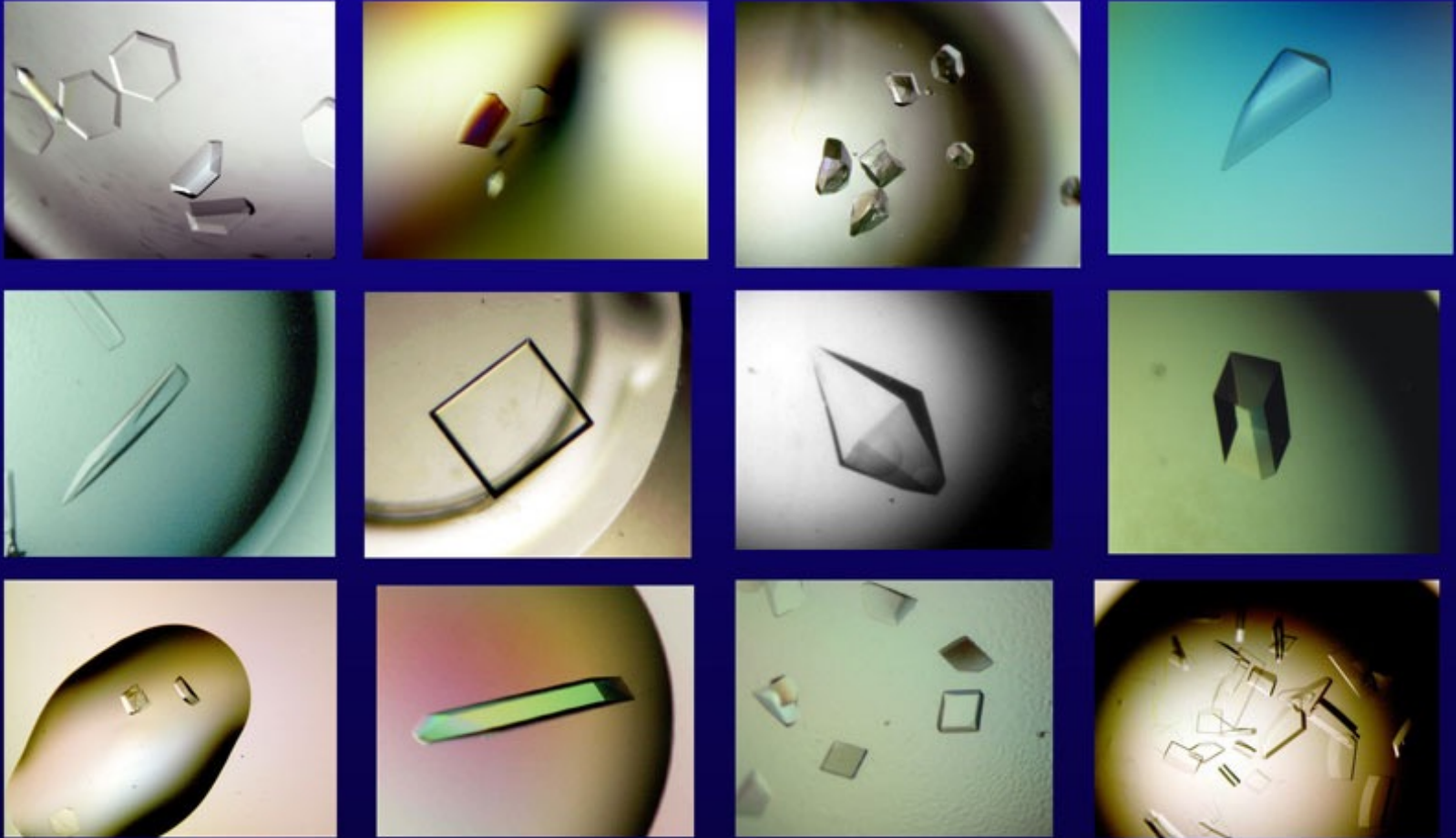
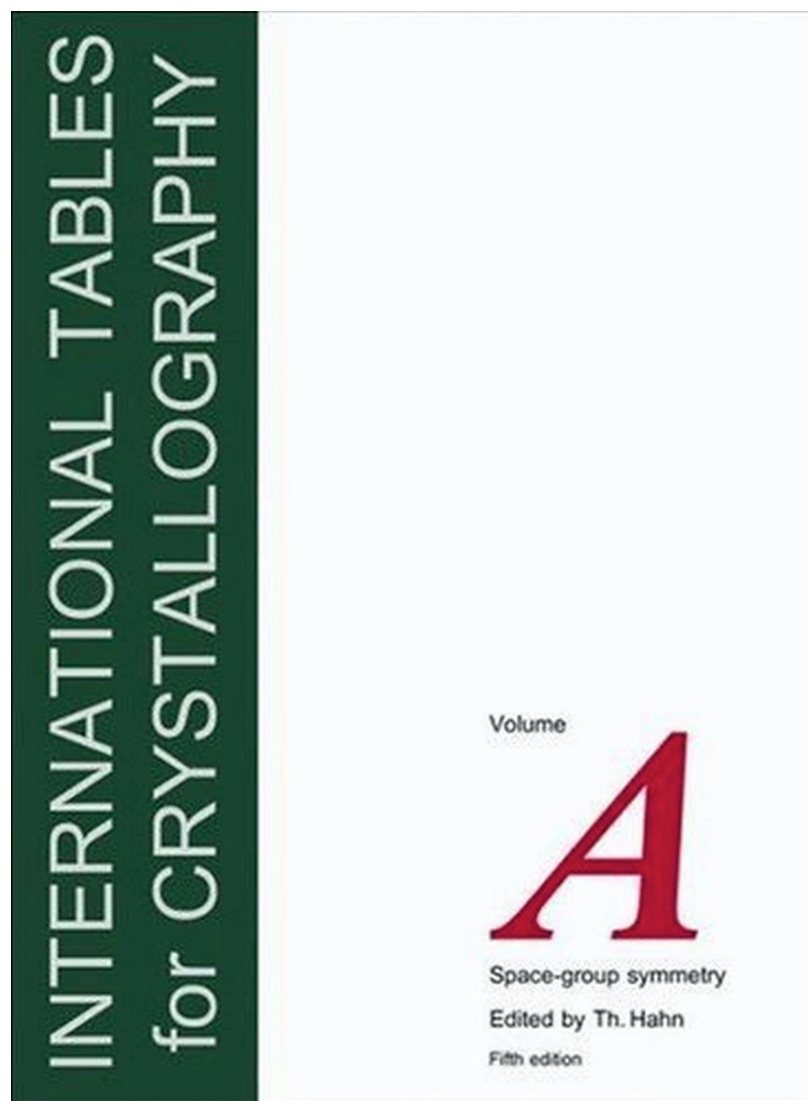


Introduction to space groups

Andrey Lebedev, CCP4





Further referred
to as ITC-A

Space group representation in ITC-A

$P2_12_12_1$

No. 19

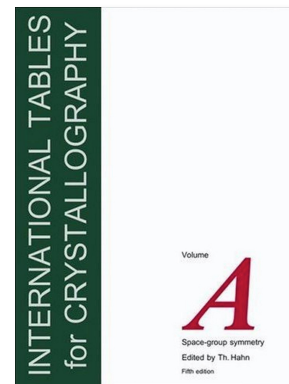
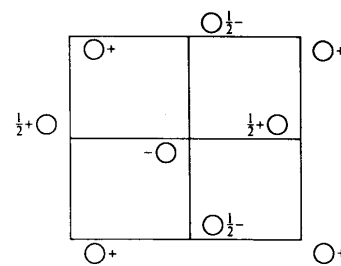
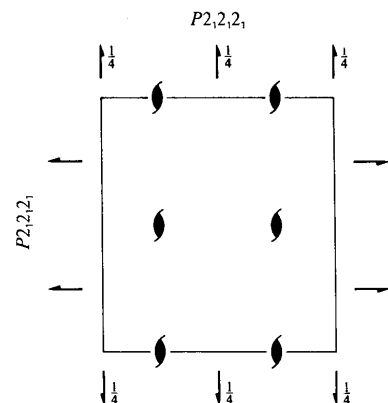
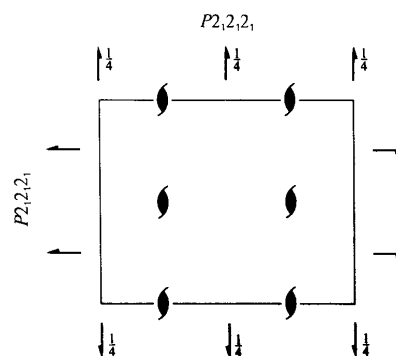
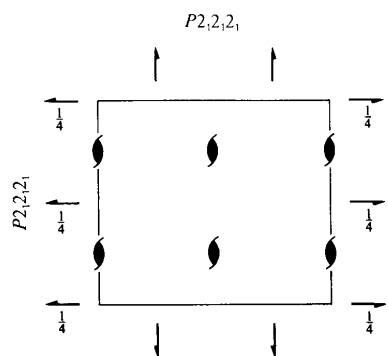
D_2^4

$P2_12_12_1$

222

Orthorhombic

Patterson symmetry $Pmmm$



Space group representation in ITC-A

$P2_12_12_1$

No. 19

D_2^4

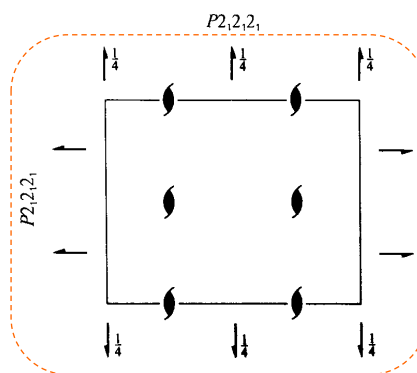
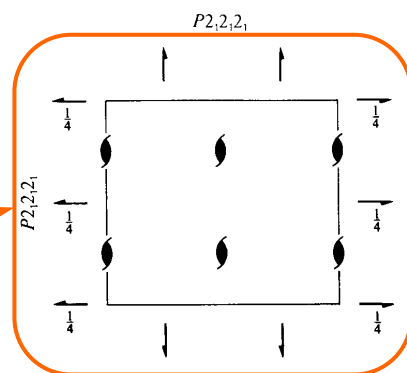
$P2_12_12_1$

222

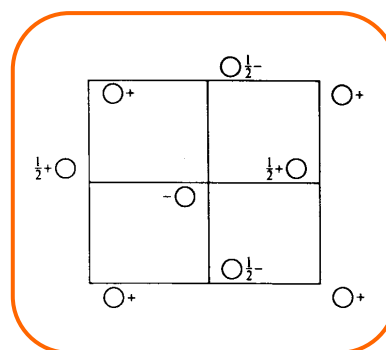
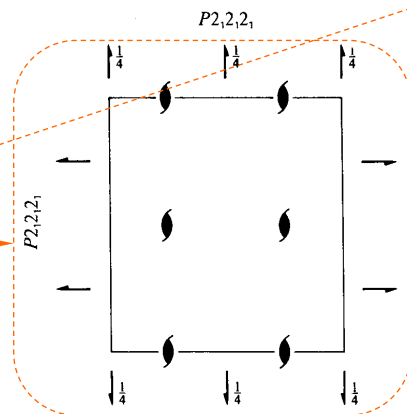
Orthorhombic

Patterson symmetry $Pmmm$

Location of
symmetry
elements



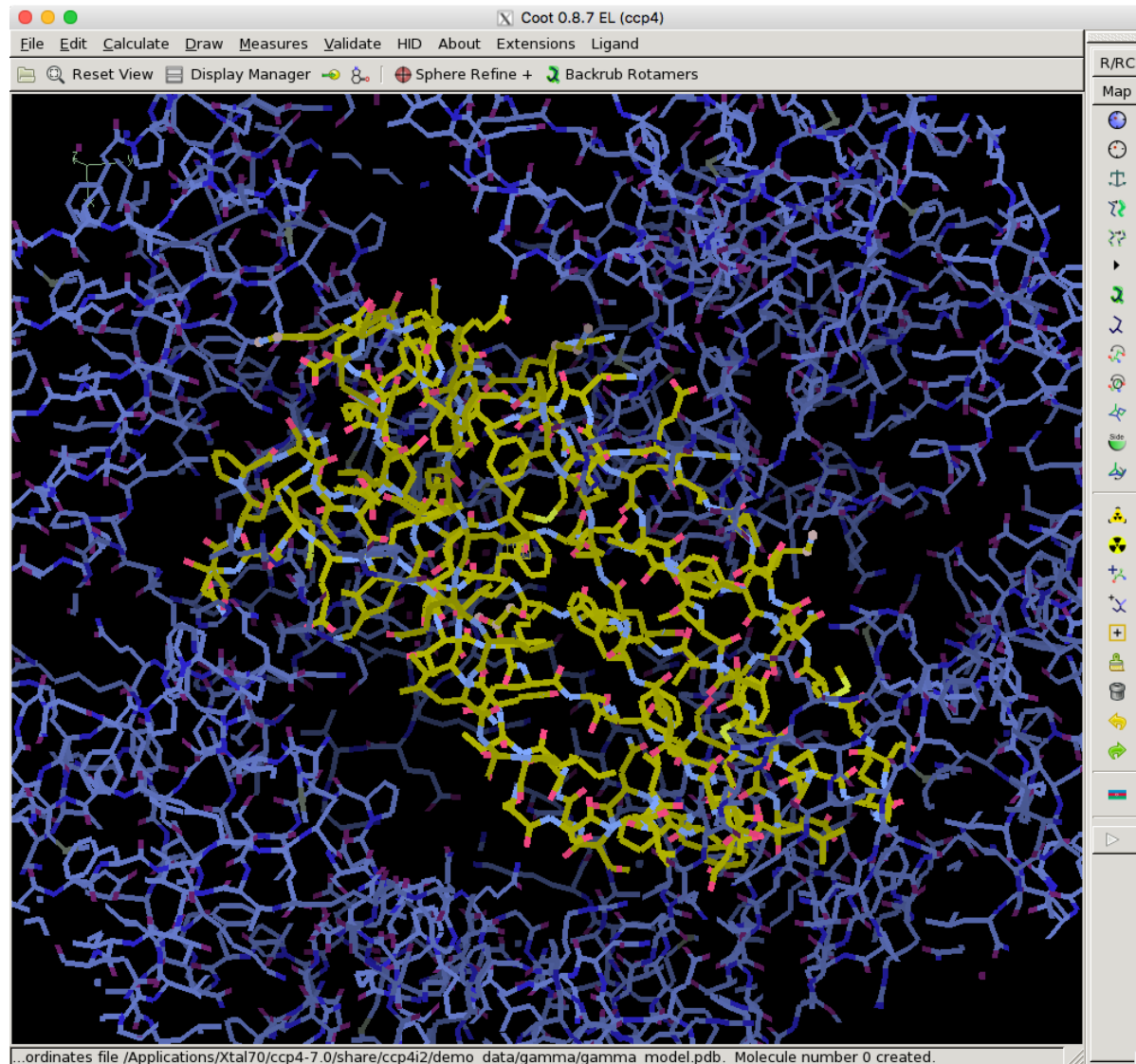
Two other projections
are also shown for this
space group



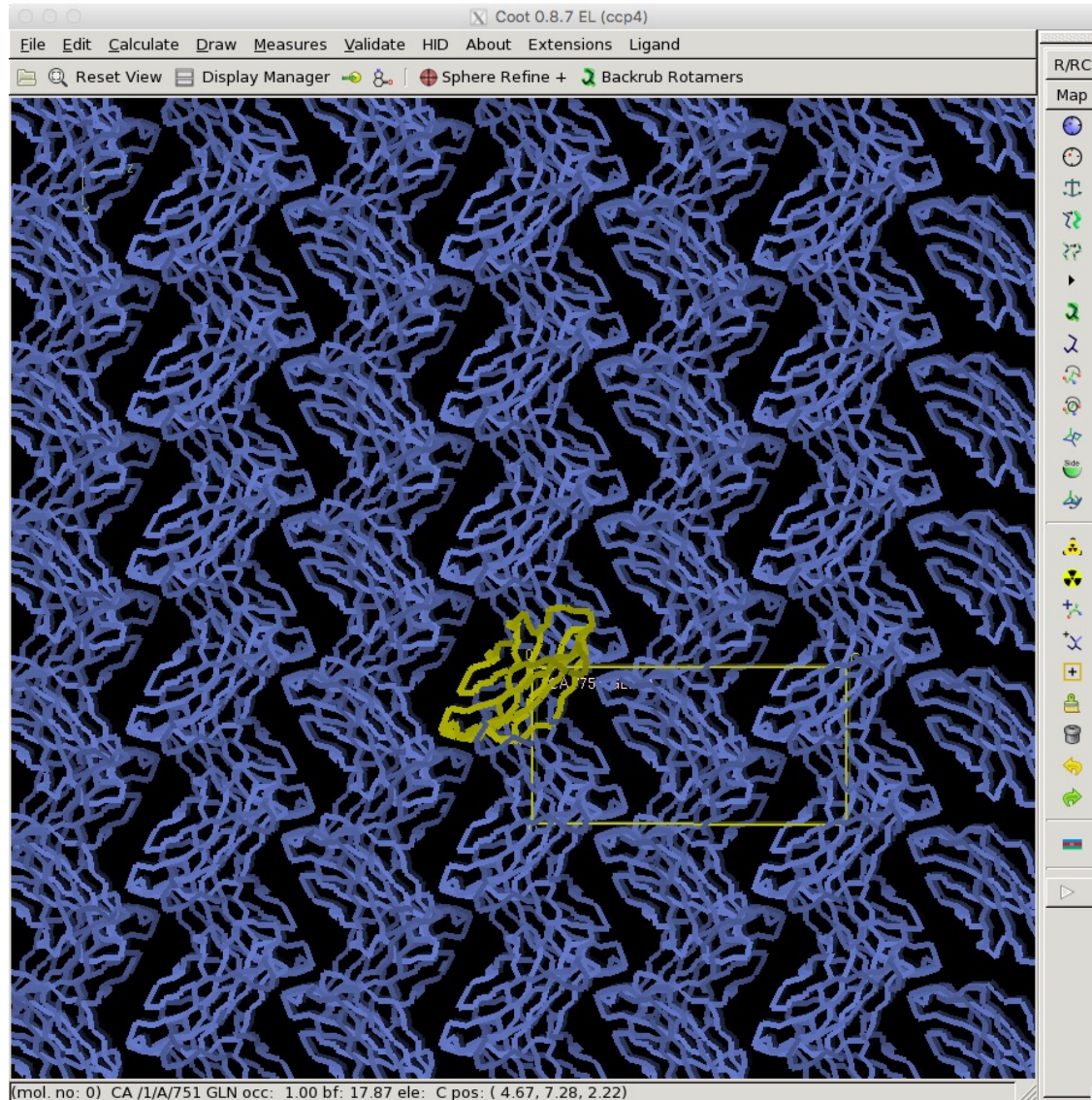
Set of equivalent
points in general
position.

We will be looking at
"molecular wallpaper"
instead

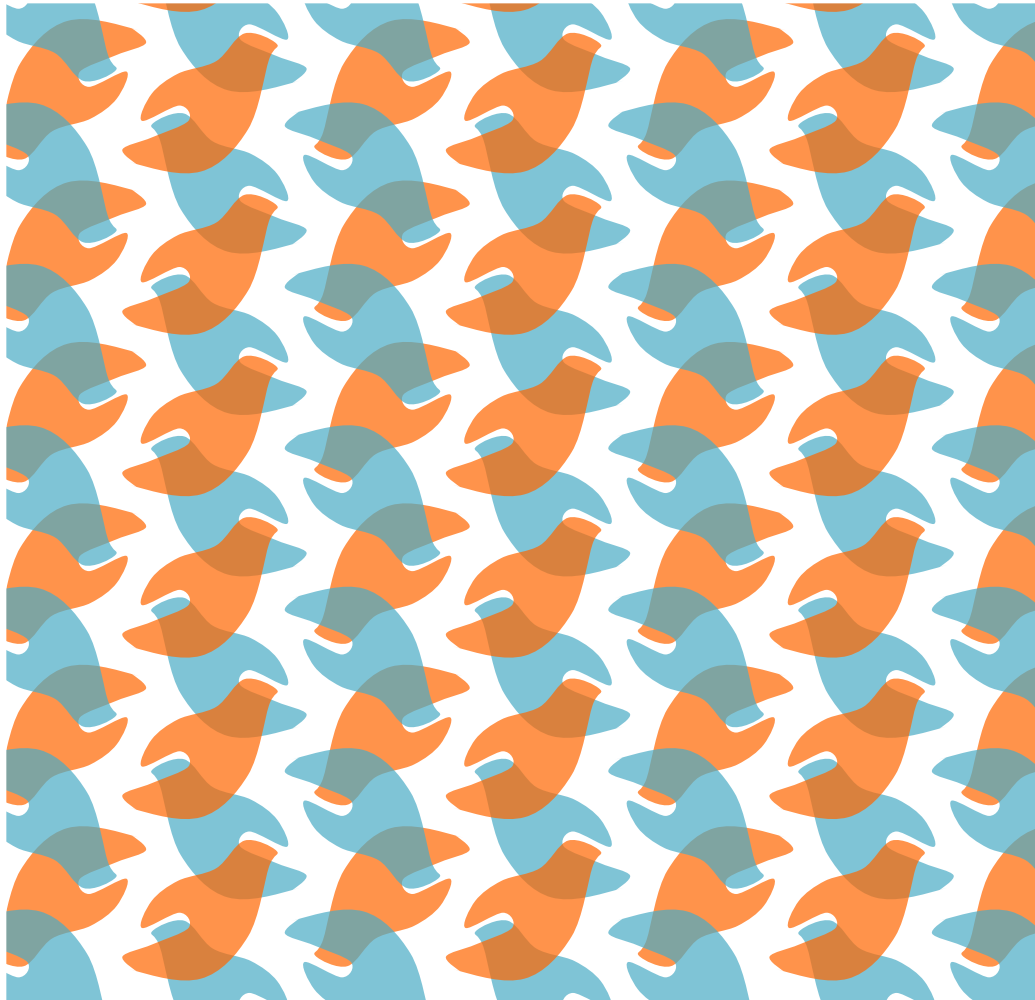
Examine structure in Coot



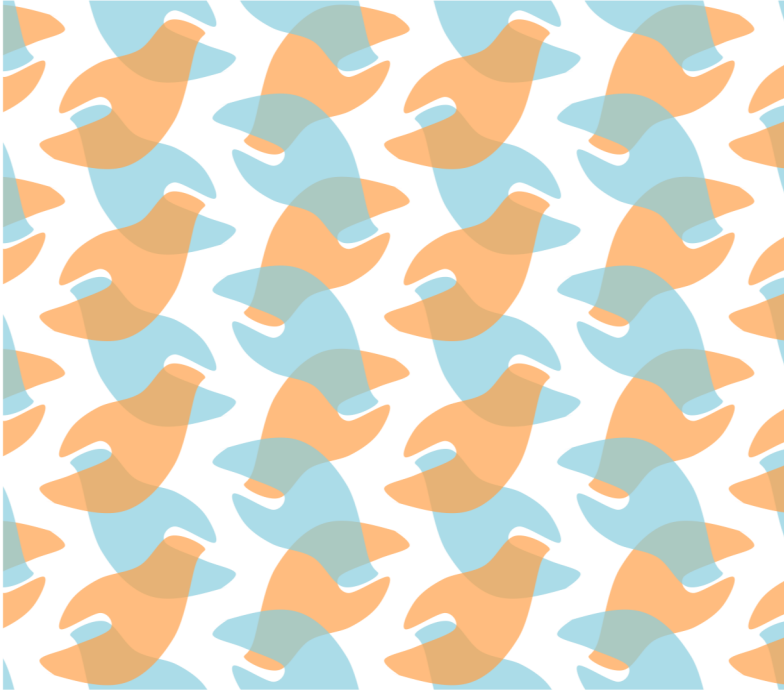
Symmetry view in Coot



Simplified representation

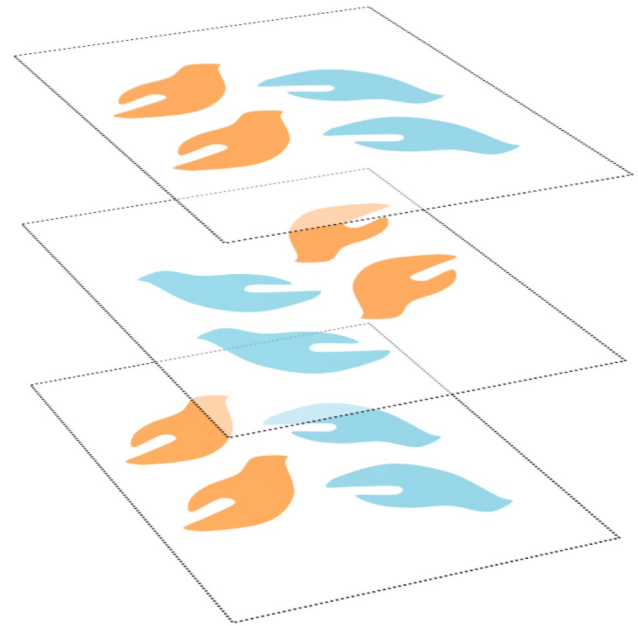


Simplified representation

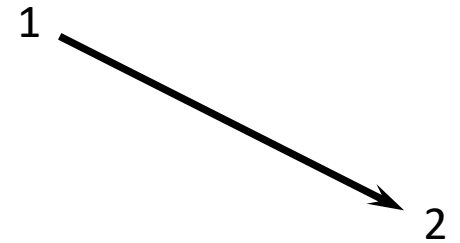
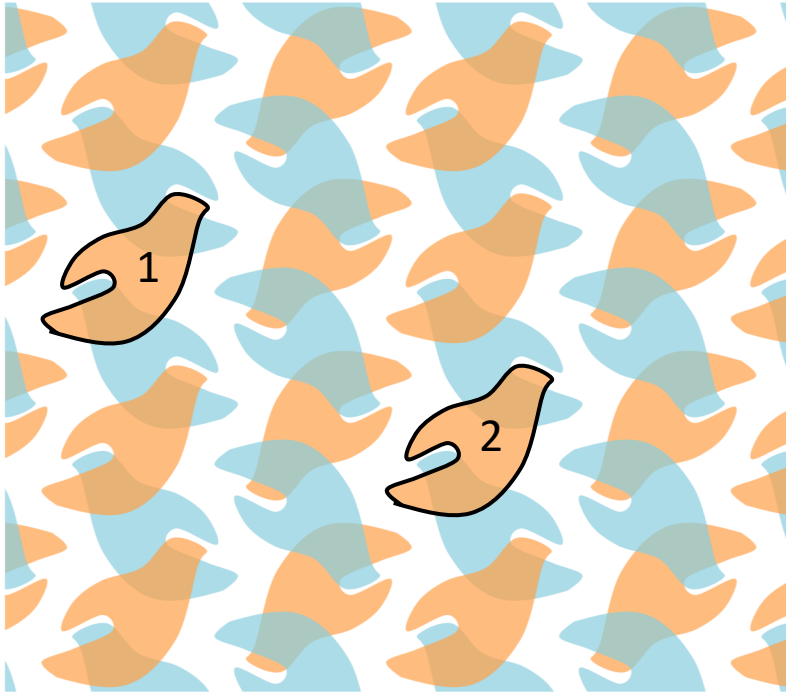


View from the top

There is a third dimension.

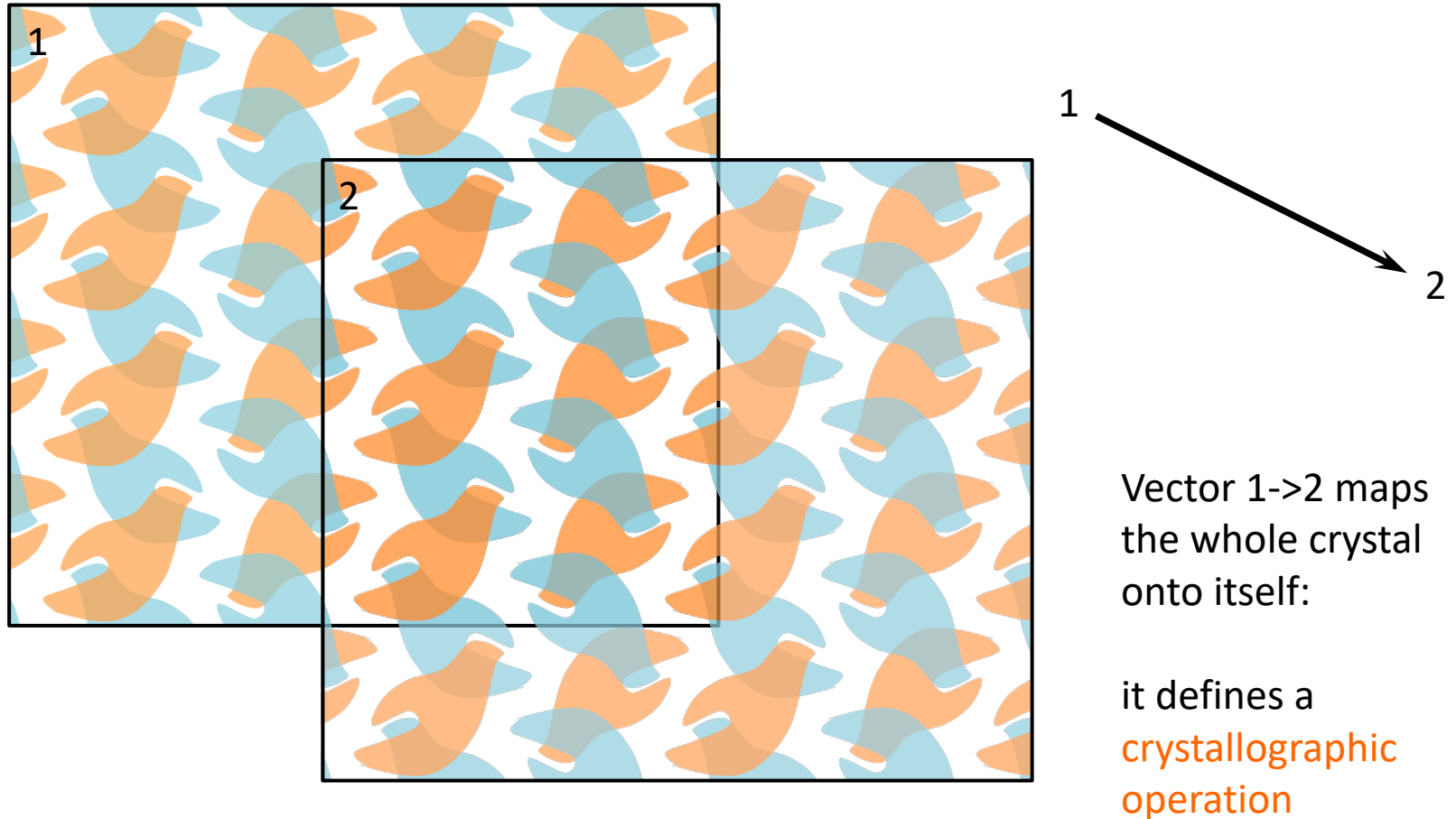


Translation 1-2

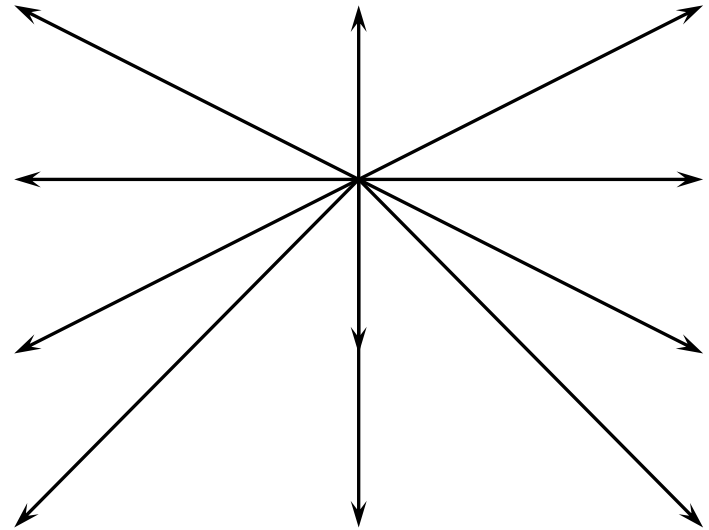
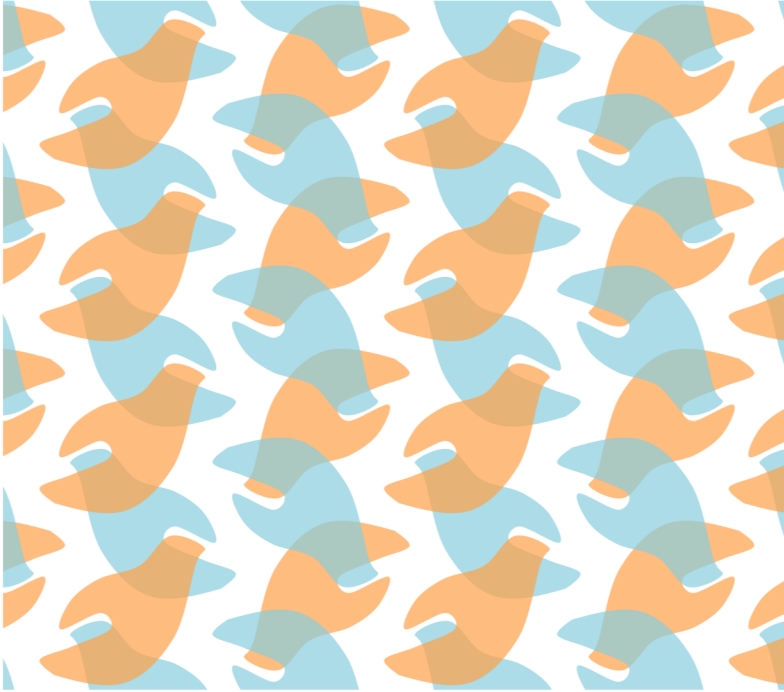


Vector maps 1 -> 2

Translation 1-2 is global



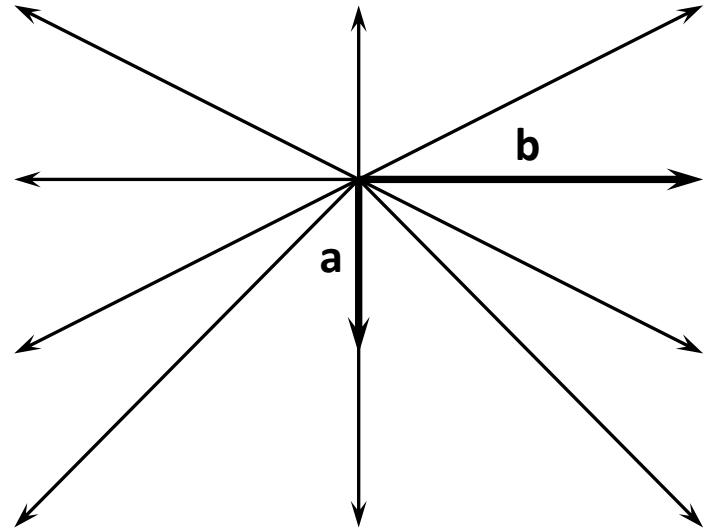
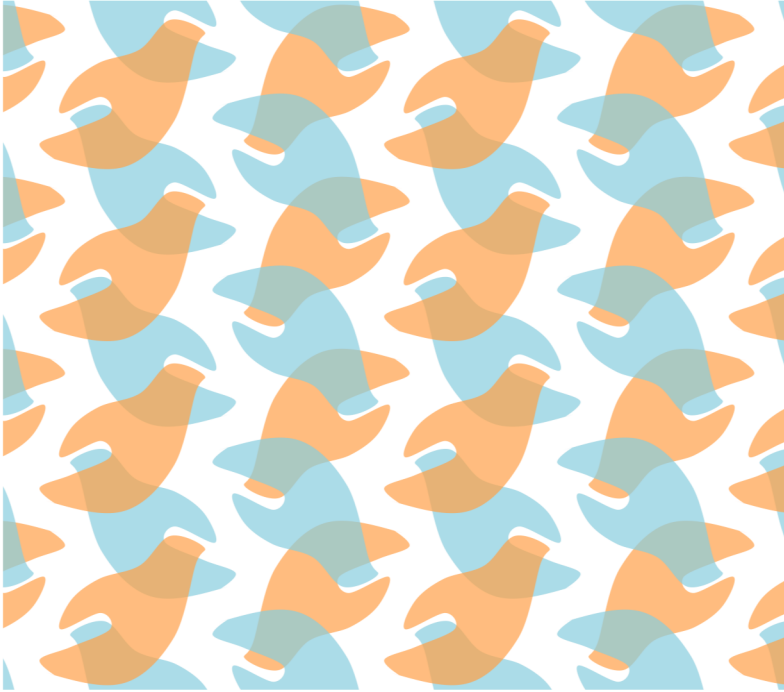
All translations form an infinite group



An infinite group (over vector sum):

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

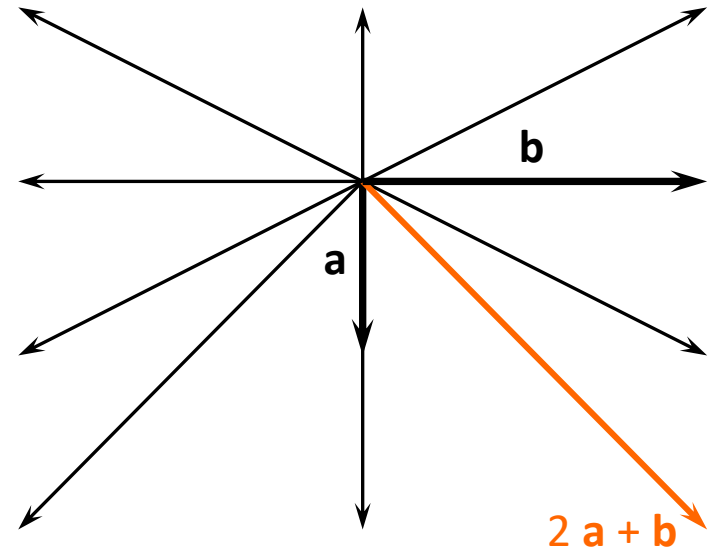
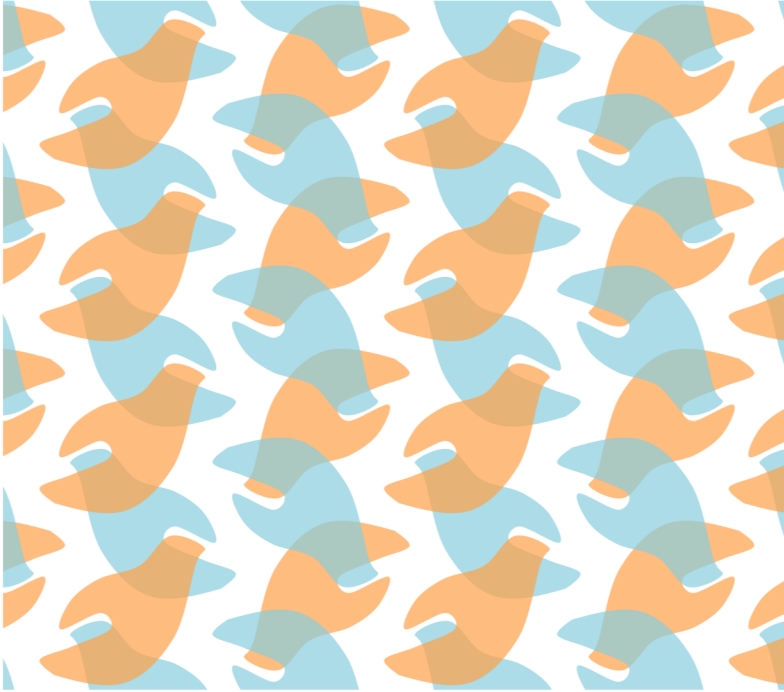
Basis vectors



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

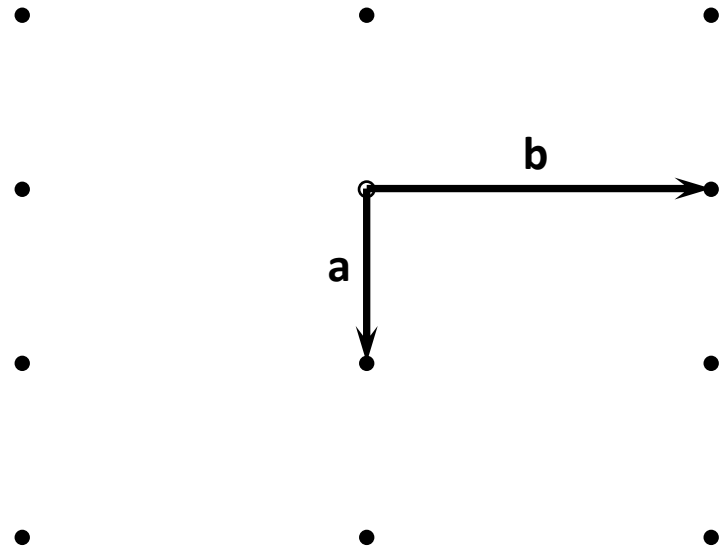
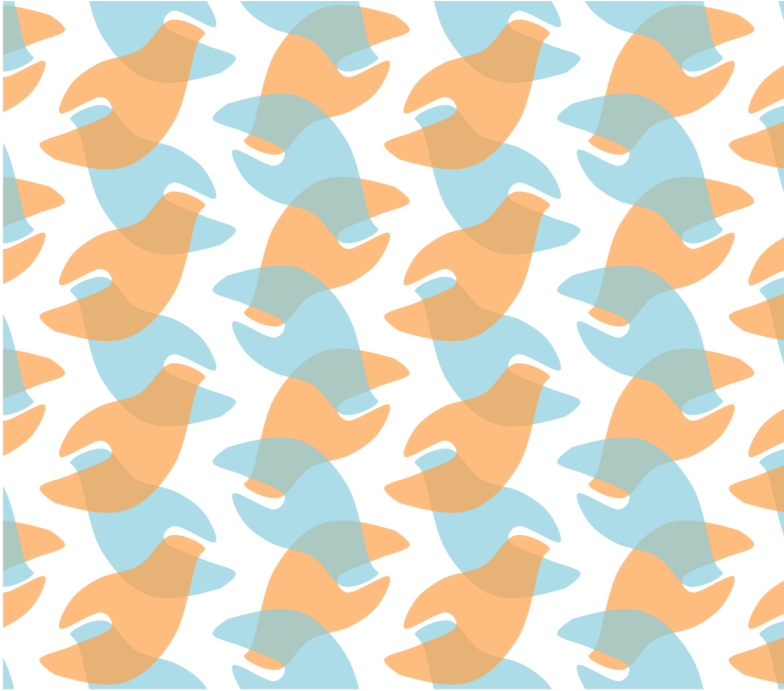
(**c** is perpendicular to the plane)

Basis vectors



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

Lattice

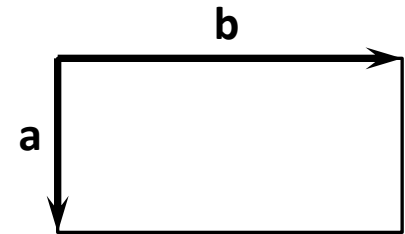
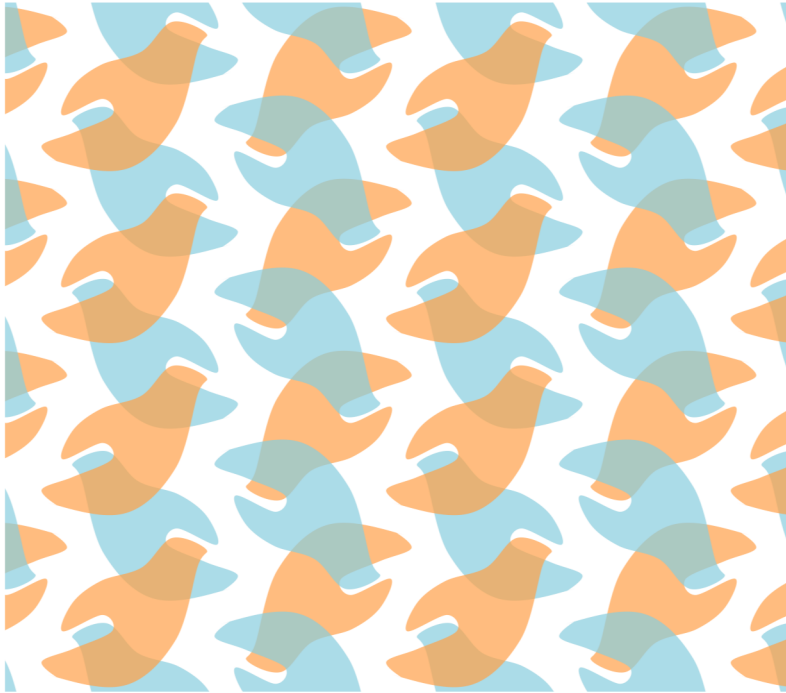


All the crystallographic translations can be represented as a lattice.

Translations, crystal lattice and unit cell live in a separate space.

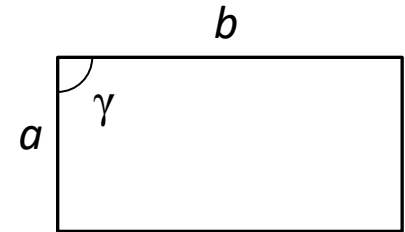
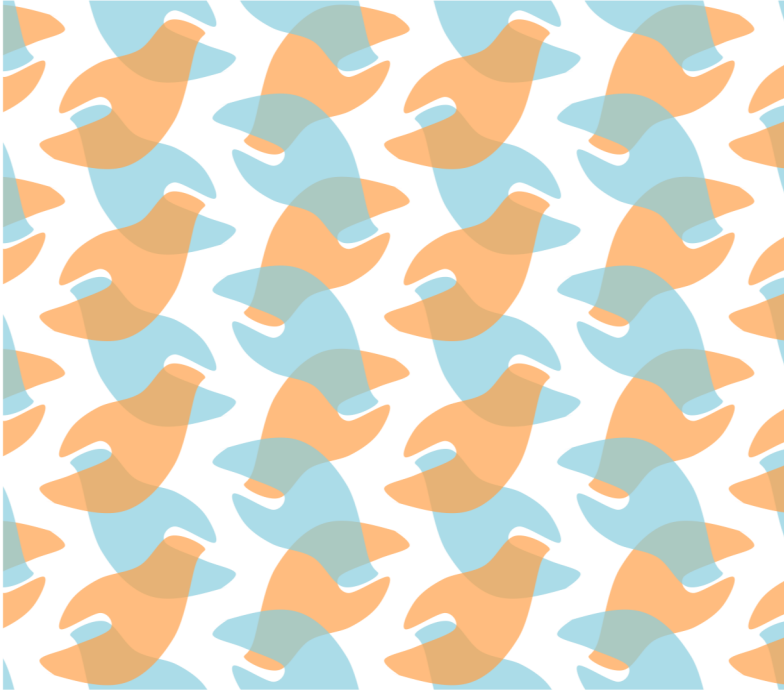
Coordinates in that space do not define coordinates of atoms but relation between equivalent atoms

Unit cell



A compact representation of translational symmetry and base vectors.

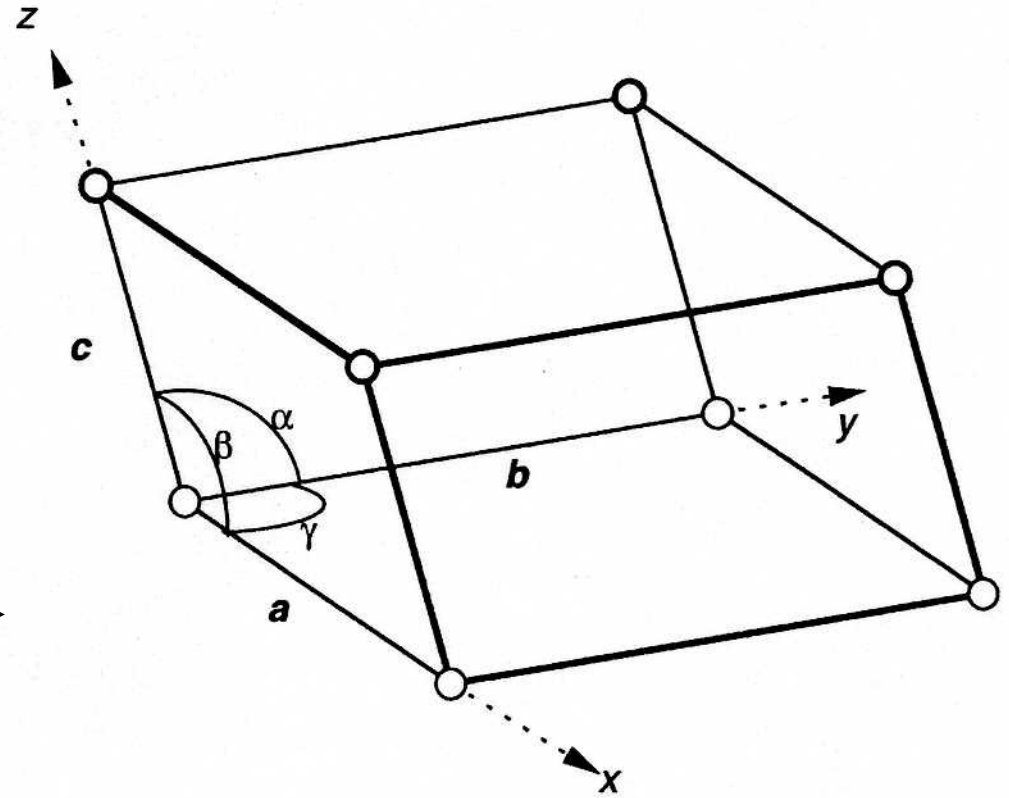
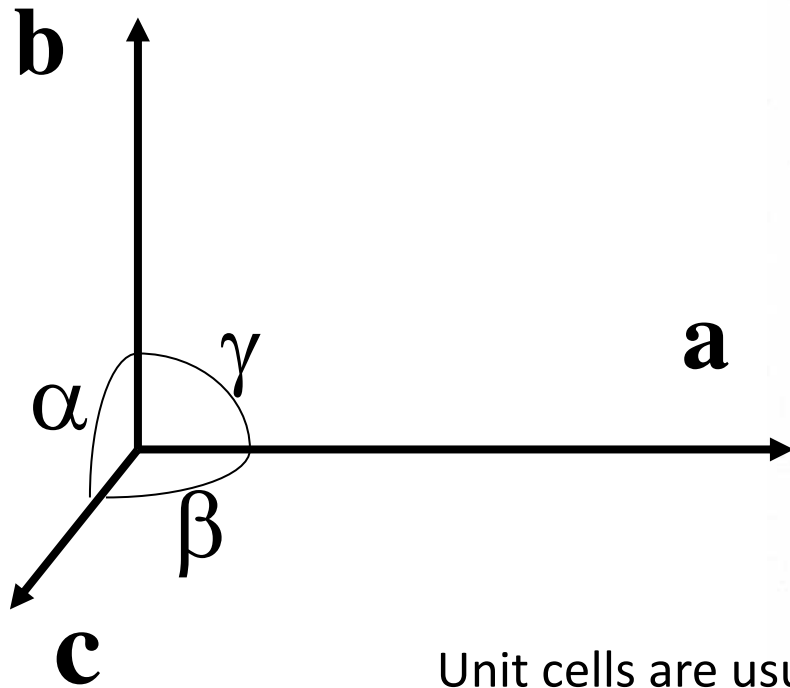
Unit cell



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

Unit cell parameters (3D view)

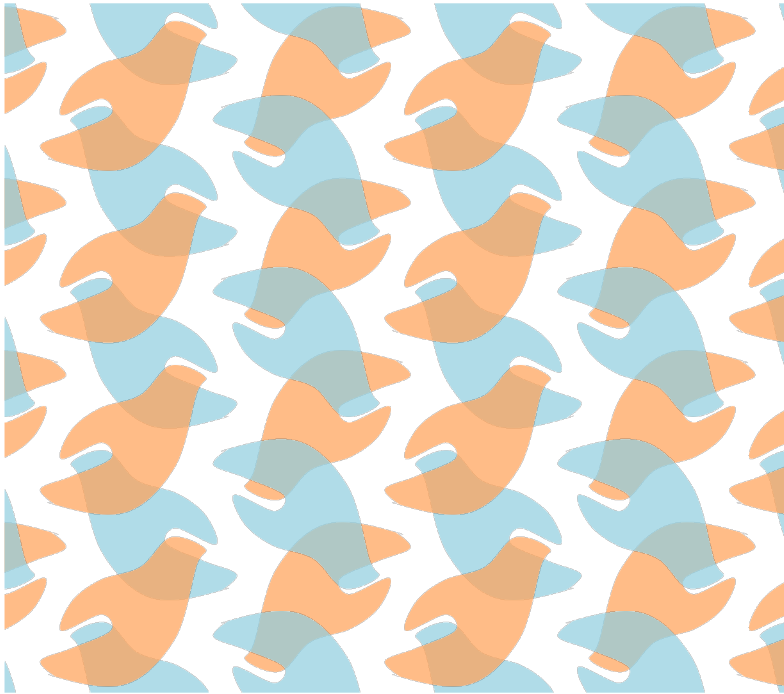
Translation symmetry is defined by three base vectors **a**, **b**, and **c**.



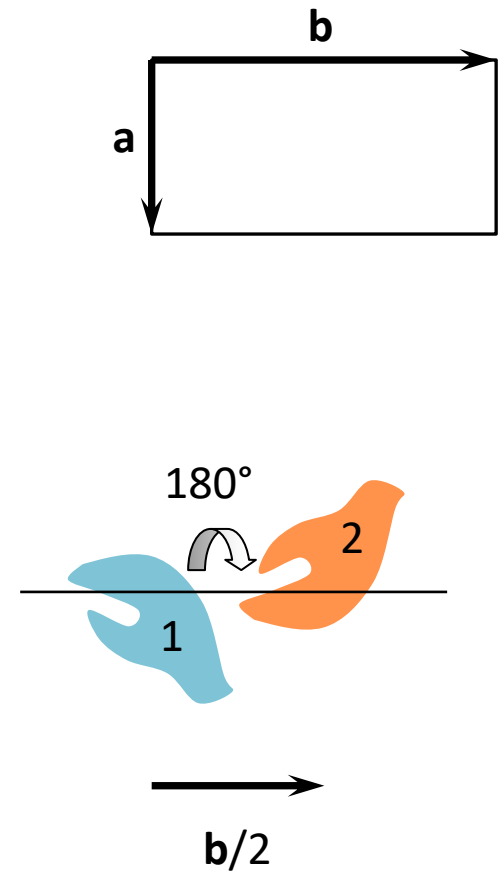
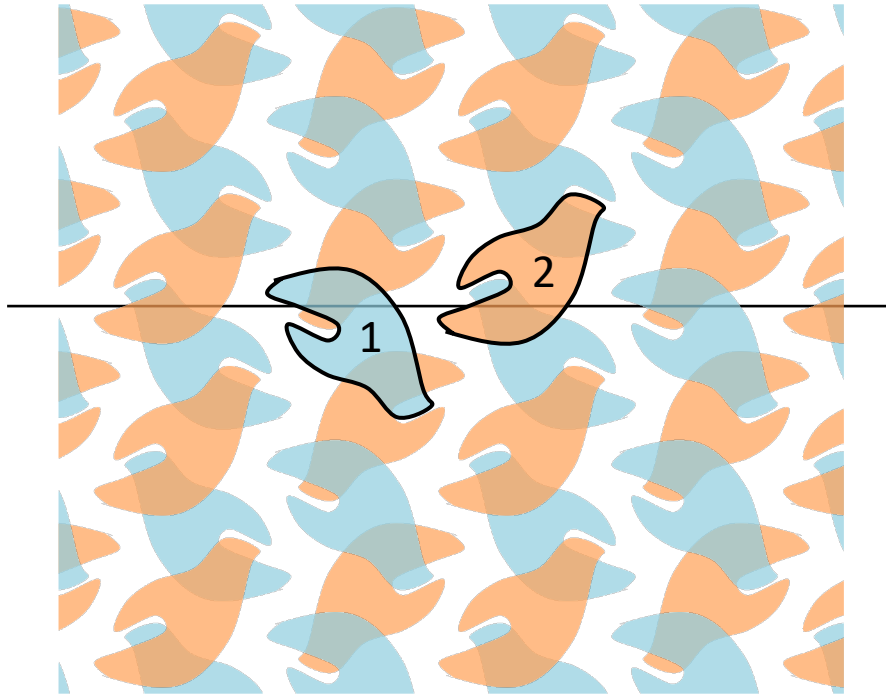
Unit cells are usually defined in terms of the *lengths* of these vectors and angles between them. For example,

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

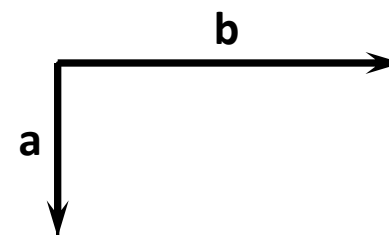
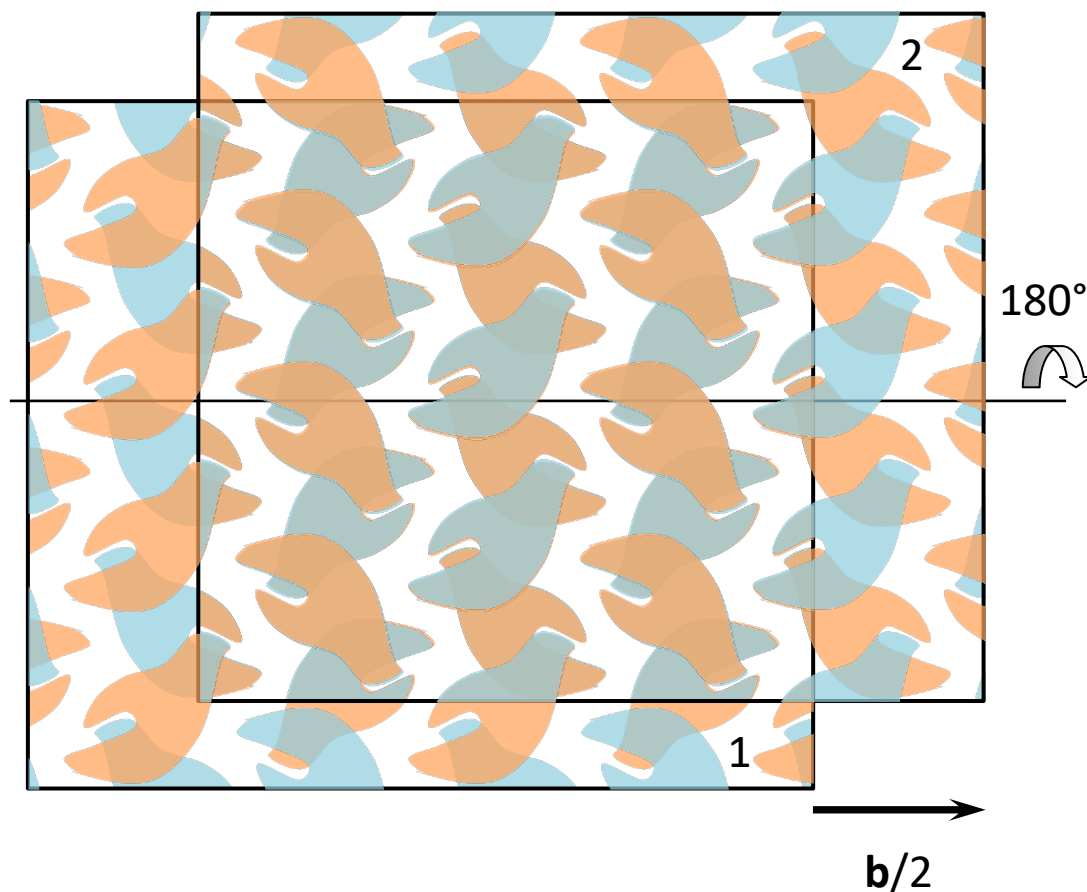
Back to example



Screw rotation



Screw rotation axis



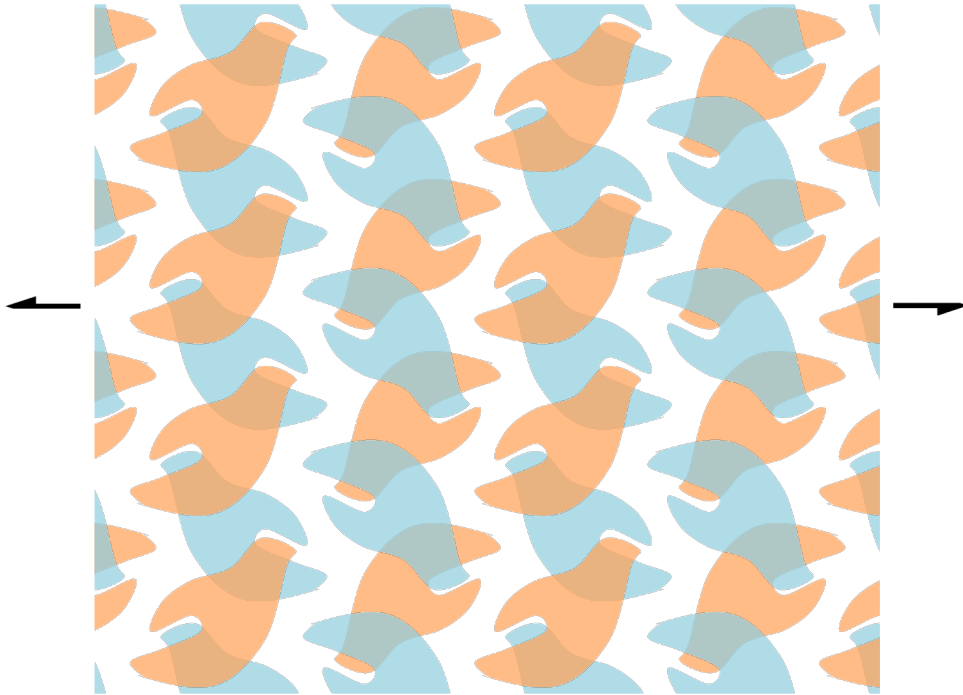
Operation 1→2
maps the whole crystal
onto itself:

this is a **crystallographic
operation**

The axis is a
crystallographic
symmetry element,

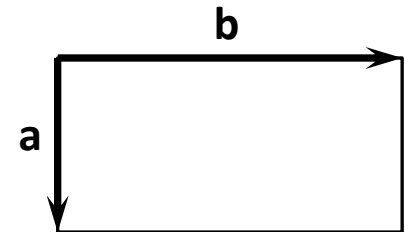
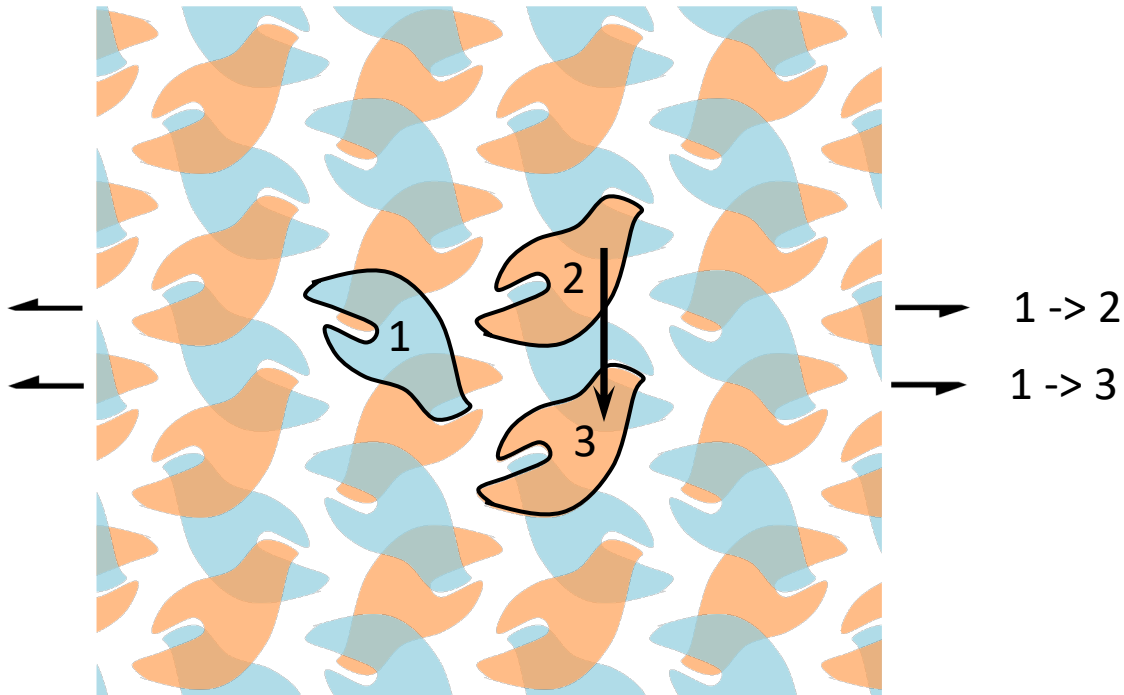
it can be **mapped into
the structure**

Screw rotation - symbol



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

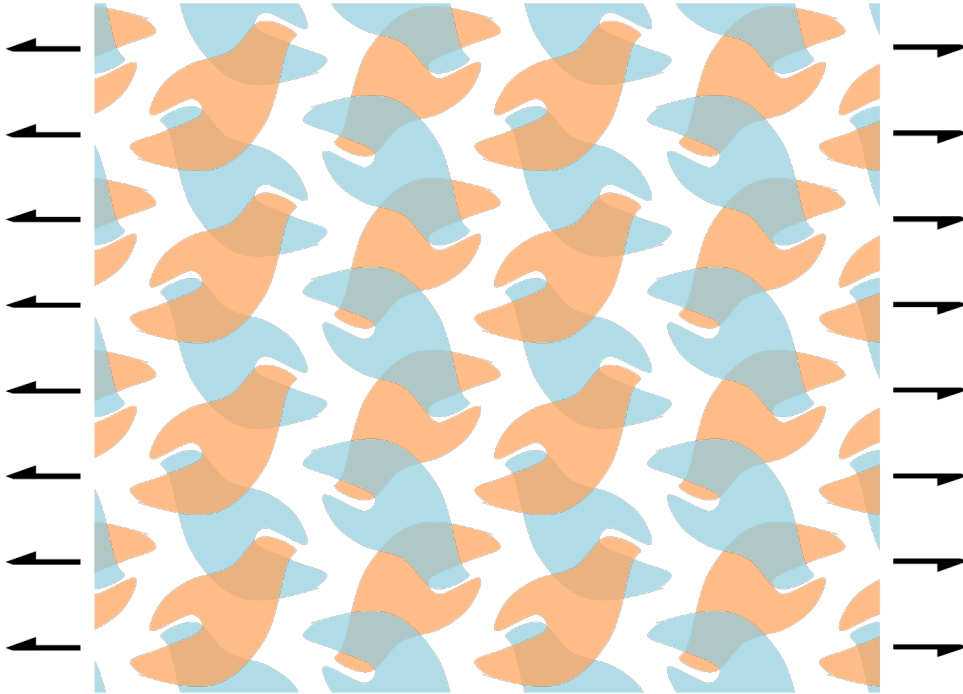
Screw rotation - repeats



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

(elements of a group)

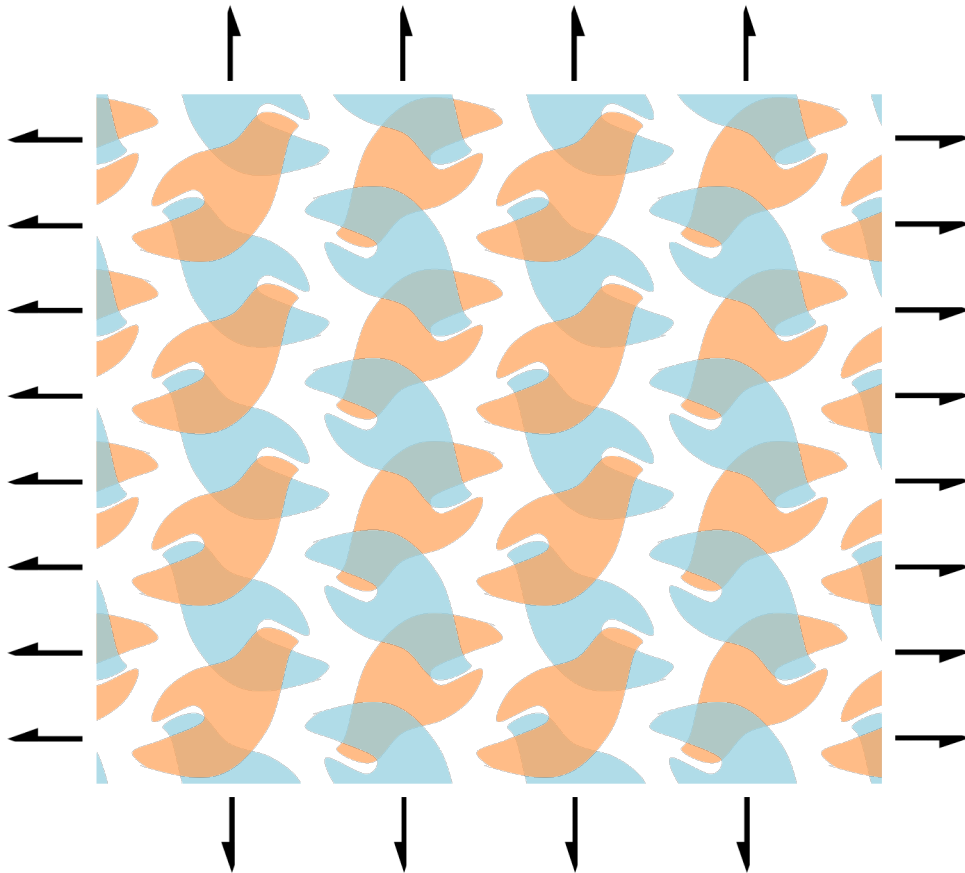
Screw rotation 1 - repeats



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

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

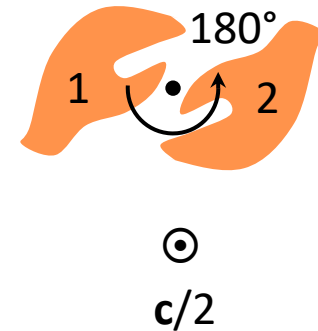
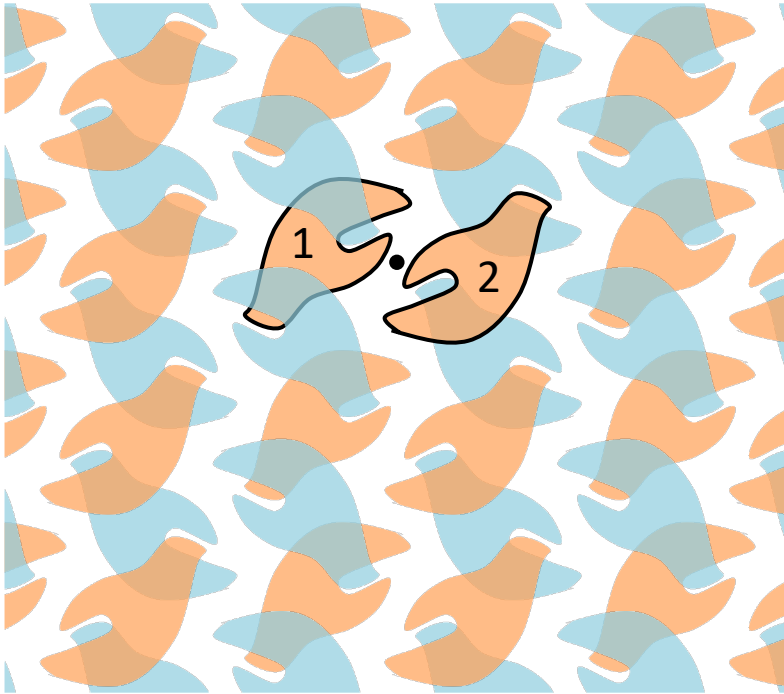
Screw rotations parallel to **a** and **b**



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

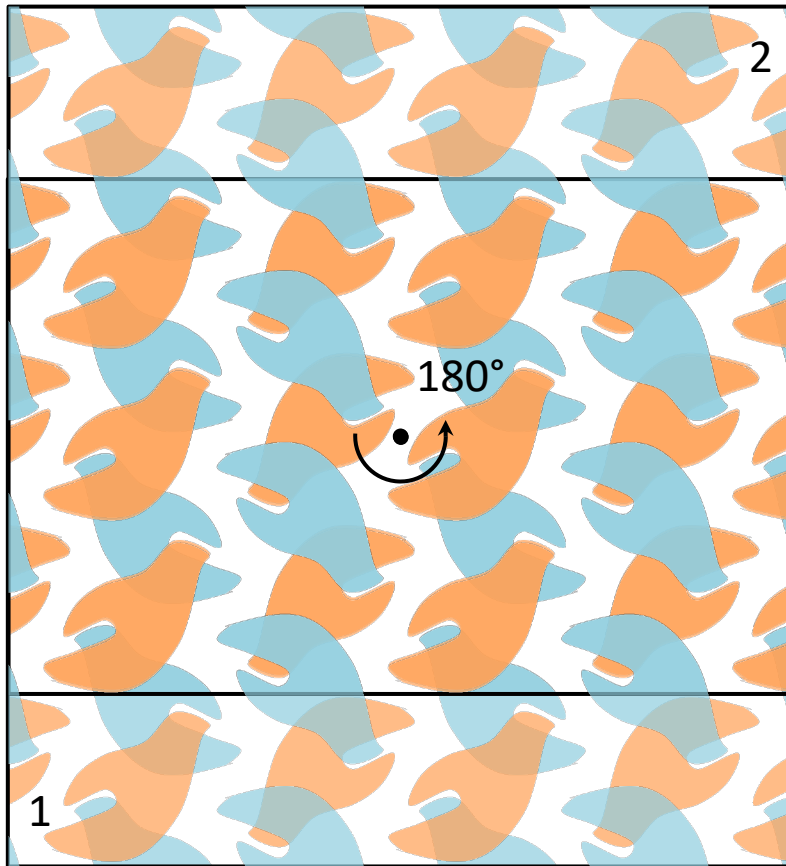
Series of 2_1 axes offset by $\frac{1}{2}$ unit cell from each other.

Screw rotation – into plane

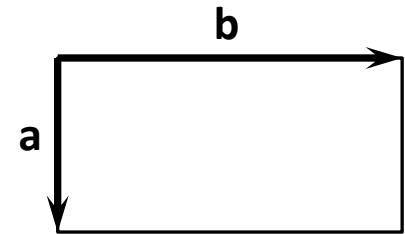


A rotation of 180° with a translation of $\frac{1}{2}$ unit cell from the figure.

Screw rotation 3 is global



⊙
 $c/2$



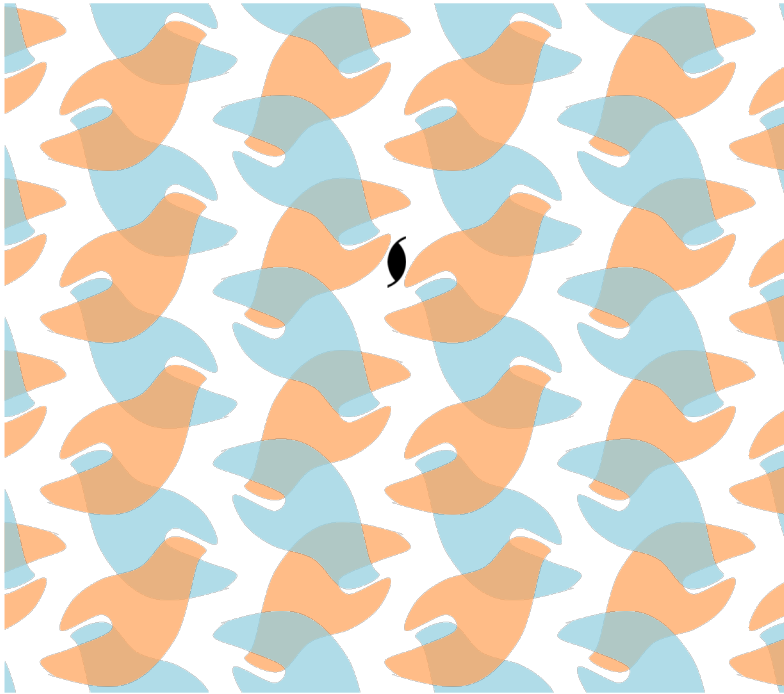
Screw rotation 3
maps the whole crystal
onto itself:

this is a **crystallographic
operation**

The rotation axis is a
crystallographic
symmetry element,

it can be **mapped into
the structure**

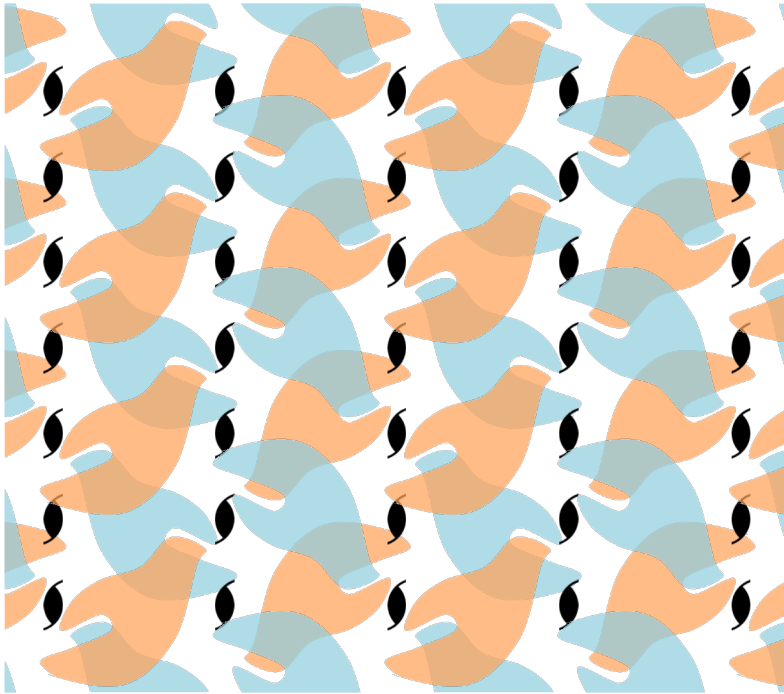
Screw rotation 3 - symbol



2_1 (along view):



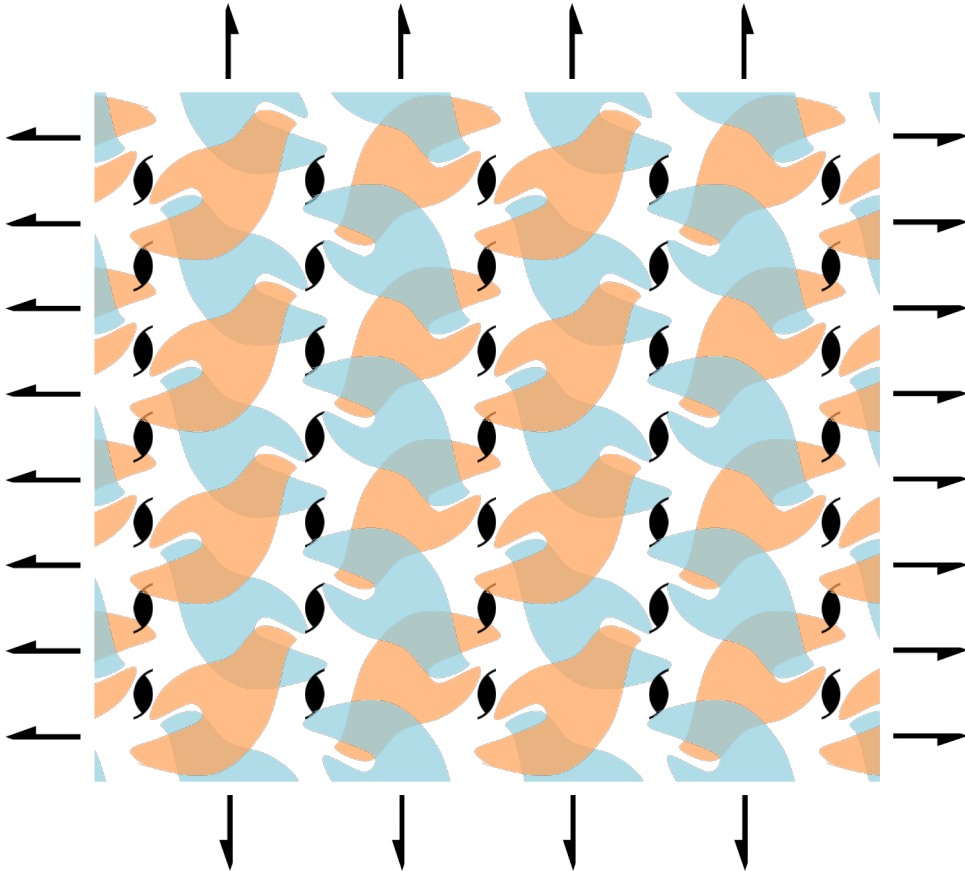
Screw rotation 3 - repeats



2_1 (along view): 

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

All axes together

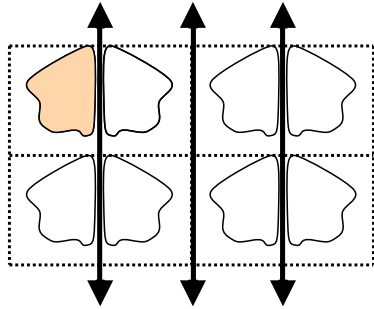


2_1 (plane of figure):

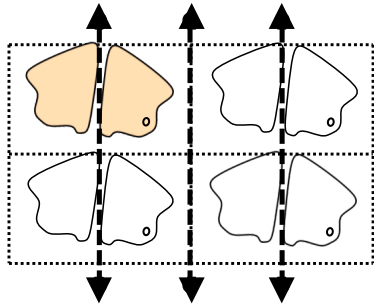
2_1 (along view):

we have built
a **space group**

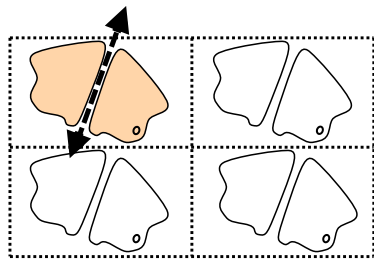
Crystallographic Symmetry, Pseudosymmetry and Non-Crystallographic Symmetry (NCS)



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

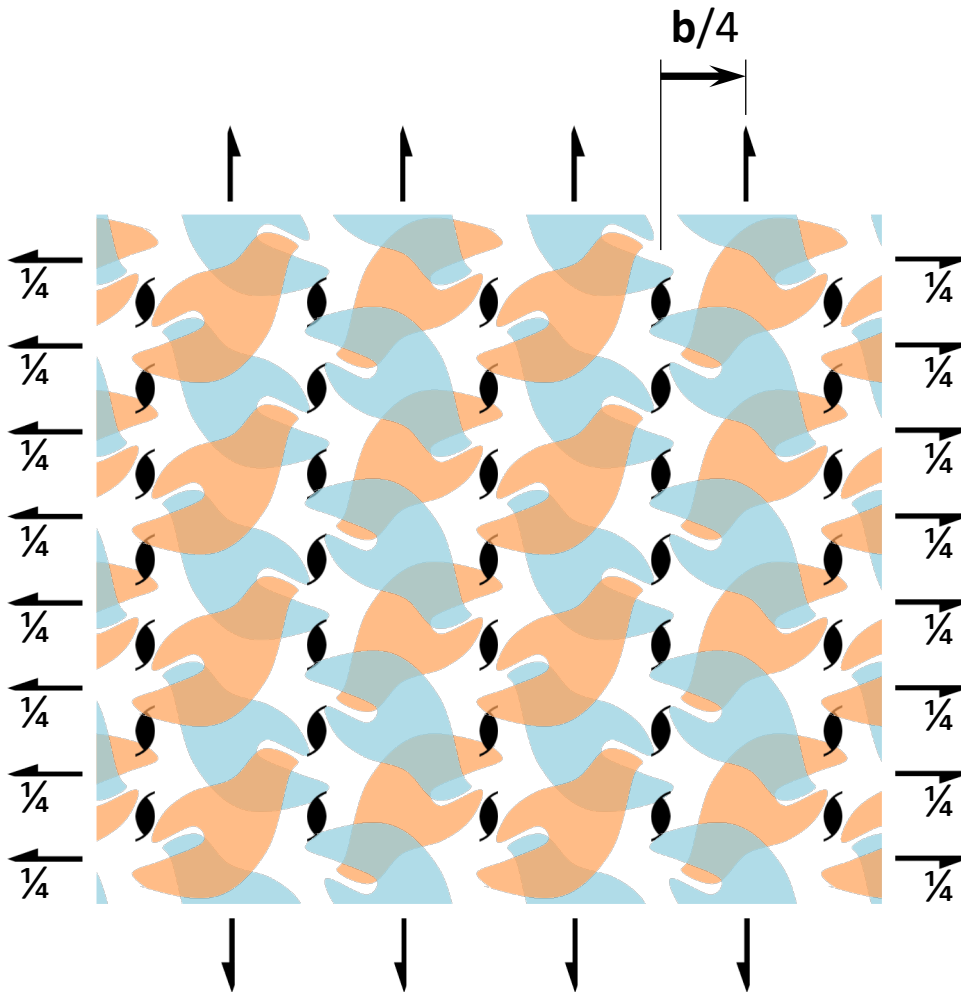


Pseudosymmetry (a limiting case of NCS)
- symmetry is **global** and **approximate**



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

Relative positions of axes



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

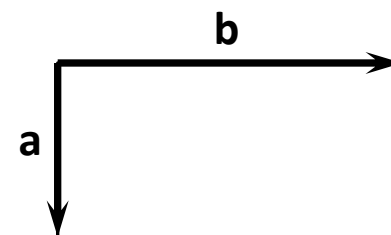
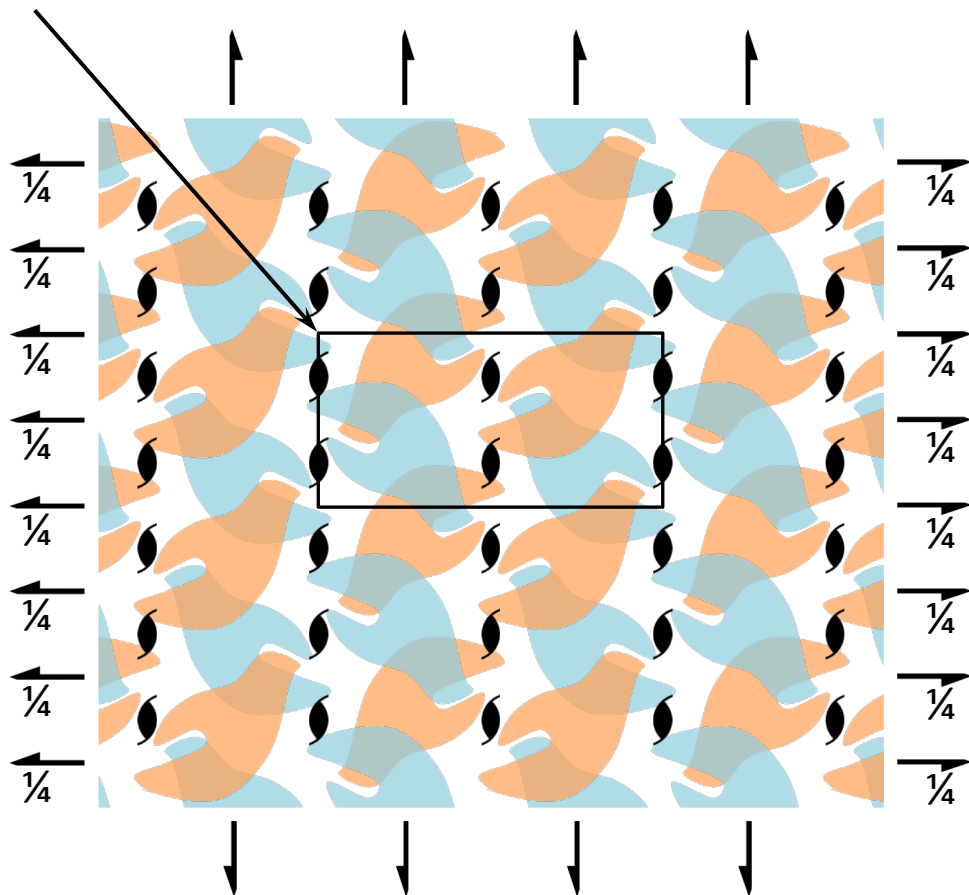
2_1 (along view): \curvearrowright

The adjacent axes running in different directions are offset by $\frac{1}{4}$ of corresponding base vector.

The horizontal $\frac{1}{4}$ indicates a offset of $(\frac{1}{2} n + \frac{1}{4}) \mathbf{c}$ into the figure.

Choice of origin is a convention. Notation

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



2_1 (plane of figure): \longleftrightarrow

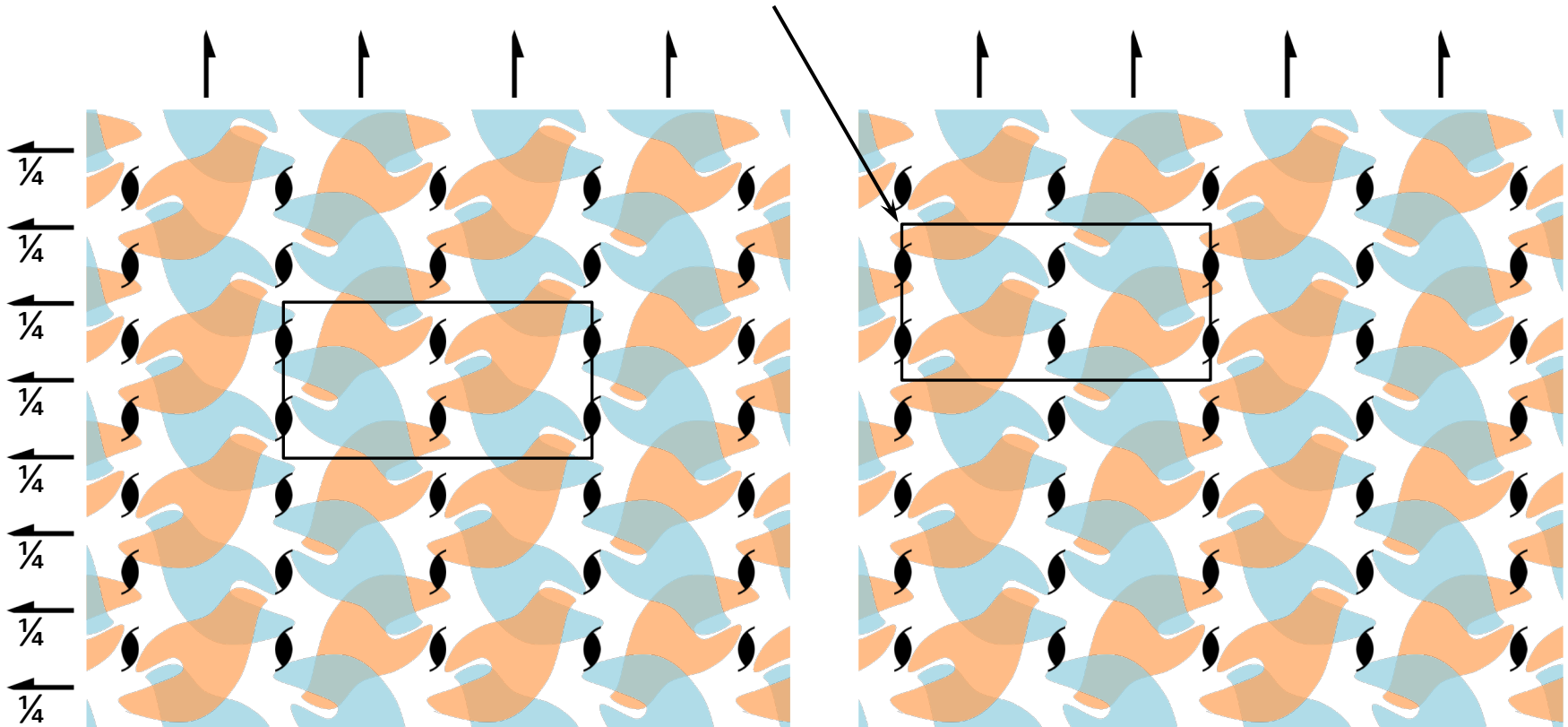
2_1 (along view): \curvearrowright

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**.

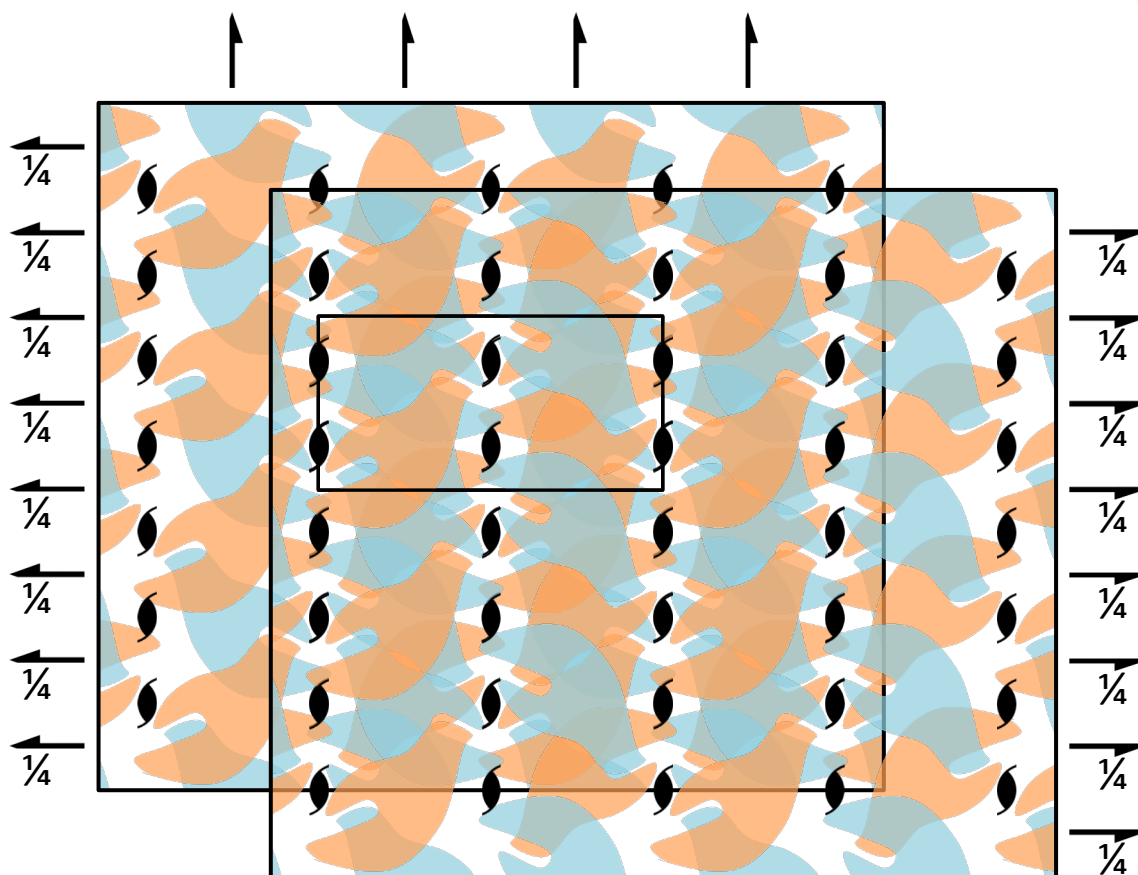
Alternative origins

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



Structures "solved in alternative origins"

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



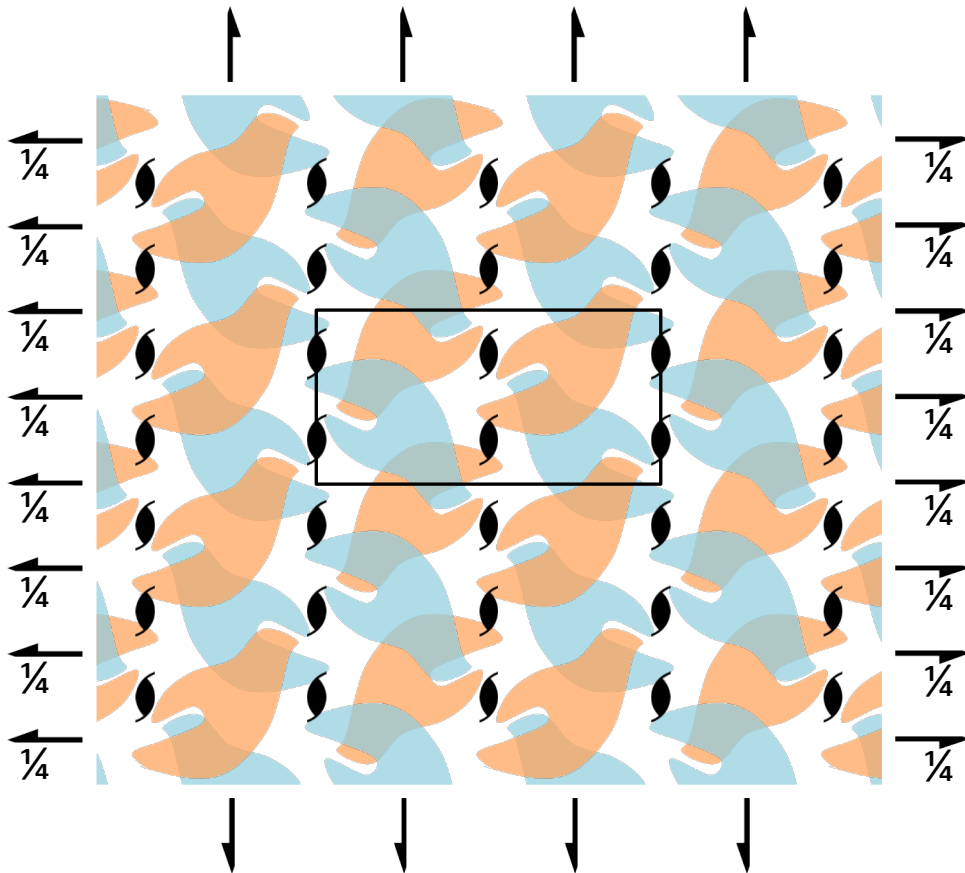
The structures do not match.

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

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

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

Complete picture



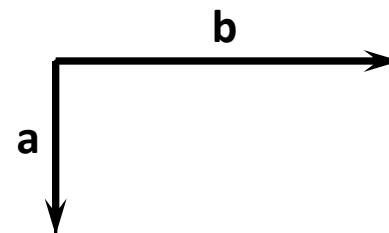
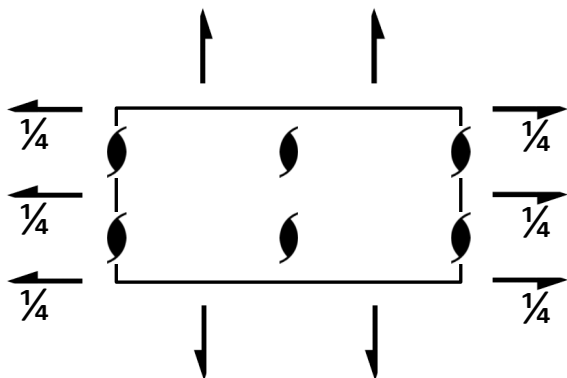
2_1 (plane of figure): \longleftrightarrow

2_1 (along view): \curvearrowright

Compact representation

$P2_12_12_1$

No. 19



2_1 (plane of figure):

2_1 (along view):

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

Space group representation in ITC-A

$P2_12_12_1$

No. 19

D_2^4

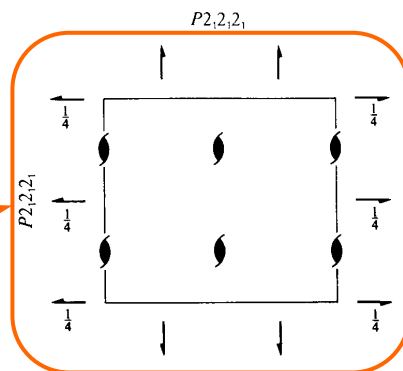
$P2_12_12_1$

222

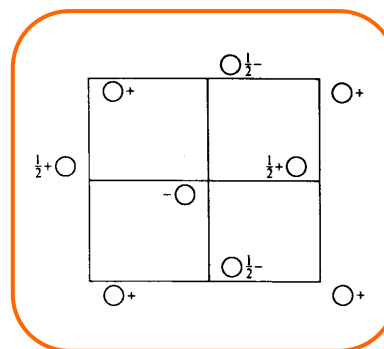
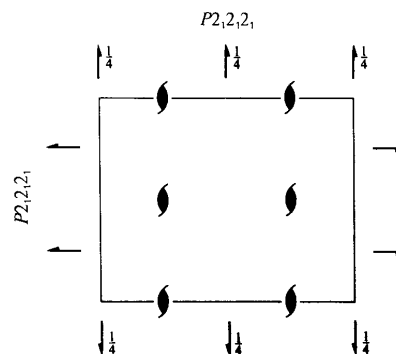
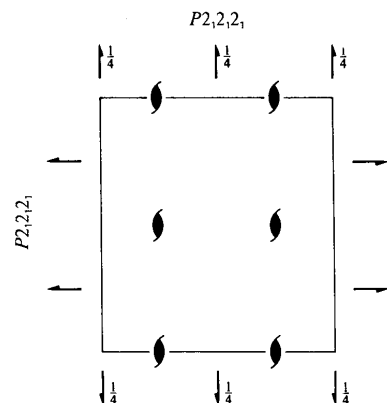
Orthorhombic

Patterson symmetry $Pmmm$

Location of
symmetry
elements



Two other projections
are also shown for this
space group



Set of equivalent
points in general
position.

We will be looking at
"molecular wallpaper"
instead

Space group representation in ITC-A

Crystal
system

$P2_12_12_1$

No. 19

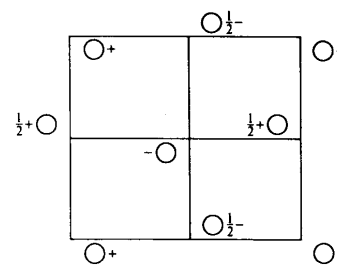
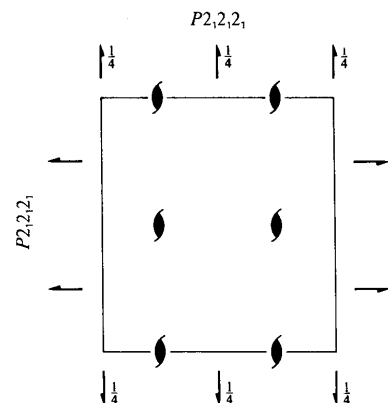
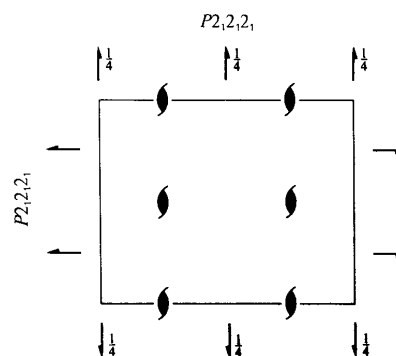
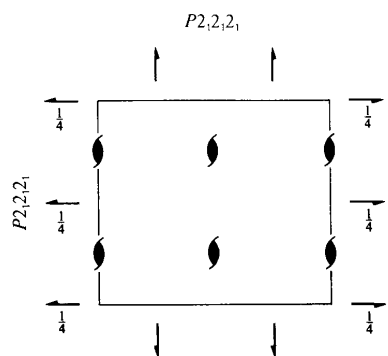
D_2^4

$P2_12_12_1$

222

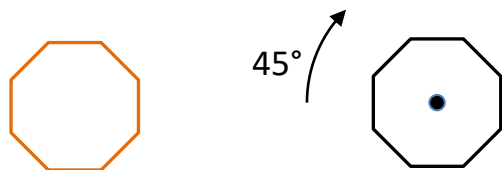
Orthorhombic

Patterson symmetry $Pmmm$



Rotational symmetry

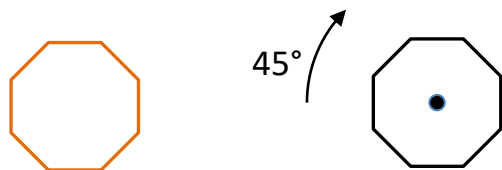
An **N**-fold rotational symmetry implies that if a rotation of $360^\circ/\mathbf{N}$ degrees is applied, the transformed object is identical to the original.



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

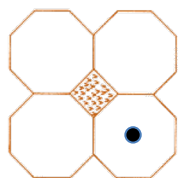
Rotational symmetry

An **N**-fold rotational symmetry implies that if a rotation of $360^\circ/\mathbf{N}$ degrees is applied, the transformed object is identical to the original.

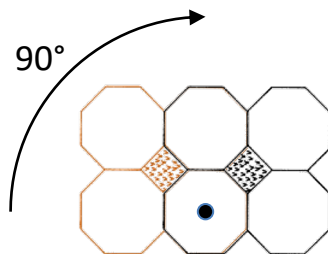


This object has **8**-fold rotational symmetry

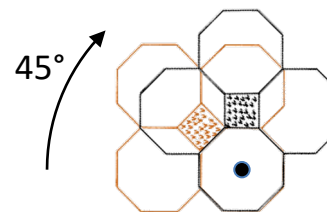
The only rotational symmetries possible in a **crystal** are **2**, **3**, **4** and **6**.



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



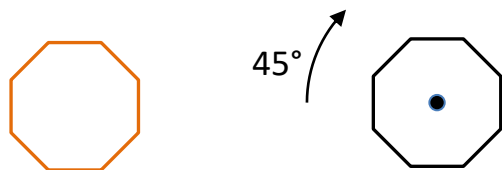
4-fold rotational **crystal** symmetry



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

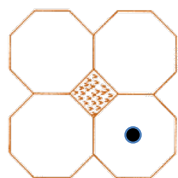
Rotational symmetry

An **N**-fold rotational symmetry implies that if a rotation of $360^\circ/\mathbf{N}$ degrees is applied, the transformed object is identical to the original.

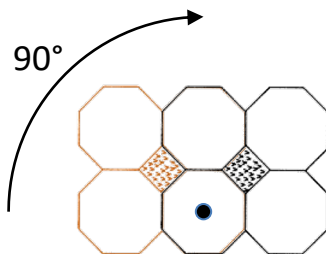


This object has **8**-fold rotational symmetry

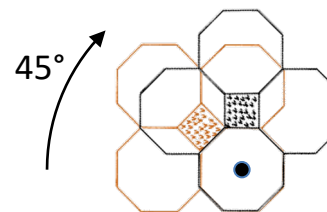
The only rotational symmetries possible in a **crystal** are **2**, **3**, **4** and **6**.



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



4-fold rotational **crystal** symmetry

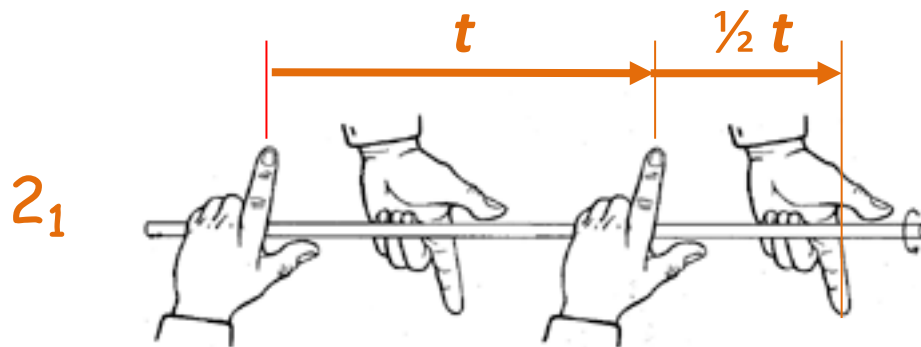


8-fold rotational **crystal** symmetry is **impossible**

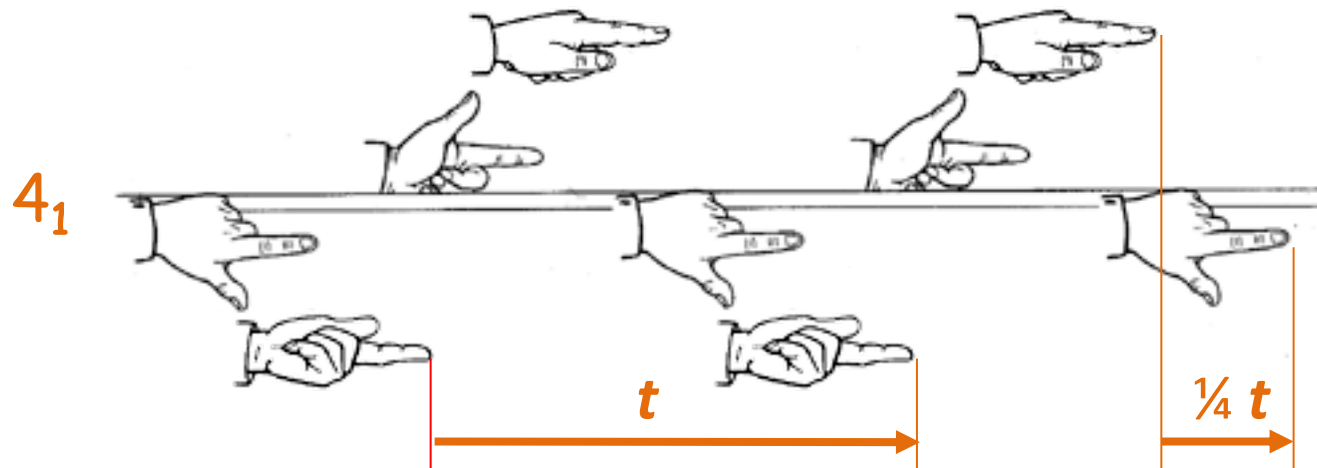
45° rotation is a **Non-Crystallographic Symmetry** (NCS)

Screw axes

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



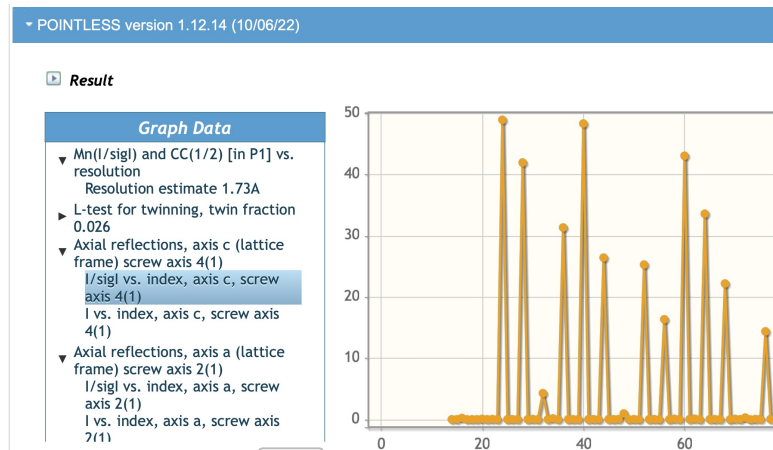
translation of $\frac{1}{2} t$
per 180° rotation



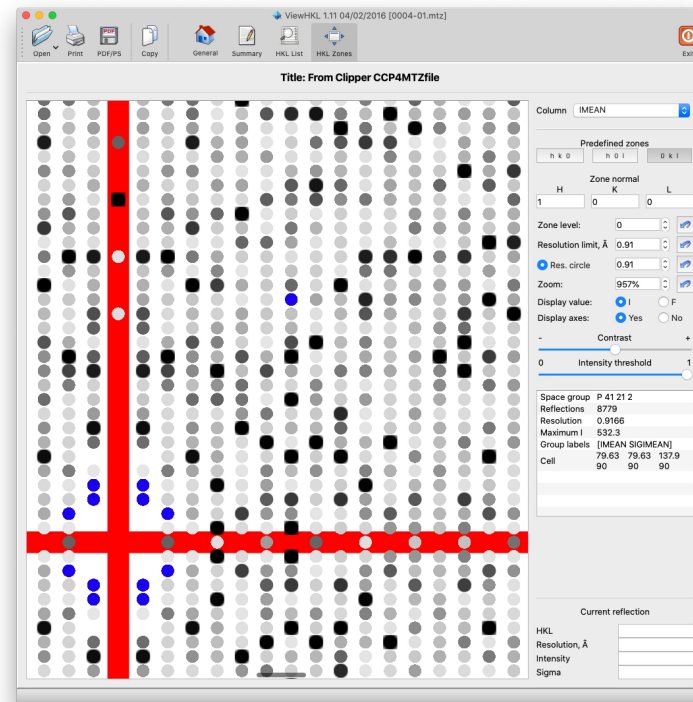
translation of $\frac{1}{4} t$
per 90° rotation

Screw axes: systematic absences

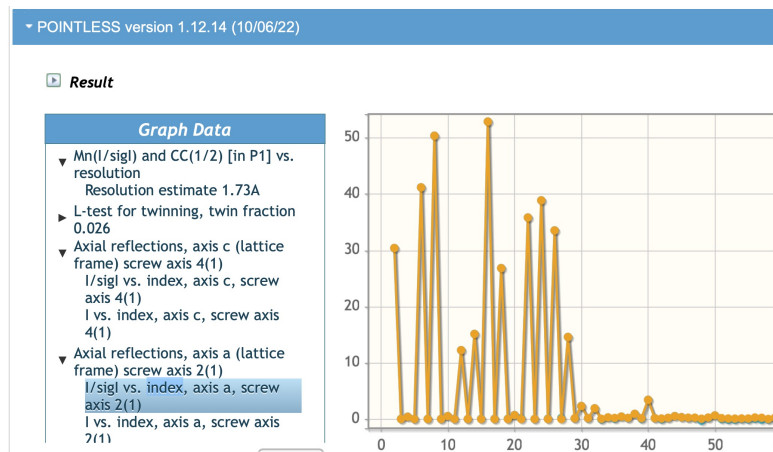
$h = k = 0$: every fourth l strong: 4_1 or 4_3



4_1 or 4_3



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



h

2_1

l

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

Screw axes: systematic absences: CCP4Cloud

↑ [0001] file import -- imported: Unmerged (1)
[0004] aimless -- Compl=83.0% CC_{1/2}=0.999 R_{meas_all}=0.258 R_{meas_ano}=0.257 Res=0.91-39.81 SpG=P 41 21 2
[0005] asymmetric unit contents
↑ [0006] file import -- imported: Sequence (1)

[0004] aimless -- completed

Input Output + [?] [↗]

Report Main Log Service Log Errors

3. Generating symmetry tables

▼ POINTLESS version 1.12.14 (10/06/22)

▶ **Result**

Graph Data

▼ Mn(I/sigI) and CC(1/2) [in P1] vs. resolution
Resolution estimate 1.73A

▶ L-test for twinning, twin fraction 0.026

▶ Axial reflections, axis c (lattice frame) screw axis 4(1)

[0004] aimless -- completed

Input Output + [?] [↗]

Report Main Log Service Log Errors

Created Reflection Data Set (merged)

Assigned name: [0004-01] aimless [XDSproject/

▶ **Reflection data** ViewHKL


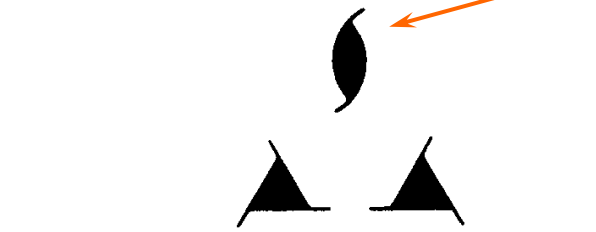






[0004] References

The following programs were used:

- **Pointless:**
 - Evans, P.R. (2006) *Scaling and assessment* doi:10.1107/S0907444905036693

Symmetry elements allowed in chiral structures

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

Proper Rotations	Screw Rotations
 2	 2_1
 3	 $3_1, 3_2$
 4	 $4_1, 4_2, 4_3$
 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 $\bar{1}$ followed by inversion

Space groups

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

Crystal Systems

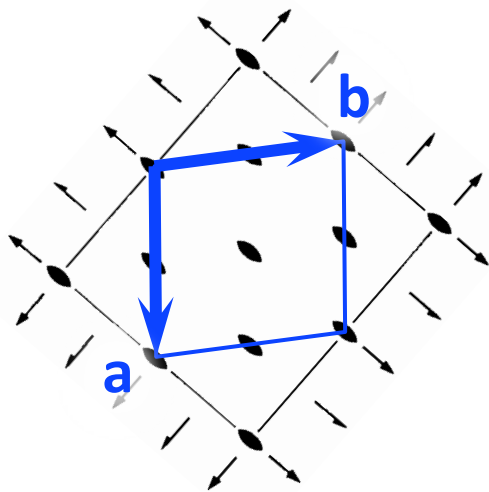
Crystal System	Characteristic symmetry elements	Convention	Bravais lattices	Constraints on unit cell parameters
1. Triclinic	Translations only		1. Primitive (<i>P</i>)	$\alpha \neq \beta \neq \gamma \neq 90^\circ$
2. Monoclinic	2-fold axes, all parallel	along b	2. Primitive (<i>P</i>) 3. Base-Centered (<i>C</i>)	$\alpha = \gamma \neq \beta \neq 90^\circ$
3. Orthorhombic	2-fold axes in three perpendicular directions (example)	along a , b and c	4. Primitive (<i>P</i>) 5. Base-Centered (<i>C</i>) 6. Body-Centered (<i>I</i>) 7. Face-Centered (<i>F</i>)	$\alpha = \beta = \gamma \neq 90^\circ$
4. Tetragonal	4-fold axes, all parallel	along c	8. Primitive (<i>P</i>) 9. Body-Centered (<i>I</i>)	$a = b \neq c$ $\alpha = \beta = \gamma = 90^\circ$
5. Trigonal	3-fold axes, all parallel	along c	10. Primitive (<i>P</i>) 11. Rhombohedral (<i>R</i> / <i>H</i>)	$a = b = c \neq 0$ $\alpha = \beta = \gamma \neq 90^\circ$
6. Hexagonal	6-fold axes, all parallel	along c	10. Primitive (<i>P</i>)	$a = b \neq c$ $\alpha = \beta = 90^\circ; \gamma = 120^\circ$
7. Cubic	3-fold axes in four different orientations	along body diagonals	12. Primitive (<i>P</i>) 13. Body-Centered (<i>I</i>) 14. Face-Centered (<i>F</i>)	$a = b = c \neq 0$ $\alpha = \beta = \gamma = 90^\circ$

Crystal Systems

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

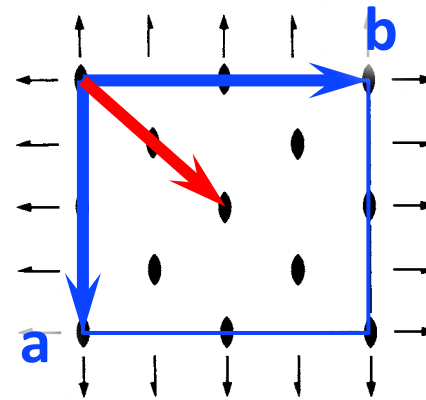
C222: an example of a centred cell

If we were using
a primitive cell



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

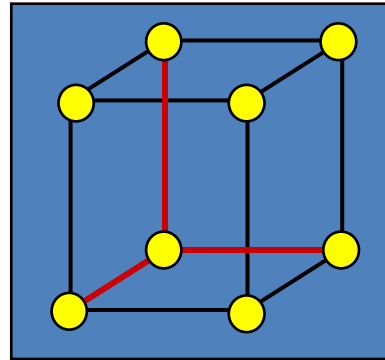
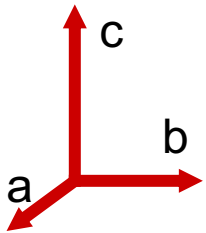
Standard setting;
C means additional
translation $\frac{1}{2}(\mathbf{a} + \mathbf{b})$



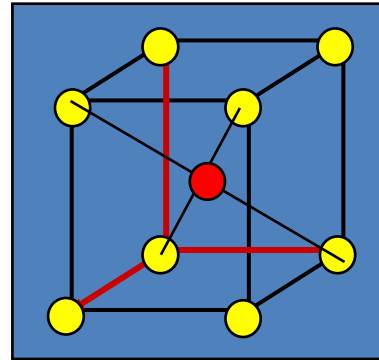
2-fold axes are
along **a**, **b** and **c**
(**conventional**
setting)

Centred unit cells in pictures

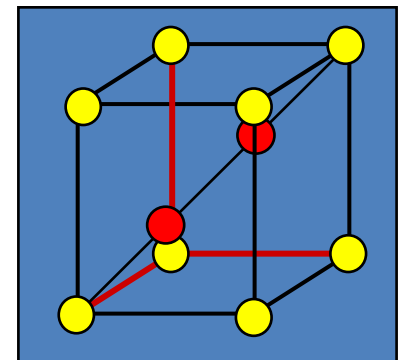
Our convention dictates that direction(s) of rotation axes define **a**, **b** and **c**
As a result, the crystal lattice of some space groups contains "additional" nodes (red) that represent "additional" translations



P – Primitive

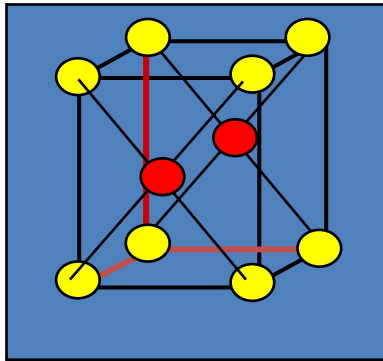


I – Body centred



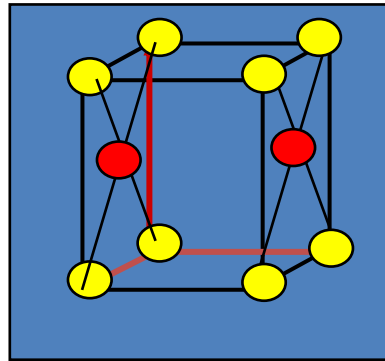
H – Hexagonal

(non-standard)

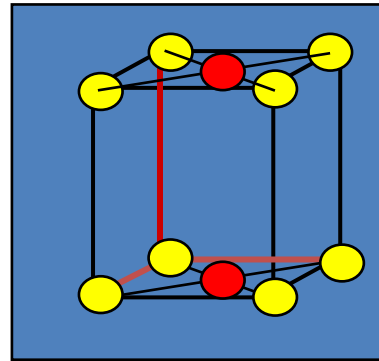


A – Face centred (A)

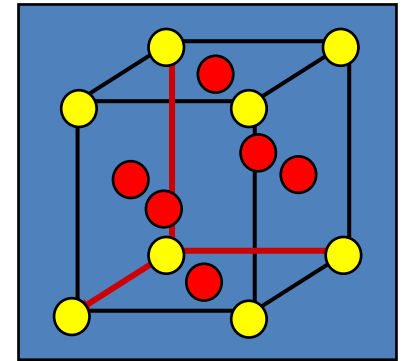
(non-standard)



B – Face centred (B)



C – Face centred (C)

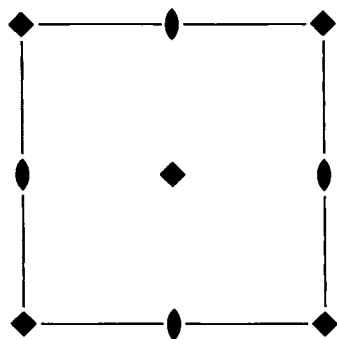


F – Face centred (all)

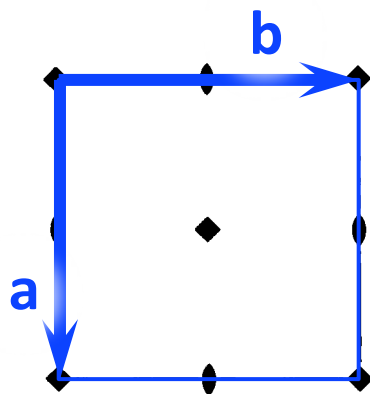
C4: an example of a redundant space group symbol

P4

as presented in the
International Tables
for Crystallography

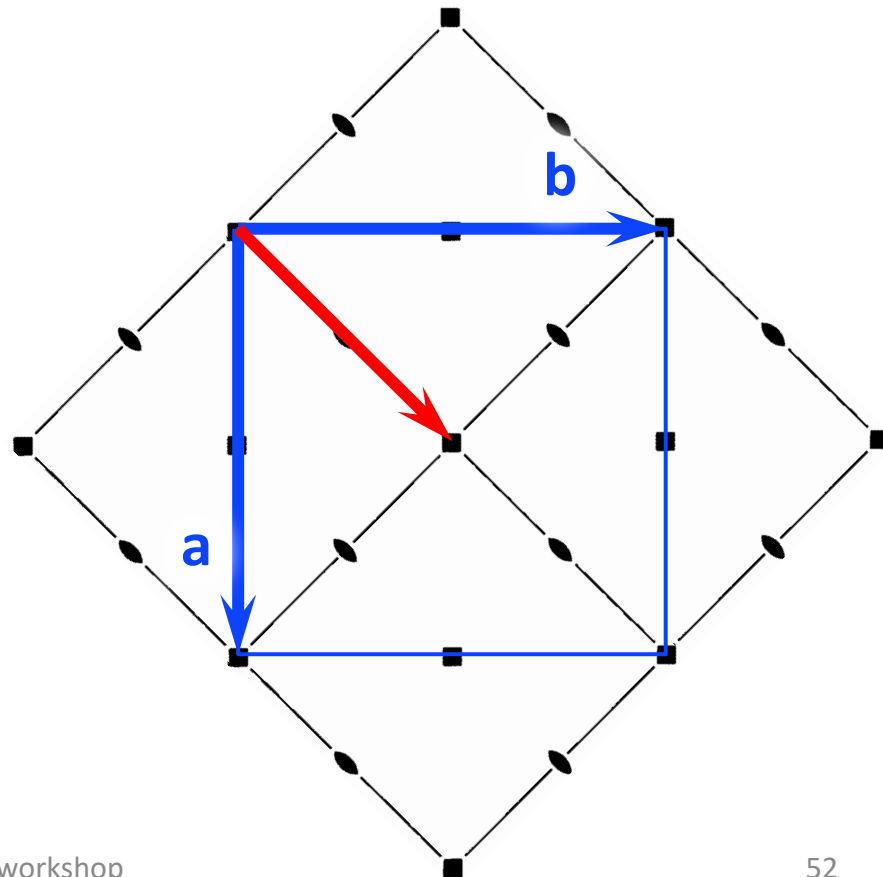


and with base
vectors shown



C4

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



Bravais lattices

- 7 crystal systems, combined with some of the centring types (P, C, I, F or H) give 14 Bravais lattices
- Not included:
 - impossible combinations (*e.g.* A4)
 - redundant combinations (*e.g.* P4 is kept, C4 is excluded)

Crystal Systems

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

Crystal Systems

Crystal System	Characteristic symmetry elements	Convention	Bravais lattices	Constraints on unit cell parameters
1. Triclinic	Translations only		1. Primitive (<i>P</i>)	$\alpha \neq \beta \neq \gamma \neq 90^\circ$
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3. Orthorhombic	2-fold axes in three perpendicular directions	along a , b and c	4. Primitive (<i>P</i>) 5. Base-Centered (<i>C</i>) 6. Body-Centered (<i>I</i>) 7. Face-Centered (<i>F</i>)	$\alpha = \beta = \gamma \neq 90^\circ$
4. Tetragonal	4-fold axes, all parallel	along c	8. Primitive (<i>P</i>) 9. Body-Centered (<i>I</i>)	$a = b \neq c$ $\alpha = \beta = \gamma = 90^\circ$
5. Trigonal	3-fold axes, all parallel	along c	10. Primitive (<i>P</i>) 11. Rhombohedral (<i>R</i> / <i>H</i>)	$a = b = c \neq 0$ $\alpha = \beta = \gamma \neq 90^\circ$
6. Hexagonal	6-fold axes, all parallel	along c	10. Primitive (<i>P</i>)	$a = b \neq c$ $\alpha = \beta = 90^\circ \neq \gamma = 120^\circ$
7. Cubic	3-fold axes in four different orientations	along body diagonals	12. Primitive (<i>P</i>) 13. Body-Centered (<i>I</i>) 14. Face-Centered (<i>F</i>)	$a = b = c \neq 0$ $\alpha = \beta = \gamma = 90^\circ$

Crystal Systems

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

Space group representation in ITC-A

(Short) Hermann-Mauguin symbol

$P2_12_12_1$

No. 19

(Extended) Hermann-Mauguin symbol

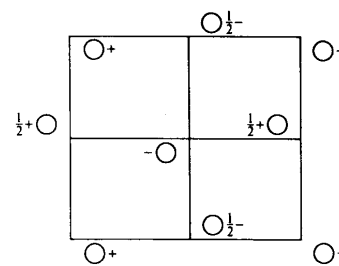
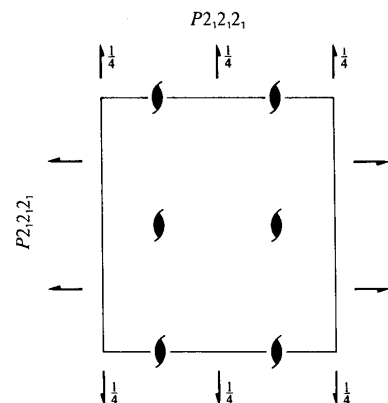
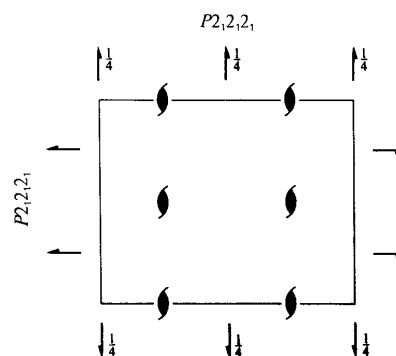
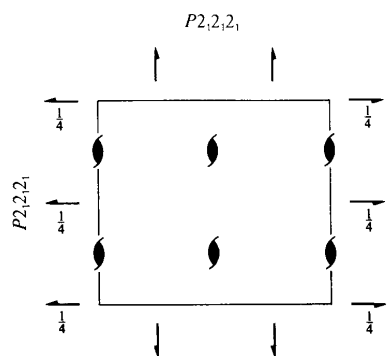
D_2^4

$P2_12_12_1$

222

Orthorhombic

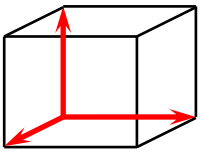
Patterson symmetry $Pmmm$



Triclinic

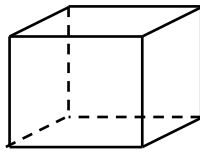
$P\ 1$

Lattice type



P

"1" means no symmetry operations except for translations



1

No constraints on
 $a, b, c, \alpha, \beta, \gamma$

Monoclinic

$P 2$
 $C 2$

$P 2_1$

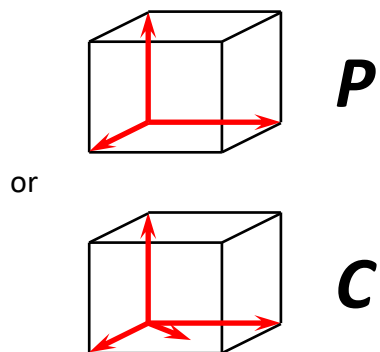
Standard HM symbols: **papers**

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

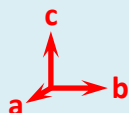
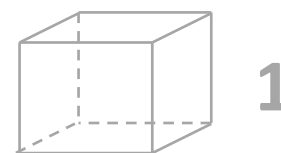
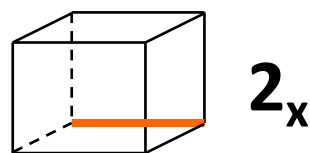
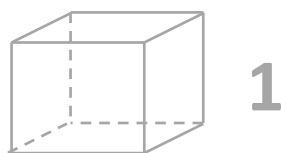
$P 1 2_1 1$

Extended HM symbols: **PDB**

Lattice type



Directions and **orders** of axes



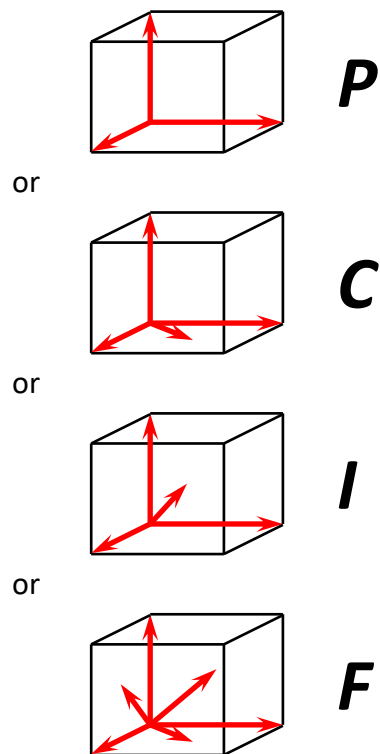
2-fold axes, all parallel

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

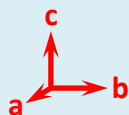
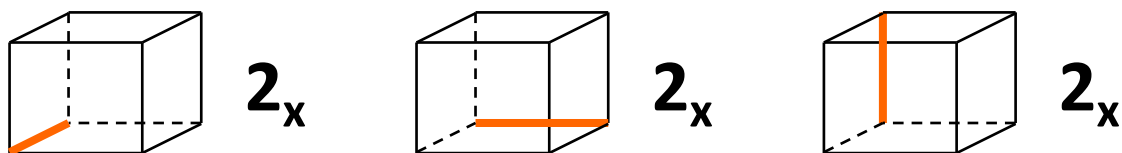
Orthorhombic

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

Lattice type



Directions and orders of axes



2-fold axes in three perpendicular directions

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

Orthorhombic

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

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

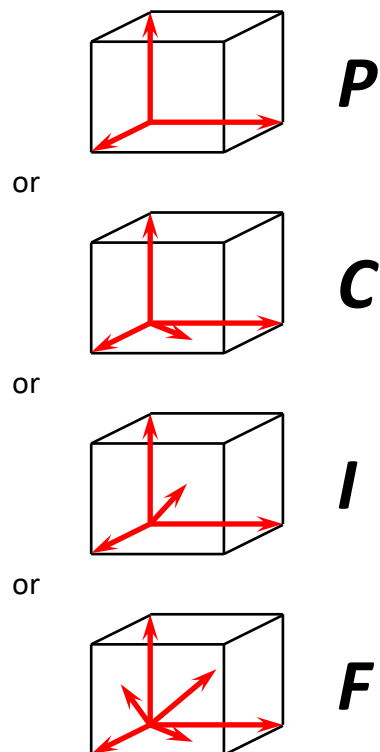
$P 2_1 2_1 2$

$P 2_1 2_1 2_1$

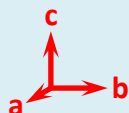
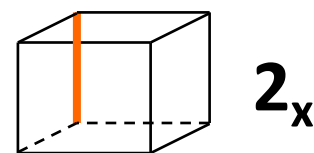
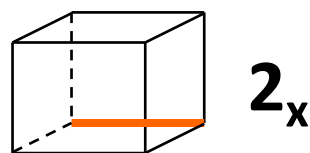
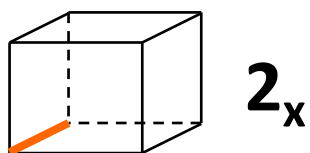
example

$I 2_1 2_1 2_1$

Lattice type



Directions and orders of axes



2-fold axes in three
perpendicular directions

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

Tetragonal

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

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

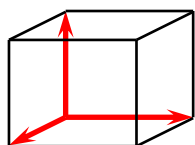
$P 4_2 2_1 2$
 $P 4_2 2 2$

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

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

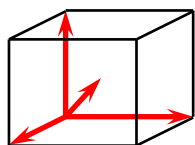
 $I 4$ $I 4_1$

Lattice type



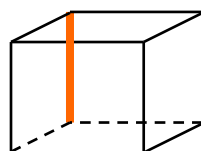
P

or

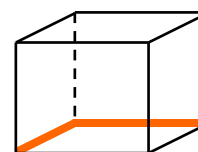


I

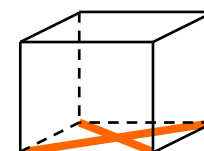
Directions and orders of axes



4_x

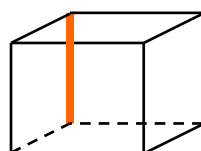


2_y

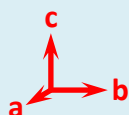


2

or



4_x



4-fold axes along c

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

Cubic

$P 4 3 2$

$I 4 3 2$

$F 4 3 2$

$P 4_1 3 2$

$I 4_1 3 2$

$F 4_1 3 2$

$P 4_2 3 2$

$P 4_3 3 2$

$P 2 3$

$I 2 3$

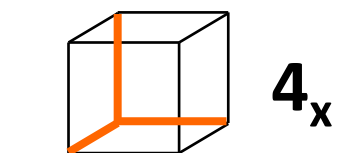
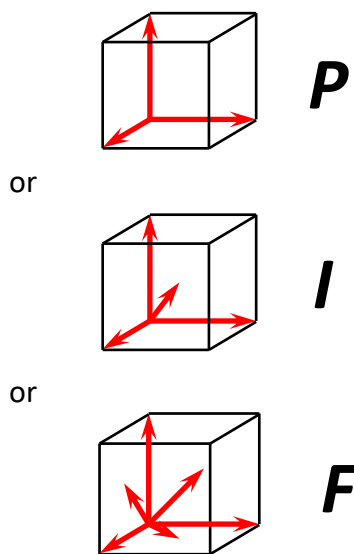
$F 2 3$

$P 2_1 3$

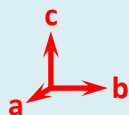
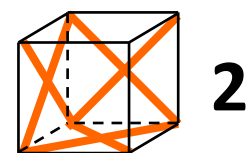
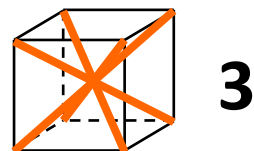
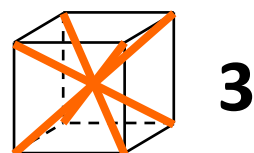
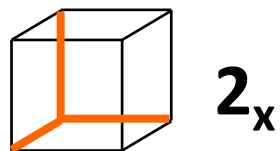
$I 2_1 3$

Lattice type

Directions and orders of axes



or



3-fold axes parallel to
the body diagonals

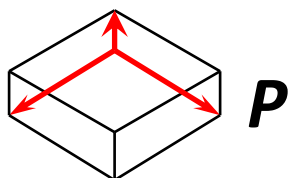
$\alpha = \beta = \gamma = 90^\circ$
 $a = b = c$

Trigonal - P

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

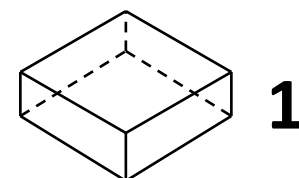
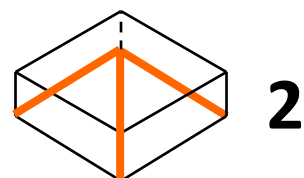
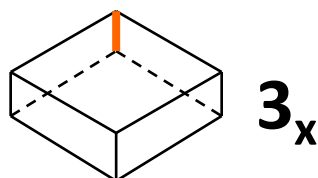
$P3$ $P3_1$ $P3_2$

Lattice type

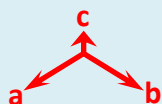
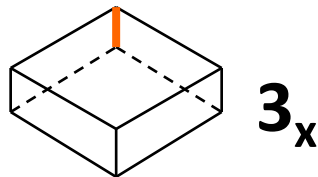
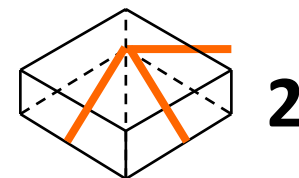
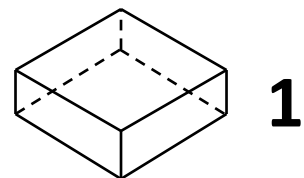
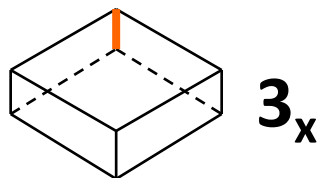


Directions and orders of axes

or



or



3-fold axes along c

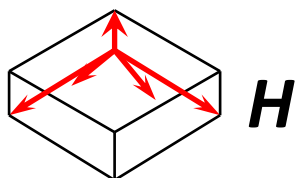
$\alpha = \beta = 90^\circ$ $a = b$
 $\gamma = 120^\circ$

Trigonal - H

$H\ 3\ 2$

$H3$

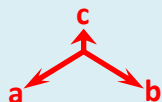
Lattice type



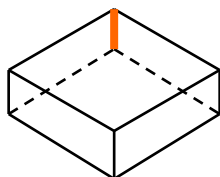
H

or

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

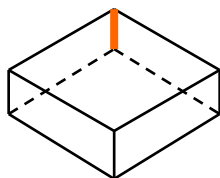


Directions and orders of axes

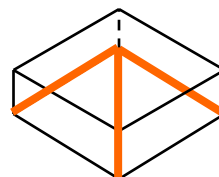


3

or



3



2

3-fold axes along **c**

$$\alpha = \beta = 90^\circ \quad a = b$$
$$\gamma = 120^\circ$$

Hexagonal

$P 6 2 2$

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

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

$P 6_3 2 2$

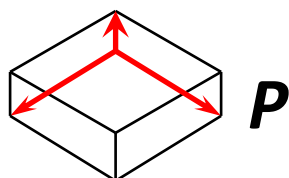
$P6$

$P6_1$
 $P6_5$

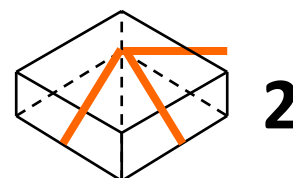
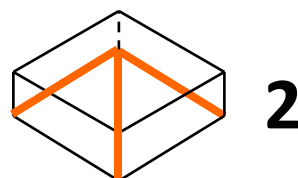
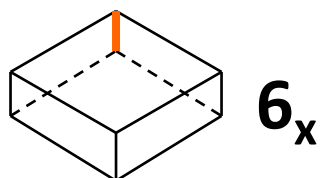
$P6_2$
 $P6_4$

$P6_3$

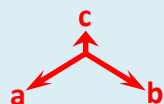
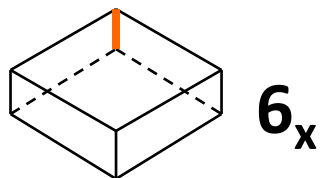
Lattice type



Directions and orders of axes



or



6-fold axes along c

$\alpha = \beta = 90^\circ$ $a = b$
 $\gamma = 120^\circ$

Ones

~~$P 1 1 1$~~

$P 1$

$P 1 2 1$

$P 2$

~~$P 4 1 1$~~

$P 4$

~~$P 3 1 1$~~

$P 3$

$P 3 2 1$

~~$P 3 2$~~

$P 3 1 2$

~~$P 3 2$~~

Subscripts

P43212

P 43 21 2

P 4(3) 2(1) 2

*P*4₃2₁2

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

Symmetry based setting: $\alpha = \gamma = 90^\circ$

C 1 2 1

Lattice based setting: $\alpha = \gamma = 90^\circ$
 $\beta < 120^\circ$

C 1 2 1 or / 1 2 1

- the same space group
- different crystal setting

Symmetry based setting vs. lattice based setting: primitive orthorhombic

Symmetry based setting: $\alpha = \beta = \gamma = 90^\circ$

$P 2 2 2_1$

$P 2_1 2_1 2$

Lattice based setting: $\alpha = \beta = \gamma = 90^\circ$
 $a < b < c$

$P 2 2 2_1$

$P 2_1 2_1 2$

$P 2 2_1 2$

$P 2_1 2 2_1$

$P 2_1 2 2$

$P 2 2_1 2_1$

each of the two columns:

- the same space group
- different crystal setting

Space group representation in ITC-A

Crystal Class
(point group)

222

Orthorhombic

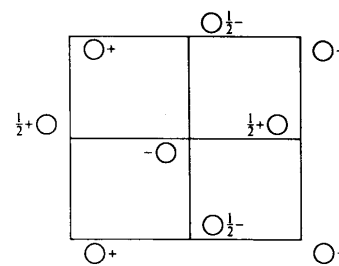
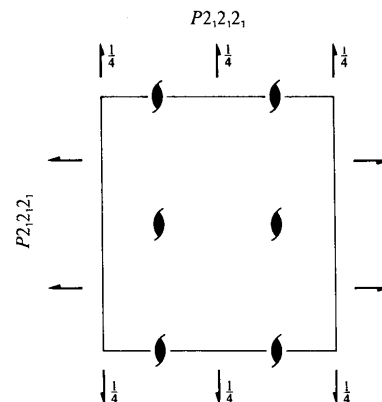
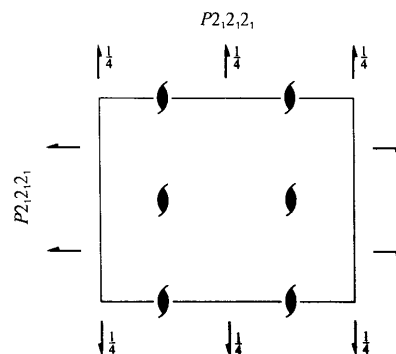
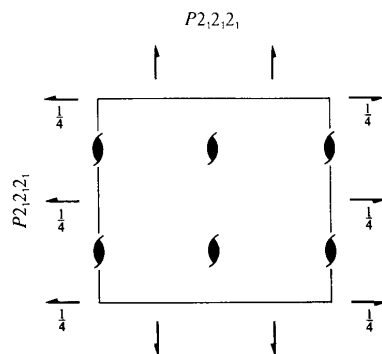
Patterson symmetry $Pmmm$

$P2_12_12_1$

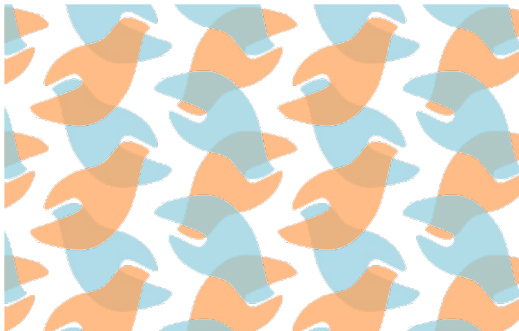
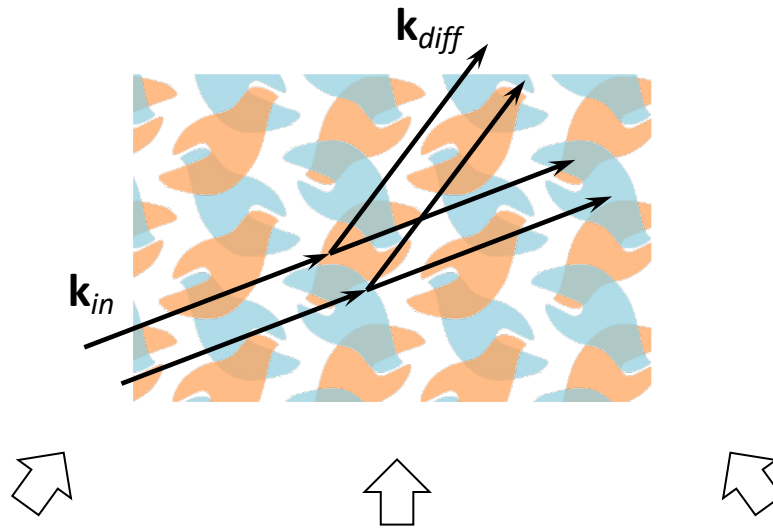
No. 19

D_2^4

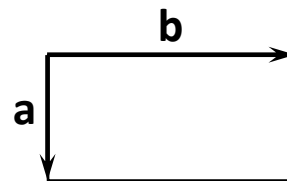
$P2_12_12_1$



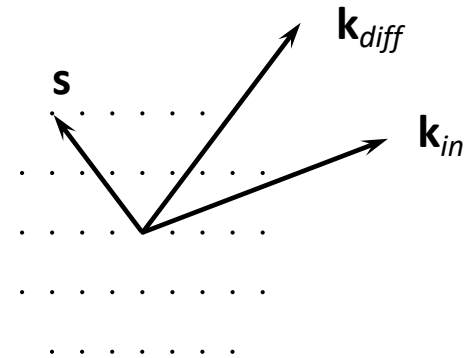
Conventional diffraction scheme



real space



Bragg planes



reciprocal space

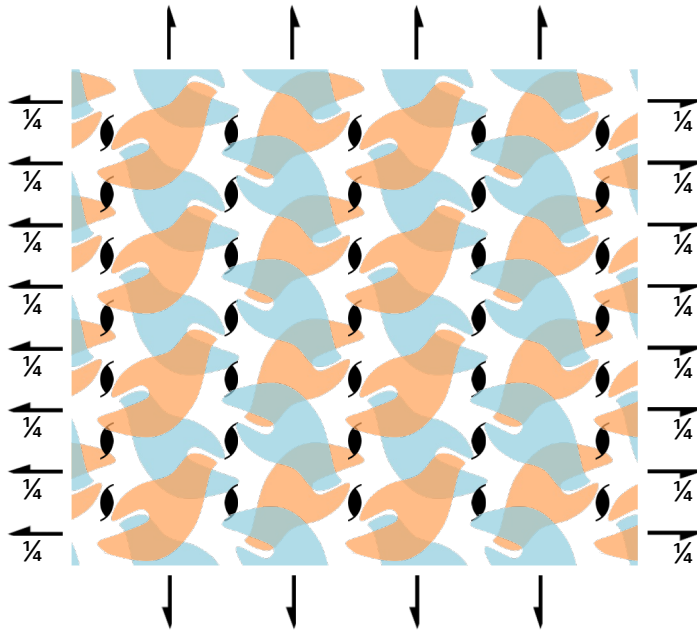
Symmetry of intensities

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

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

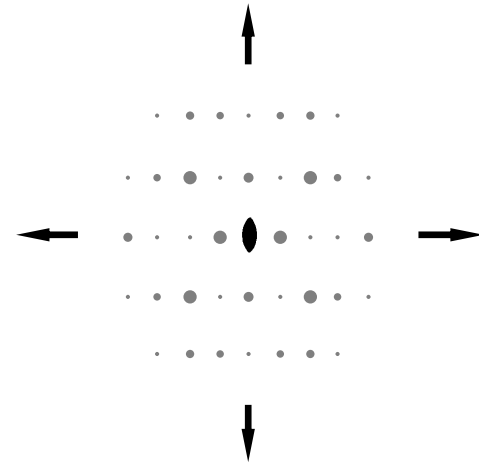
Symmetry of intensities

real space



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

reciprocal space



to give an element of a point group.

Symmetry of intensities

Real space

Crystal structure

Space group operation

The same crystal structure

Reciprocal space

Intensities at Bragg points

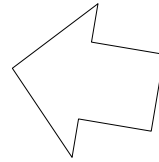
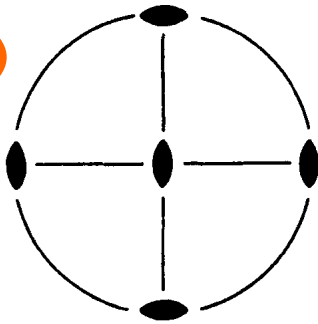
Strip any translation component from the space group operation:

Point group operation

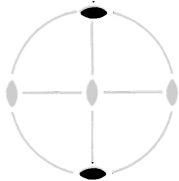
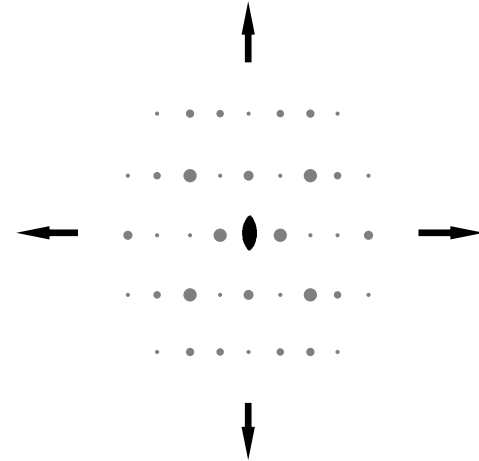
The same set of intensities (within σ)

Point group scheme

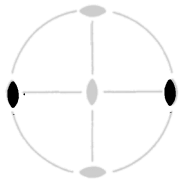
222



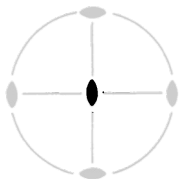
reciprocal space



vertical 2-fold axis



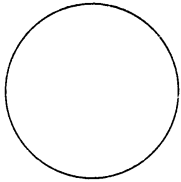
horizontal 2-fold axis



2-fold axis into plane

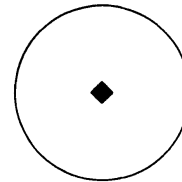
The point groups that can exist in protein crystals

1

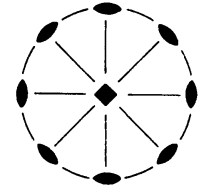


If it helps view as sphere

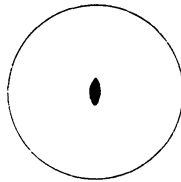
4



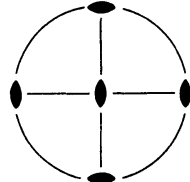
422



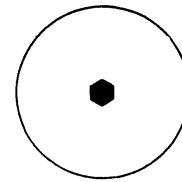
2



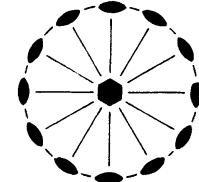
222



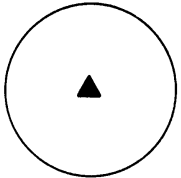
6



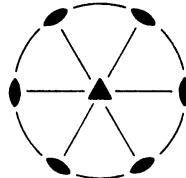
622



3



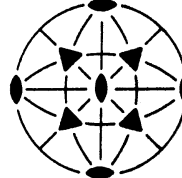
321



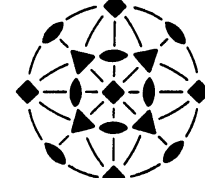
312



23



432



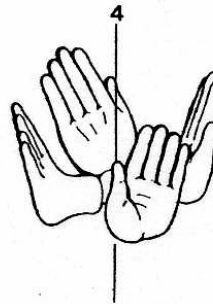
The point groups that can exist in protein crystals

1

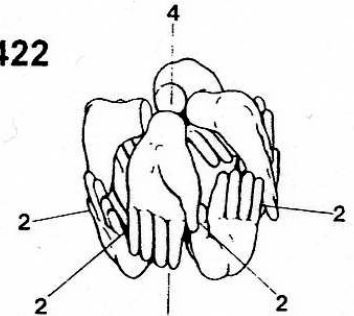


maybe an easier
representation

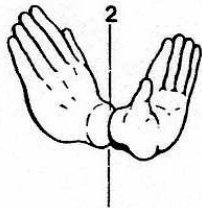
4



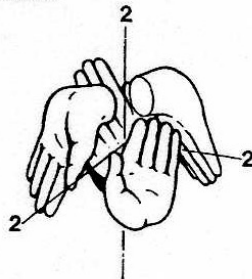
422



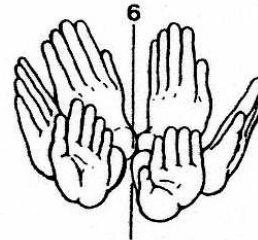
2



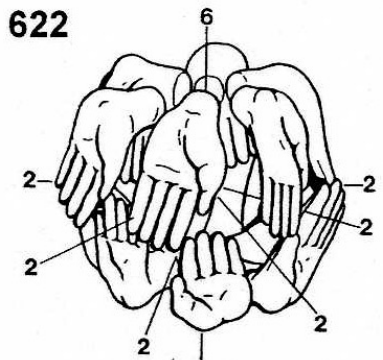
222



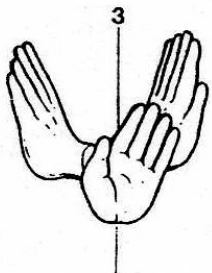
6



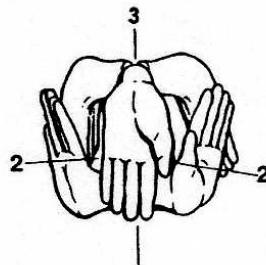
622



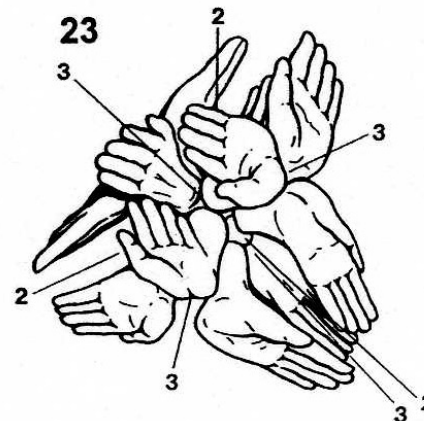
3



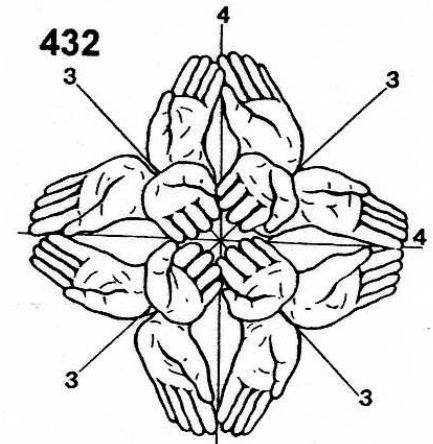
32



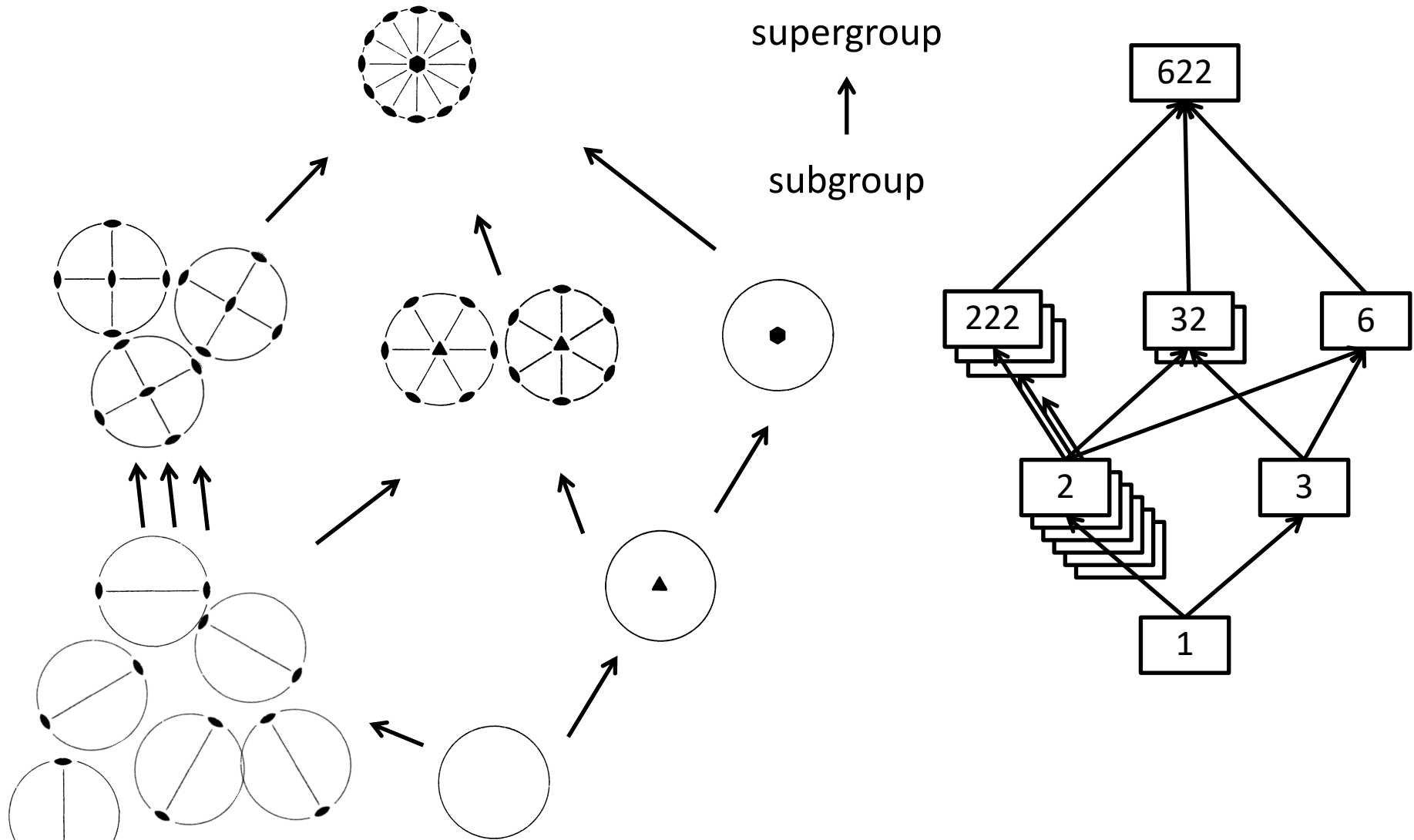
23



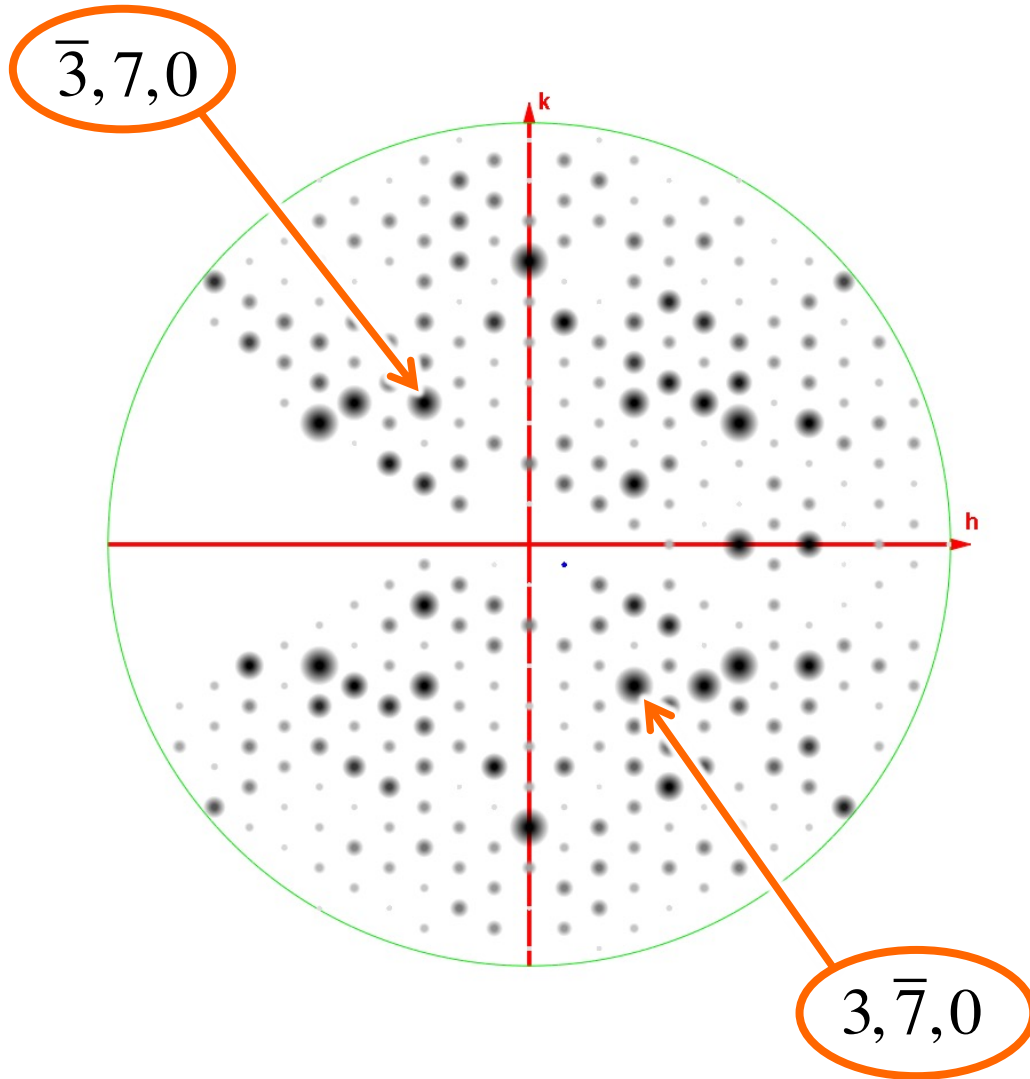
432



Subgroups of the point group 622



Friedel's law



(no anomalous signal)

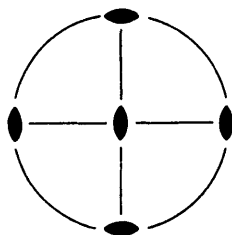
$$I(\bar{3}, 7, 0) = I(3, \bar{7}, 0)$$

Point group and Laue group

+ inversion =

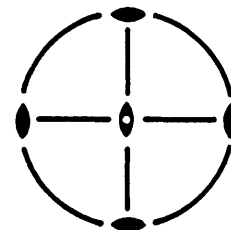
Crystal point group

222



Laue point group

m m m

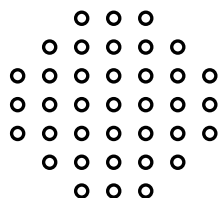


The eleven Laue point groups or crystal classes

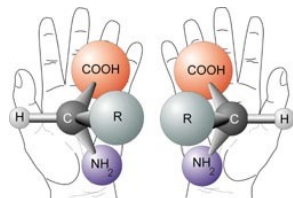
Crystal system	Laue point group experiment (no anomalous data)	Non-centrosymmetric point groups belonging to the Laue point group
Cubic	$m\bar{3}m$ $m\bar{3}$	432 $\bar{4}3m$ 23
Tetragonal	$4/mmm$ $4/m$	422 $4mm$ $\bar{4}2m$ 4 $\bar{4}$
Orthorhombic	mmm	222 $mm2$
Trigonal	$3m$ 3	32 $3m$ 3
Hexagonal	$6/mmm$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

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

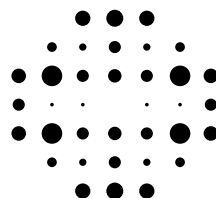
Reciprocal space lattice
(positions of reflections)



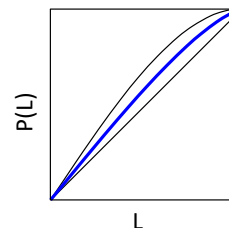
Mirror symmetry is not
allowed in biological
macromolecules



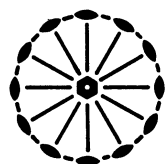
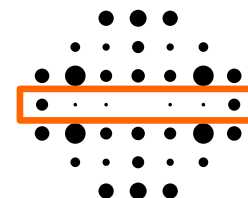
Intensities of
reflections



Twinning
test

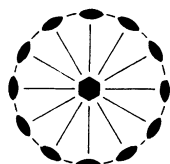


Intensities of axial
reflections



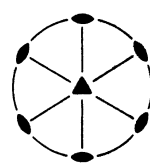
$6/mmm$

Lattice
point group



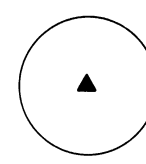
622

Highest possible
crystal point group



312

Approximate
point group of
diffraction



3

Possible
crystal point
group



$P3_1$ or $P3_2$

Possible
crystal space
group(s)

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

End

(Short) Hermann-Mauguin symbol

$P2_12_12_1$

No. 19

(Extended) Hermann-Mauguin symbol

D_2^4

$P2_12_12_1$

Crystal Class (point group)

222

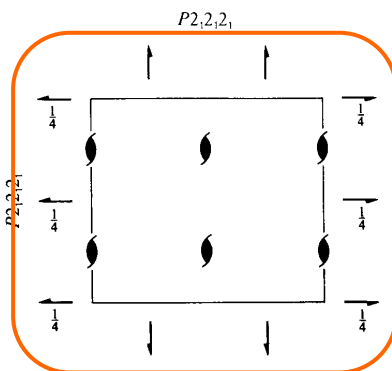
Crystal system

Orthorhombic

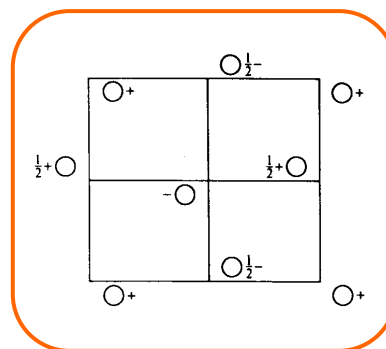
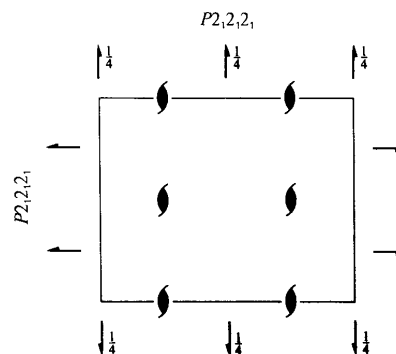
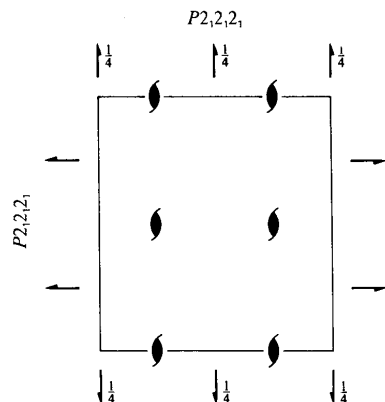
Patterson symmetry $Pmmm$

Patterson symmetry

Location of symmetry elements



Two other projections are also shown for this space group



Set of equivalent points in general position.

We were looking at "molecular wallpaper" instead