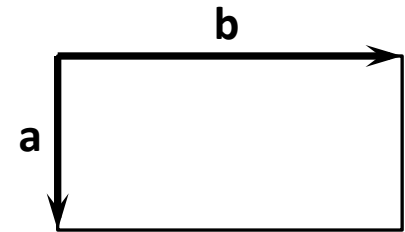
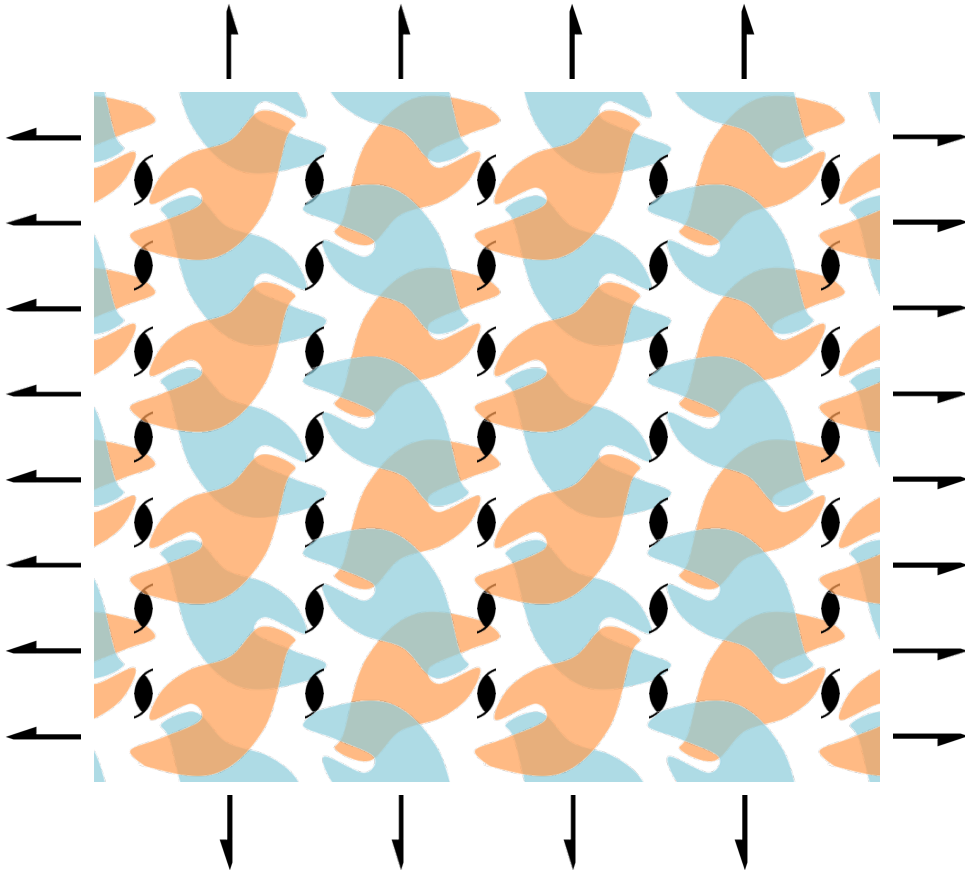
Screw rotation 3 - repeats

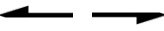


2_1 (along view): 

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

All axes together



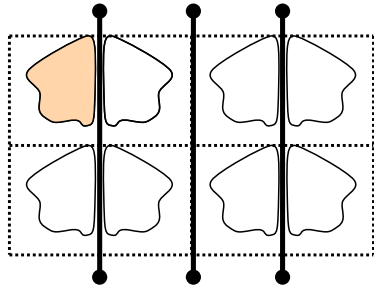
2_1 (plane of figure): 

2_1 (along view): 

we have built
a **space group**

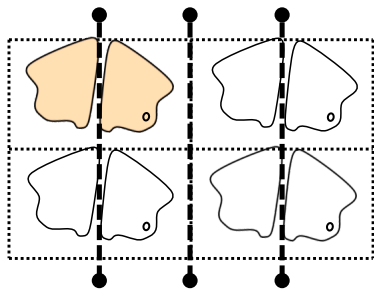
Crystallographic Symmetry, Pseudosymmetry and Non-Crystallographic Symmetry (NCS)

non-conventional
symbols for axes



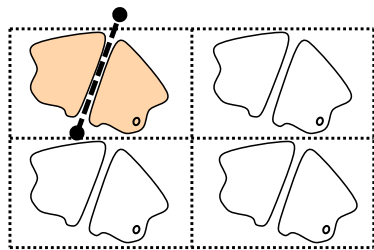
Crystallographic symmetry

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



Pseudosymmetry (a limiting case of NCS)

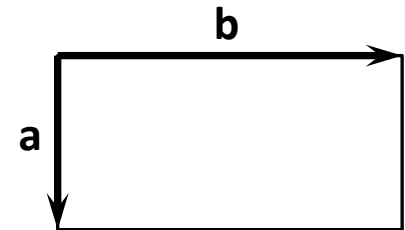
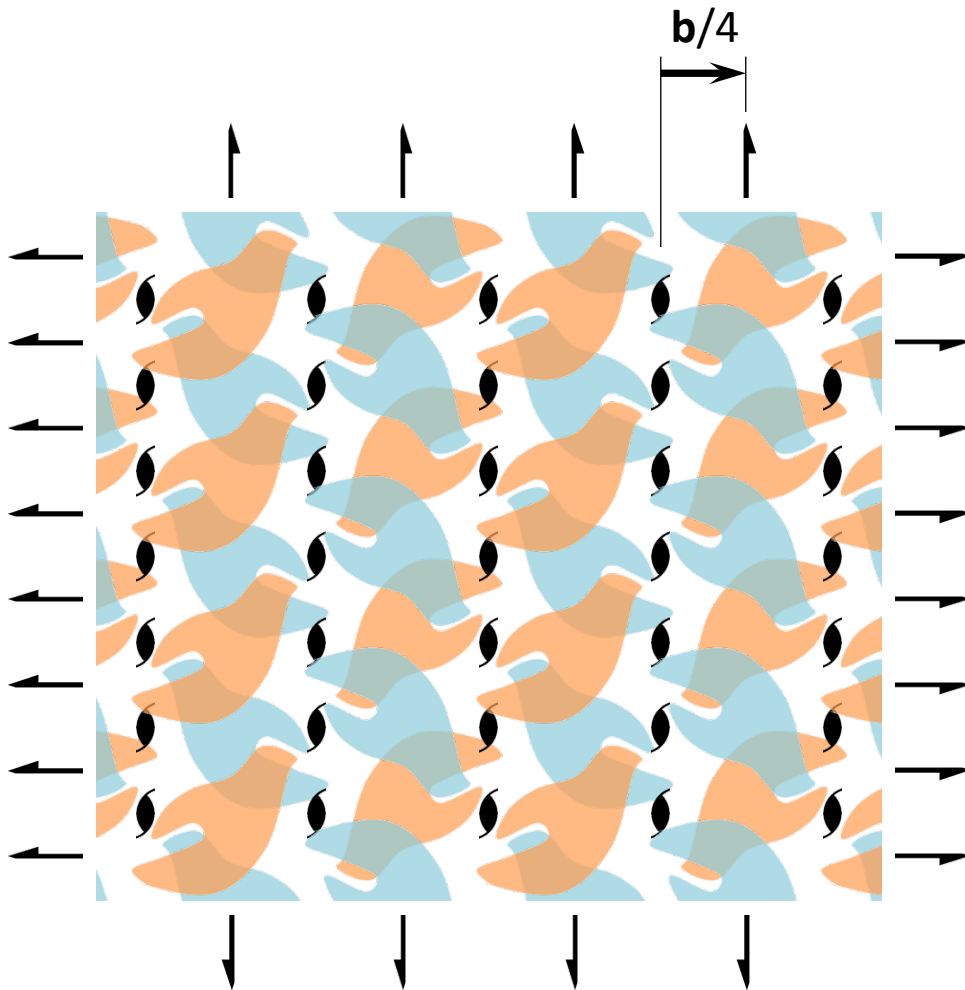
- symmetry is **global** and **approximate**



Generic Non-Crystallographic Symmetry (NCS):

- symmetry is **local** and **approximate**

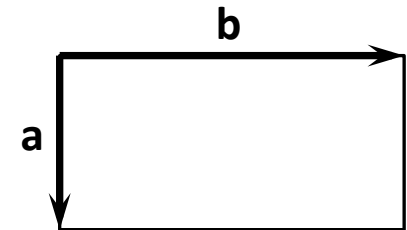
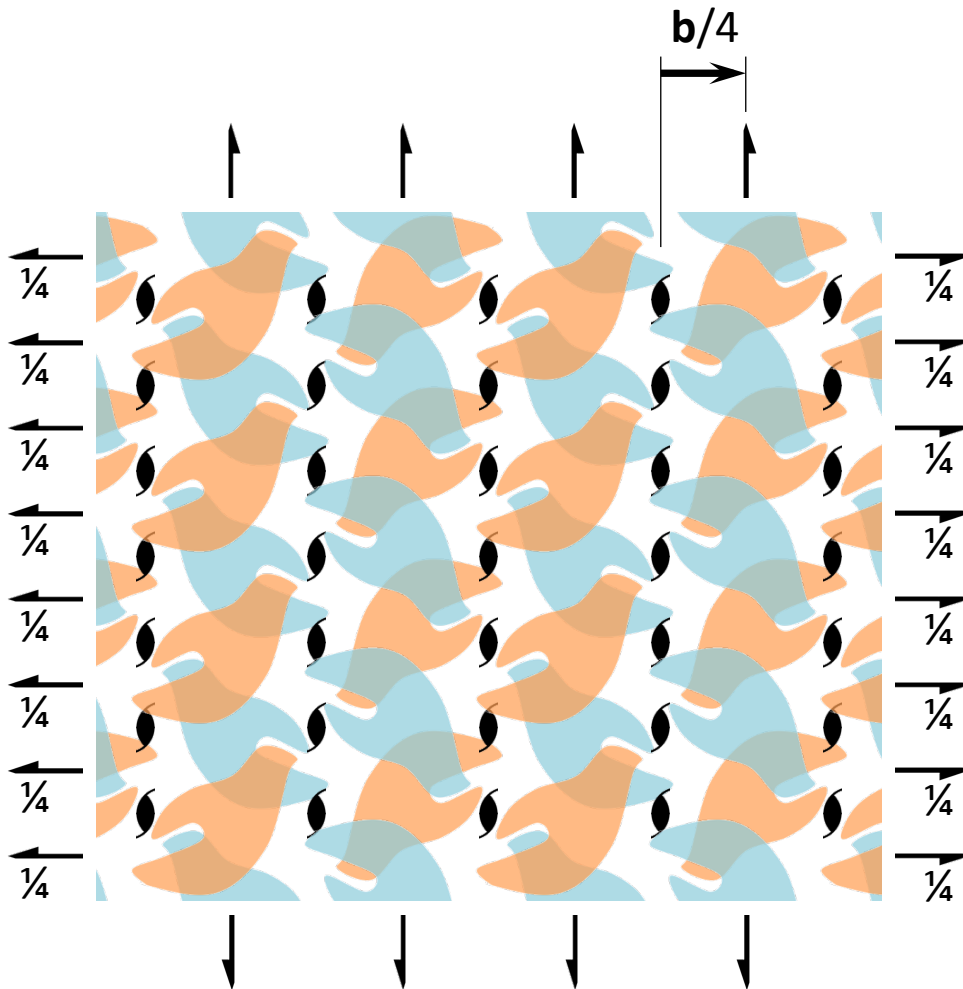
Relative positions of axes



2_1 (plane of figure): $\leftarrow \rightarrow$

2_1 (along view): $\curvearrowright$

Relative positions of axes



2_1 (plane of figure): $\longleftrightarrow$

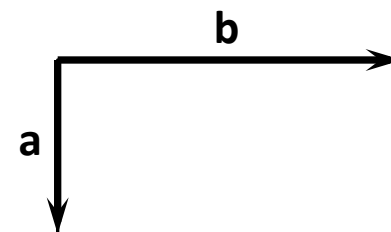
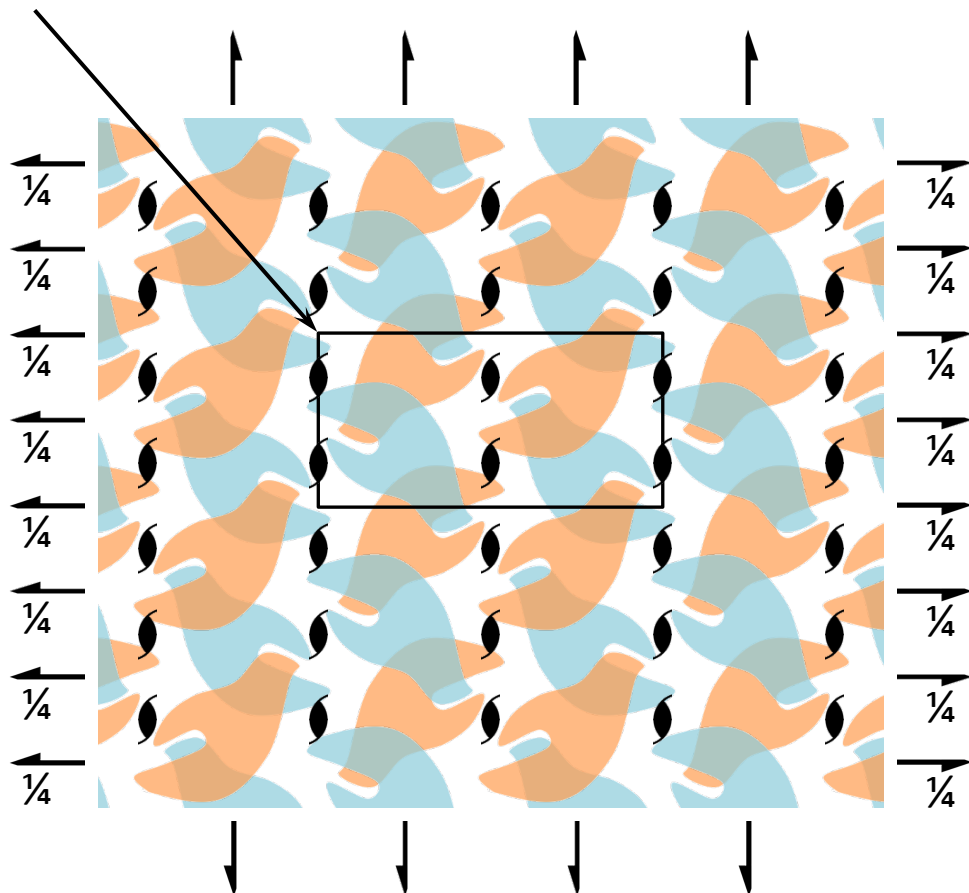
2_1 (along view): $\curvearrowright$

The adjacent axes running in different directions are offset by $1/4$ of corresponding base vector.

The horizontal $1/4$ indicates a offset of $(n + 1/4) \mathbf{c}$ into the figure.

Choice of origin is a convention. Notation

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



2_1 (plane of figure): $\longleftrightarrow$

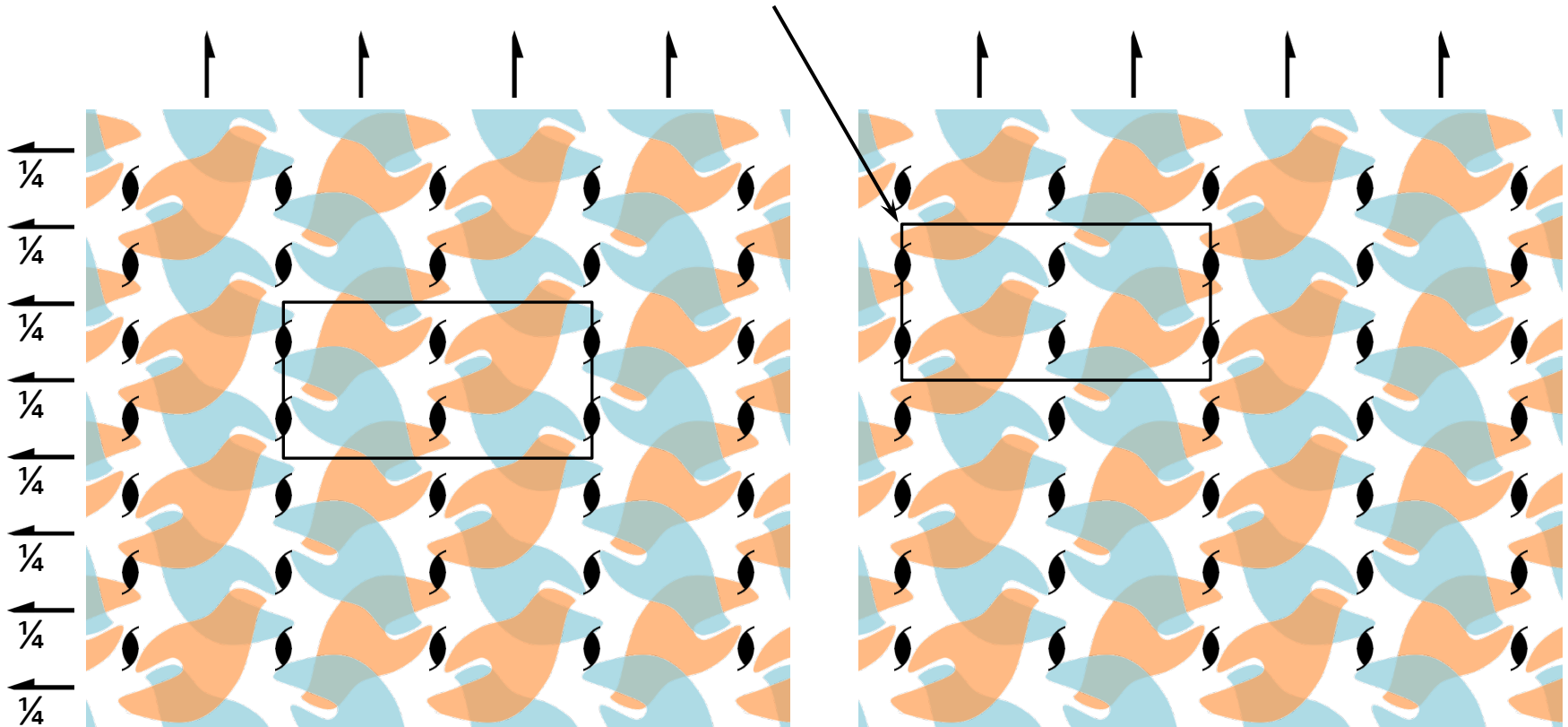
2_1 (along view): $\curvearrowright$

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

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

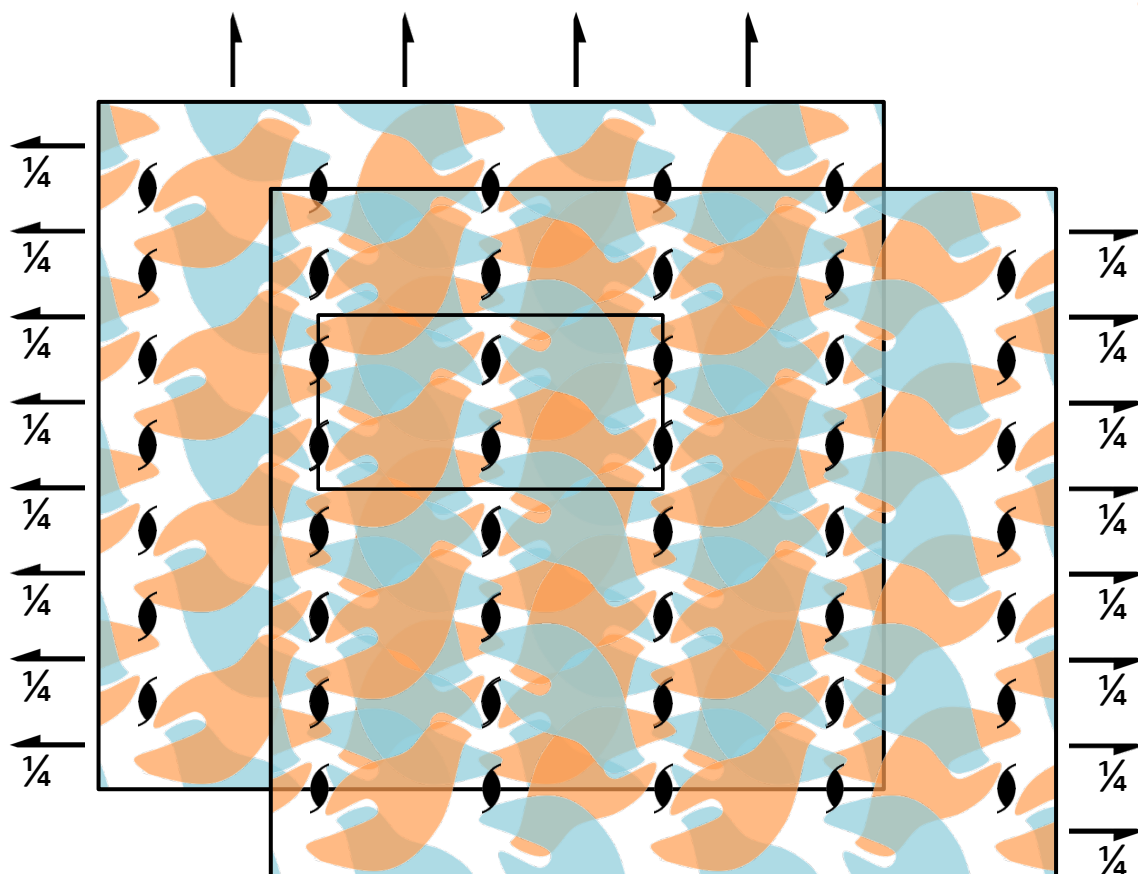
Alternative origins

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



Structures "solved in alternative origins"

Superpose two sets of coordinates. **Positions of axes match** (requirement for convention).



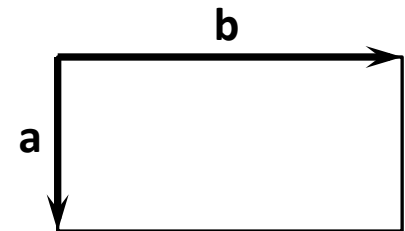
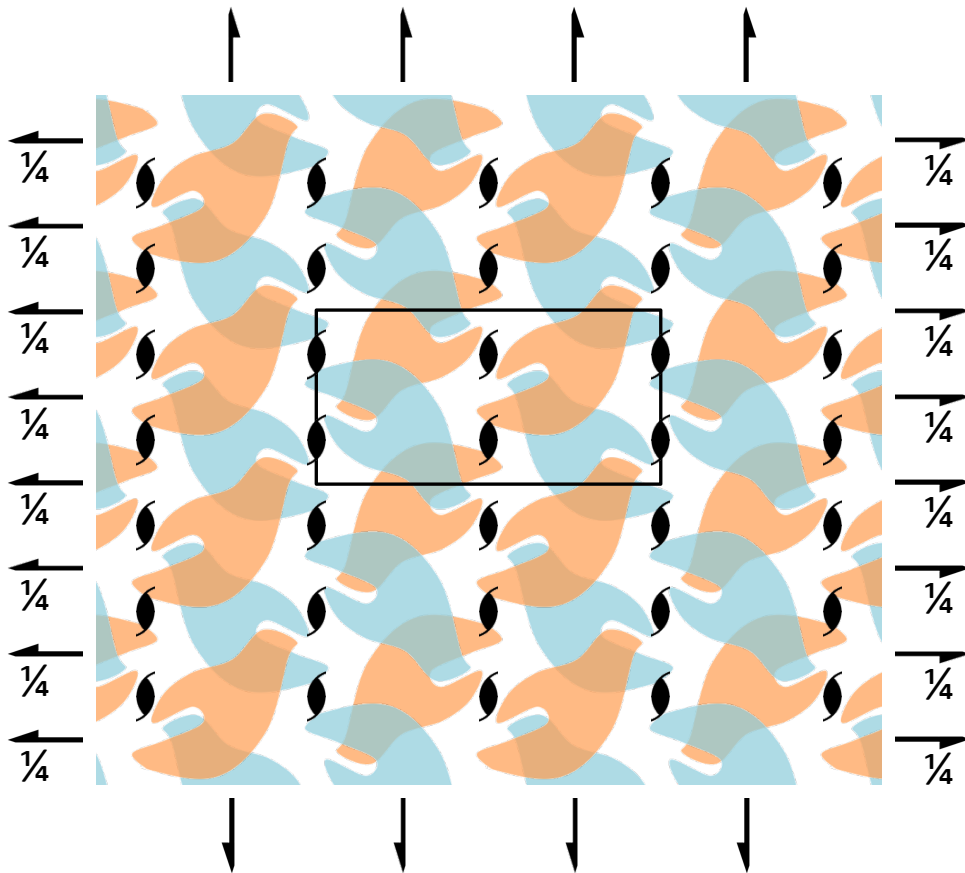
The structures do not match.

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

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

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

Complete picture



2_1 (plane of figure): $\leftarrow \rightarrow$

2_1 (along view): $\curvearrowright$

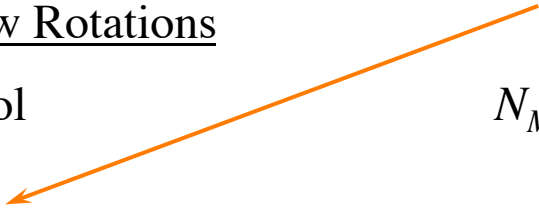
- Example structure (using Coot)
 - examine symmetry operations
 - construct space group
 - assign crystallographic origin
- **Classification of space groups**
- Space group symbols
 - identify space group of the example structure
- Space groups in the International Tables
- Symmetry of diffraction pattern
 - 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 $360^\circ / N$.

Screw rotation: Rotate by $360^\circ / N$ and translate by $(\mathbf{t} M / N)$ where $\mathbf{t}$ is the shortest crystallographic translation along the rotation axis

<u>Proper Rotations</u>			<u>Screw Rotations</u>		Example
	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

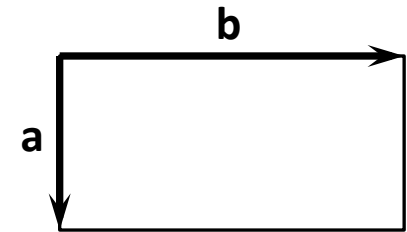
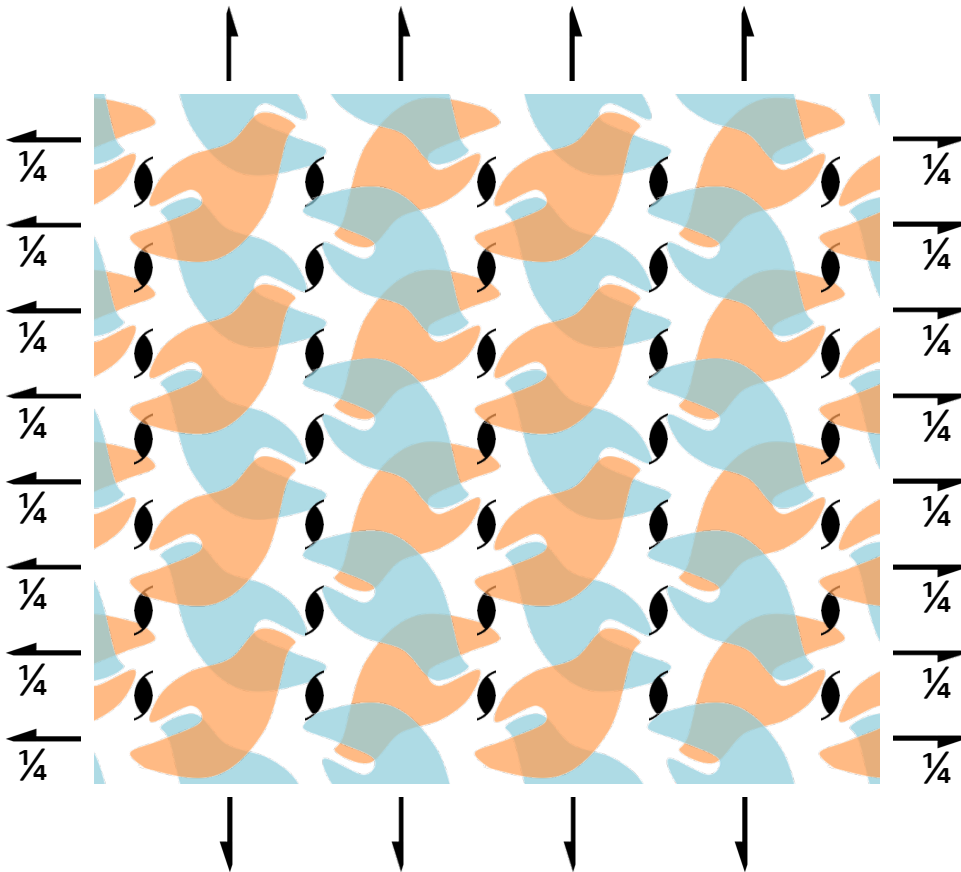
- All possible combinations of symmetry elements => 230 space groups
- Because protein and nucleic acid molecules are chiral, there are only 65 “biological” space groups.
- Space groups are divided on 7 crystal system based on
 - the presence of symmetry elements of a certain order (6, 4, 3, 2)
 - the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

Axes orders? How many different orientations?



2_1 (plane of figure): $\longleftrightarrow$

2_1 (along view): $\curvearrowright$

Crystal Systems

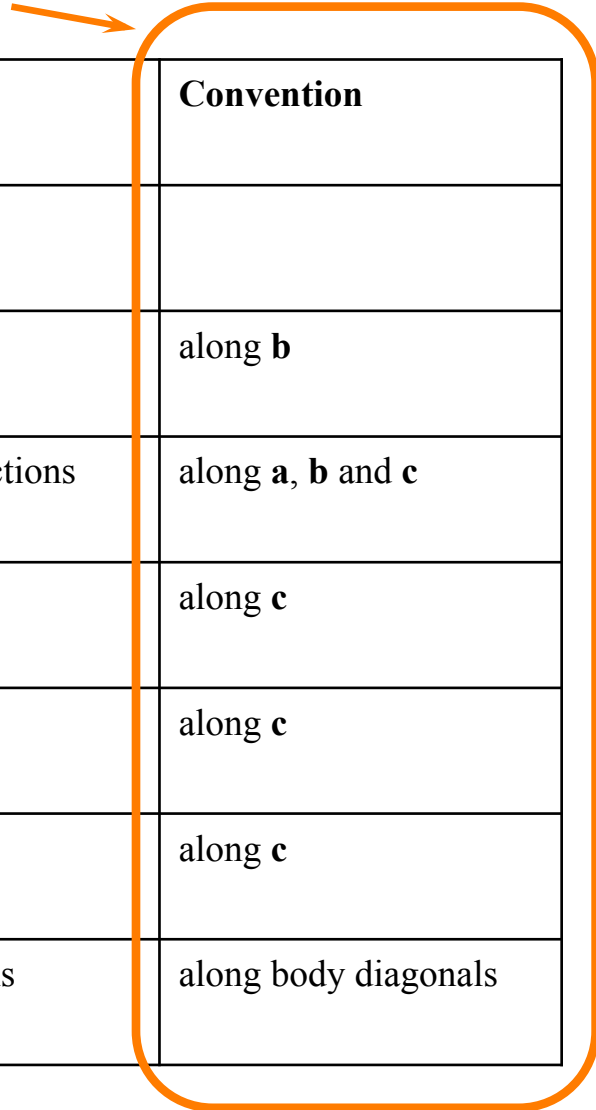
* In macromolecular crystals the symmetry elements are all rotations

Crystal System	Characteristic symmetry elements	Convention
1. Triclinic	Translations only	
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6. Hexagonal	6-fold axes, all parallel	along c
7. Cubic	3-fold axes in four different orientations	along body diagonals

example

Crystal Systems

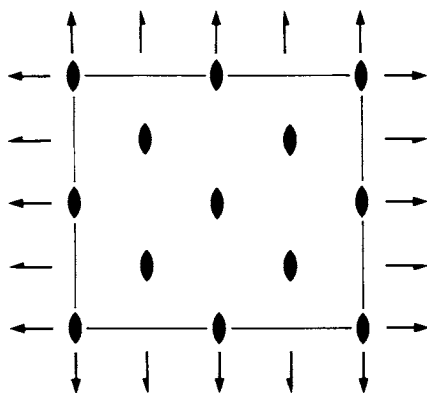
Some SGs require use of centred (**non-primitive**) unit cells



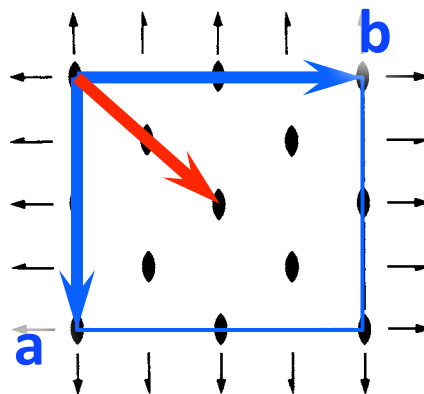
Crystal System	Characteristic symmetry elements	Convention
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5. Trigonal	3-fold axes, all parallel	along c
6. Hexagonal	6-fold axes, all parallel	along c
7. Cubic	3-fold axes in four different orientations	along body diagonals

C222: an example of a centred cell

C222
as presented in the
International Tables
for Crystallography

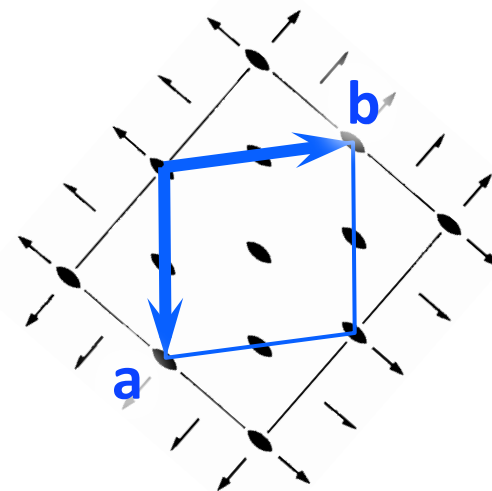


Standard setting;
C means additional
translation $\frac{1}{2}(\mathbf{a} + \mathbf{b})$



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

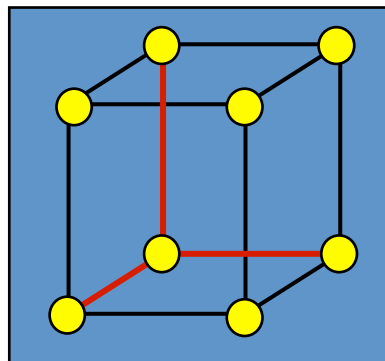
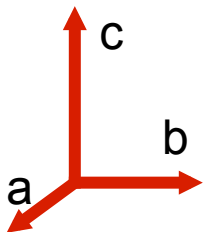
If we were using
a primitive cell



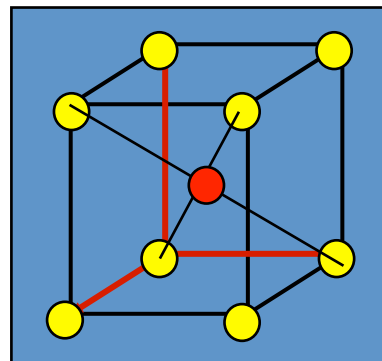
2-fold axes are along
face diagonals (non-
conventional crystal
setting)

Centred cells in pictures

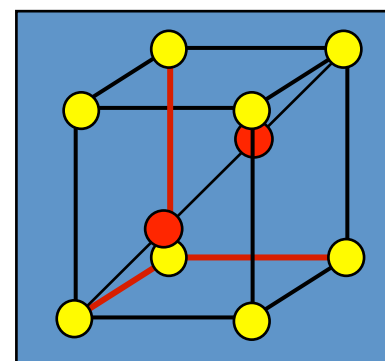
Not a natural phenomenon, but just a notion required by convention on direction of axes



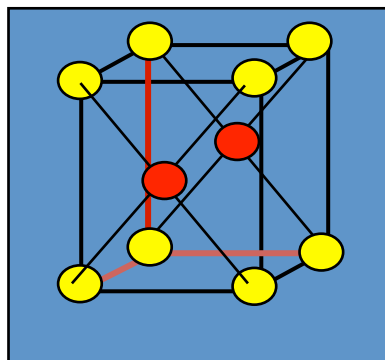
P – Primitive



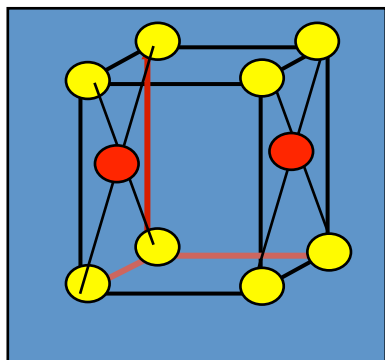
I – Body centred



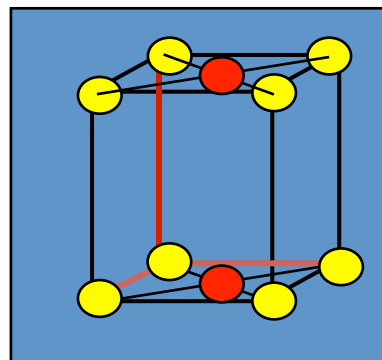
H – Hexagonal



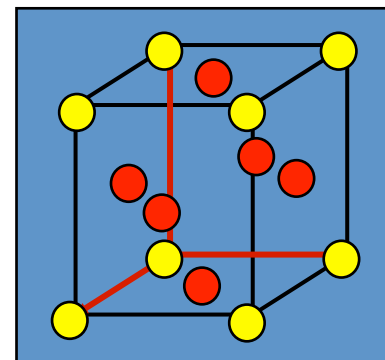
A – Face centred (A)



B – Face centred (B)



C – Face centred (C)



F – Face centred (all)

Bravais lattices

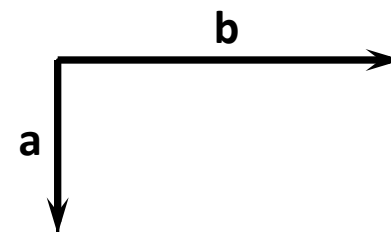
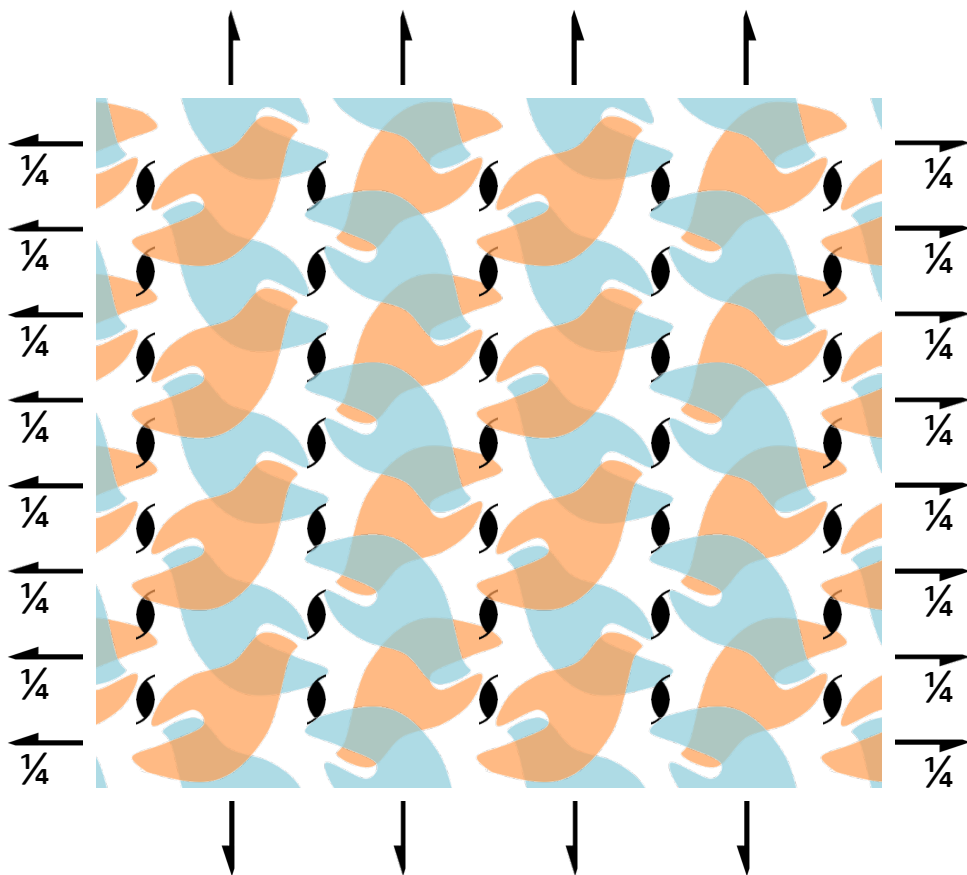
- 7 crystal systems, combined with some of the centring types (P, C, I, F or H) gives 14 Bravais lattices
 - excluded are impossible combinations (*e.g.* $A4$)
 - or one of equivalent combinations (*e.g.* $C4$ and $P4$)

Bravais lattices

example →

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

Are there additional translations?



2_1 (plane of figure): $\longleftrightarrow$

2_1 (along view): $\curvearrowright$

Bravais lattices

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

example

- Example structure (using Coot)
 - examine symmetry operations
 - construct space group
 - assign crystallographic origin
- Classification of space groups
- **Space group symbols**
 - identify space group of the example structure
- Space groups in the International Tables
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- 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
 $a, b, c, \alpha, \beta, \gamma$

Monoclinic

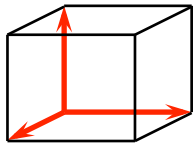
$P 2$ $P 2_1$
 $C 2$

Standard HM symbols: papers

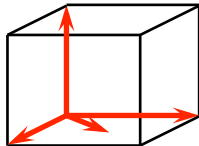
$P 1 2 1$ $P 1 2_1 1$
 $C 1 2 1$

Extended HM symbols: PDB

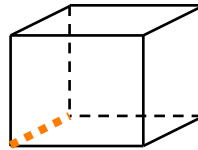
P or C



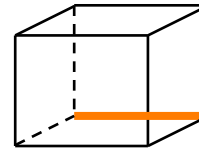
or



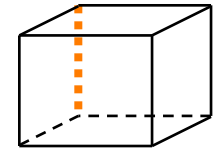
None or 1



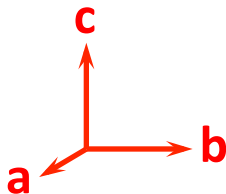
2 or 2_1



None or 1



None or "1" mean no symmetry axes in a given direction
 "2" or " 2_1 " mean 2-fold axes in a given direction



$$\alpha = \gamma = 90^\circ$$

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

Monoclinic

$P 2$

$P 2_1$

Standard HM symbols: papers

$P 2 1 1$

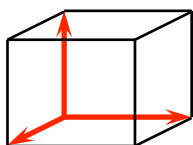
$P 2_1 1 1$

Extended HM symbols: PDB

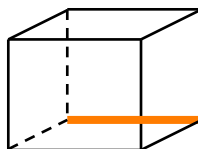
An example of a non-standard setting

Only occur in some structures solved long ago

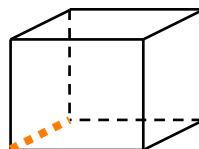
P



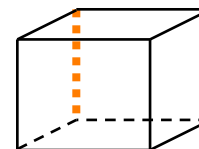
2 or 2_1



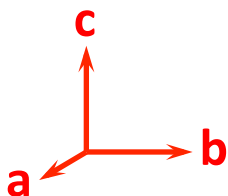
None or 1



None or 1



None or "1" mean no symmetry axes in a given direction
"2" or " 2_1 " mean 2-fold axes in a given direction



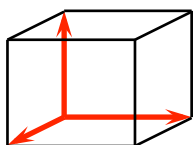
$$\beta = \gamma = 90^\circ$$

Note: non-standard setting: the 2-fold is along **a**

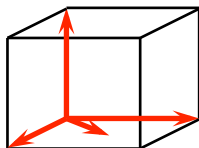
Orthorhombic

$P 2 2 2$ $P 2 2 2_1$ $P 2_1 2_1 2$ $P 2_1 2_1 2_1$
 $C 2 2 2$ $C 2 2 2_1$
 $I 2 2 2$ $I 2_1 2_1 2_1$
 $F 2 2 2$

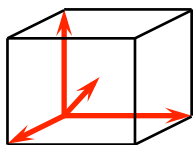
P, C, I or F



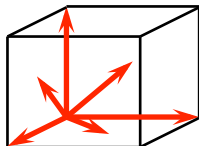
or



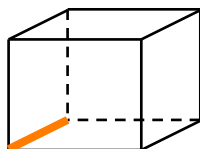
or



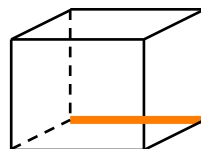
or



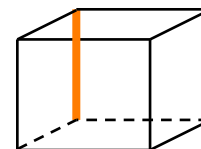
2 or 2_1



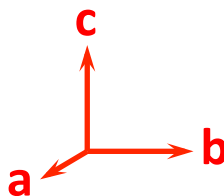
2 or 2_1



2 or 2_1

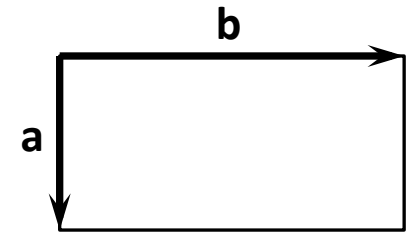
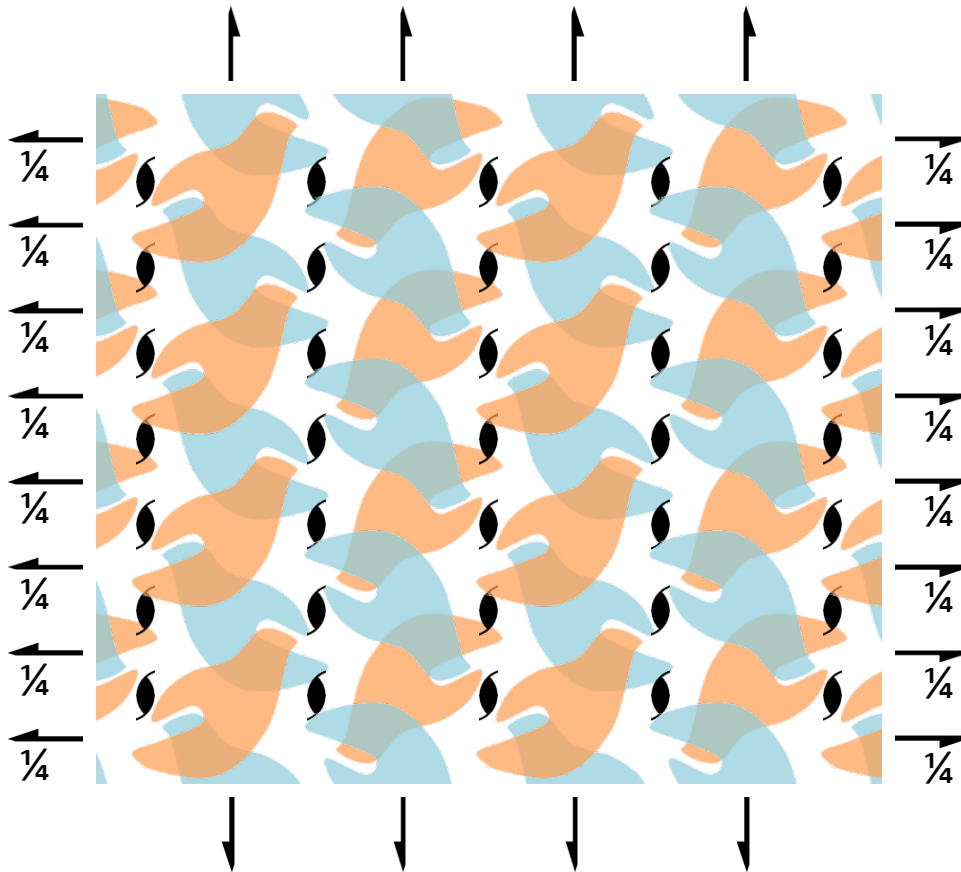


"2" or " 2_1 " means 2-fold axes in a given direction



$$\alpha = \beta = \gamma = 90^\circ$$

Are there any proper 2-fold axes?



2_1 (plane of figure): $\longleftrightarrow$

2_1 (along view): $\curvearrowright$

Orthorhombic

$P 2 2 2$
 $C 2 2 2$
 $I 2 2 2$
 $F 2 2 2$

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

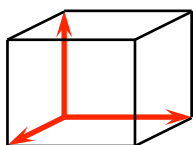
$P 2_1 2_1 2$

$P 2_1 2_1 2_1$

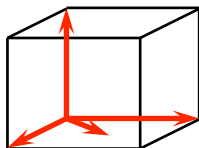
example

$I 2_1 2_1 2_1$

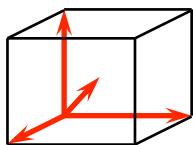
P, C, I or F



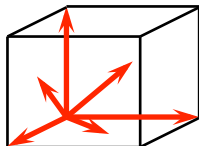
or



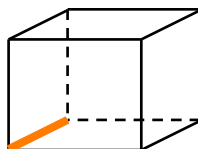
or



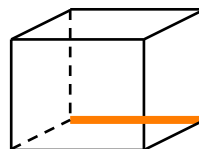
or



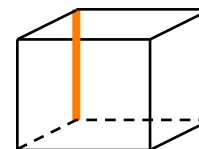
2 or 2_1



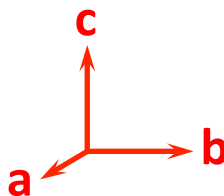
2 or 2_1



2 or 2_1



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



$$\alpha = \beta = \gamma = 90^\circ$$

Tetragonal

$P 4 2_1 2$
 $P 4 2 2$
 $I 4 2 2$

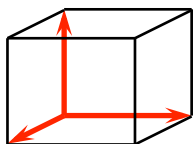
$P 4_1 2_1 2$
 $P 4_1 2 2$
 $I 4_1 2 2$

$P 4_2 2_1 2$
 $P 4_2 2 2$

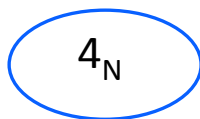
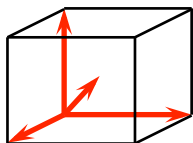
$P 4_3 2_1 2$
 $P 4_3 2 2$

$P 4$ $P 4_1$ $P 4_2$ $P 4_3$
 $I 4$ $I 4_1$

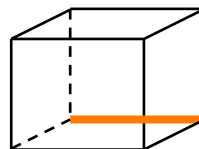
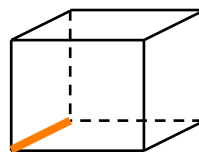
P or I



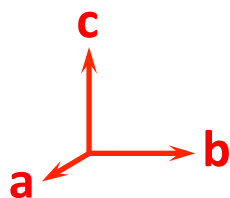
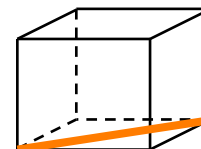
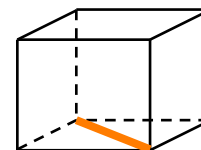
or



2 , 2_1 or None



2 or None



$$\alpha = \beta = \gamma = 90^\circ$$

$$a = b$$

$a \equiv b$ due to the 4-fold relating them

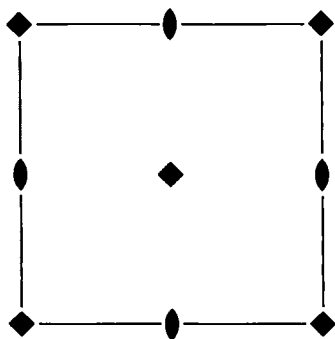
All 2-fold axes are also related via 4-fold rotations and either

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

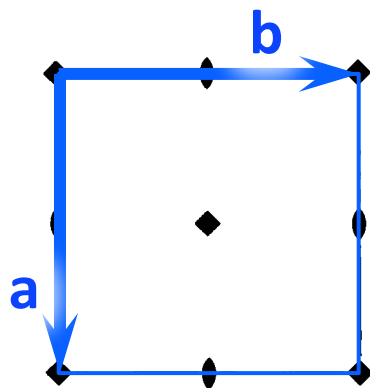
C4: an example of a redundant space group symbol

P4

as presented in the
International Tables
for Crystallography

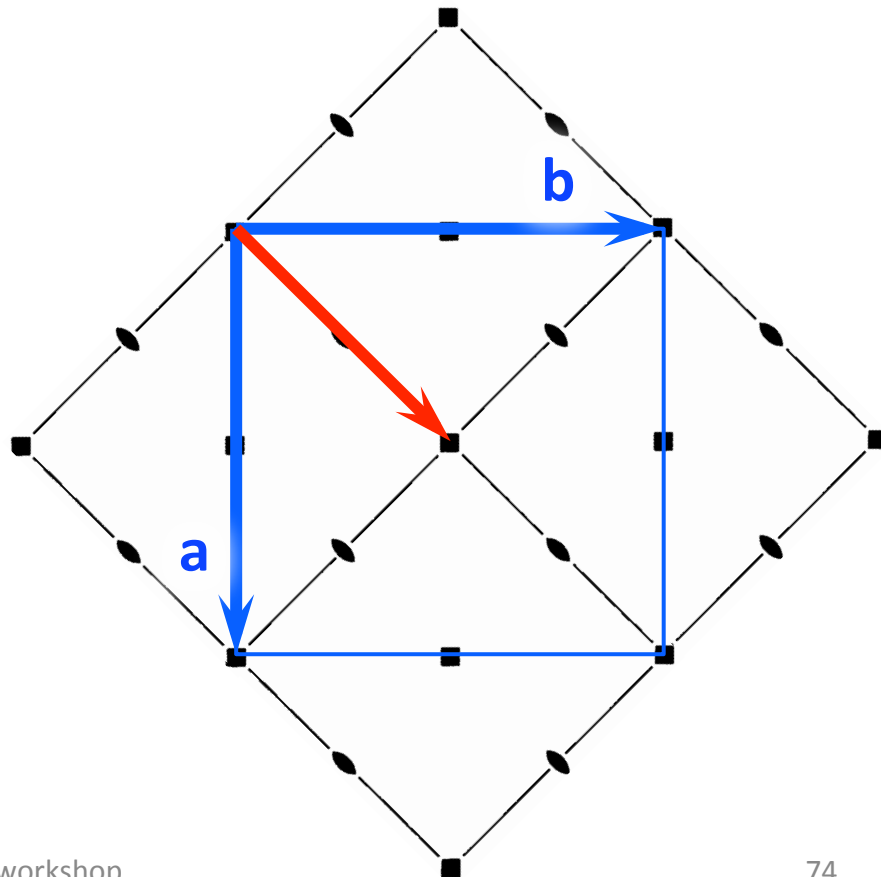


and with base
vectors shown



C4

This is just a different setting obtained
- by rotation 45° and
- redefining base vectors
- additional translation $(\mathbf{a} + \mathbf{b})/2$



Trigonal

$P 3 2 1$

$P 3_1 2 1$

$P 3_2 2 1$

$P 3$

$P 3_1$

$P 3_2$

$P 3_1 1 2$

$P 3_2 1 2$

$H 3 2$

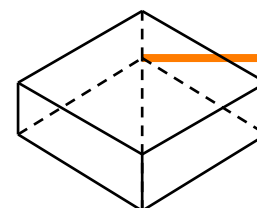
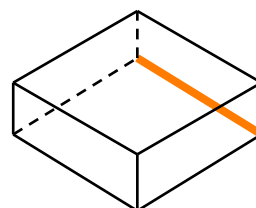
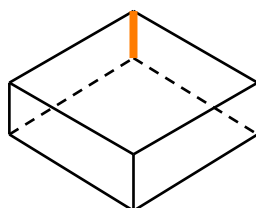
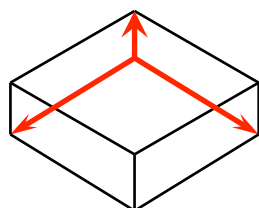
$H 3$

P or $H^{(*)}$

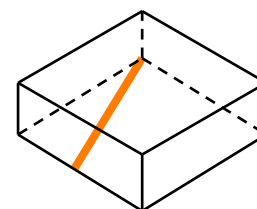
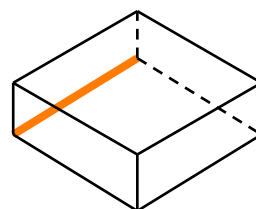
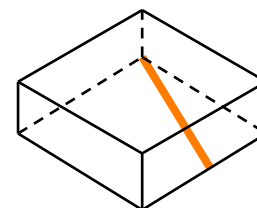
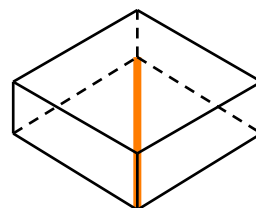
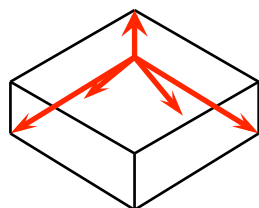
3_N

2, 1 or None

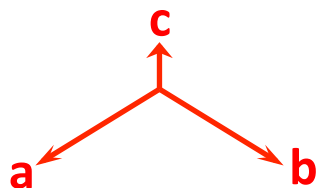
2, 1 or None



or



$$\begin{aligned}\alpha &= \beta = 90^\circ \\ \gamma &= 120^\circ \\ a &= b\end{aligned}$$



(*) 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 4₃ 2₁ 2

Hexagonal

$P 6 2 2$

$P 6_1 2 2$
 $P 6_5 2 2$

$P 6_2 2 2$
 $P 6_4 2 2$

$P 6_3 2 2$

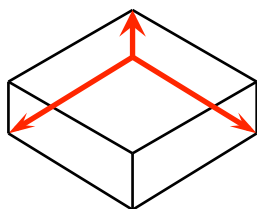
$P 6$

$P 6_1$
 $P 6_5$

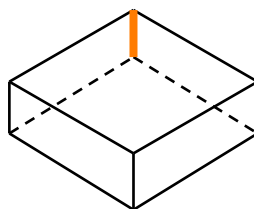
$P 6_2$
 $P 6_4$

$P 6_3$

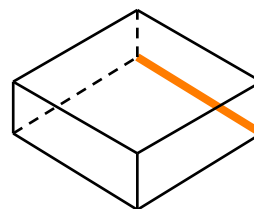
P



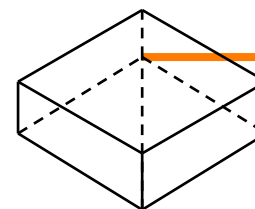
6_N



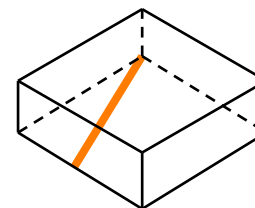
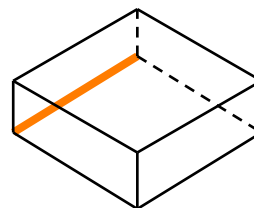
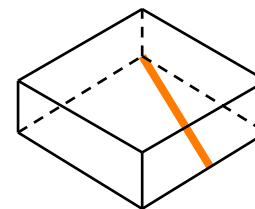
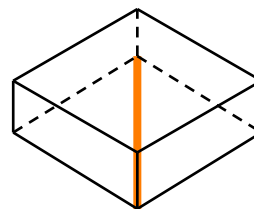
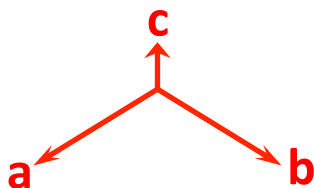
2 or None



2 or None



$$\begin{aligned}\alpha &= \beta = 90^\circ \\ \gamma &= 120^\circ \\ a &= b\end{aligned}$$



Cubic

$P 4 3 2$
 $I 4 3 2$
 $F 4 3 2$

$P 4_1 3 2$
 $I 4_1 3 2$
 $F 4_1 3 2$

$P 4_2 3 2$

$P 4_3 3 2$

$P 2 3$
 $I 2 3$
 $F 2 3$

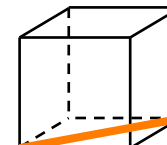
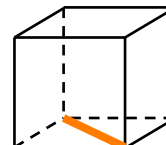
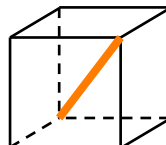
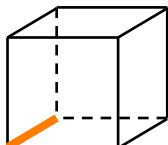
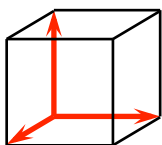
$P 2_1 3$
 $I 2_1 3$

P, I or F

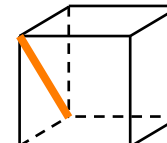
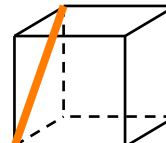
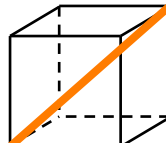
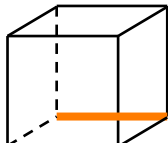
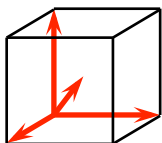
4_N or 2_N

3

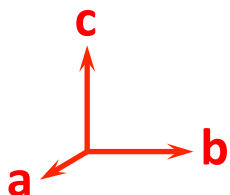
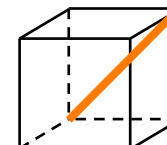
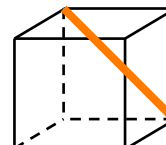
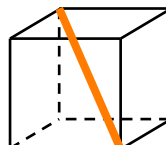
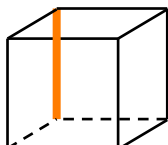
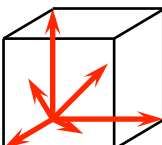
2 or None



or

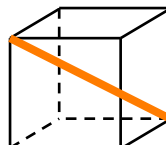


or



$$\alpha = \beta = \gamma = 90^\circ$$

$$a = b = c$$



Monoclinic (lattice based setting)

$$\alpha = \gamma = 90^\circ$$

additional condition:
 $\beta < 120^\circ$

P 1 2 1 *P* 1 2₁ 1

C 1 2 1

I 1 2 1

In orange frame:

- the same space group
- different crystal setting

Orthorhombic (lattice based setting)

$$\alpha = \beta = \gamma = 90^\circ$$

additional condition:
 $a < b < c$

$P 2 2 2$

$P 2 2 2_1$

$P 2 2_1 2$

$P 2_1 2 2$

$P 2_1 2_1 2$

$P 2_1 2 2_1$

$P 2 2_1 2_1$

$P 2_1 2_1 2_1$

$C 2 2 2$

$C 2 2 2_1$

$I 2 2 2$

$I 2_1 2_1 2_1$

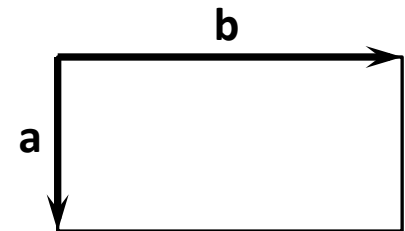
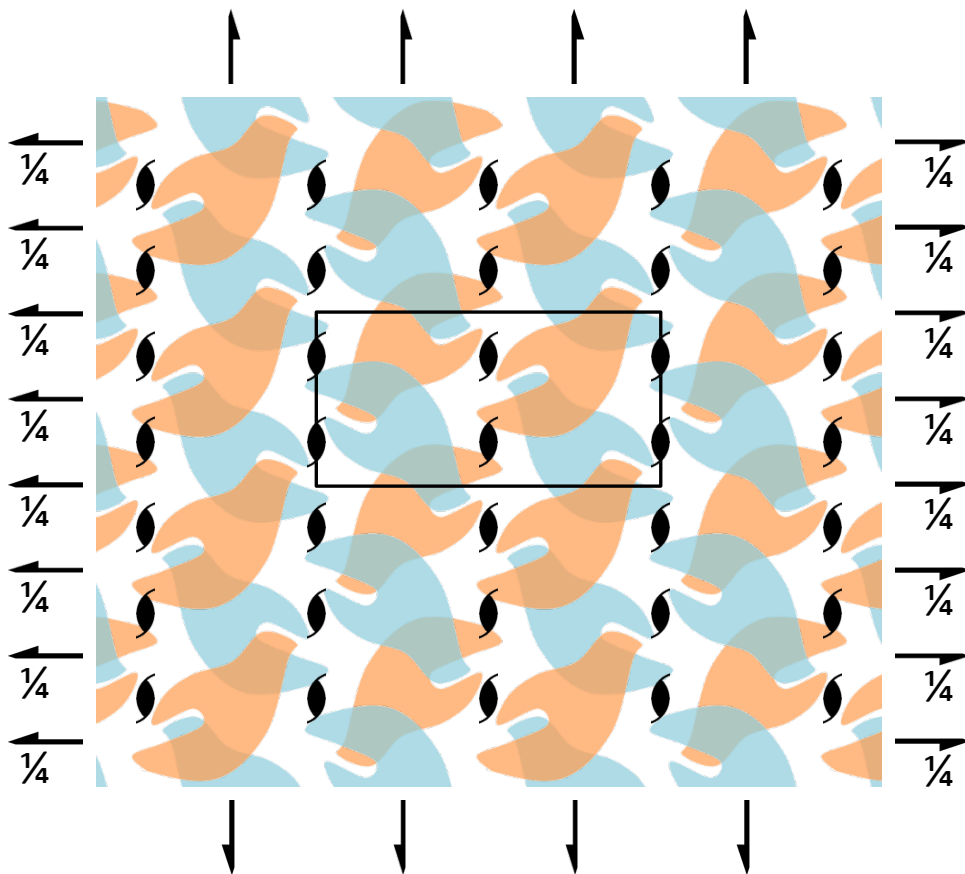
$F 2 2 2$

In orange frames:

- the same space group
- different crystal setting (orientation)

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

Now we know the name: $P2_12_12_1$

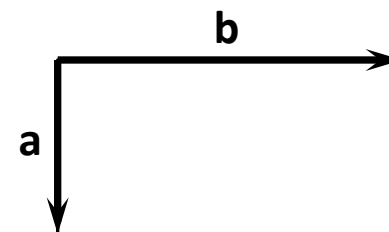
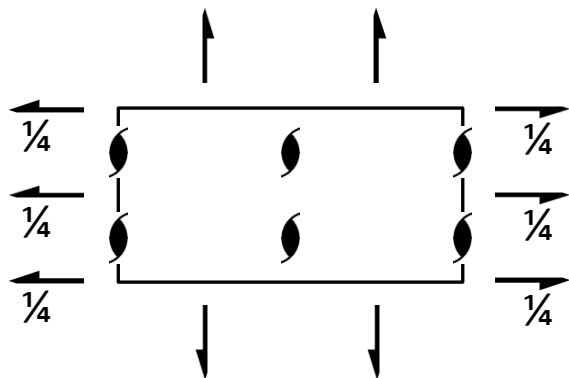


2_1 (plane of figure): $\leftarrow \rightarrow$

2_1 (along view): $\curvearrowright$

Compact representation

$P2_12_12_1$



2_1 (plane of figure):

2_1 (along view):

Presentation in International Tables

$P2_12_12_1$

No. 19

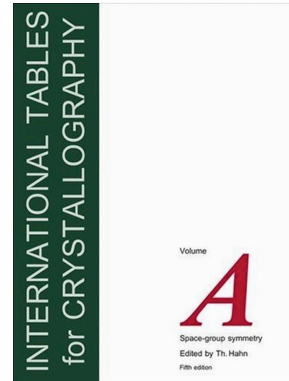
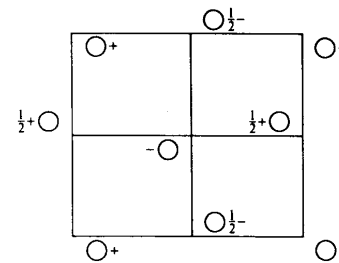
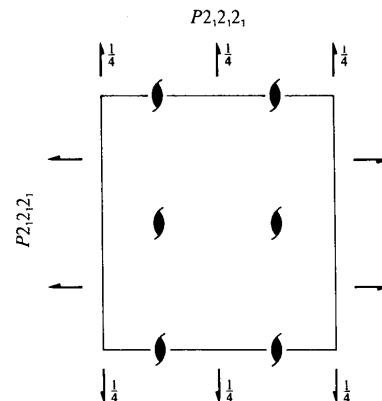
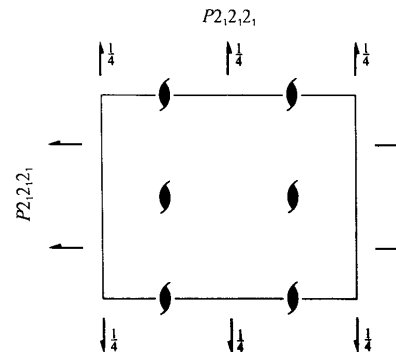
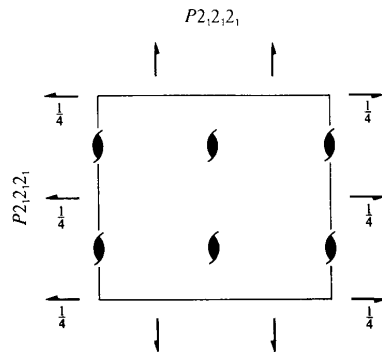
D_2^4

$P2_12_12_1$

222

Orthorhombic

Patterson symmetry $Pmmm$



Has been discussed

(Short) Hermann-Mauguin symbol

$P2_12_12_1$

No. 19

(Extended) Hermann-Mauguin symbol

D_2^4

$P2_12_12_1$

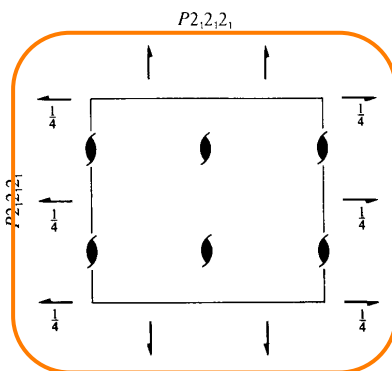
222

Orthorhombic

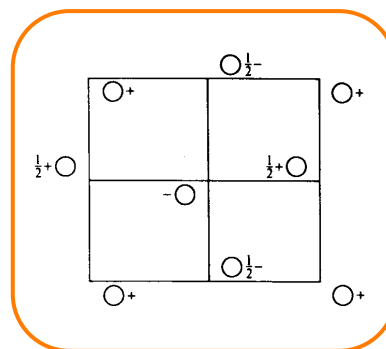
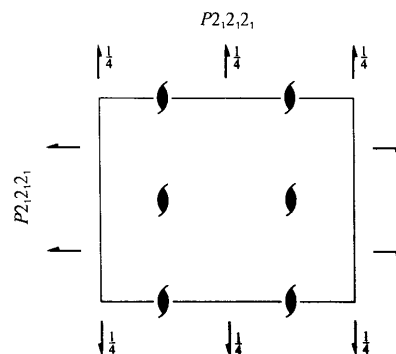
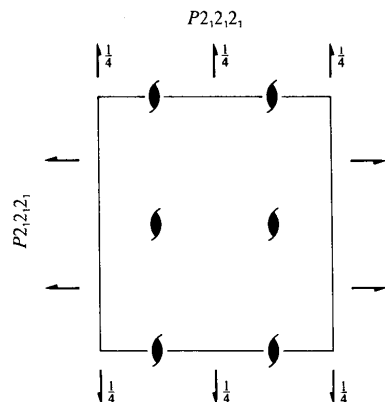
Patterson symmetry $Pmmm$

Crystal system

Location of symmetry elements



Two other projections are also shown for this space group



Set of equivalent points in general position.

We were looking at "molecular wallpaper" instead

Remain to be discussed

Crystal Class
(point group)

222

Orthorhombic

Patterson symmetry **Pmmm**

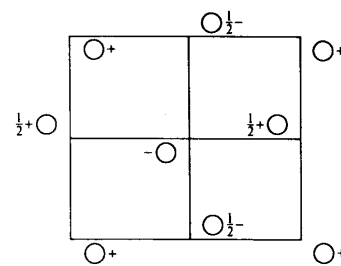
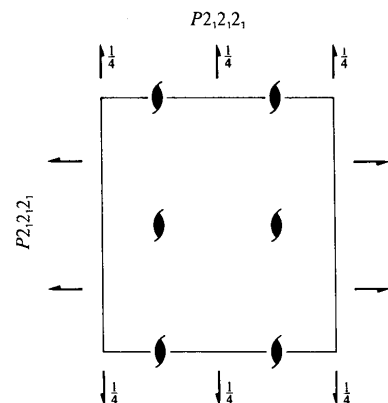
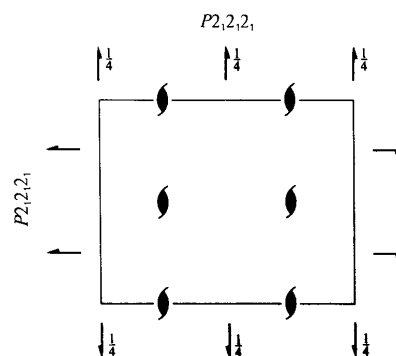
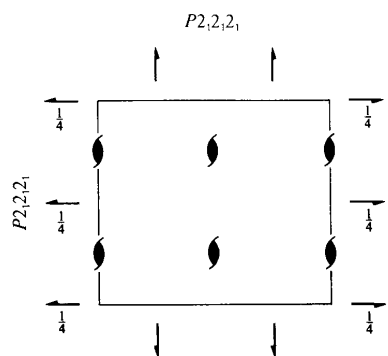
Patterson
symmetry

$P2_12_12_1$

No. 19

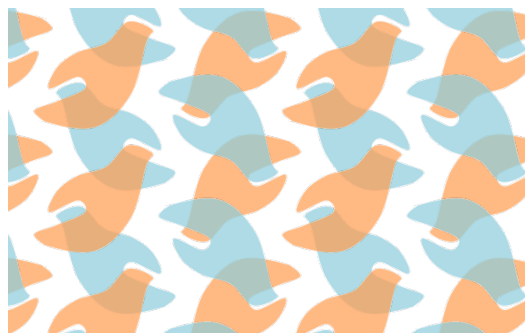
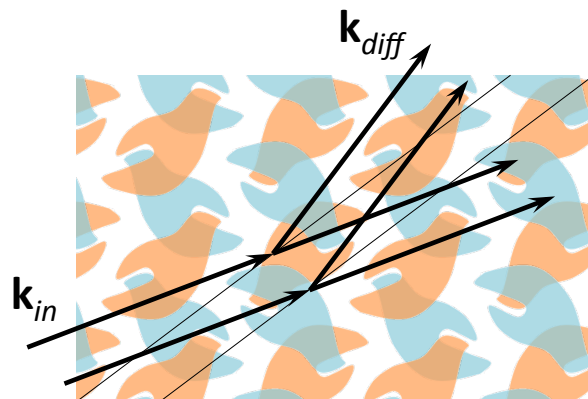
D_2^4

$P2_12_12_1$

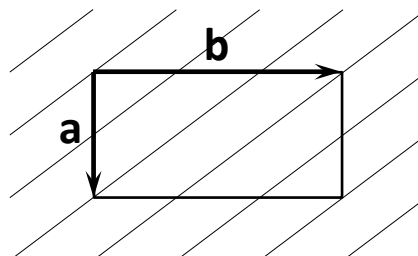


- Example structure (using Coot)
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- **Symmetry of diffraction pattern**
 - point groups
- SG determination in structure solution process

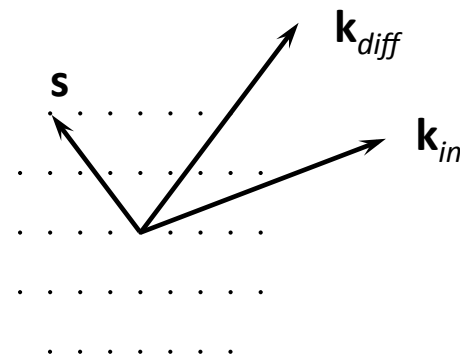
Conventional diffraction scheme



real space



Bragg planes



reciprocal space

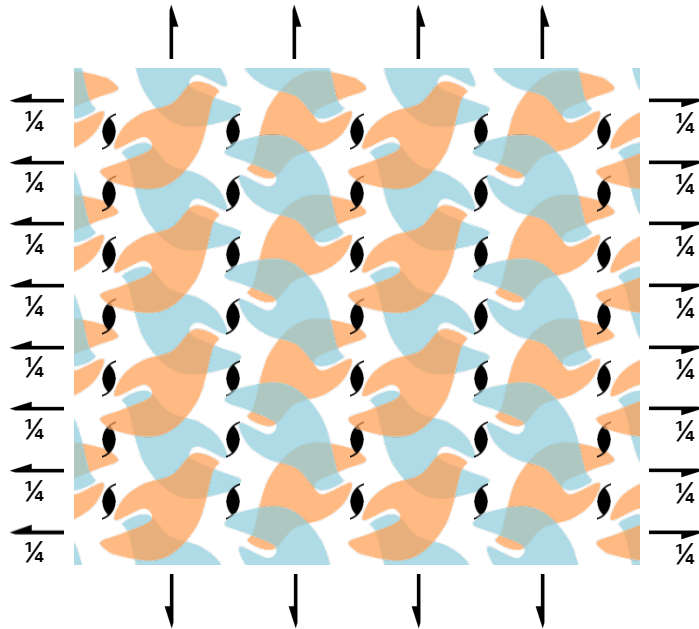
Symmetry of intensities

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

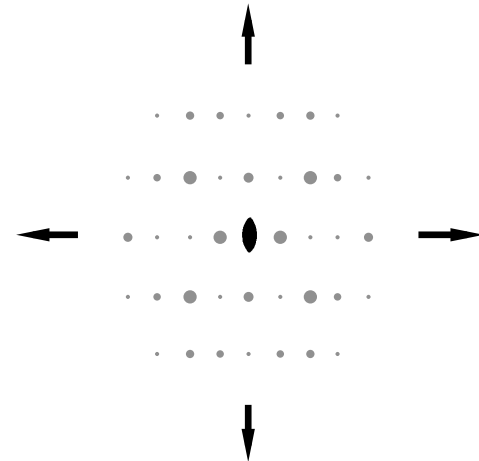
Symmetry of intensities

real space



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

reciprocal space



to give an element of a point group.

Symmetry of intensities

Real space

Crystal structure

Space group operation

The same crystal structure

Reciprocal space

Intensities at Bragg points

Strip any translation component from the space group operation:

Point group operation

The same set of intensities

Space group and point group

Crystal space group

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

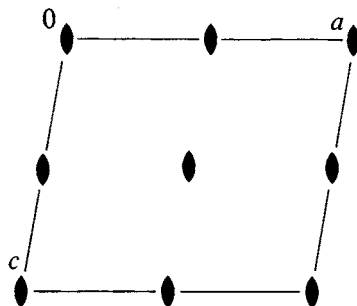
P2

No. 3

UNIQUE AXIS *b*

C_2^1

P121

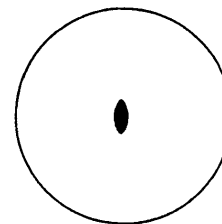


Arithmetic crystal class

2P

Crystal point group

2



Space group and point group

Crystal space group

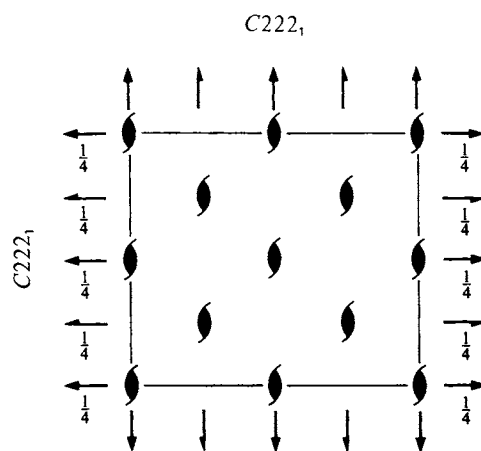
International Tables for Crystallography (2006). Vol. A,

$C222_1$

No. 20

D_2^5

$C222_1$

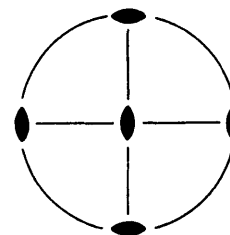


Arithmetic crystal class

222C

Crystal point group

222



Space group and point group

Crystal space group

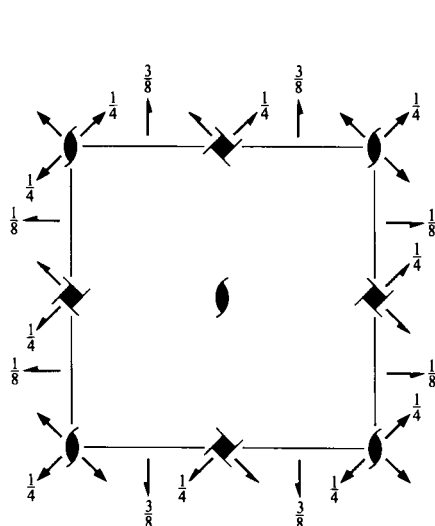
International Tables for Crystallography (2006). Vol. A,

$P4_12_12$

No. 92

D_4^4

$P4_12_12$

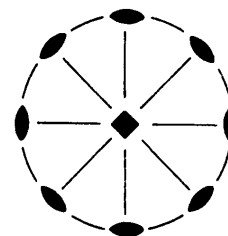


Arithmetic crystal class

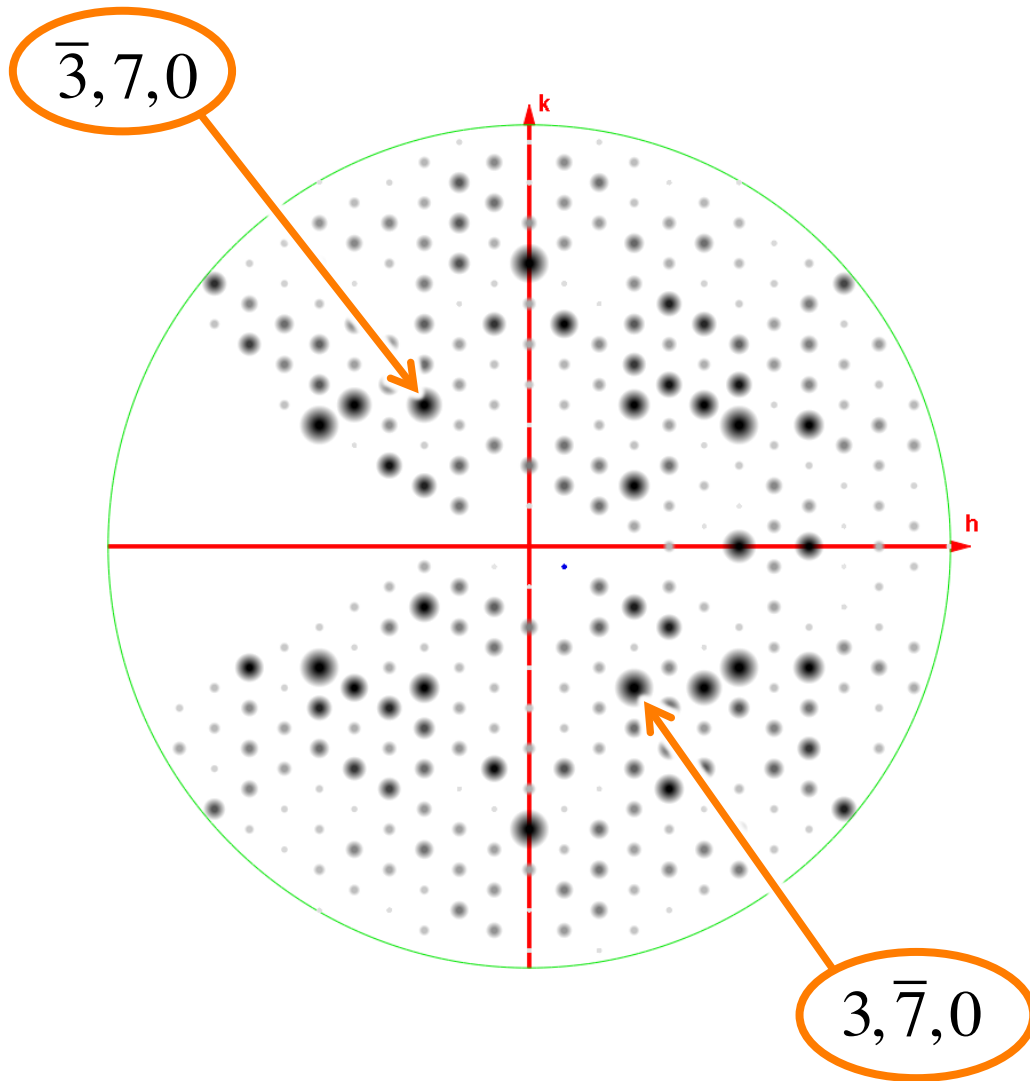
$422P$

Crystal point group

422



Friedel's law



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

Point group and Laue group

+ inversion =

Arithmetic crystal class

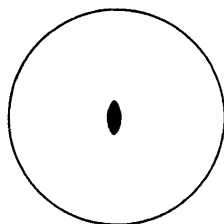
$2P$

Patterson space group

$P\ 1\ 2/m\ 1$

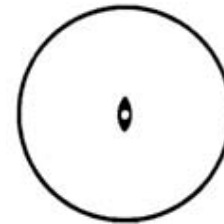
Crystal point group

2



Laue point group

$2/m$



Point group and Laue group

+ inversion =

Arithmetic crystal class

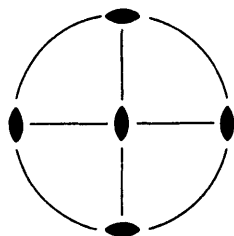
222C

Patterson space group

C m m m

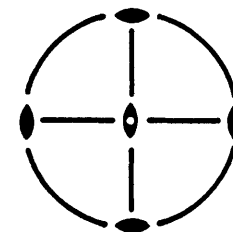
Crystal point group

222



Laue point group

m m m



Point group and Laue group

+ inversion =

Arithmetic crystal class

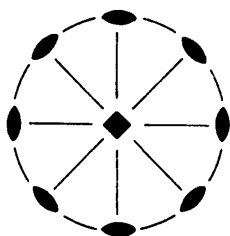
422P

Patterson space group

P 4/m m m

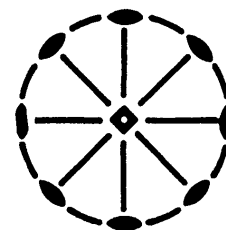
Crystal point group

422



Laue point group

4/m m m



The eleven Laue point groups or crystal classes

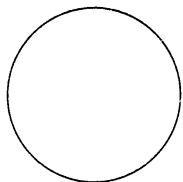
Crystal system	Laue point group (experiment)	Non-centrosymmetric point groups belonging to the Laue point group
Cubic	$m\bar{3}m$ $m\bar{3}$	432 $\bar{4}3m$ 23
Tetragonal	$4/mmm$ $4/m$	422 $4mm$ $\bar{4}2m$ 4 $\bar{4}$
Orthorhombic	mmm	222 $mm2$
Trigonal	$3m$ 3	32 $3m$ 3
Hexagonal	$6/mmm$ $6/m$	622 $6mm$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

The eleven Laue point groups or crystal classes

Crystal system	Laue point group (experiment)	Non-centrosymmetric point groups belonging to the Laue point group
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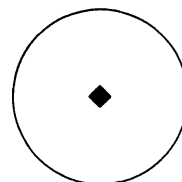
The point groups that can exist in protein crystals

1

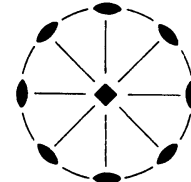


If it helps view as sphere

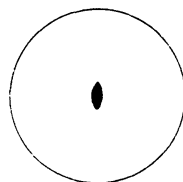
4



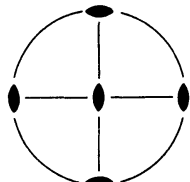
422



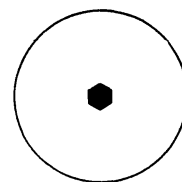
2



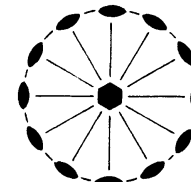
222



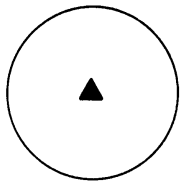
6



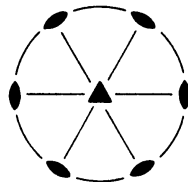
622



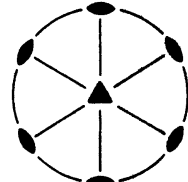
3



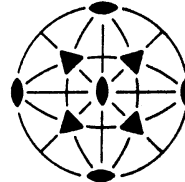
321



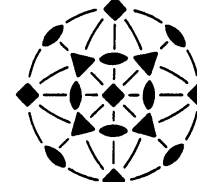
312



23



432



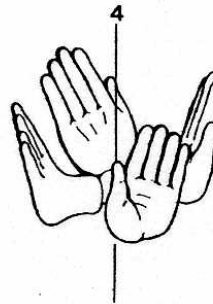
The point groups that can exist in protein crystals

1

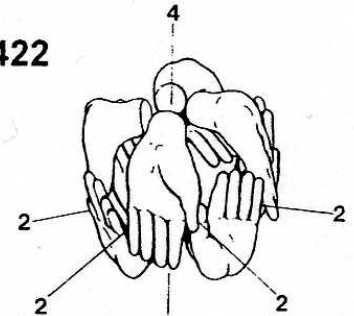


maybe an easier
representation

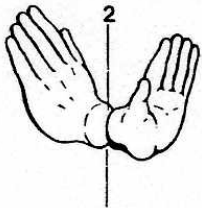
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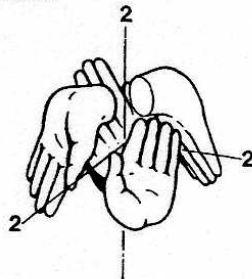
422



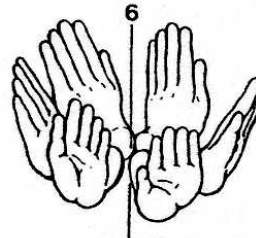
2



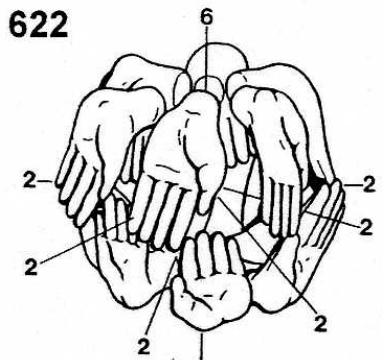
222



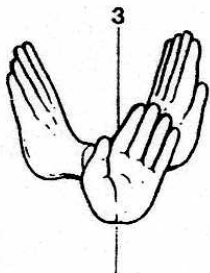
6



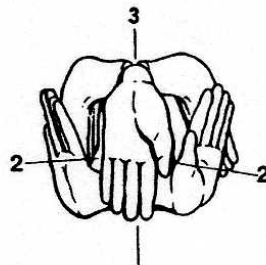
622



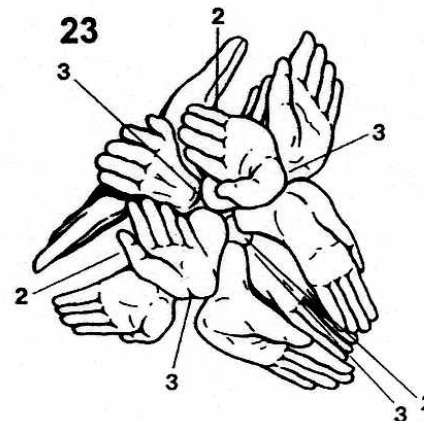
3



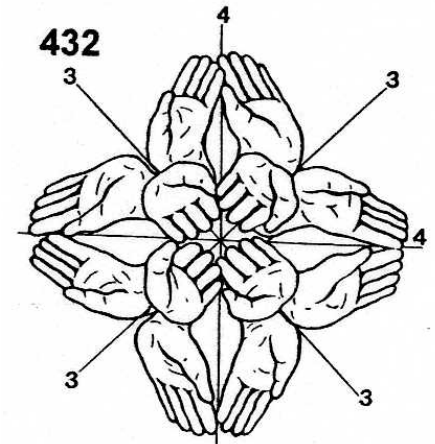
32



23



432



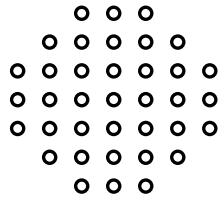
- Example structure (using Coot)
 - examine symmetry operations
 - construct space group
 - assign crystallographic origin
- Classification of space groups
- Space group symbols
 - identify space group of the example structure
- Space groups in the International Tables
- Symmetry of diffraction pattern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

How do we deduce the Space Group in practice?

- We start in reciprocal space (Laue 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

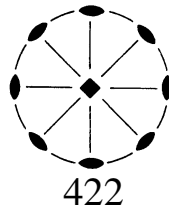
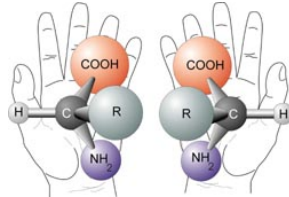
Space group assignment (e.g. *Pointless*)

Reciprocal space lattice
(positions of reflections)



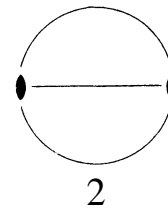
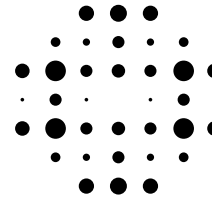
(Approximate)
Laue point group

Mirror symmetry is not
allowed in biological
macromolecules



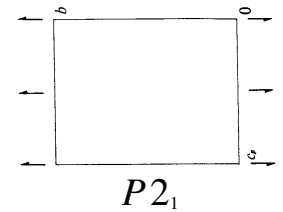
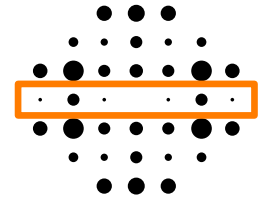
Highest possible
crystal point group

Intensities of
reflections



Probable
crystal point group

Intensities of axial
reflections



Probable
crystal space group

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

End