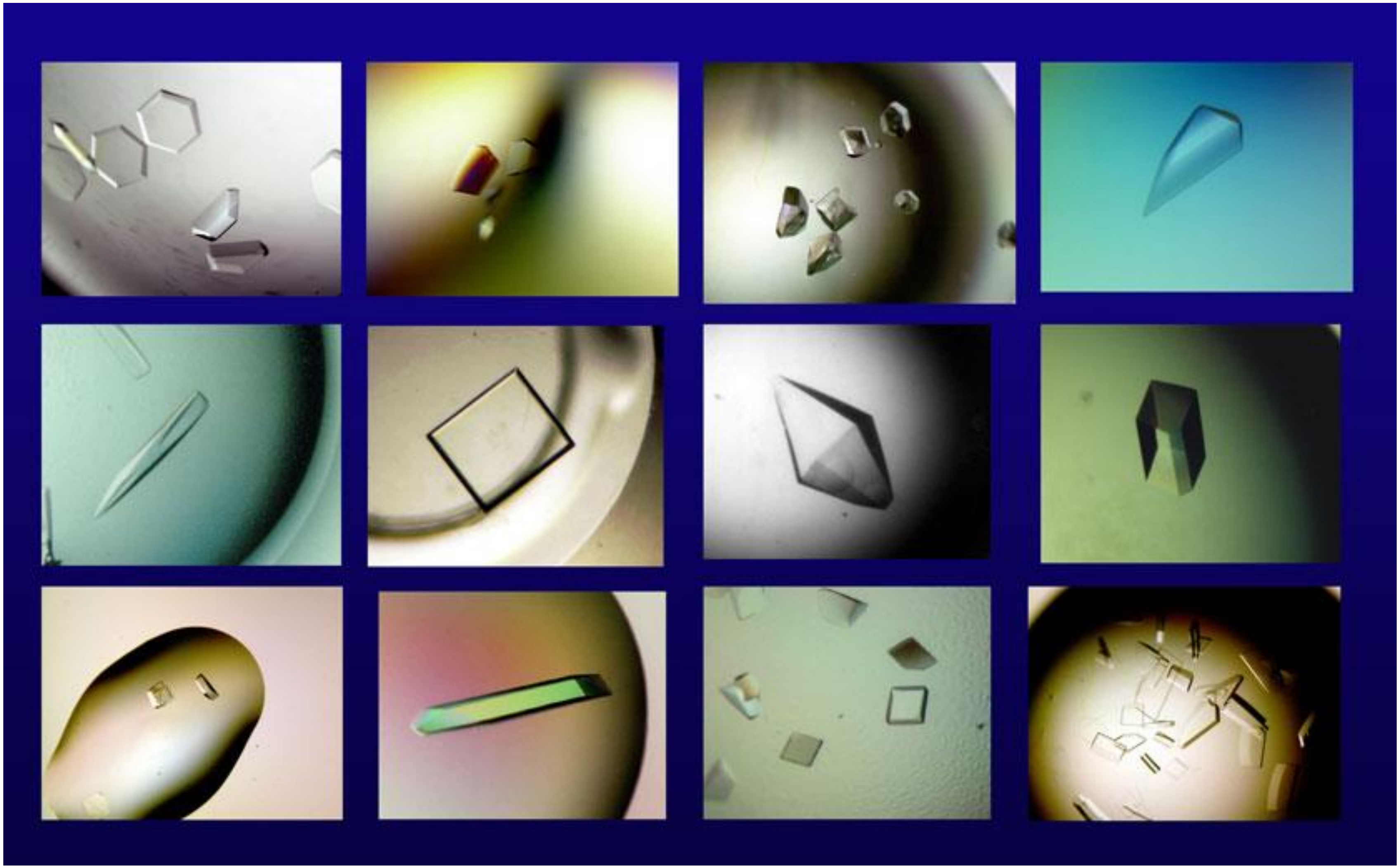
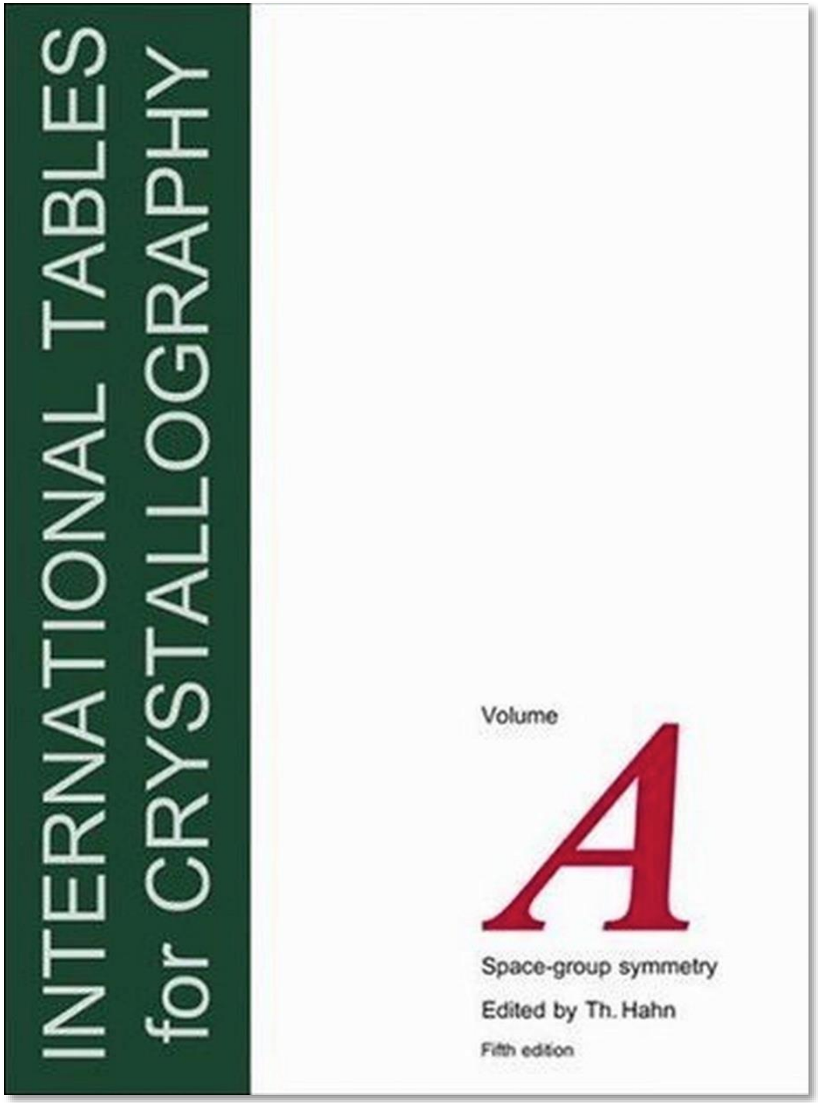
Introduction to space groups

Andrey Lebedev, CCP4

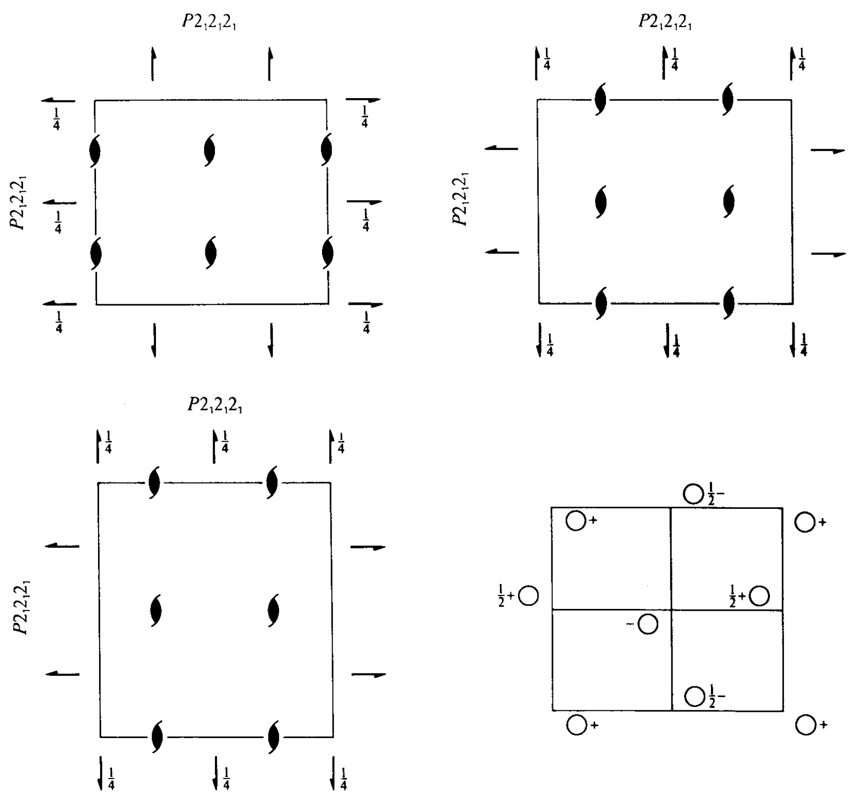




Further referred
to as ITC-A

Space group representation in ITC-A

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

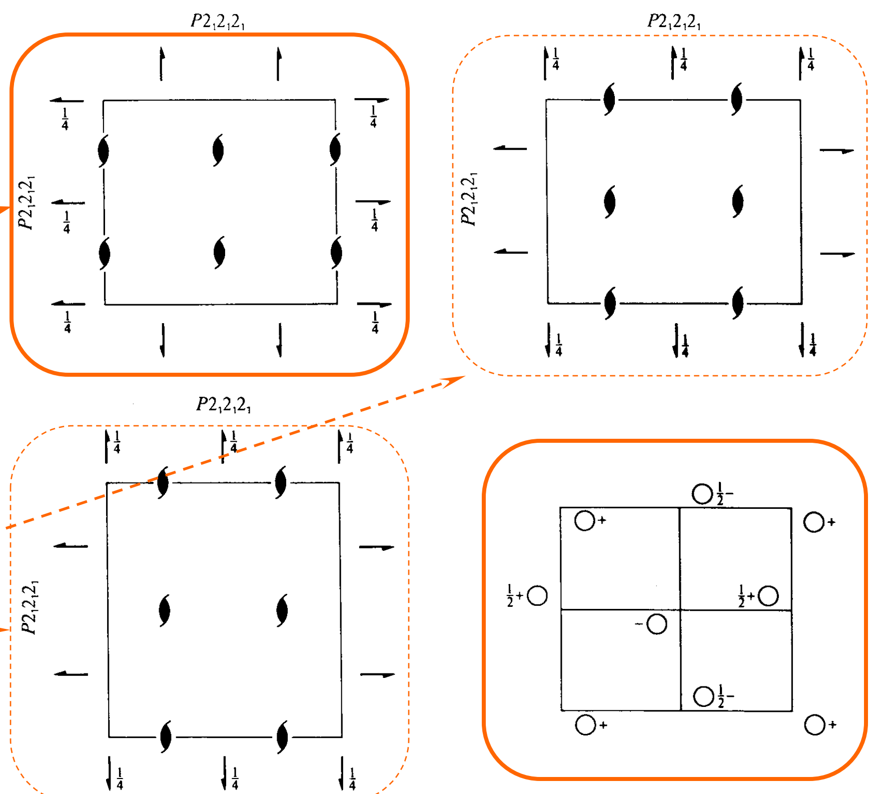


Space group representation in ITC-A

$P2_12_12_1$ D_2^4 222 Orthorhombic

No. 19 $P2_12_12_1$ Patterson symmetry $Pmmm$

Location of symmetry elements

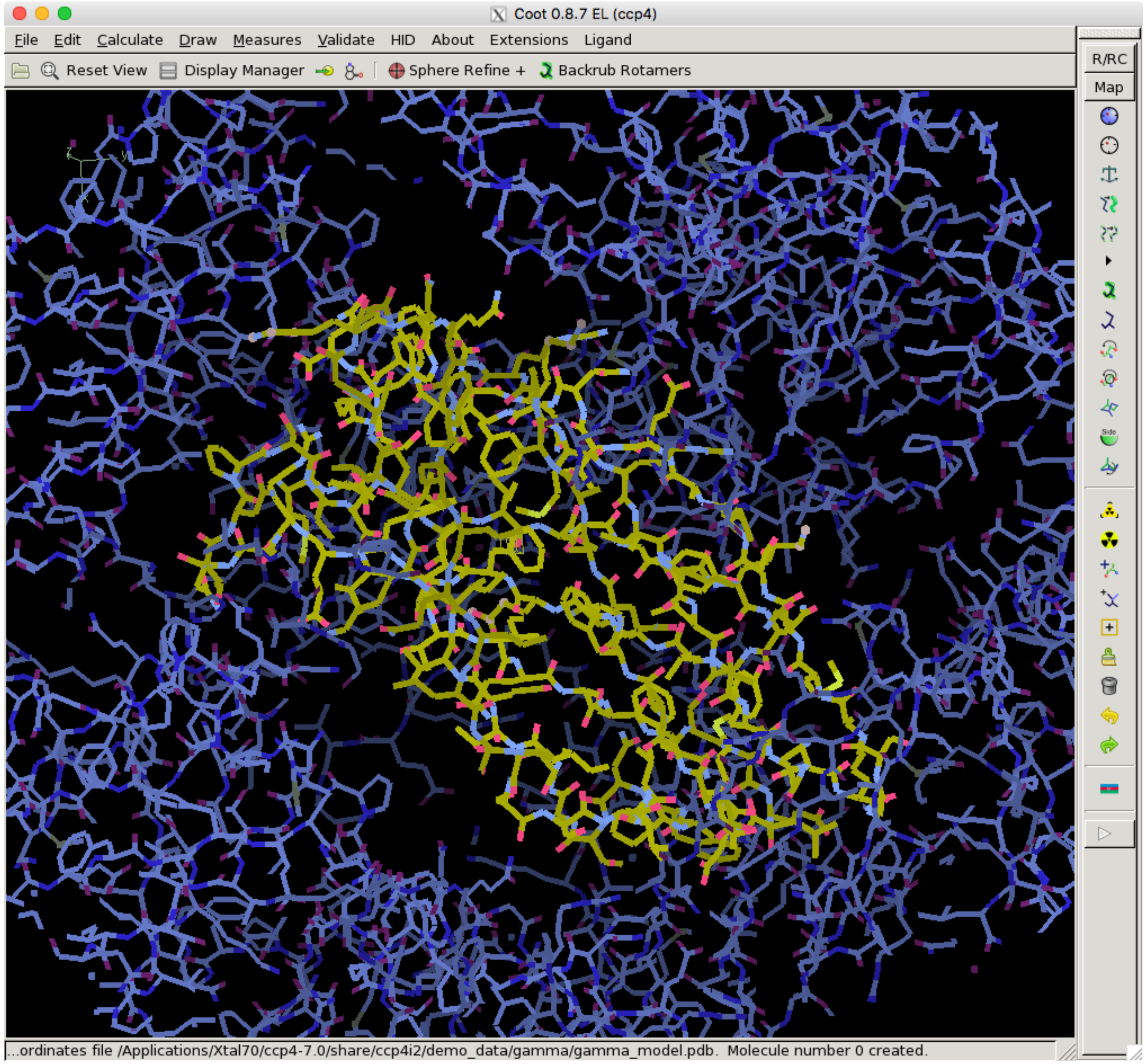


Two other projections are also shown for this space group

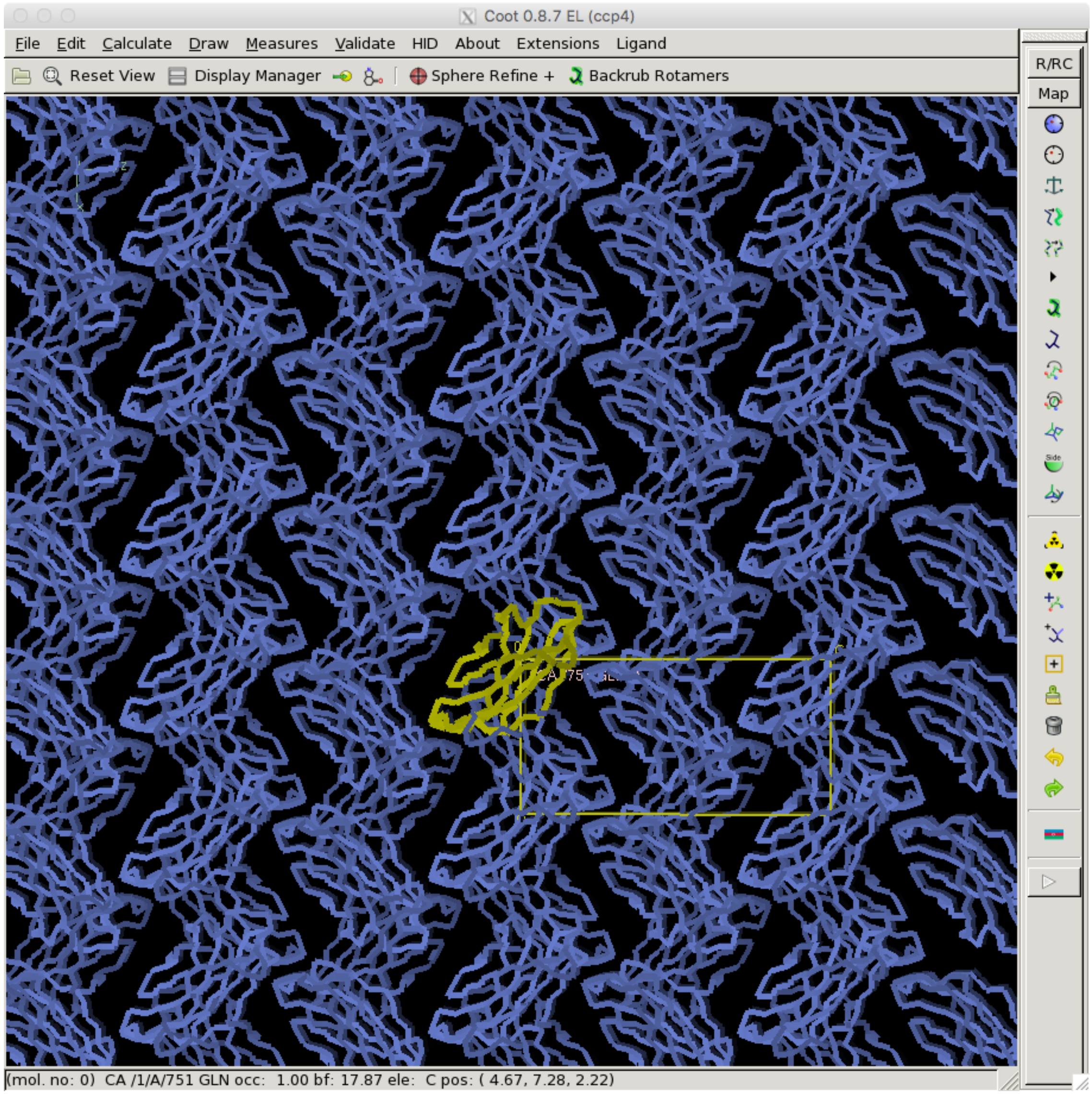
Set of equivalent points in general position.

We will be looking at "molecular wallpaper" instead

Examine structure in Coot



Symmetry view in Coot

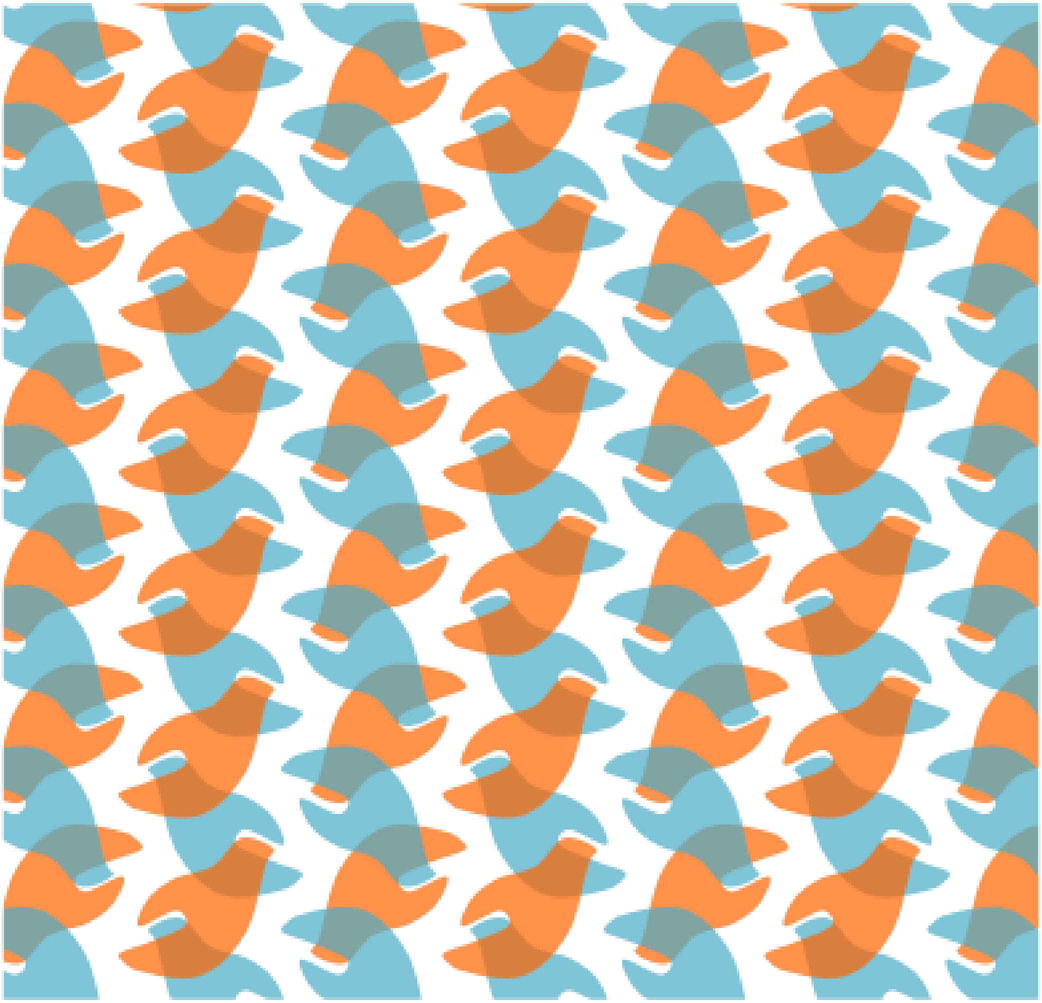


- Helps learning – compare you structure with the space group scheme in the International tables

- Helps building correct perception of what is the physical object and what is an “annotation”.

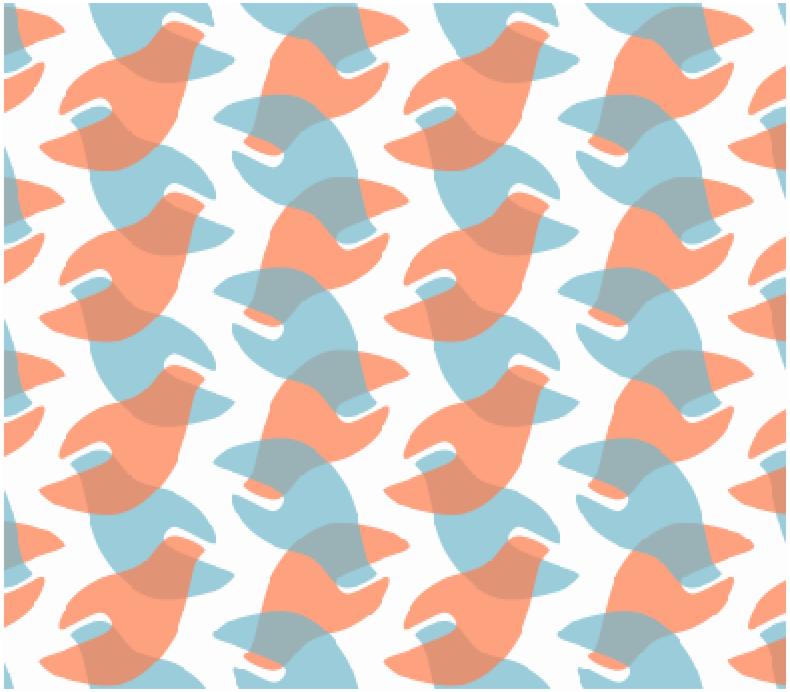
(e.g. molecules are real, and unit cell is just a label; crystal is built of molecules not of unit cells!)

Simplified representation



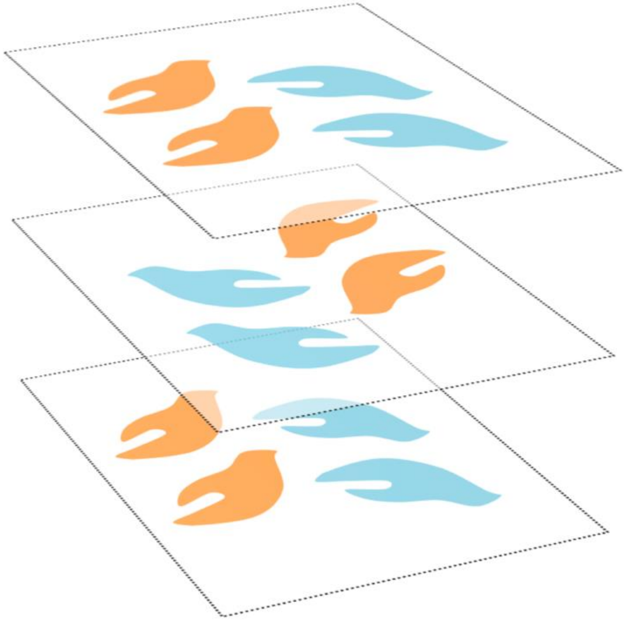
Each “molecule” has two sides, blue and orange

Simplified representation

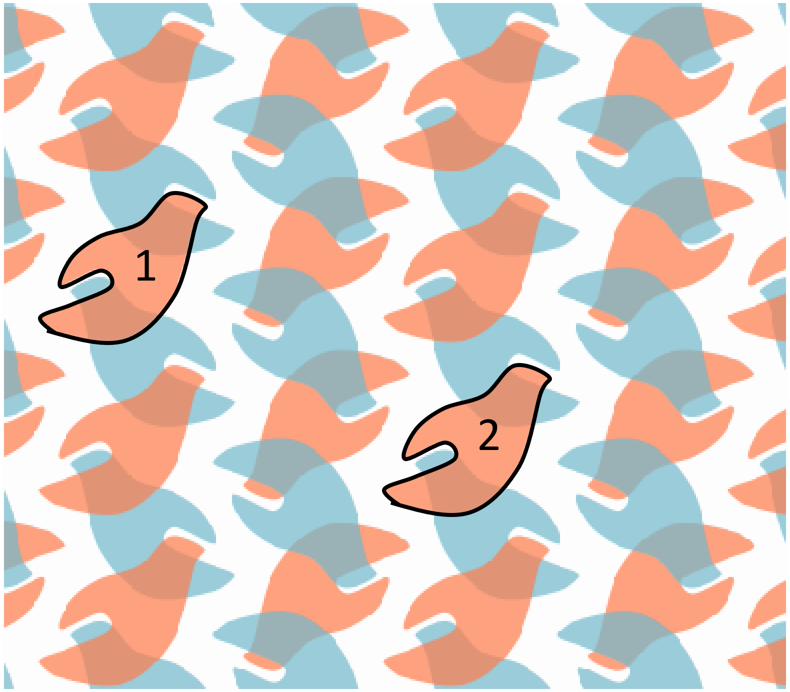


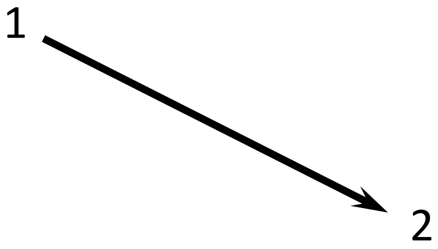
View from the top

There is a third dimension.



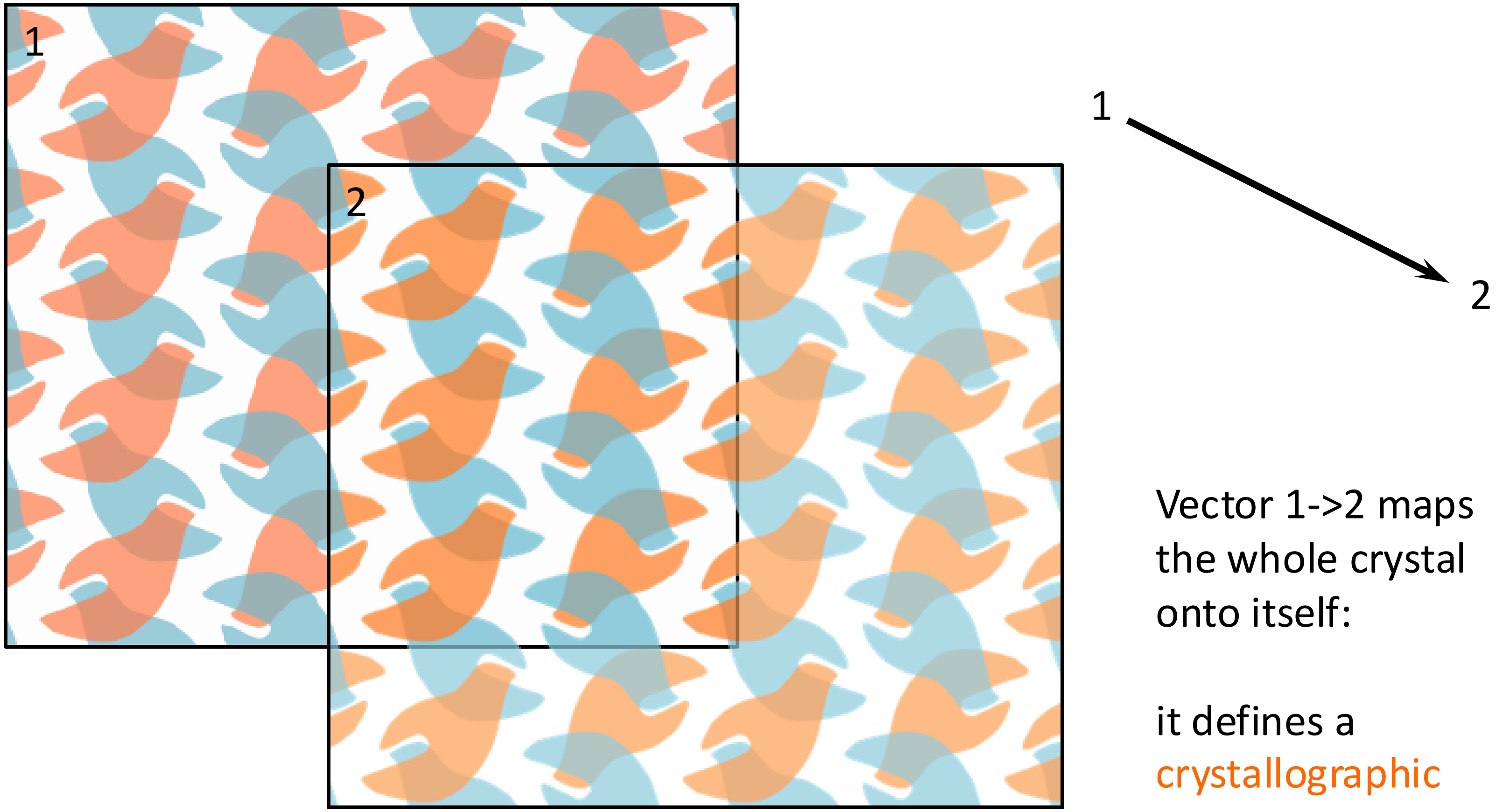
Translation 1-2





Vector maps 1 -> 2

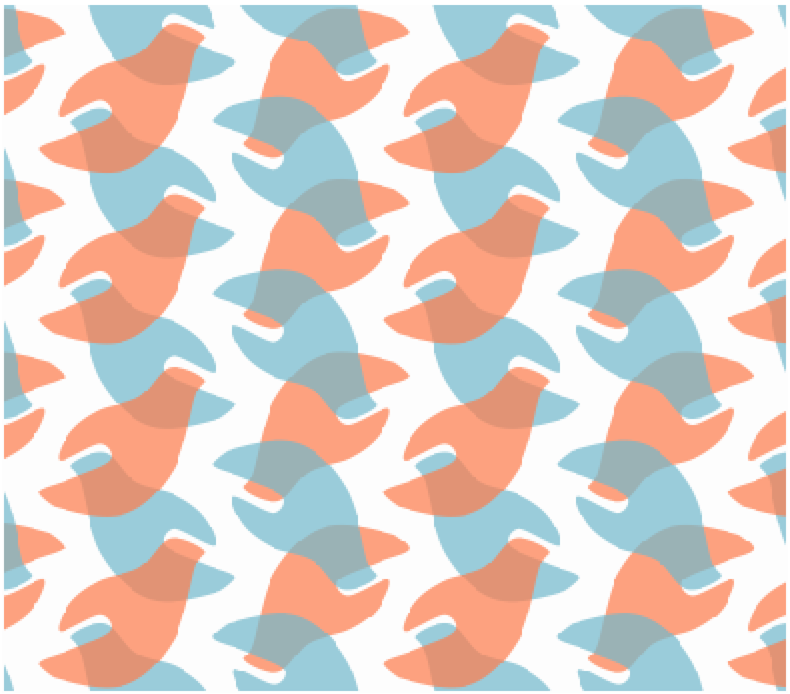
Translation 1-2 is global

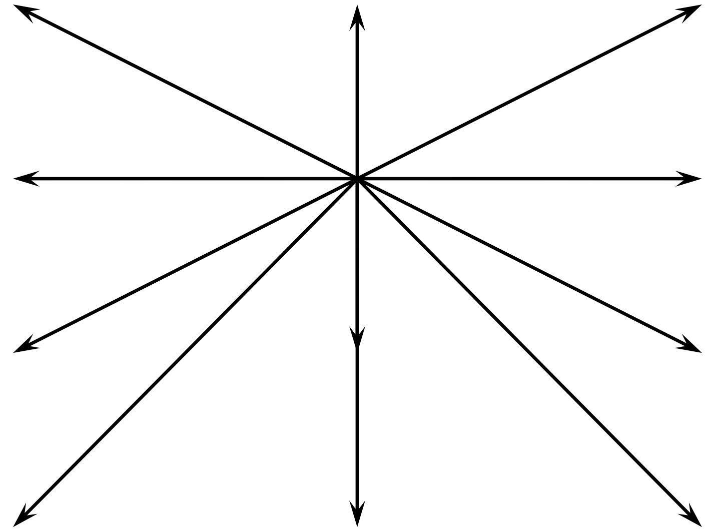


Vector 1->2 maps the whole crystal onto itself:

it defines a crystallographic operation

All translations form an infinite group

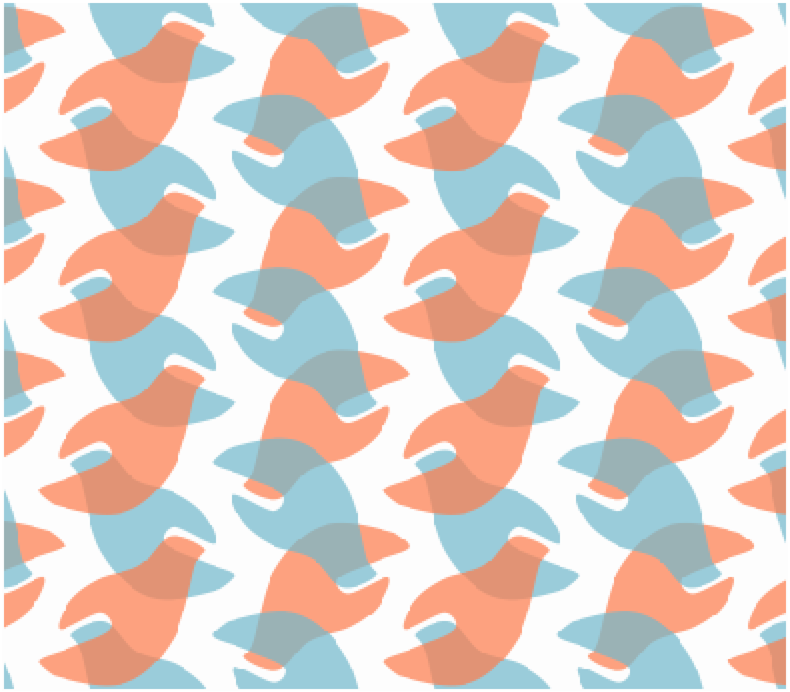


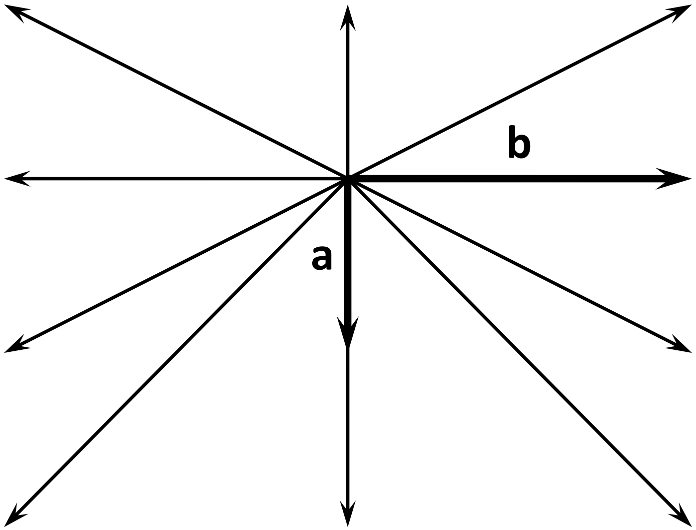


An infinite group (over vector sum):

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

Basis vectors

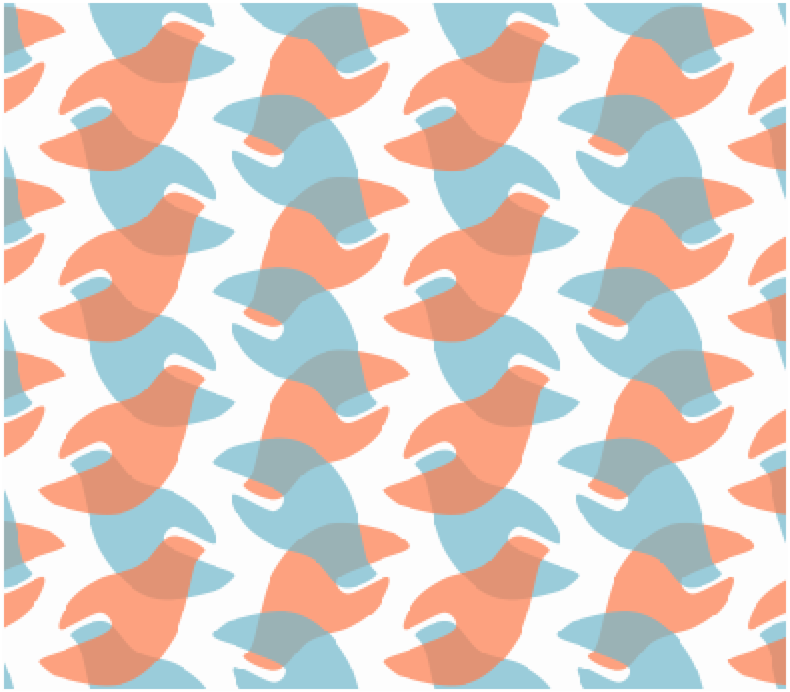


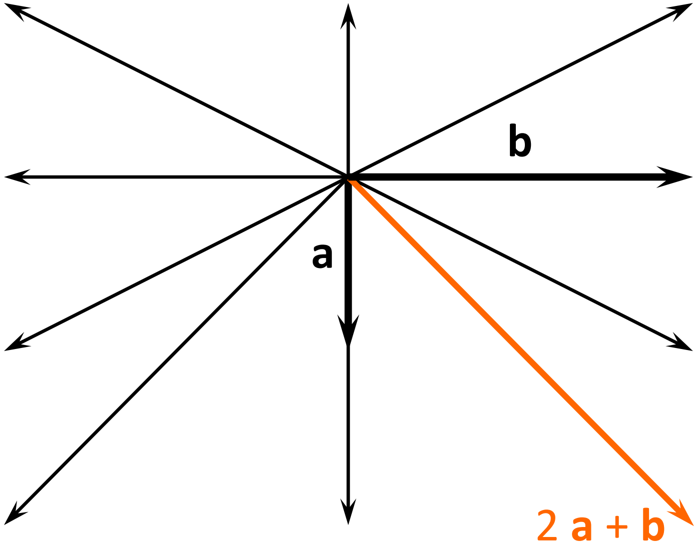


All the translations that map the crystal onto itself can be produced from a basis set: **a**, **b**, **c**

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

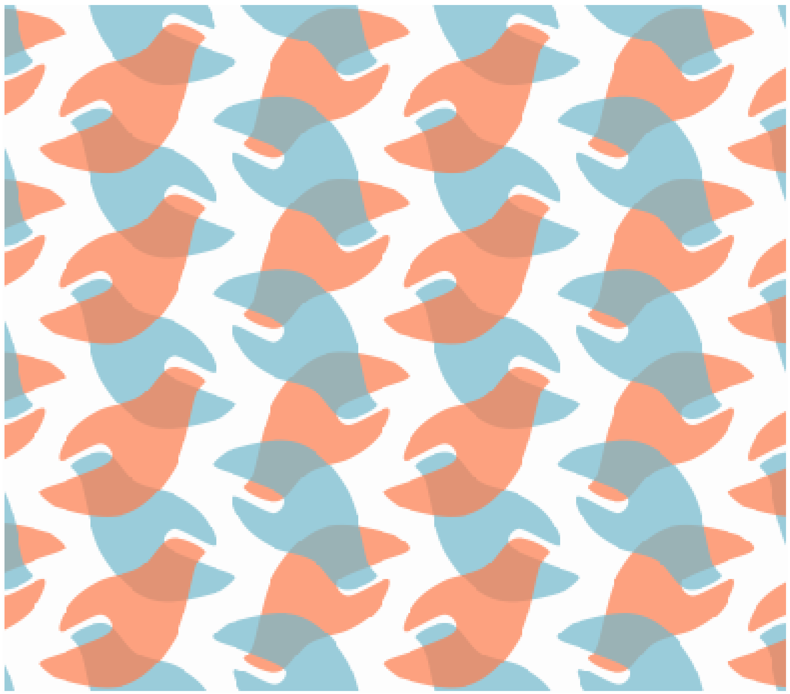
Basis vectors

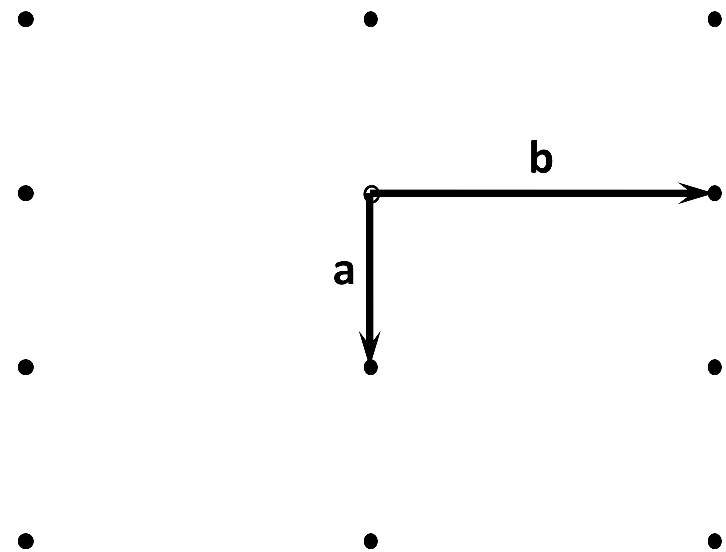




For example, the highlighted vector is expressed as 2 **a** + **b**.

Lattice

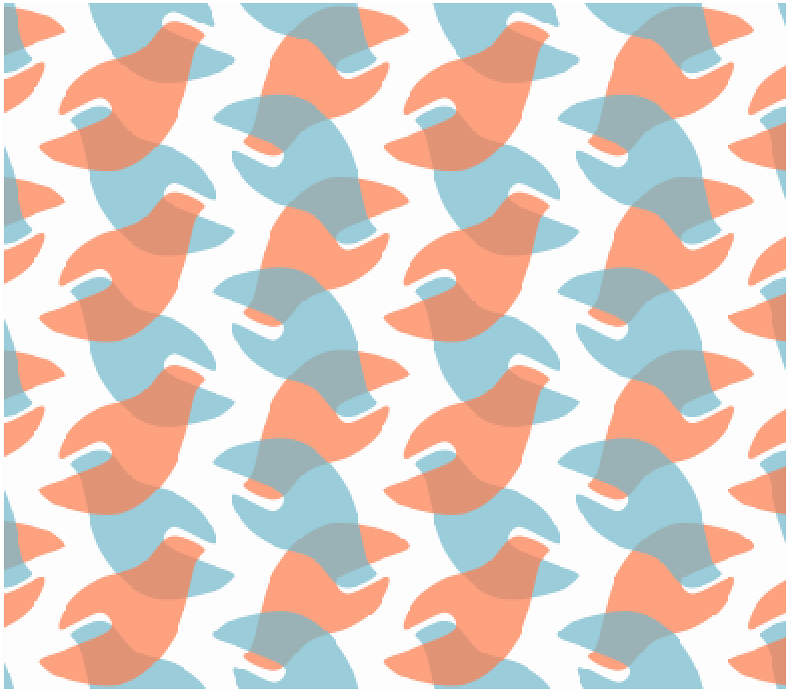


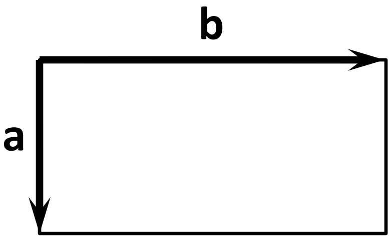


All the crystallographic translations can be represented as a lattice.

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

Unit cell

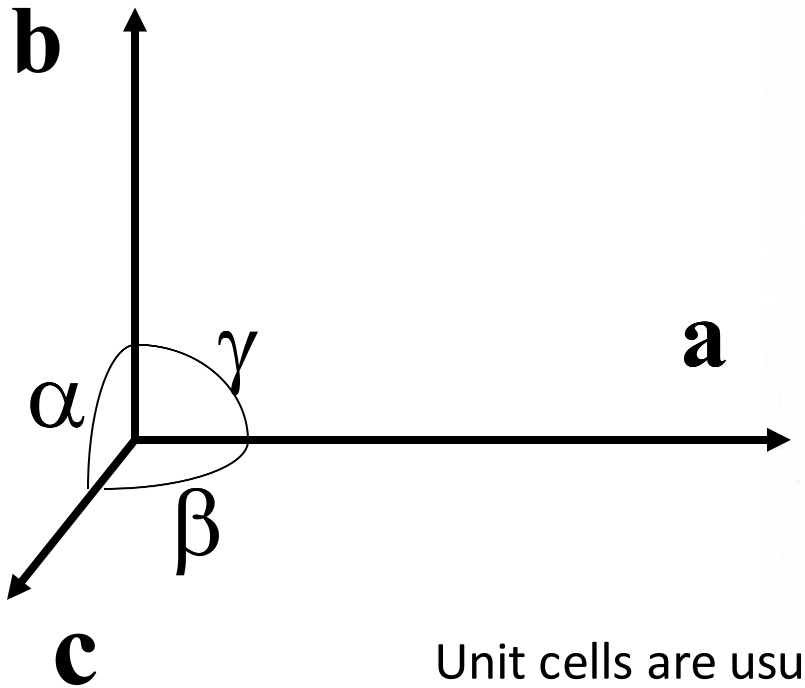


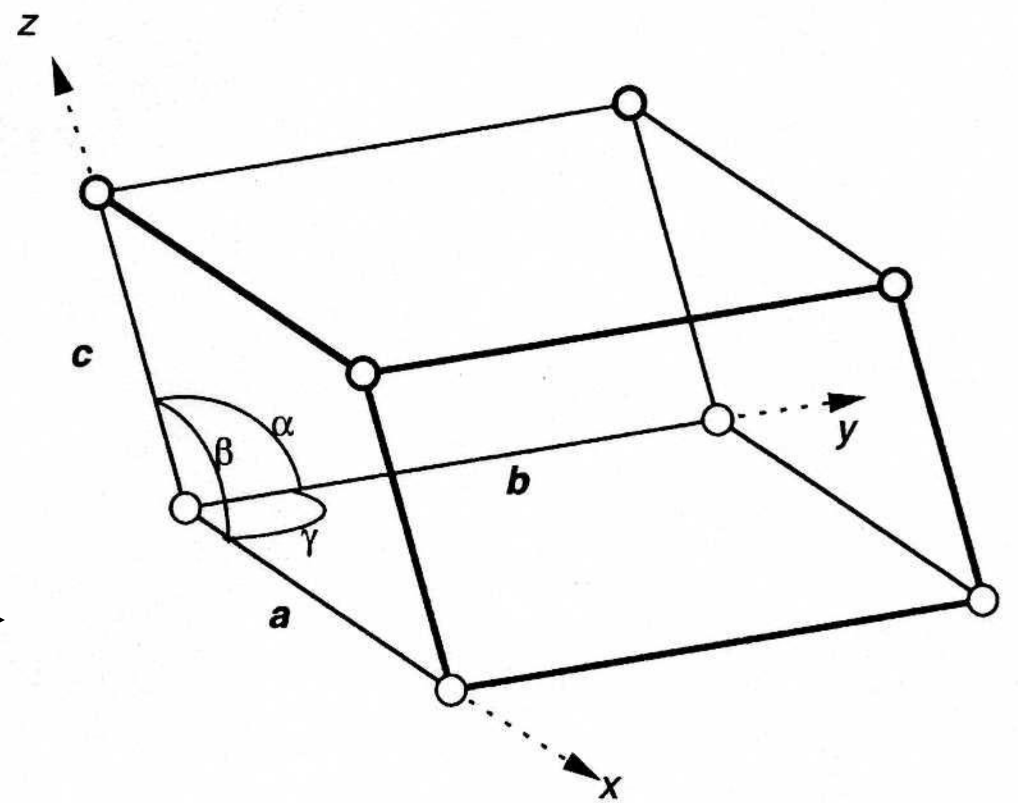


A compact representation of translational symmetry and base vectors.

Unit cell parameters (3D view)

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

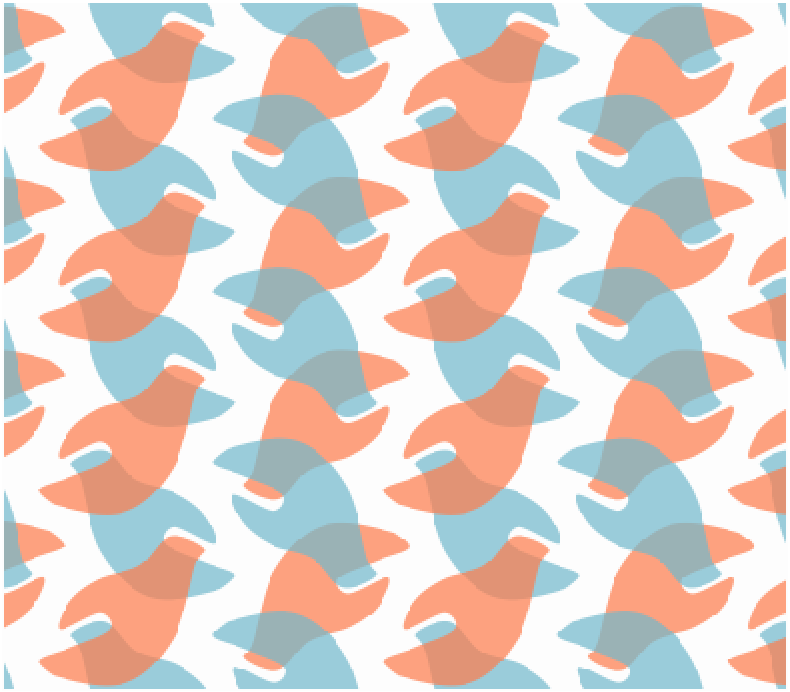


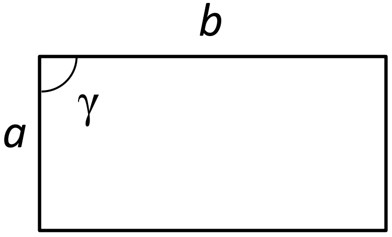


Unit cells are usually defined in terms of the *lengths* of these vectors and angles between them. For example,

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

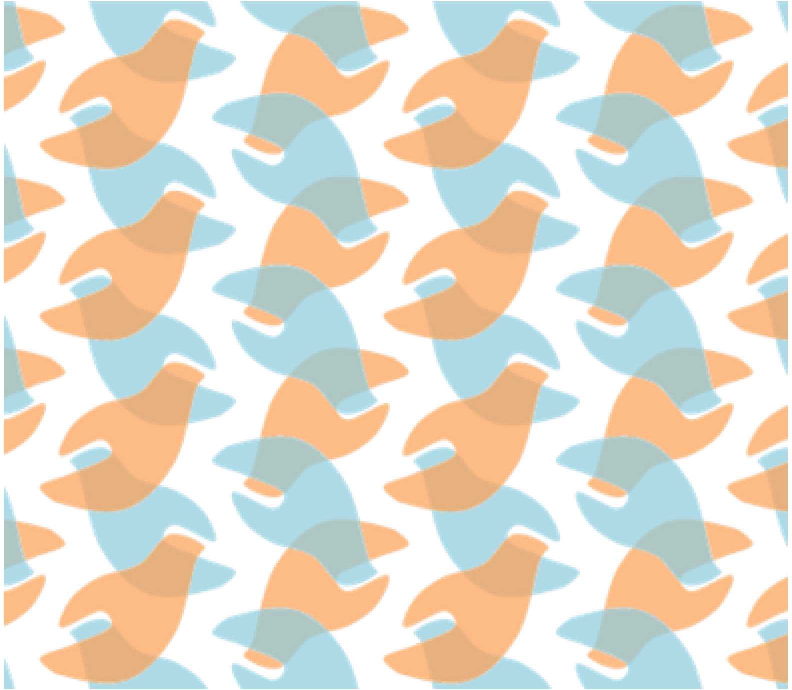
Unit cell

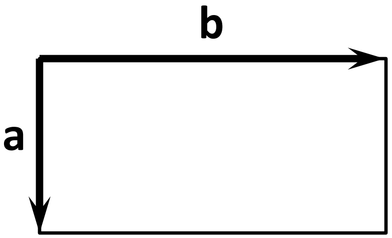




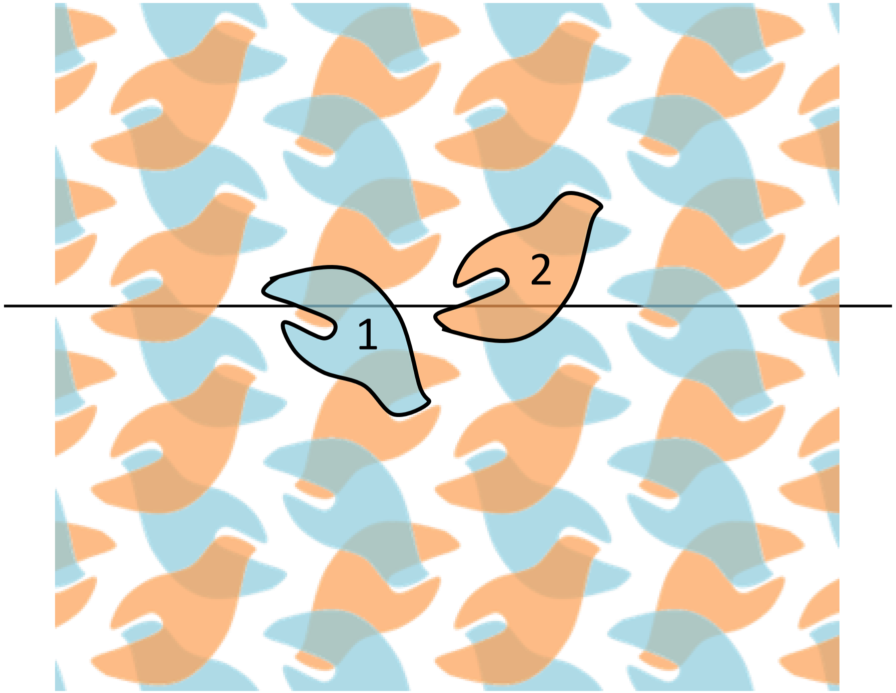
Can be fully characterised by six numbers
(the third dimension is not shown here)

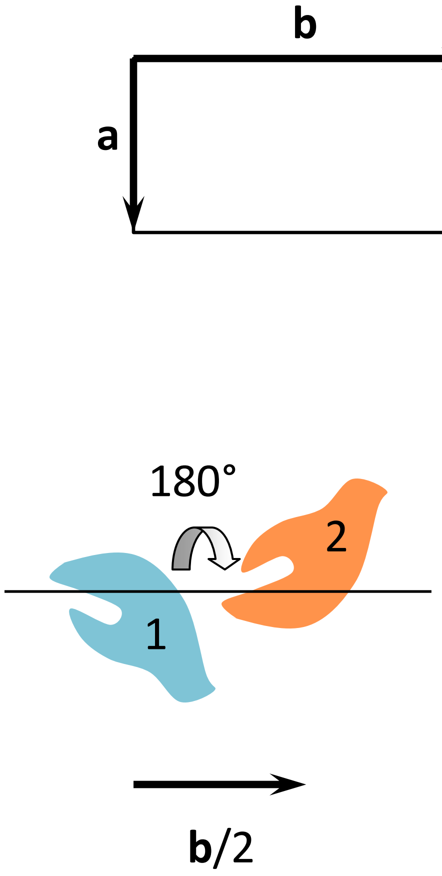
Back to example



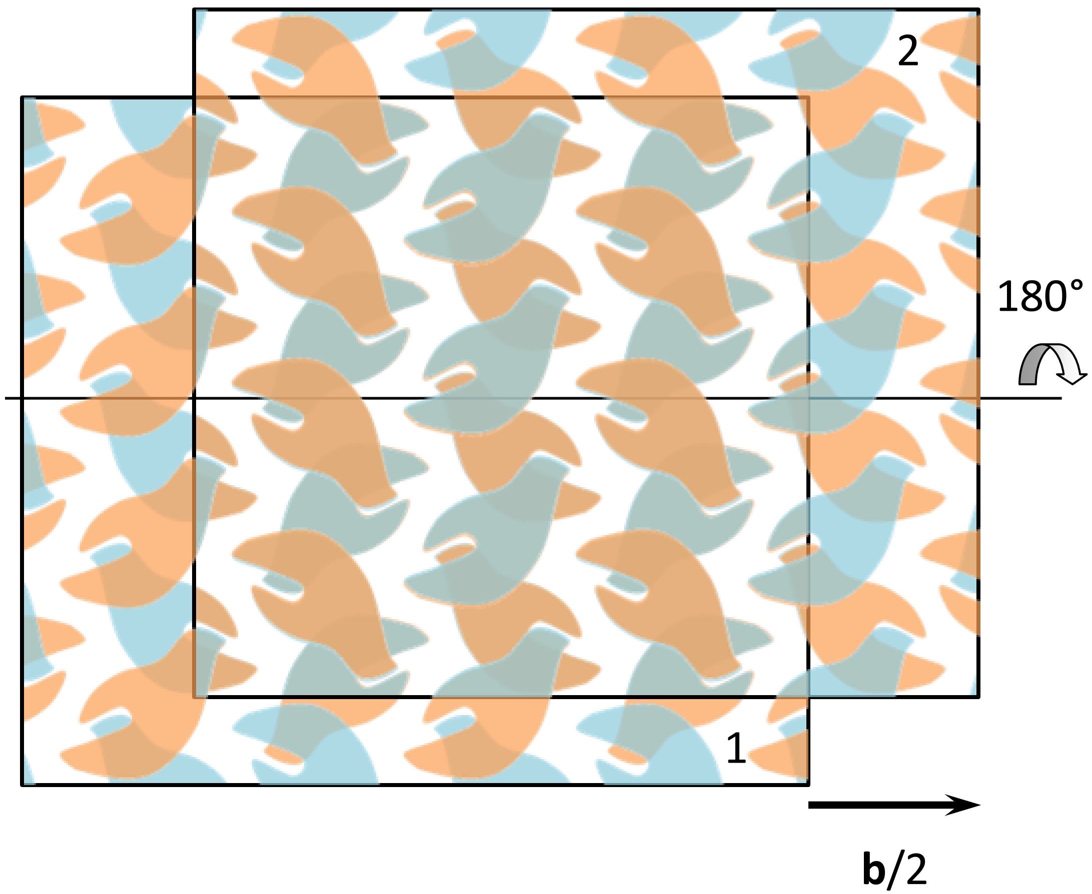


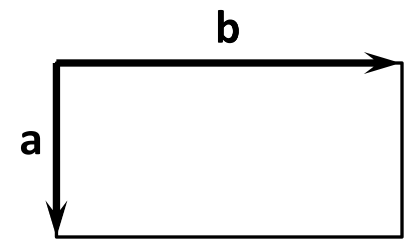
Screw rotation





Screw rotation axis





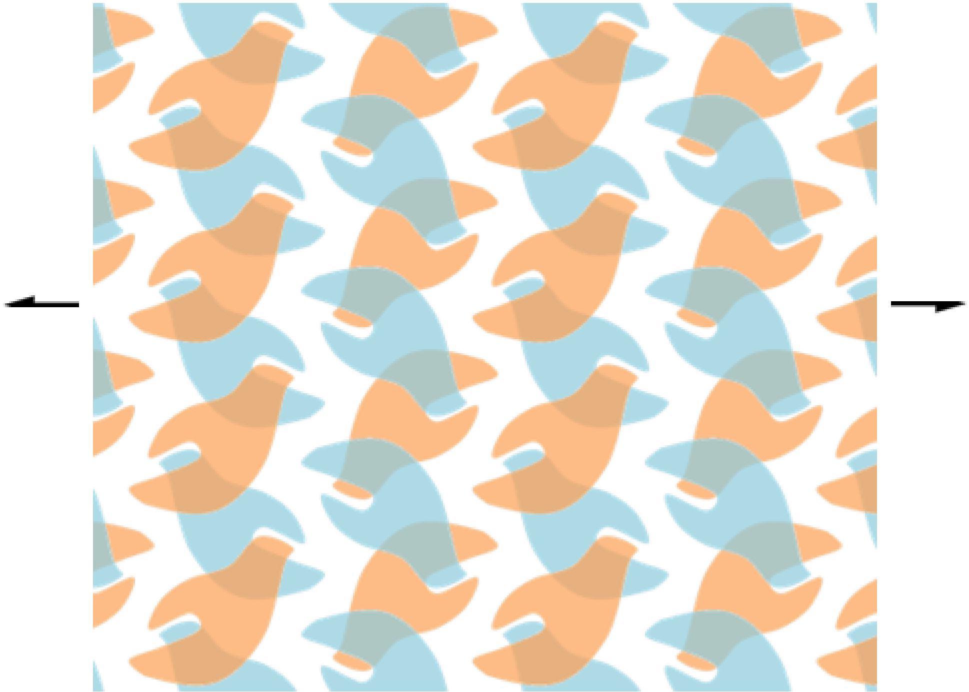
Operation 1->2
maps the whole crystal
onto itself:

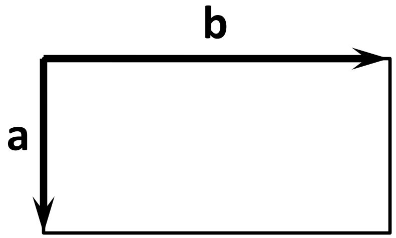
this is a crystallographic
operation

The axis is a
crystallographic
symmetry element,

it can be mapped into
the structure

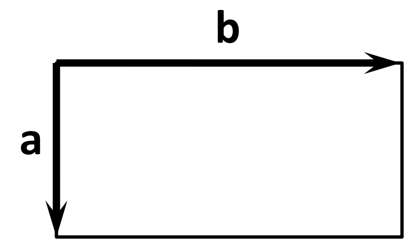
Screw rotation - symbol

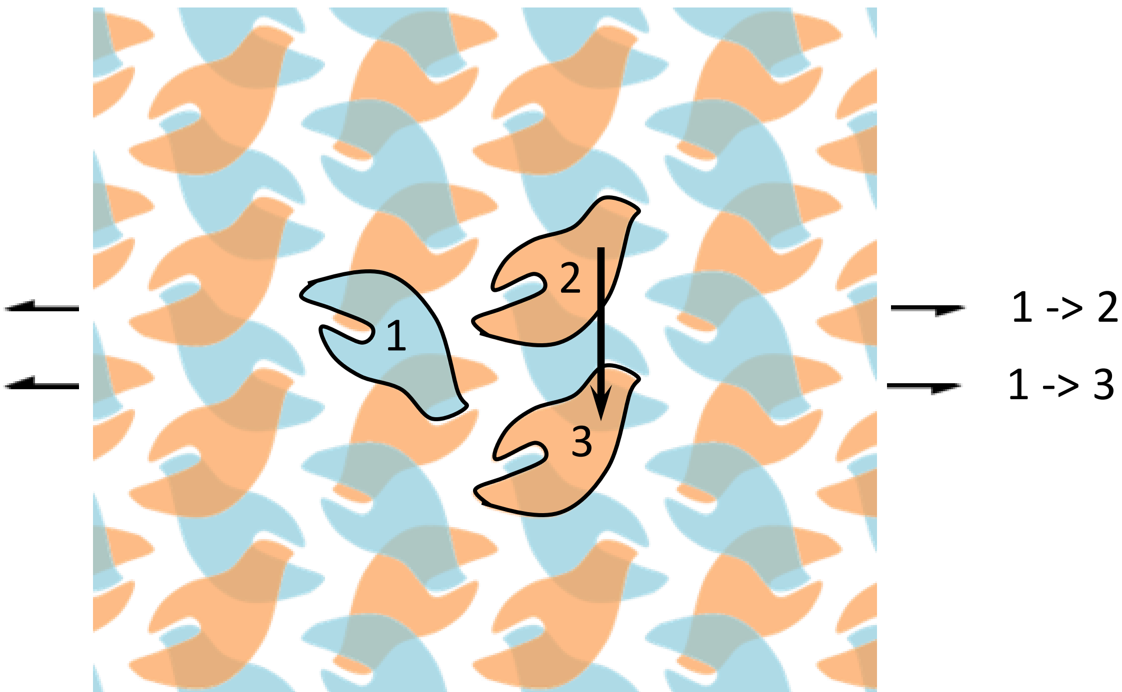




2_1 (plane of figure):

Screw rotation - repeats

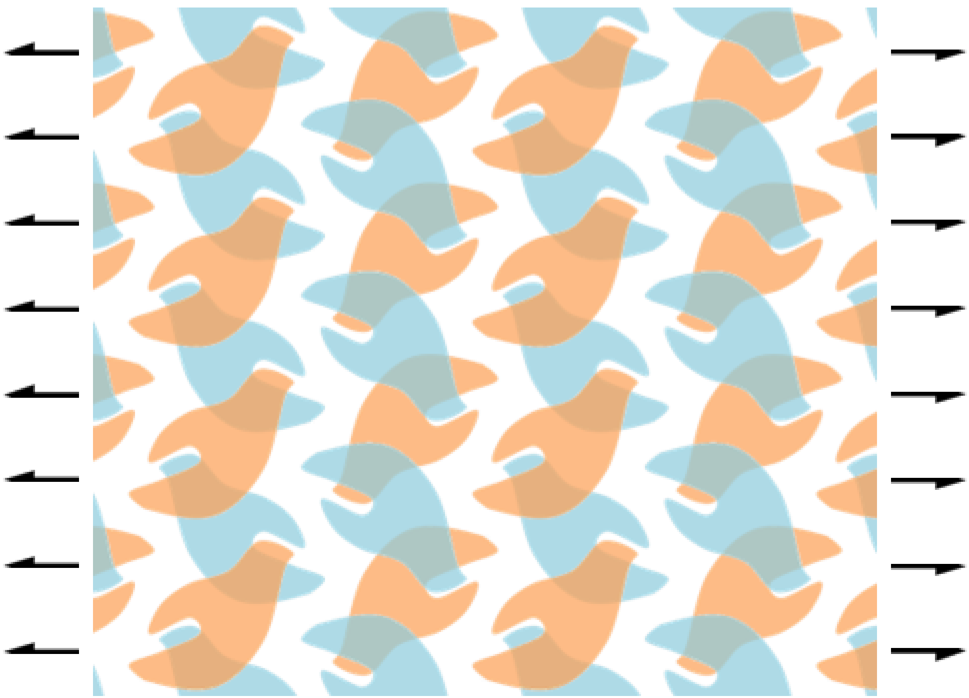


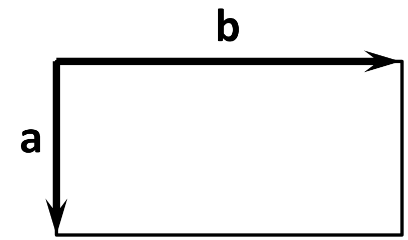


action of top axis
×
translation **a**
=
action of bottom axis

(elements of a group)

Screw rotation 1 - repeats

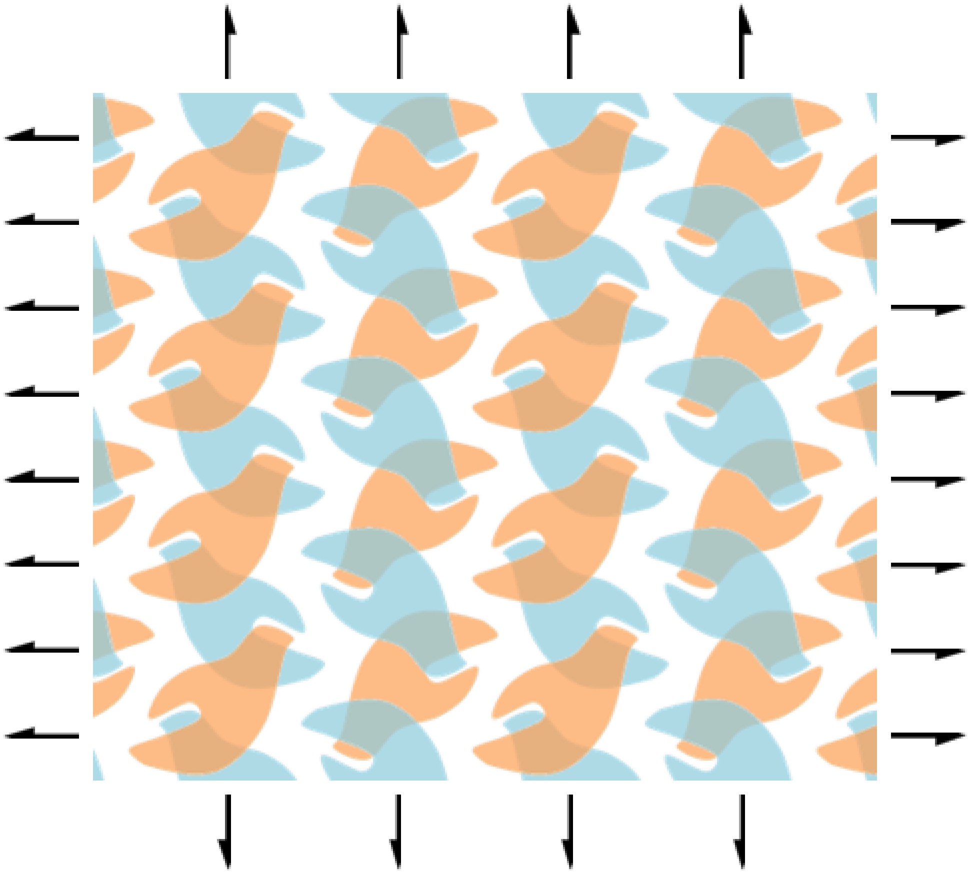


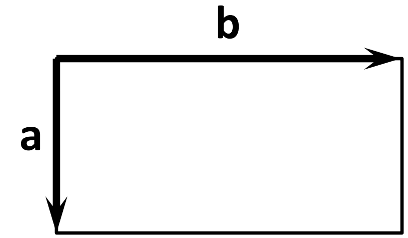


2_1 (plane of figure):

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

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

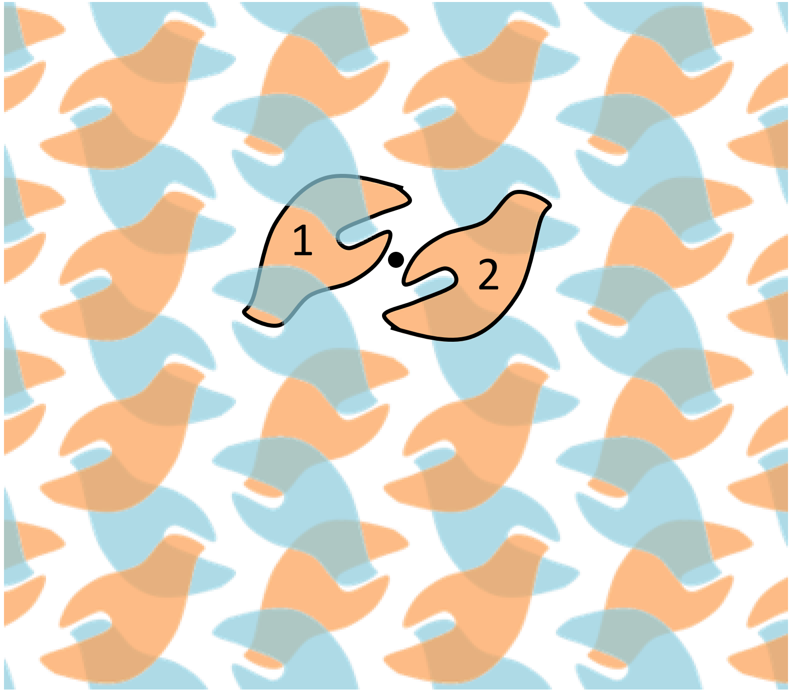


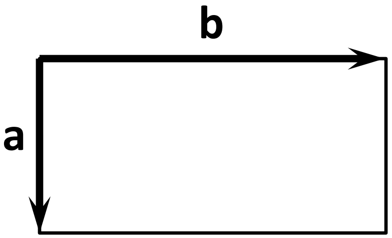


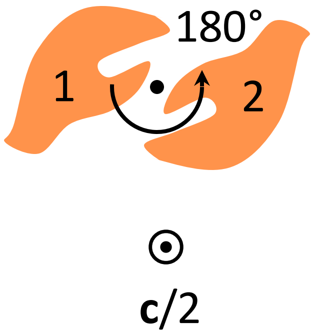
2_1 (plane of figure):

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

Screw rotation – into plane

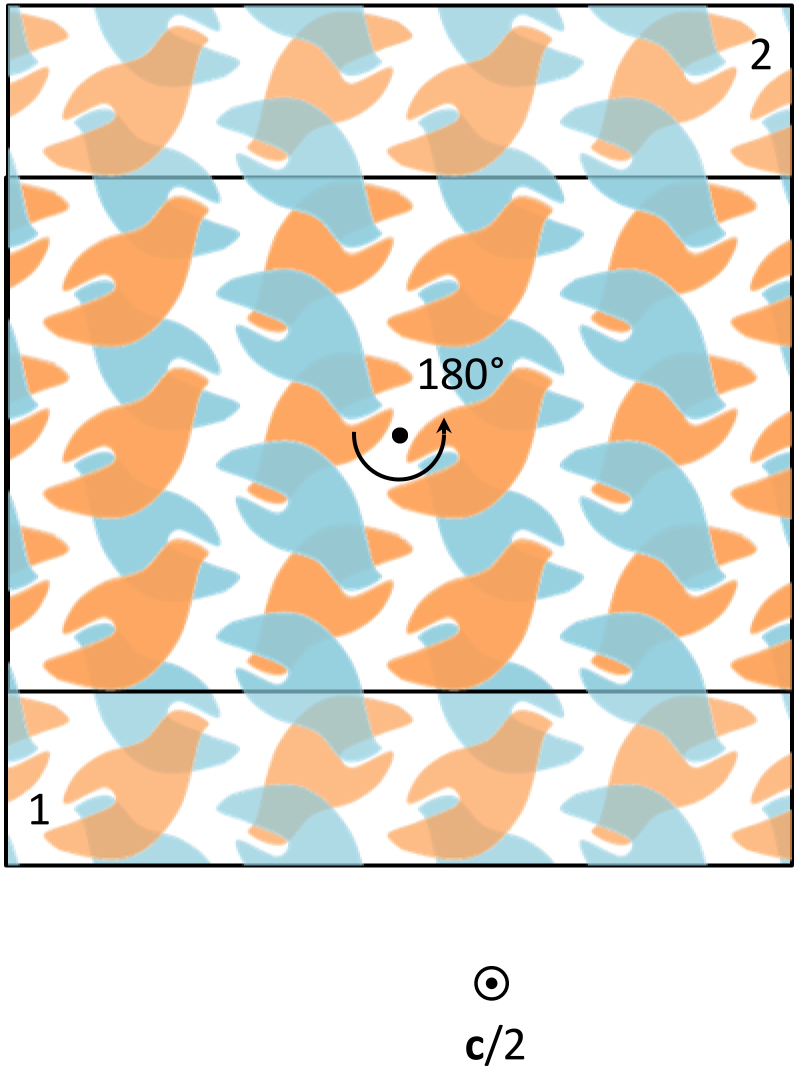


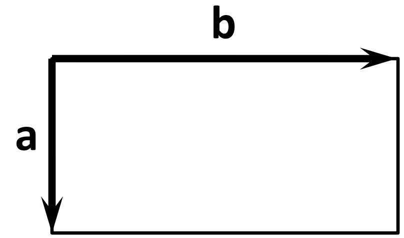




A rotation of 180° with a translation of ½ unit cell from the figure.

Screw rotation 3 is global





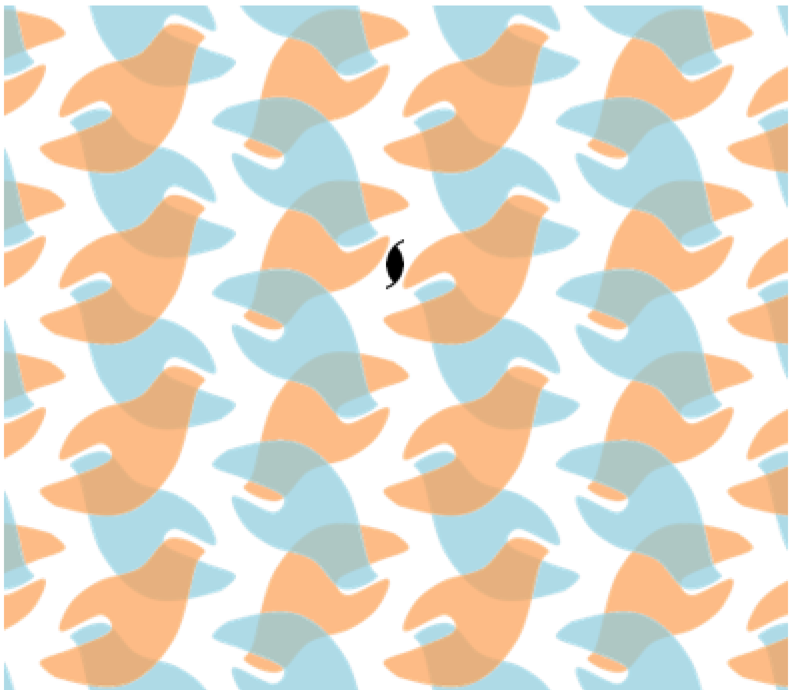
Screw rotation 3 maps the whole crystal onto itself:

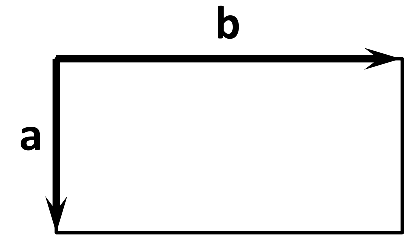
this is a crystallographic operation

The rotation axis is a crystallographic symmetry element,

it can be mapped into the structure

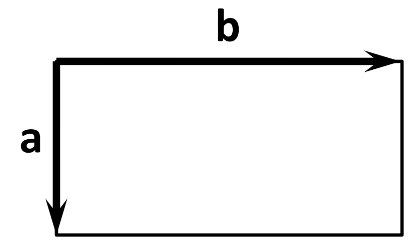
Screw rotation 3 - symbol

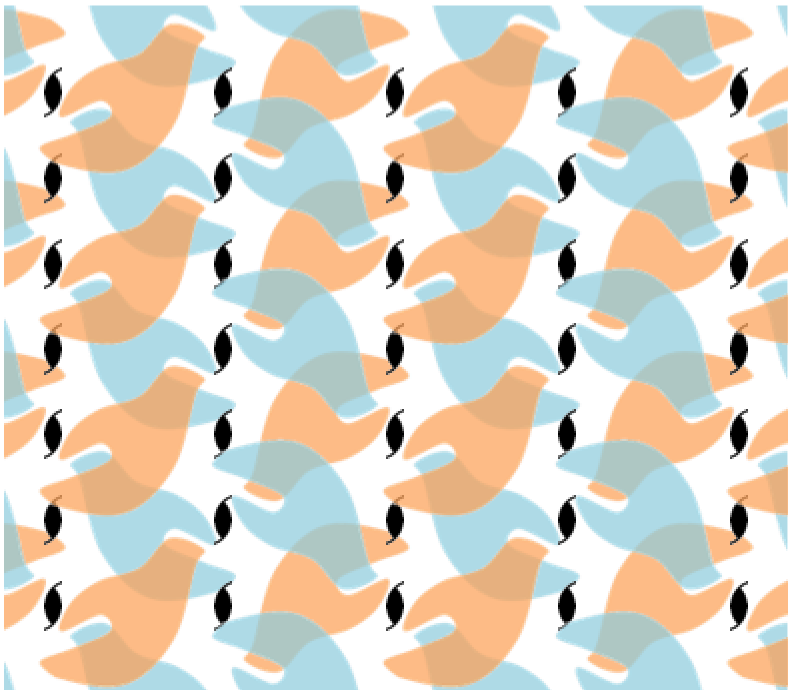




2_1 (along view):

Screw rotation 3 - repeats

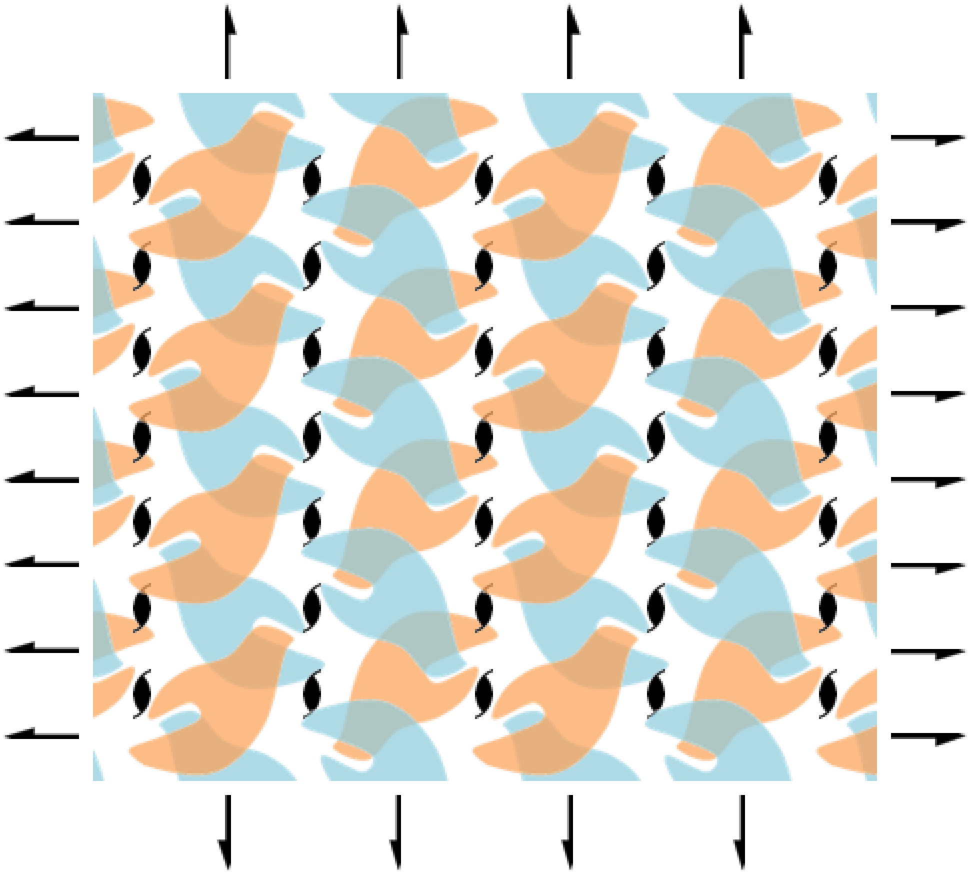


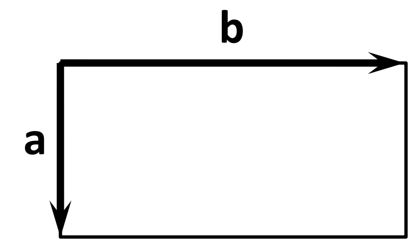


2_1 (along view):

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

All axes together





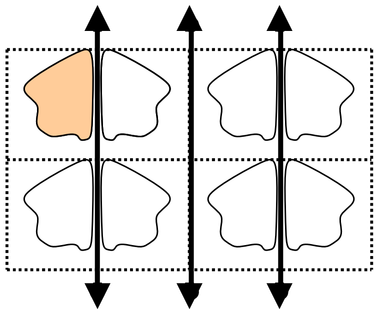
2_1 (plane of figure):

2_1 (along view):

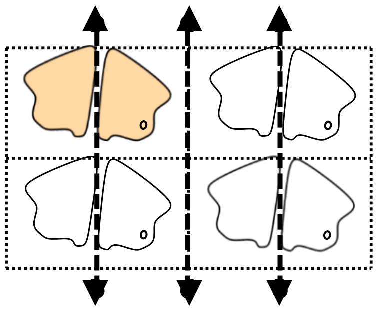
we have built a
space group

- identity
- inverse
- multiplication

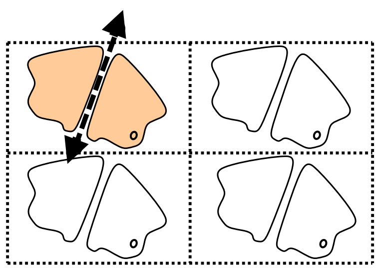
Crystallographic Symmetry, Pseudosymmetry and Non-Crystallographic Symmetry (NCS)



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

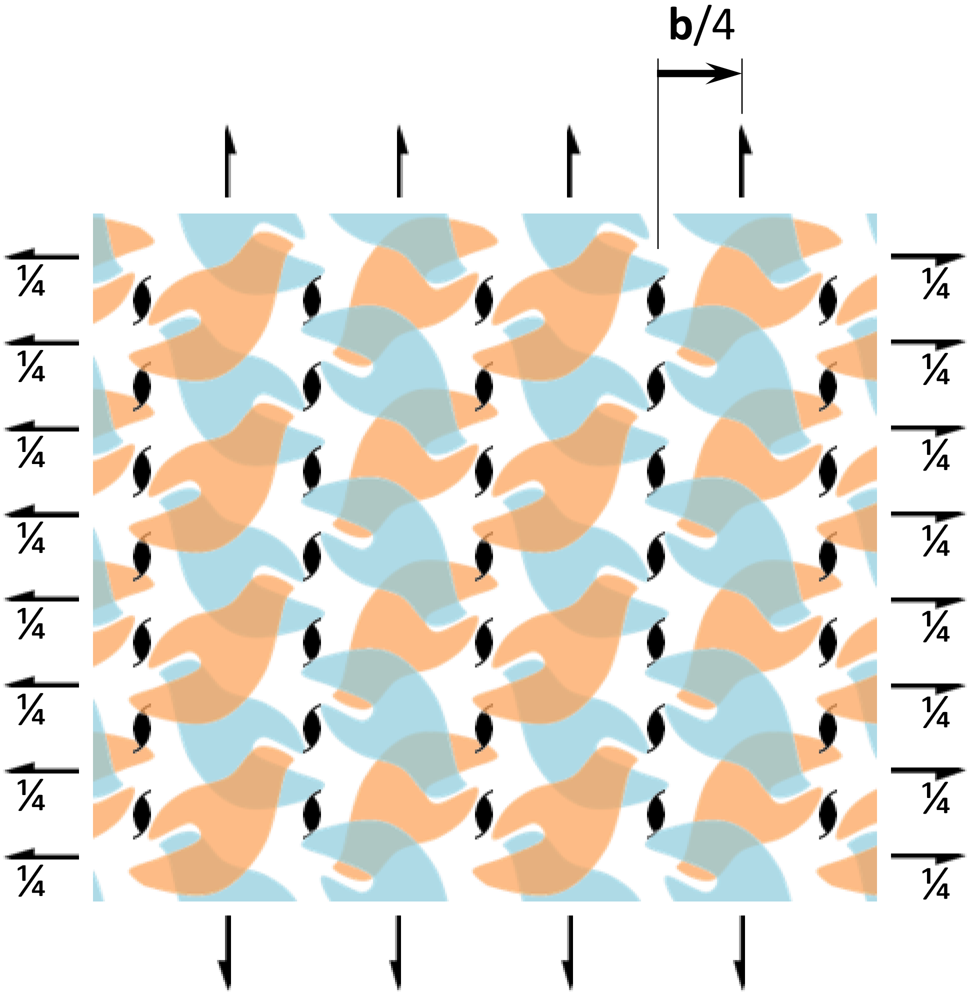


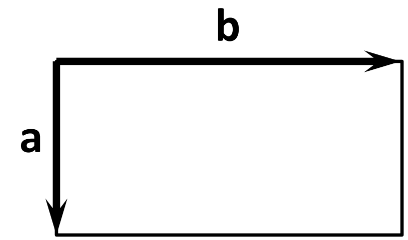
Pseudosymmetry (a limiting case of NCS)
- symmetry is **global** and **approximate**



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

Relative positions of axes





2_1 (plane of figure):

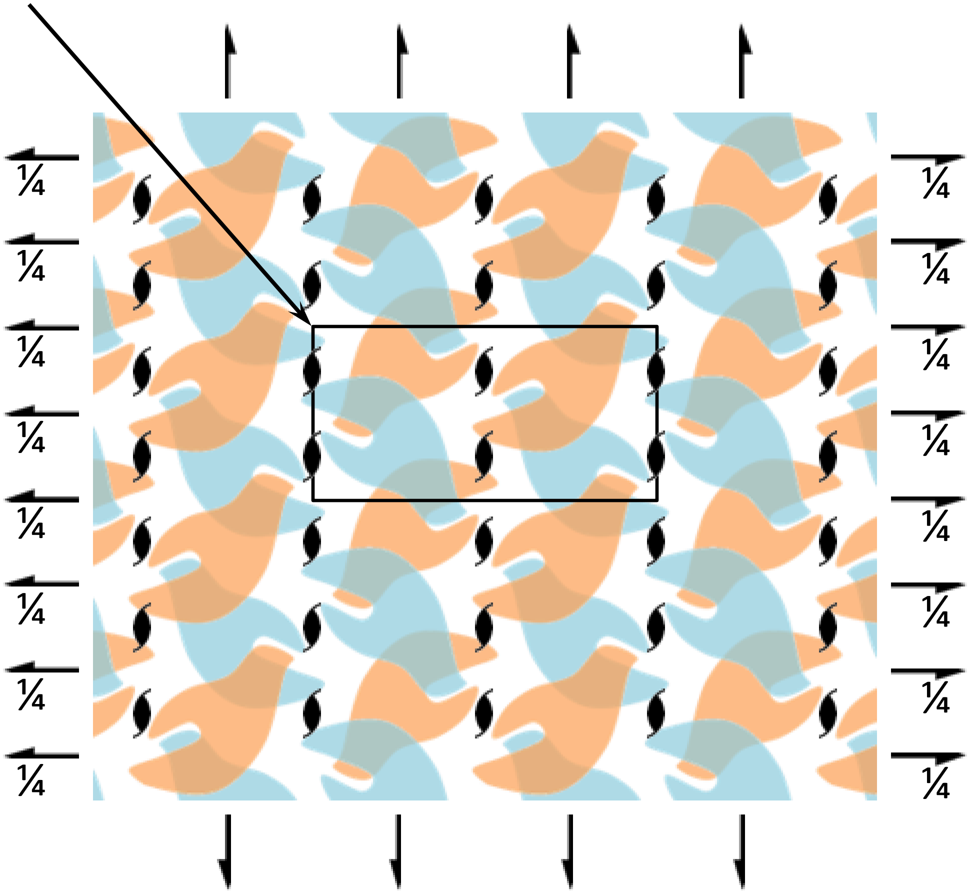
2_1 (along view):

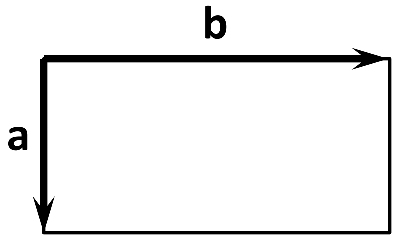
The adjacent axes running in different directions are offset by ¼ of corresponding base vector.

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

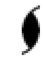
Choice of origin is a convention. Notation

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





2_1 (plane of figure): 

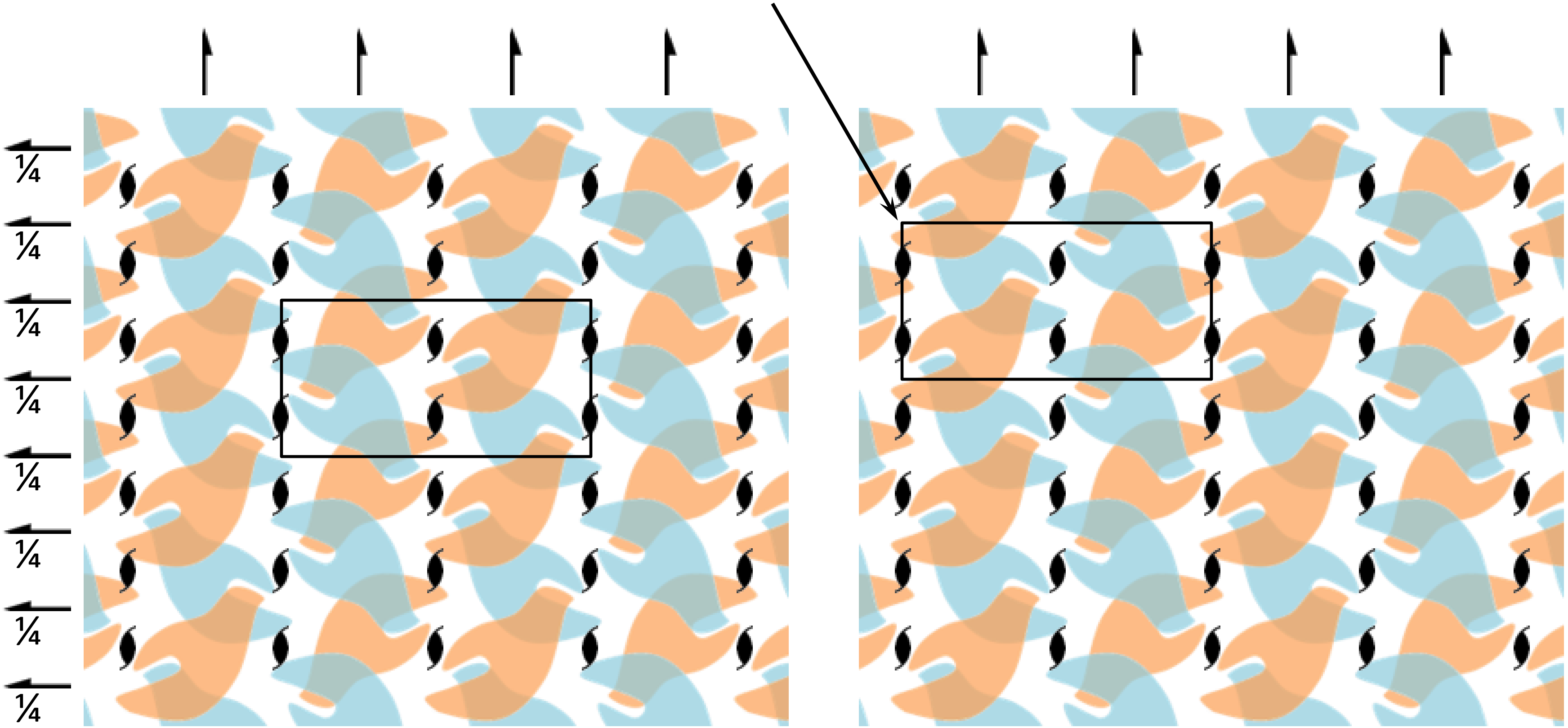
2_1 (along view): 

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.

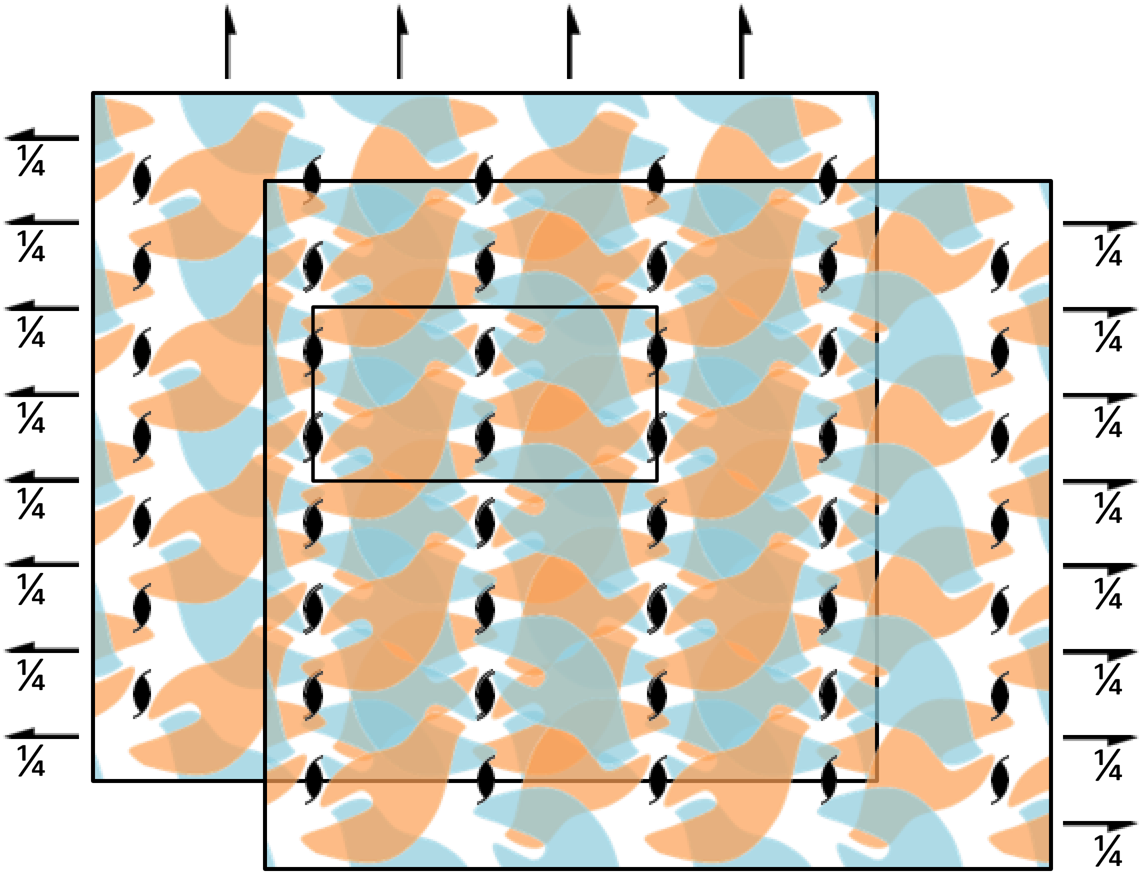
Alternative origins

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. The structures do not match.

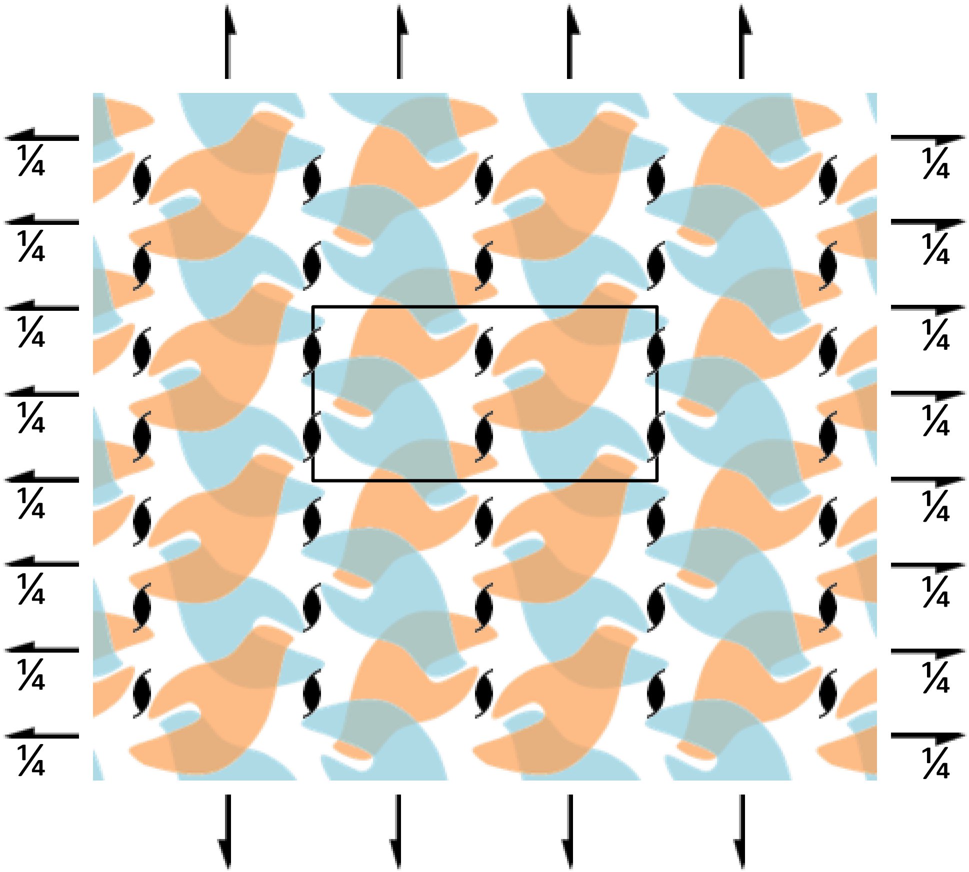


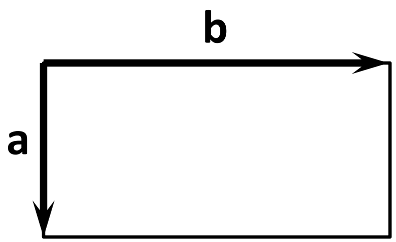
Conventions regarding the choice of crystallographic origin are expressed in terms of position relative to crystallographic axes.

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

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

Complete picture





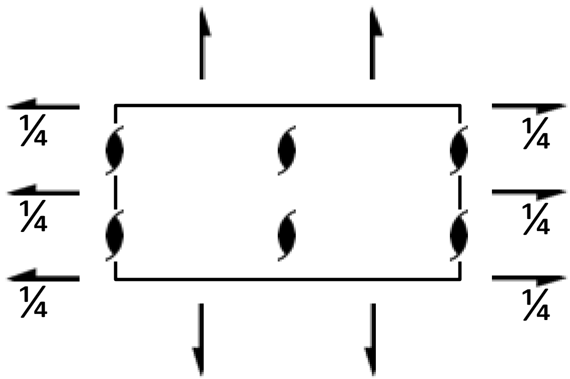
2_1 (plane of figure):

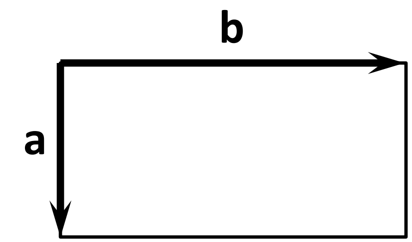
2_1 (along view):

Compact representation

$P2_12_12_1$

No. 19





2_1 (plane of figure): 

2_1 (along view): 

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

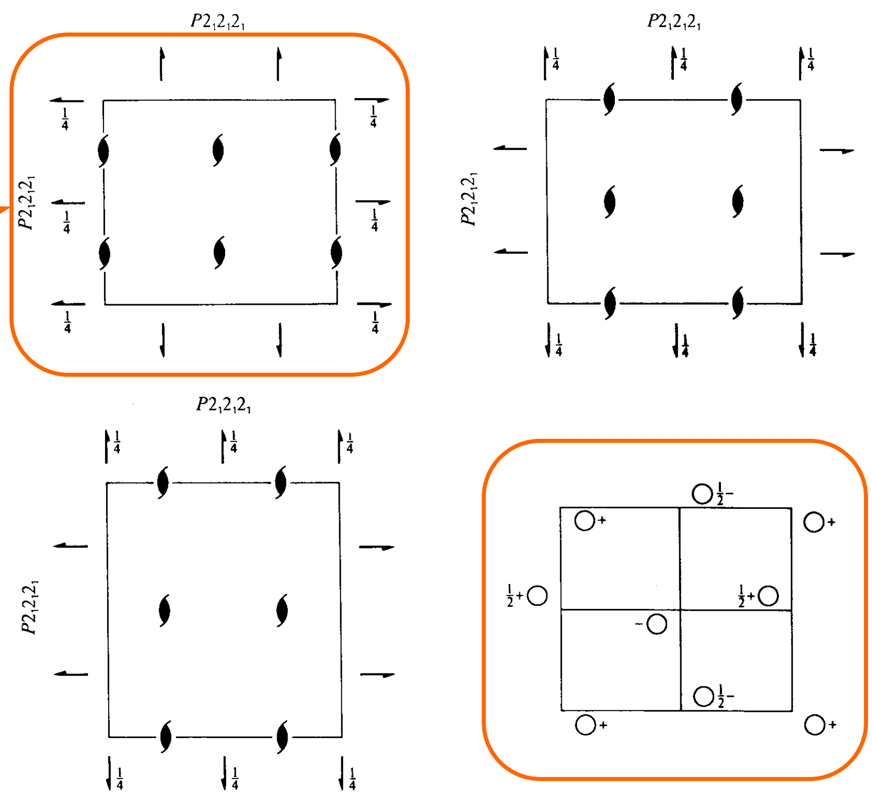
Space group representation in ITC-A

$P2_12_12_1$ D_2^4 222 Orthorhombic

No. 19 $P2_12_12_1$ Patterson symmetry $Pmmm$

Location of symmetry elements

Two other projections are also shown for this space group



Set of equivalent points in general position.

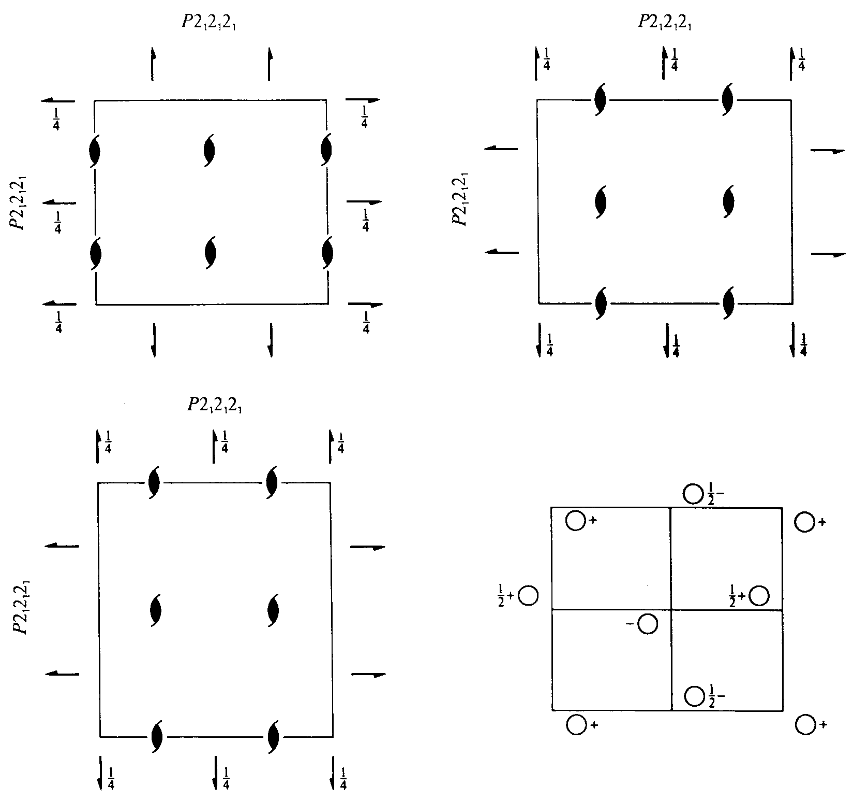
We will be looking at "molecular wallpaper" instead

Space group representation in ITC-A

Crystal system

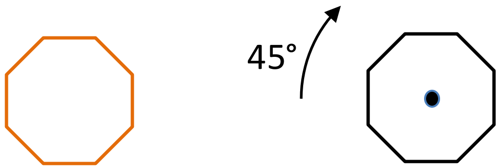
$P2_12_12_1$ $\quad D_2^4 \quad$ 222 $\quad \boxed{\text{Orthorhombic}}$

No. 19 $\quad P2_12_12_1 \quad$ Patterson symmetry $Pmmm$



Rotational symmetry

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



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

Rotational symmetry

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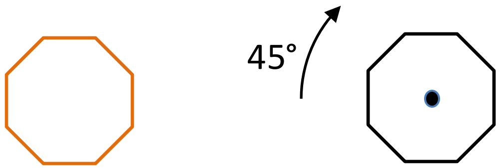
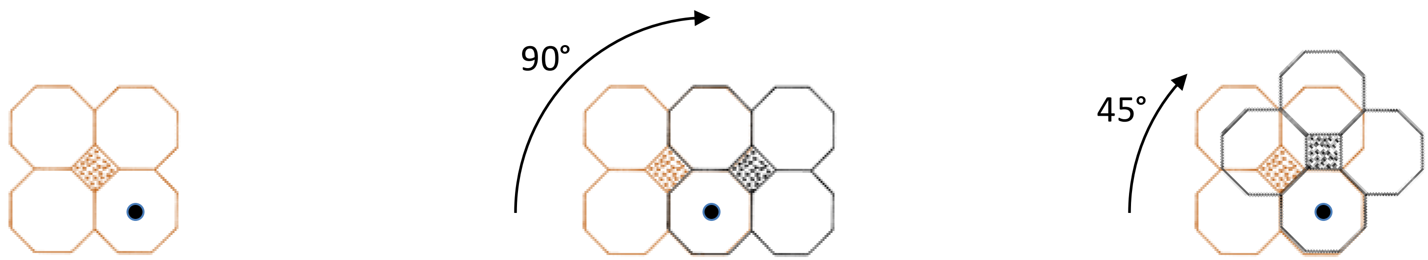


This object has **8**-fold rotational symmetry

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



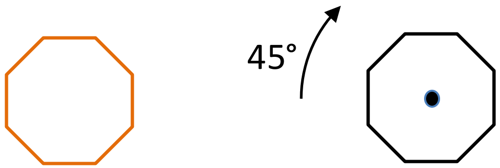
Wallpaper: objects with **8**-fold symmetry

4-fold rotational **crystal** symmetry

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

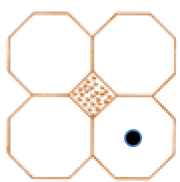
Rotational symmetry

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

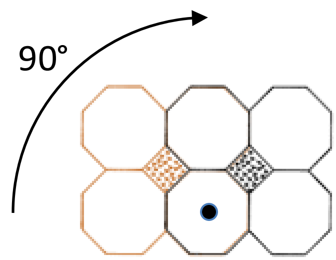


This object has **8**-fold rotational symmetry

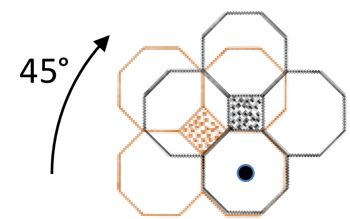
The only rotational symmetries possible in a **crystal** are **2**, **3**, **4** and **6**.



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



4-fold rotational **crystal** symmetry



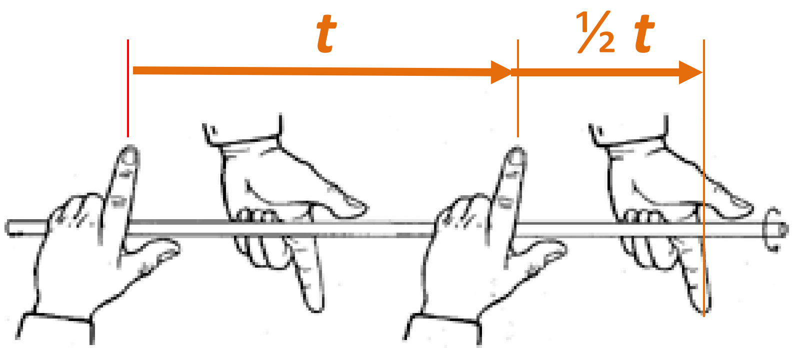
8-fold rotational **crystal** symmetry is **impossible**

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

Screw axes

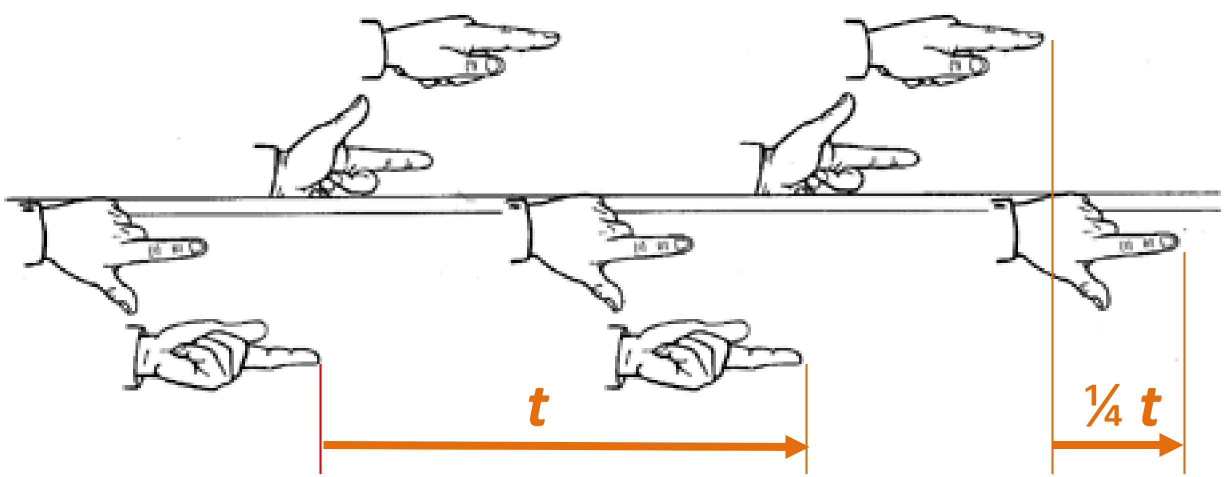
- Rotate clockwise about an axis (1, 2, 3, 4 or 6-fold rotation)
- Translate along this axis by a fraction of the shortest crystallographic translation along the rotation axis

2_1



translation of ½ t per 180° rotation

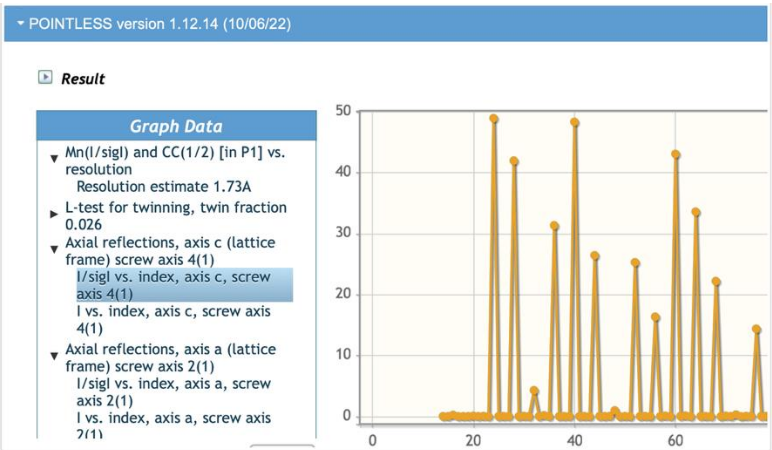
4_1



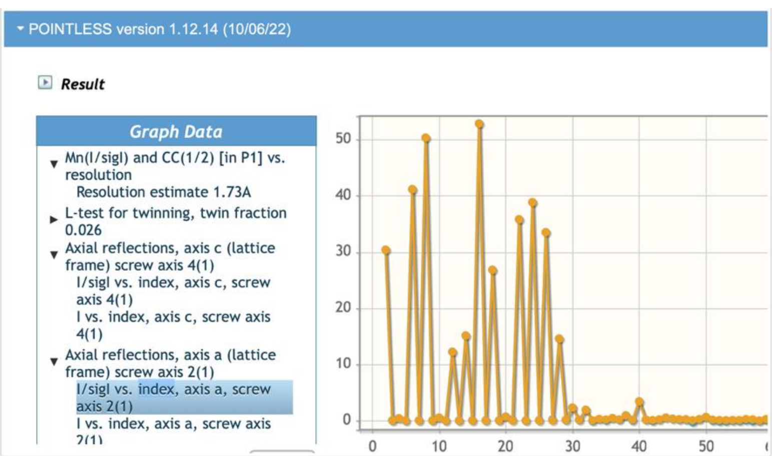
translation of ¼ t per 90° rotation

Screw axes: systematic absences

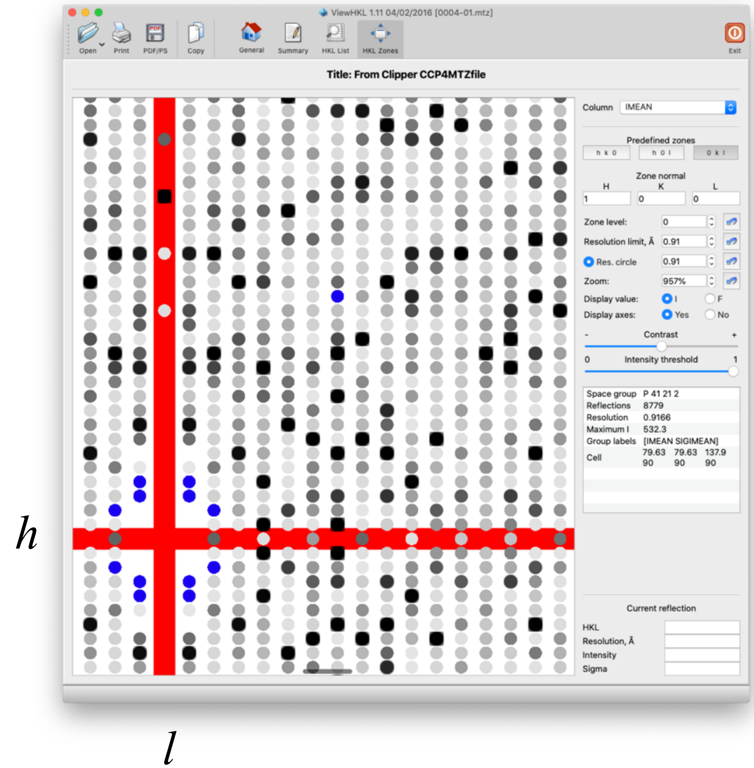
h = k = 0: every fourth l strong: 4_1 or 4_3



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



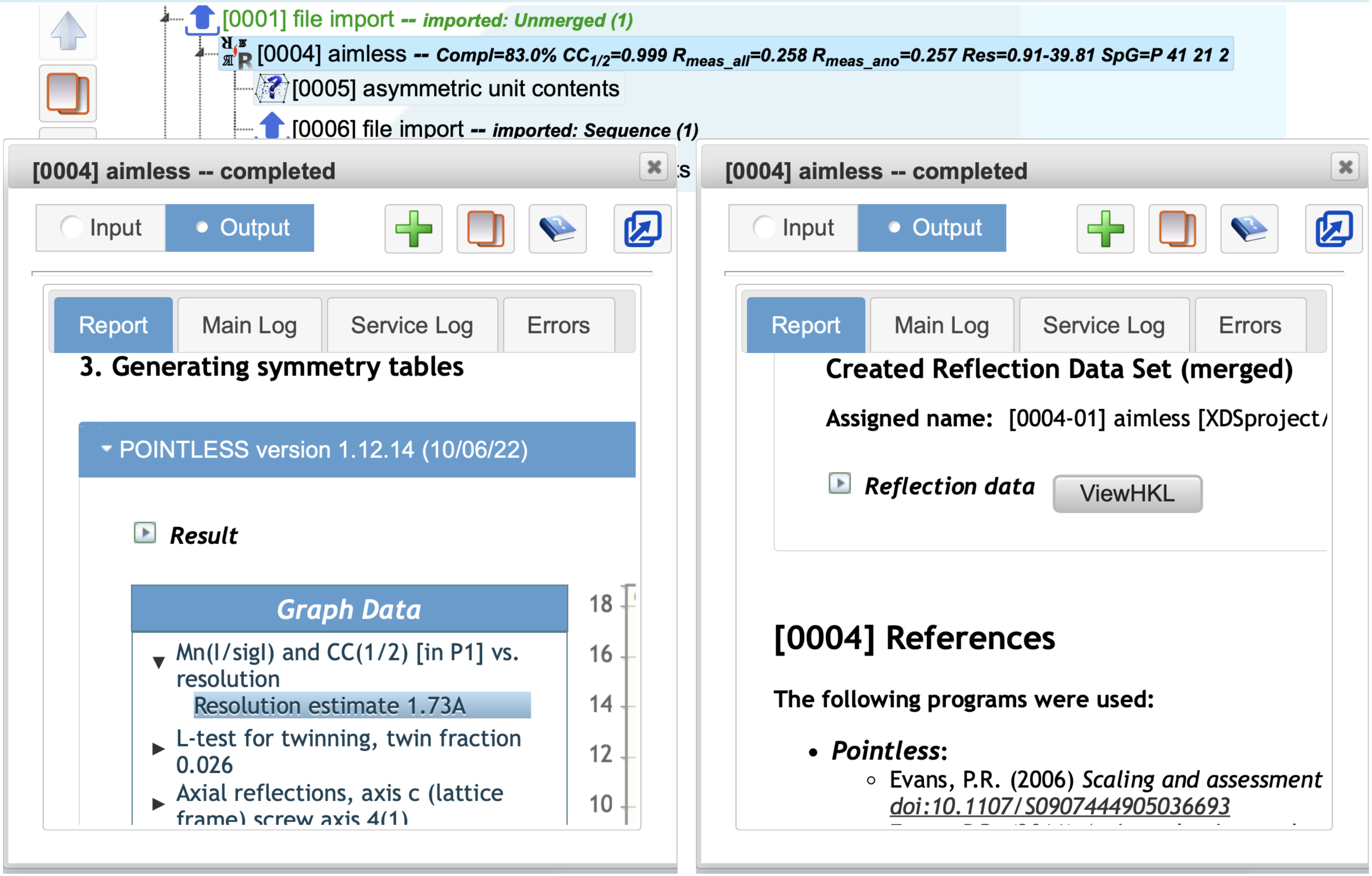
4_1 or 4_3



2_1

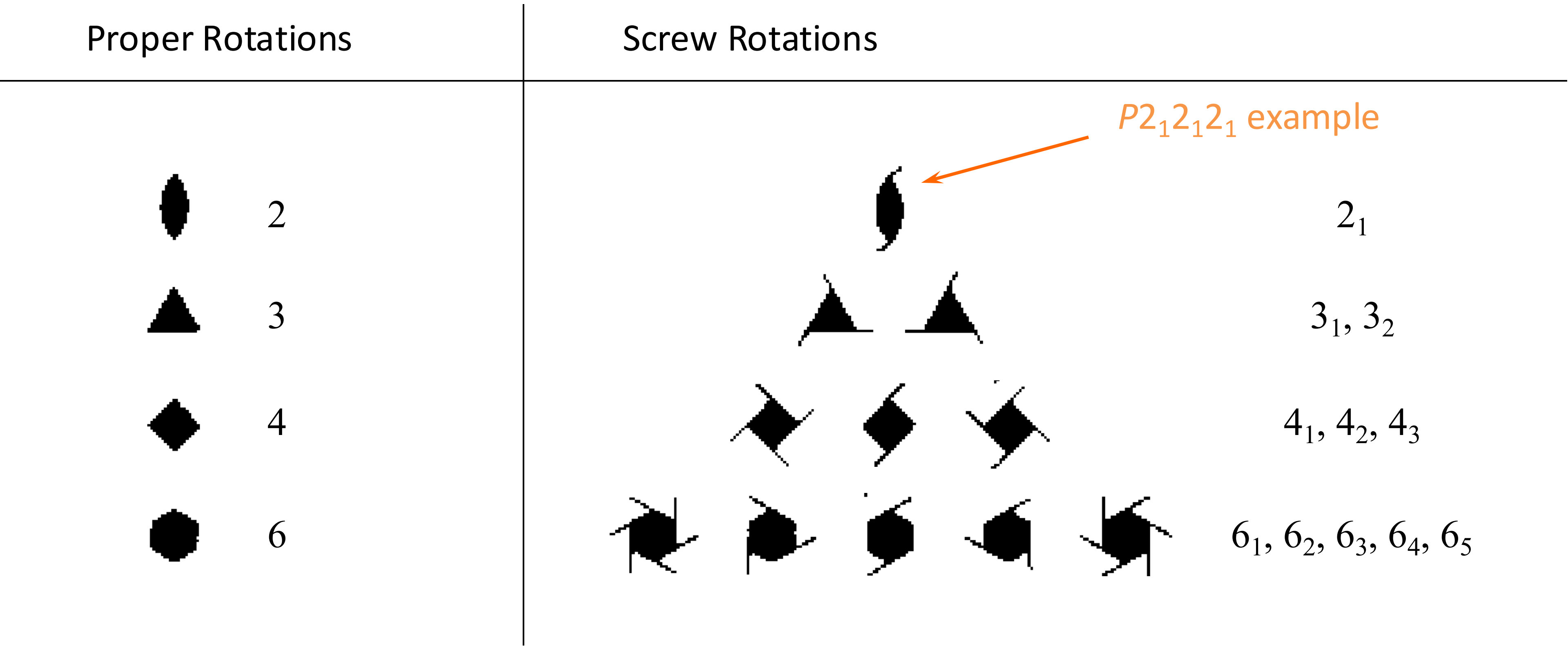
- might not be very clear with noisy data
- enantiomorph not resolved: $P4_12_12$ or $P4_32_12$

Screw axes: systematic absences: CCP4Cloud



Symmetry elements allowed in chiral structures

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



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

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

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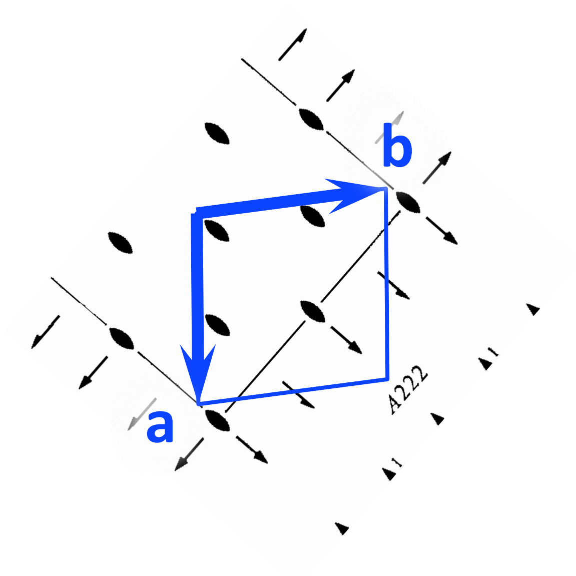
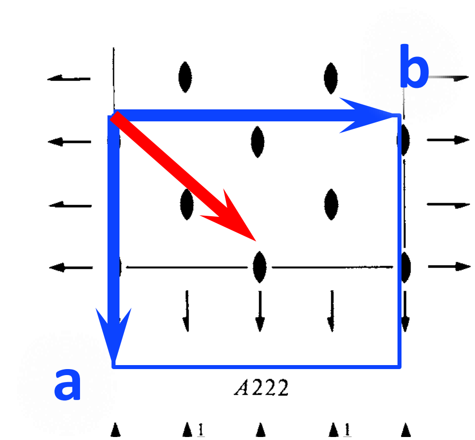
*C*222: an example of a centred cell

If we were using
a primitive cell



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

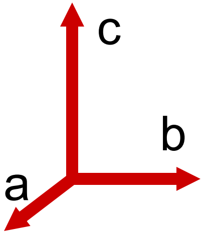
Standard setting;
C means additional
translation ½ (**a** + **b**)

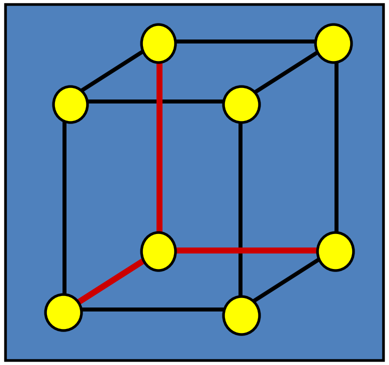


2-fold axes are
along **a**, **b** and **c**
(conventional
setting)

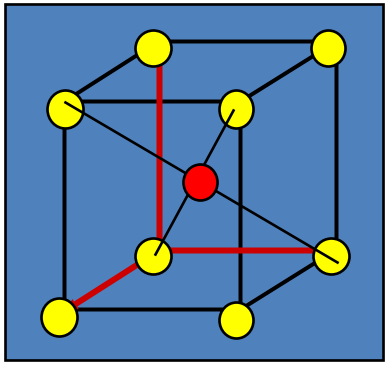
Centred unit cells in pictures

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

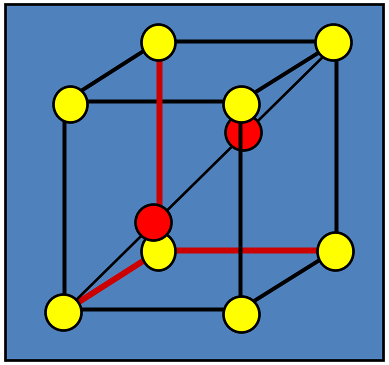




P – Primitive

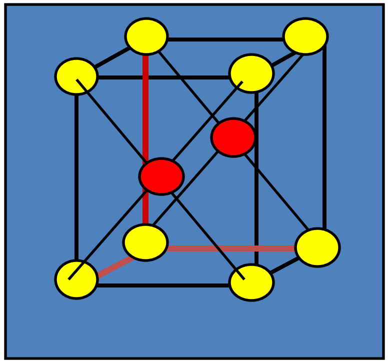


I – Body centred



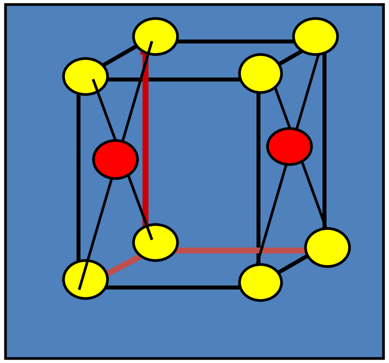
H – Hexagonal

(non-standard)

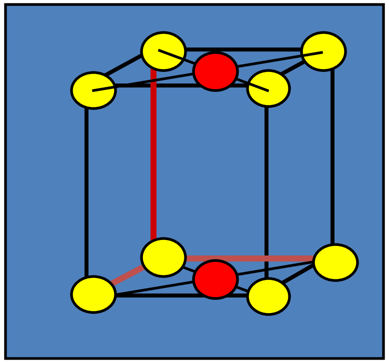


A – Face centred (A)

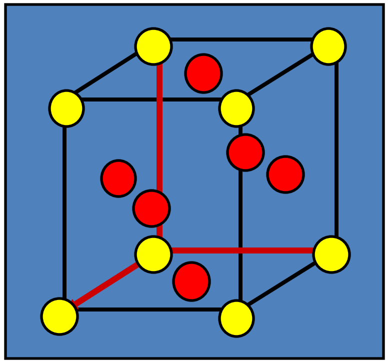
(non-standard)



B – Face centred (B)



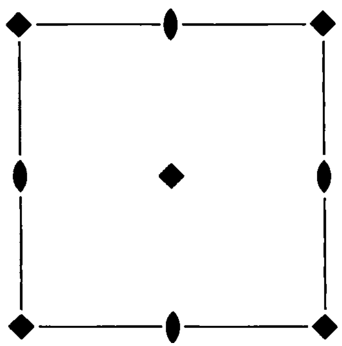
C – Face centred (C)



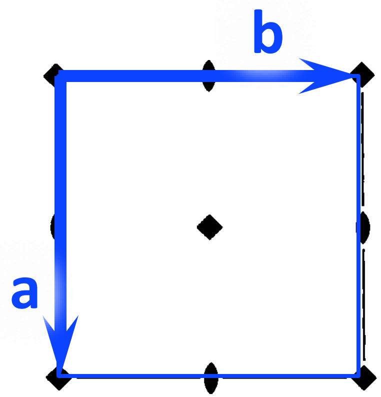
F – Face centred (all)

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

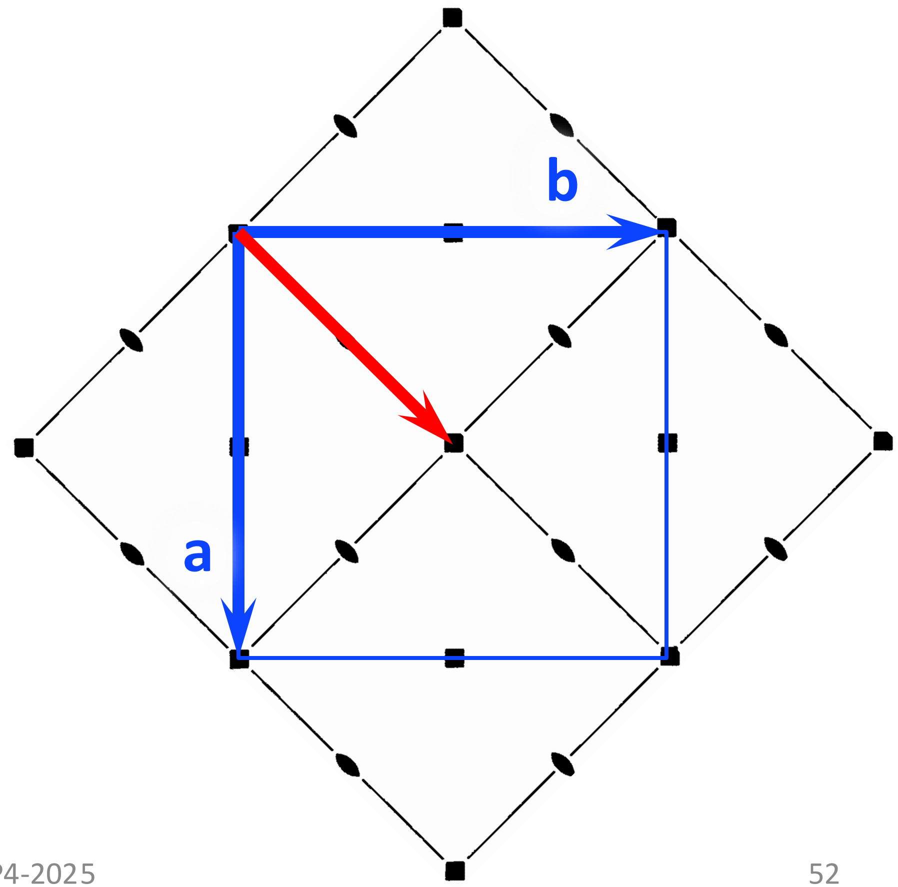
*P*4
as presented in the International Tables for Crystallography



and with base vectors shown



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



Bravais lattices

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

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

Crystal Systems

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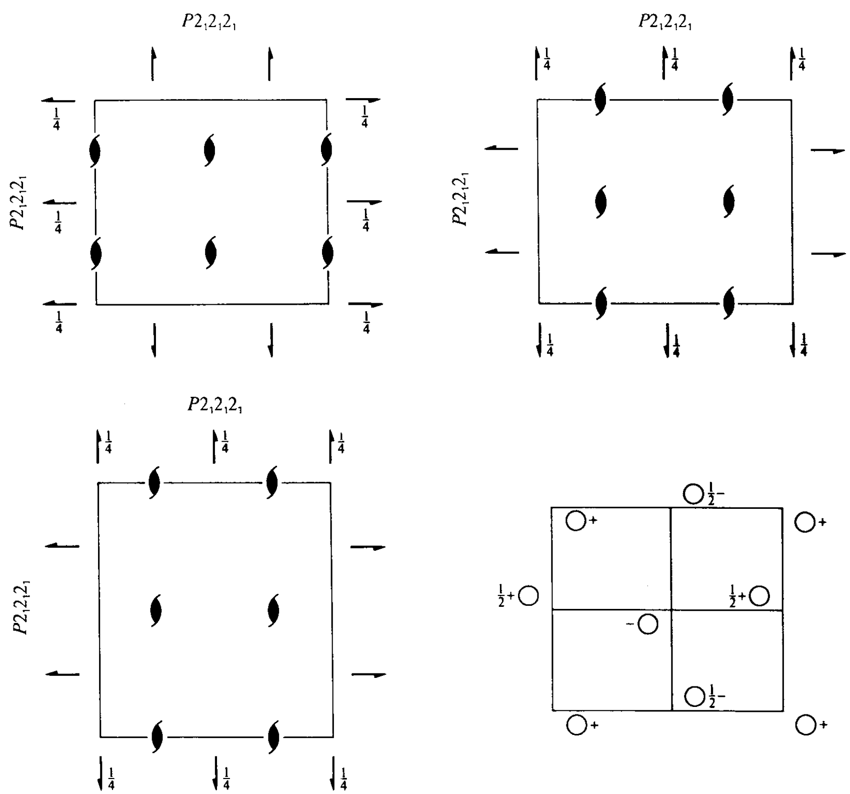
Space group representation in ITC-A

(Short) Hermann-Mauguin symbol

(Extended) Hermann-Mauguin symbol

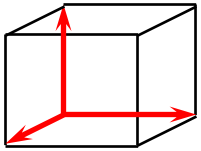
$\boxed{P2_12_12_1}$ D_2^4 222 Orthorhombic

No. 19 $\boxed{P2_12_12_1}$ Patterson symmetry $Pmmm$



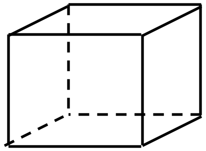
Triclinic $P\,1$

Lattice type



P

"1" means no symmetry operations except for translations



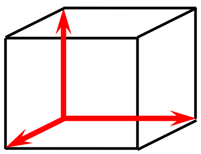
1

No constraints on
a, b, c, α, β, γ

Monoclinic

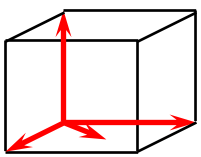
Standard HM symbols: **papers**		Extended HM symbols: **PDB**	
P 2	*P* 2_1	*P* 1 2 1	*P* 1 $2_1$1
C 2		*C* 1 2 1	

Lattice type



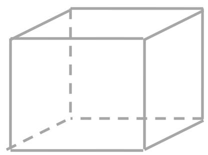
P

or

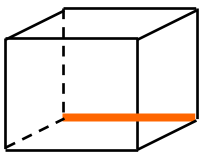


C

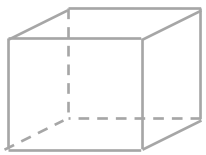
Directions and **orders** of axes



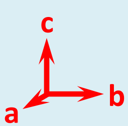
1



2_x



1



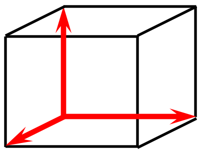
2-fold axes, all parallel

α = γ = 90°

Orthorhombic

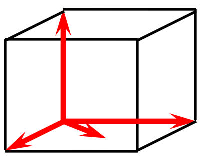
$P\,2\,2\,2$ $\quad P\,2\,2\,2_1$ $\quad P\,2_12_12$ $\quad P\,2_12_12_1$
$C\,2\,2\,2$ $\quad C\,2\,2\,2_1$
$I\,2\,2\,2$ $\quad I\,2_12_12_1$
$F\,2\,2\,2$

Lattice type



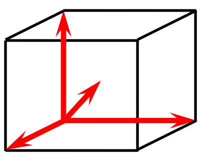
P

or



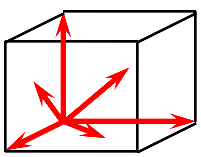
C

or



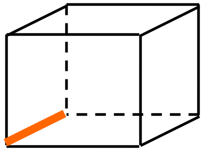
I

or

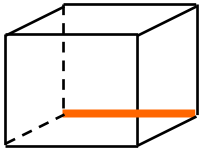


F

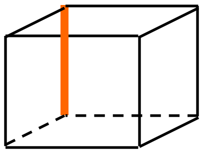
Directions and **orders** of axes



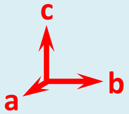
$\mathbf{2_x}$



$\mathbf{2_x}$



$\mathbf{2_x}$



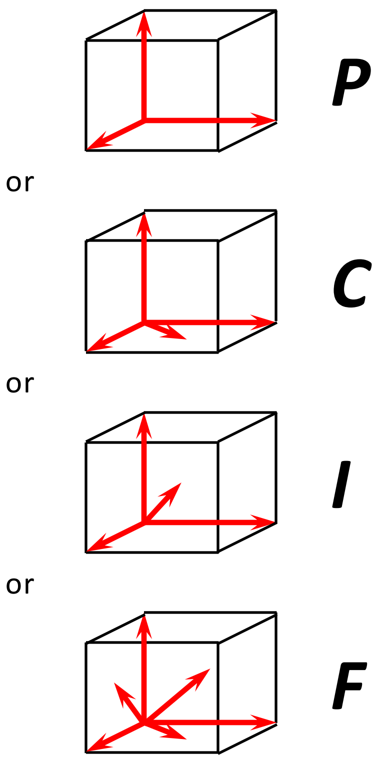
2-fold axes in three perpendicular directions

$\alpha = \beta = \gamma = 90°$

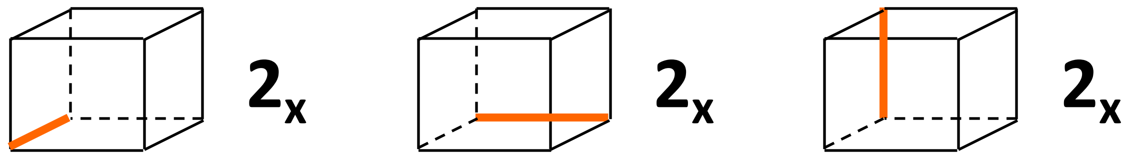
Orthorhombic

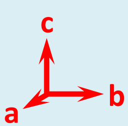
$P\,2\,2\,2$	$P\,2\,2\,2_1$	$P\,2_1 2_1 2$	$P\,2_1 2_1 2_1$	example
$C\,2\,2\,2$	$C\,2\,2\,2_1$			
$I\,2\,2\,2$			$I\,2_1 2_1 2_1$	
$F\,2\,2\,2$				

Lattice type



Directions and **orders** of axes





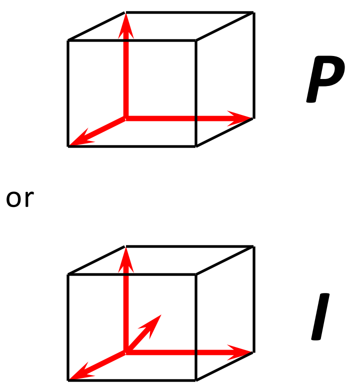
2-fold axes in three perpendicular directions

$\alpha = \beta = \gamma = 90°$

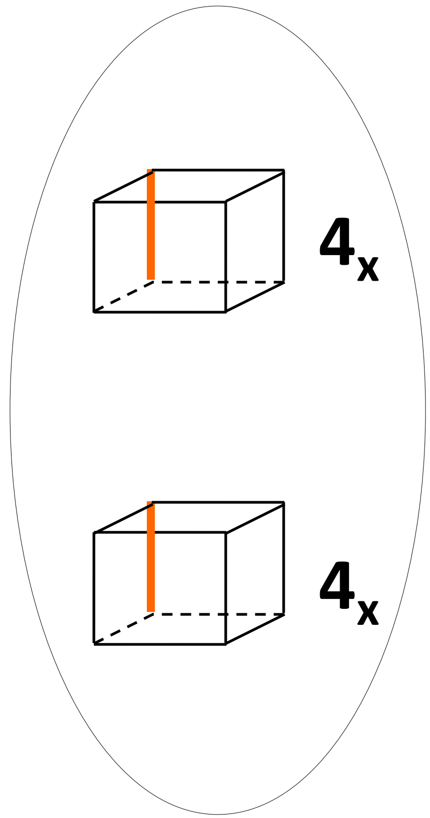
Tetragonal

$P\,4\,2_1 2$ $P\,4_1 2_1 2$ $P\,4_2 2_1 2$ $P\,4_3 2_1 2$ $P4$ $P4_1$ $P4_2$ $P4_3$
$P\,4\,2\,2$ $P\,4_1 2\,2$ $P\,4_2 2\,2$ $P\,4_3\,2\,2$
$I\,4\,2\,2$ $I\,4_1 2\,2$ $I\,4$ $I\,4_1$

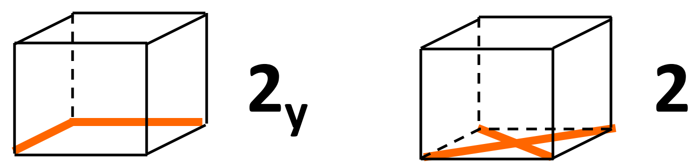
Lattice type

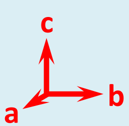


or



Directions and **orders** of axes





4-fold axes along **c**

α = β = γ = 90°
a = *b*

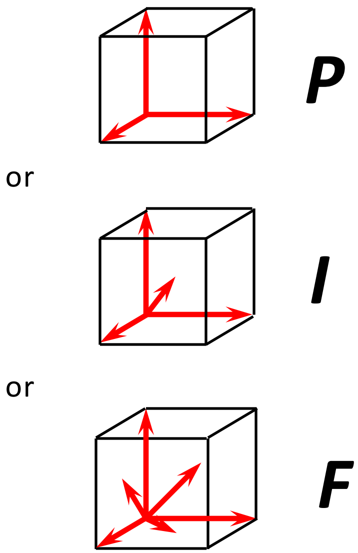
Cubic

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

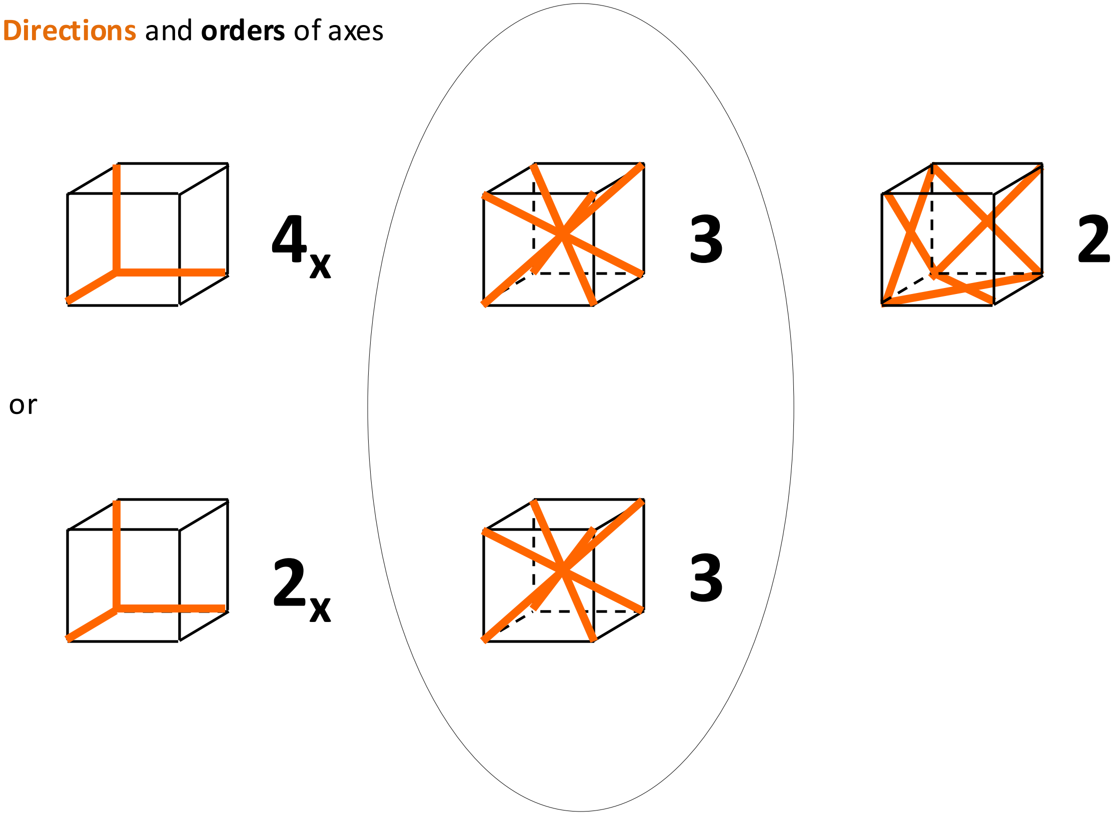
$I\,4\,3\,2$ $I\,4_1 3\,2$ $I\,2\,3$ $I\,2_1 3$

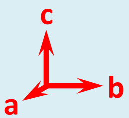
$F\,4\,3\,2$ $F\,4_1 3\,2$ $F\,2\,3$

Lattice type



Directions and orders of axes





3-fold axes parallel to the body diagonals

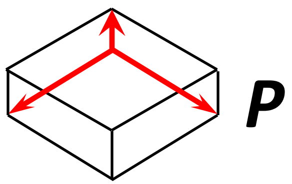
$\alpha = \beta = \gamma = 90°$
$a = b = c$

Trigonal - P

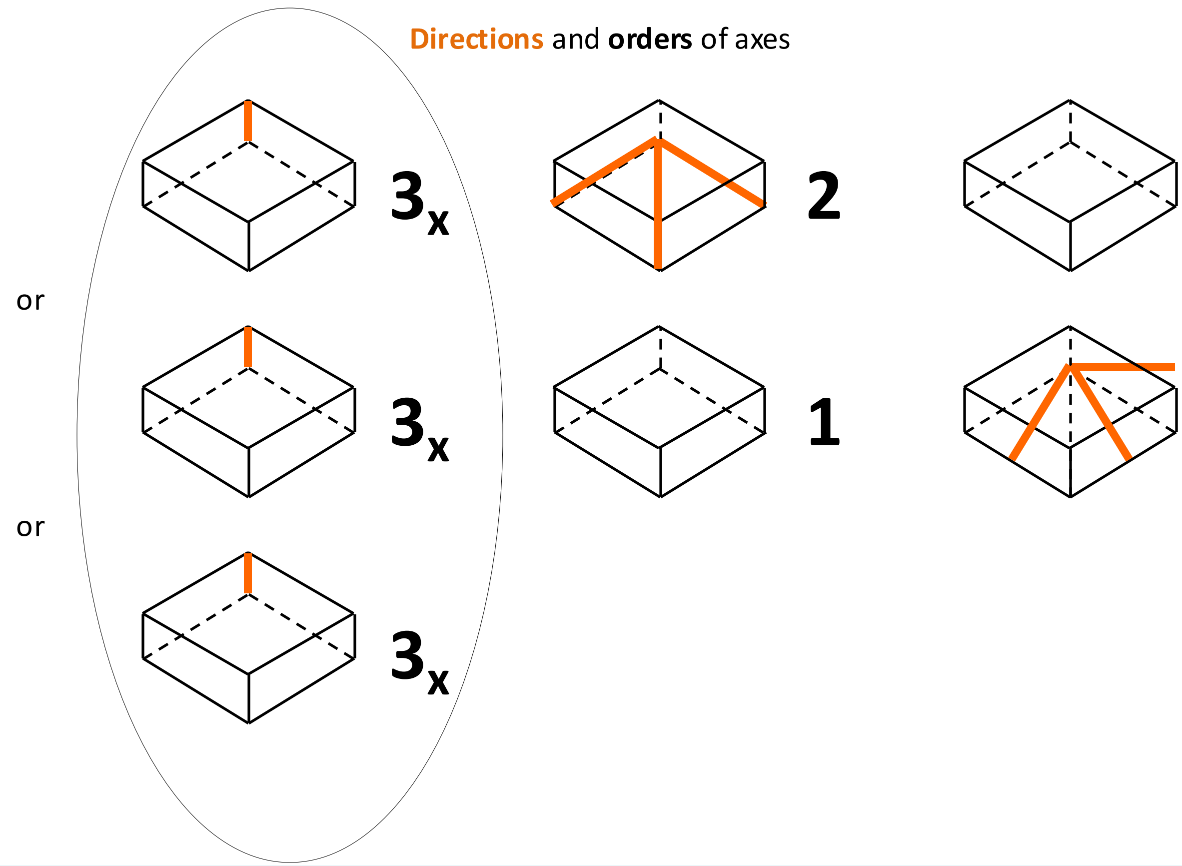
P 3 2 1   *P* $3_1$2 1   *P* $3_2$2 1   *P*3   *P*3_1 *P*3_2

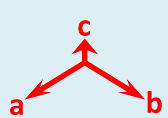
P 3 1 2   *P* $3_1$1 2   *P* $3_2$1 2

Lattice type



Directions and **orders** of axes





3-fold axes along **c**

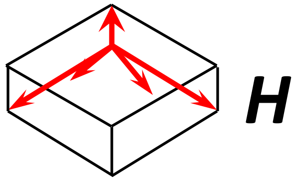
$\alpha = \beta = 90°$ $a = b$
$\gamma = 120°$

Trigonal - H

H 3 2

*H*3

Lattice type

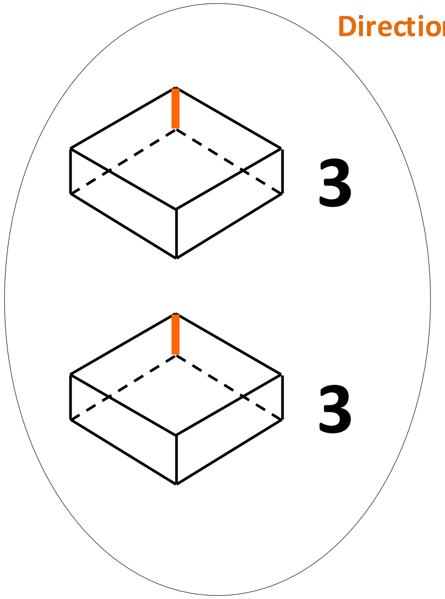


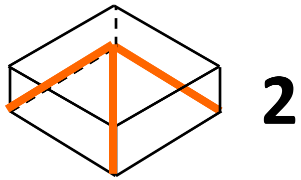
or

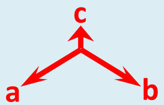
Rhombohedral setting ***R*** is an alternative to setting ***H***

Directions and **orders** of axes

or







3-fold axes along **c**

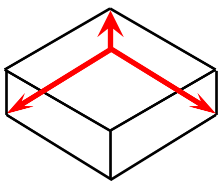
α = β = 90° *a* = *b*
γ = 120°

Hexagonal

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

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

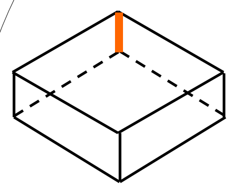
Lattice type

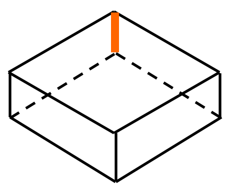


P

or

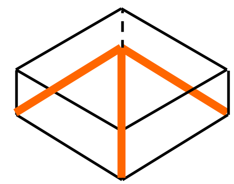
Directions and **orders** of axes





$\mathbf{6_x}$

$\mathbf{6_x}$



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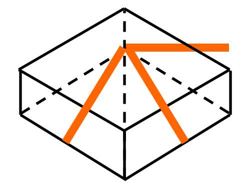

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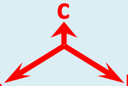


6-fold axes along **c**

$\alpha = \beta = 90°$ $a = b$

$\gamma = 120°$

Ones

~~*P* 1 1 1~~	*P* 1
P 1 2 1	*P* 2
~~*P* 4 1 1~~	*P* 4
~~*P* 3 1 1~~	*P* 3
P 3 2 1	~~*P* 3 2~~
P 3 1 2	~~*P* 3 2~~

Subscripts

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

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

Symmetry based setting:	$\alpha = \gamma = 90°$	*C* 1 2 1
Lattice based setting:	$\alpha = \gamma = 90°$ $\beta < 120°$	*C* 1 2 1 or *I* 1 2 1 - the same space group - different crystal setting

Symmetry based setting vs. lattice based setting: primitive orthorhombic

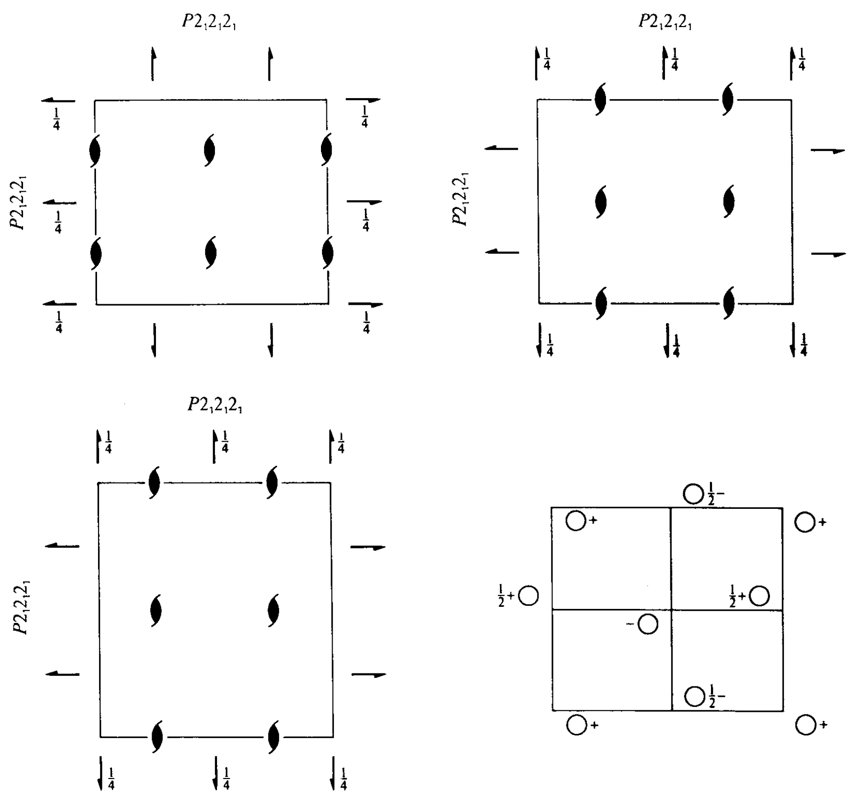
Symmetry based setting:	$\alpha = \beta = \gamma = 90°$	$P\,2\,2\,2_1$	$P\,2_12_12$
Lattice based setting:	$\alpha = \beta = \gamma = 90°$ $a < b < c$	$P\,2\,2\,2_1$ $P\,2\,2_12$ $P\,2_12\,2$	$P\,2_12_12$ $P\,2_12\,2_1$ $P\,2\,2_12_1$

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

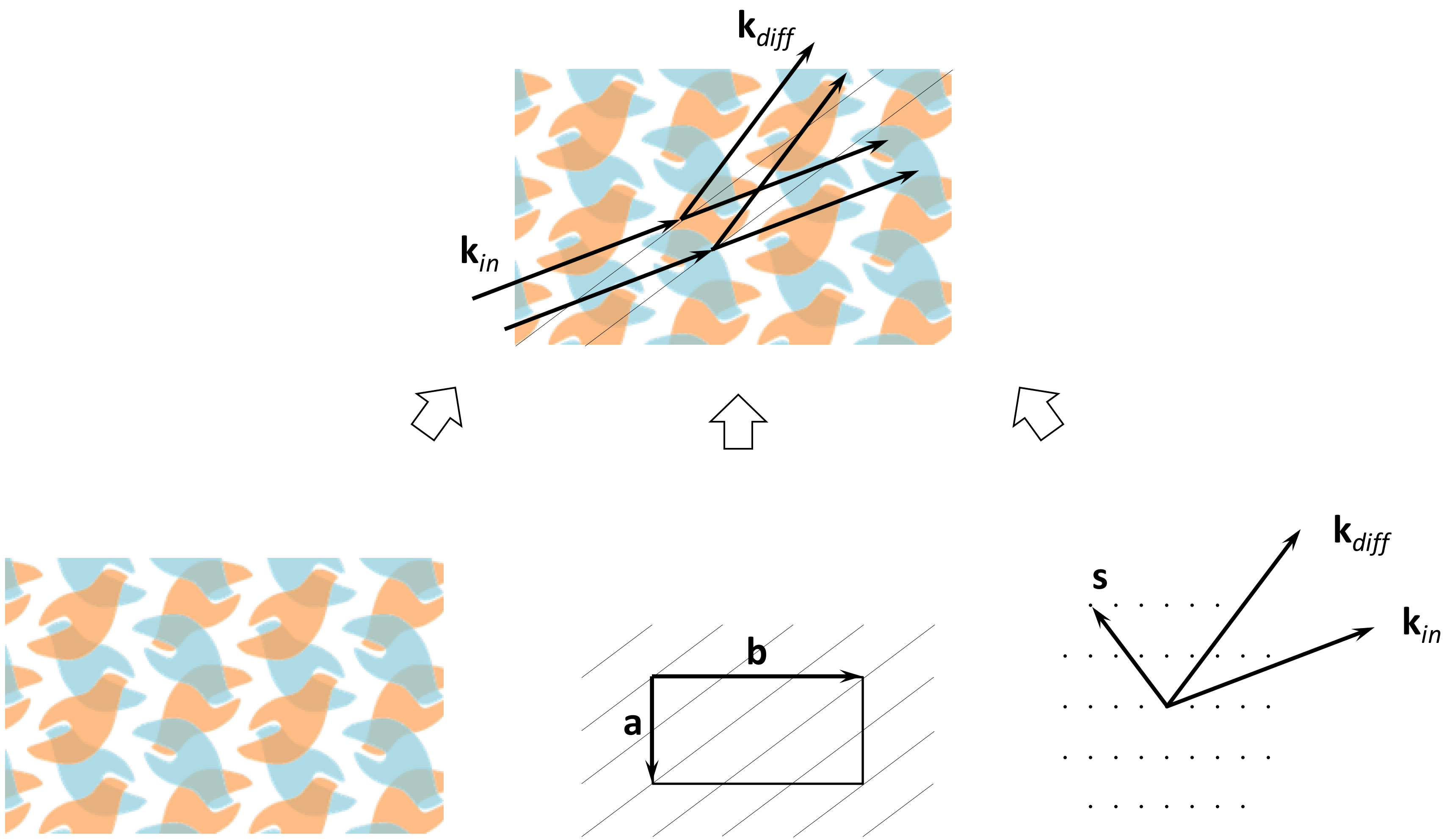
Space group representation in ITC-A

Crystal Class
(point group)

$P\,2_1\,2_1\,2_1$	D_2^4	$\boxed{222}$	Orthorhombic
No. 19	$P\,2_1\,2_1\,2_1$		Patterson symmetry $Pmmm$



Conventional diffraction scheme



real space

Bragg planes

reciprocal space

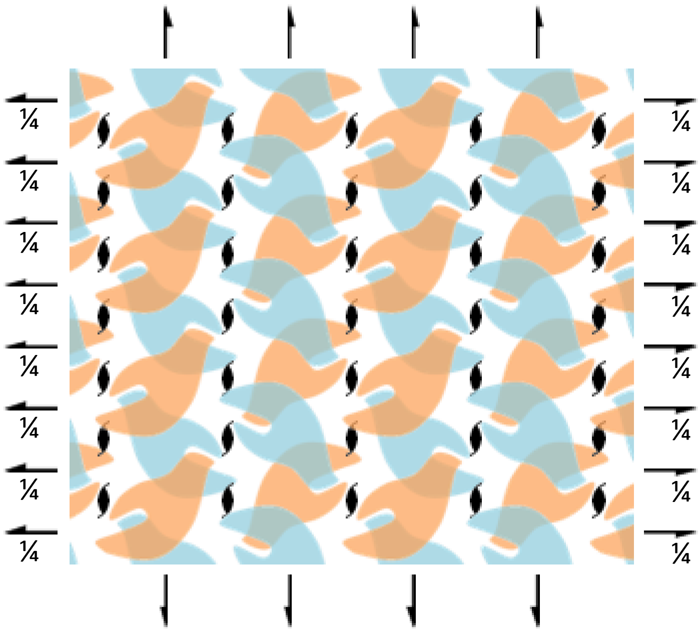
Symmetry of intensities

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

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

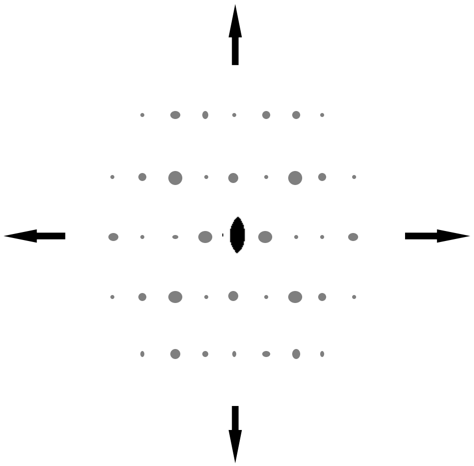
Symmetry of intensities

real space



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

reciprocal space



to give an element of a point group.

Symmetry of intensities

Real space

Crystal structure

Space group operation

The same crystal structure

Reciprocal space

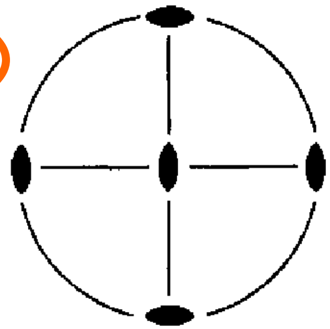
Intensities at Bragg points

Strip any translation component from the space group operation and merge identical operations:
Point group operation

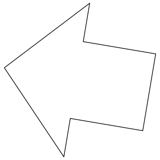
The same set of intensities (within σ)

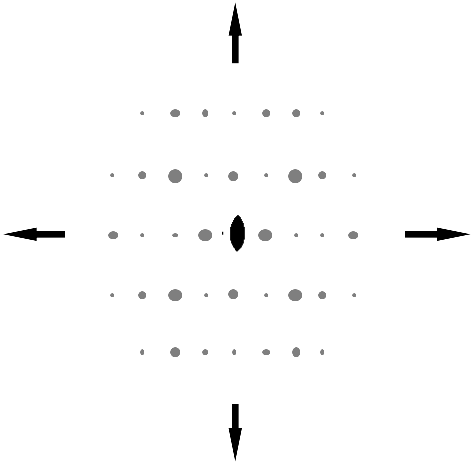
Point group scheme

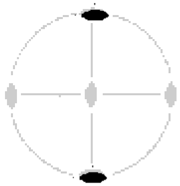
222



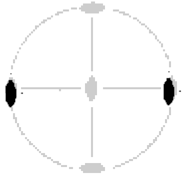
reciprocal space



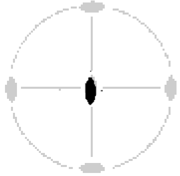




vertical 2-fold axis



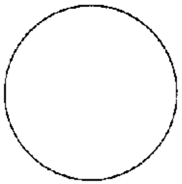
horizontal 2-fold axis



2-fold axis into plane

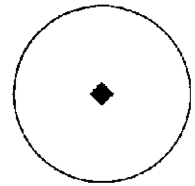
The point groups that can exist in protein crystals

1

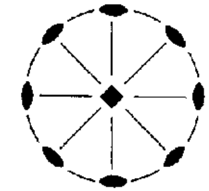


If it helps view as sphere

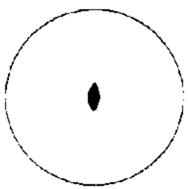
4



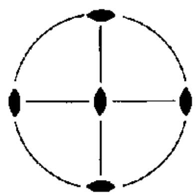
422



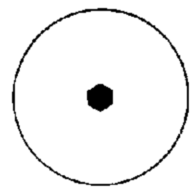
2



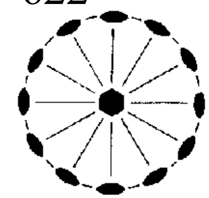
222



6



622



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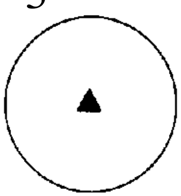
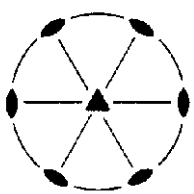
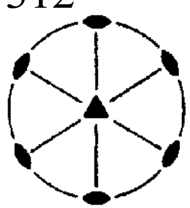


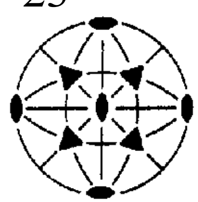
321



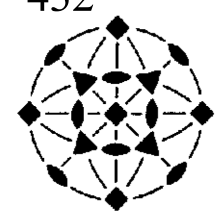
312



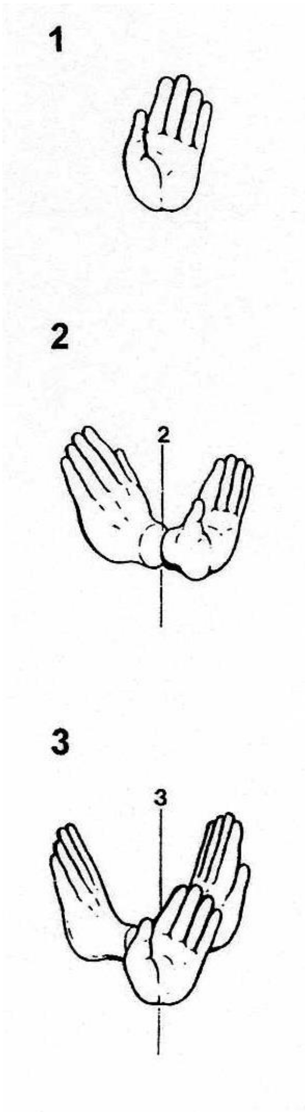
23



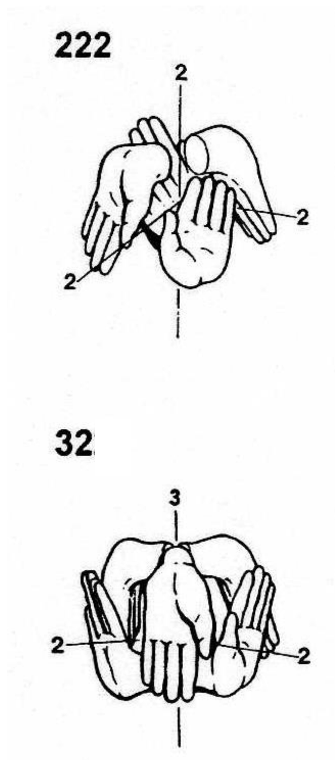
432

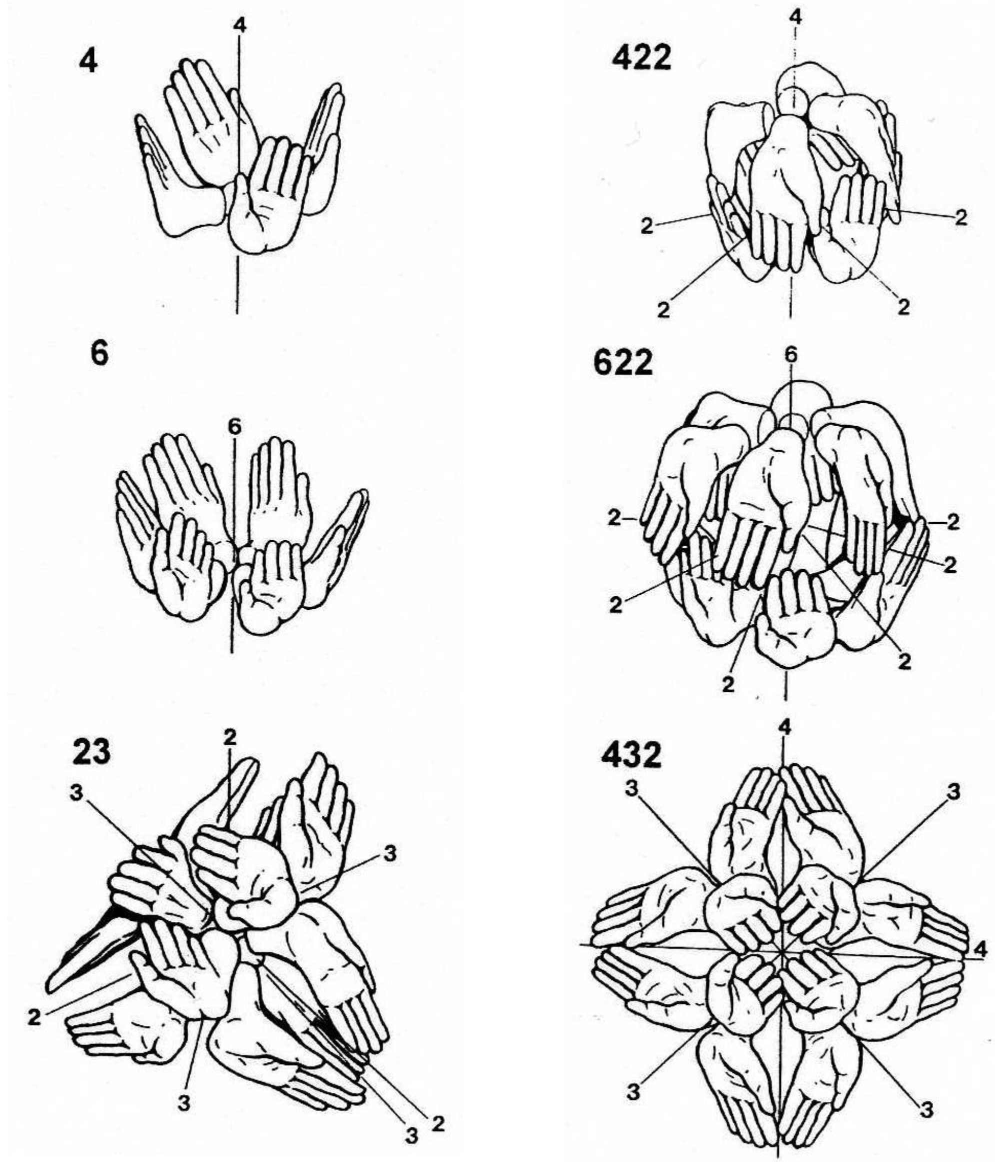


The point groups that can exist in protein crystals

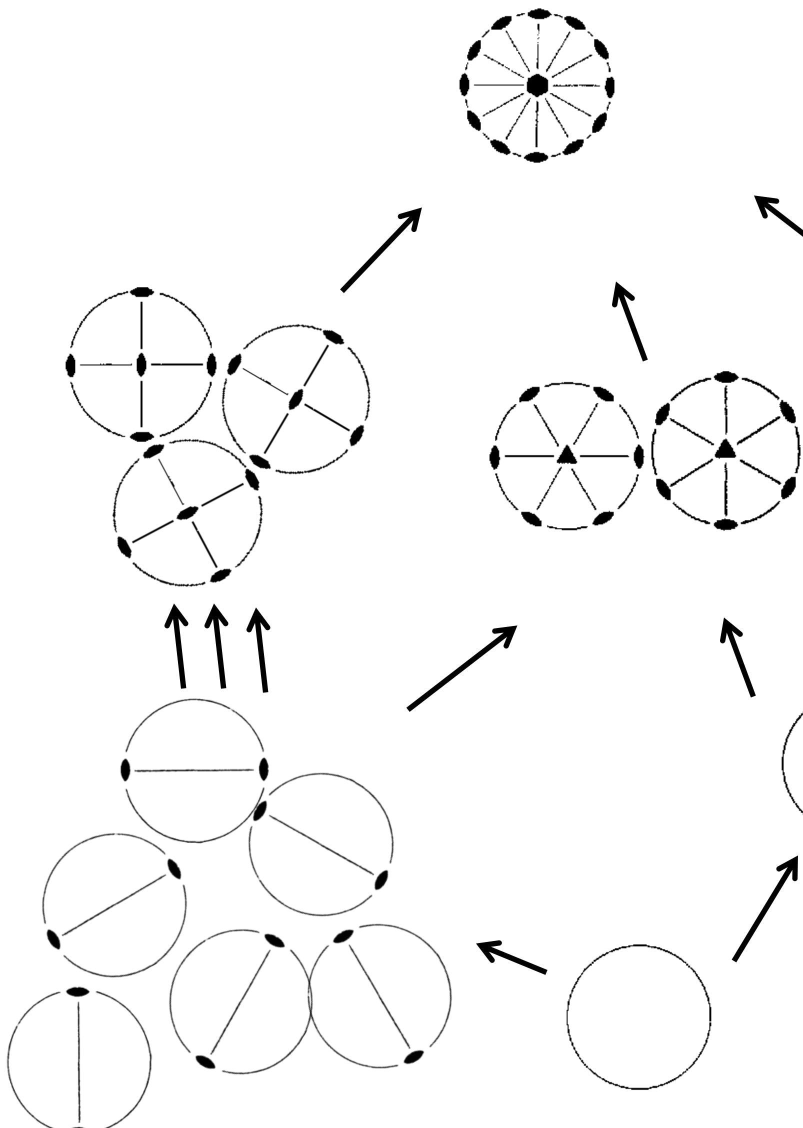


maybe an easier
representation





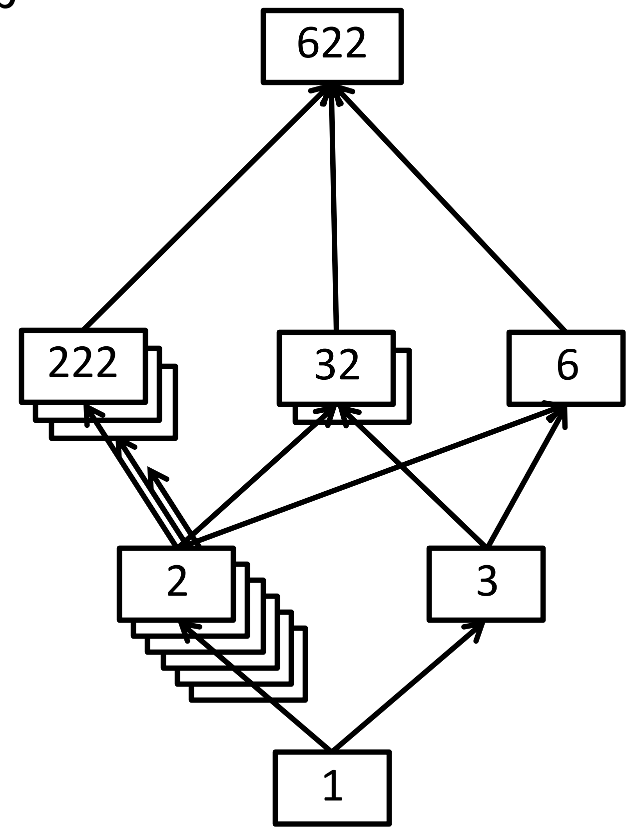
Subgroups of the point group 622



supergroup

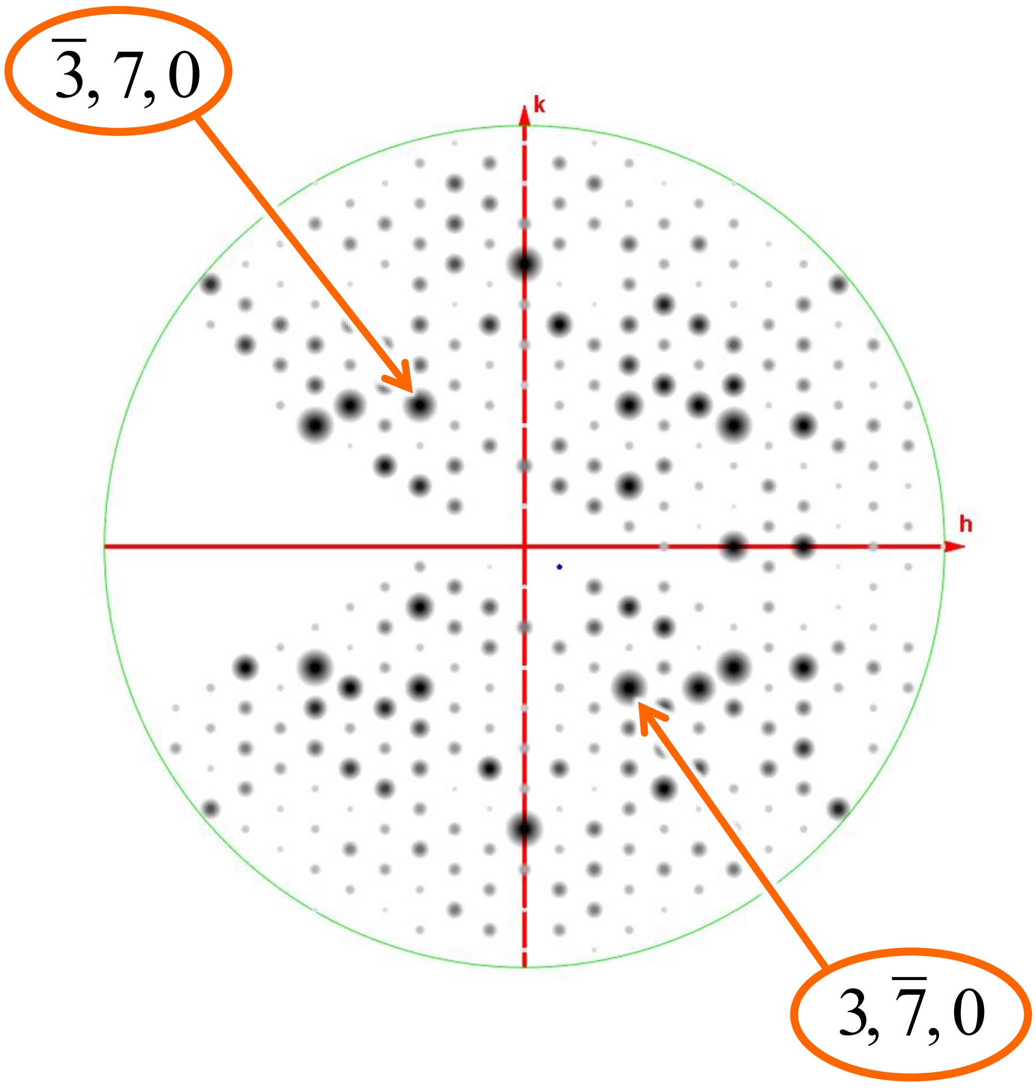
↑

subgroup



Useful for interpreting symmetry determination tables in Aimless – important for twinning

Friedel's law



(no anomalous signal)

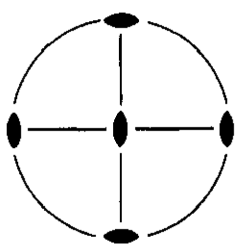
$$I\left(\bar{3},7,0\right)=I\left(3,\bar{7},0\right)$$

Point group and Laue group

+ inversion =

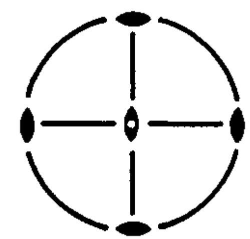
Crystal point group

222



Laue point group

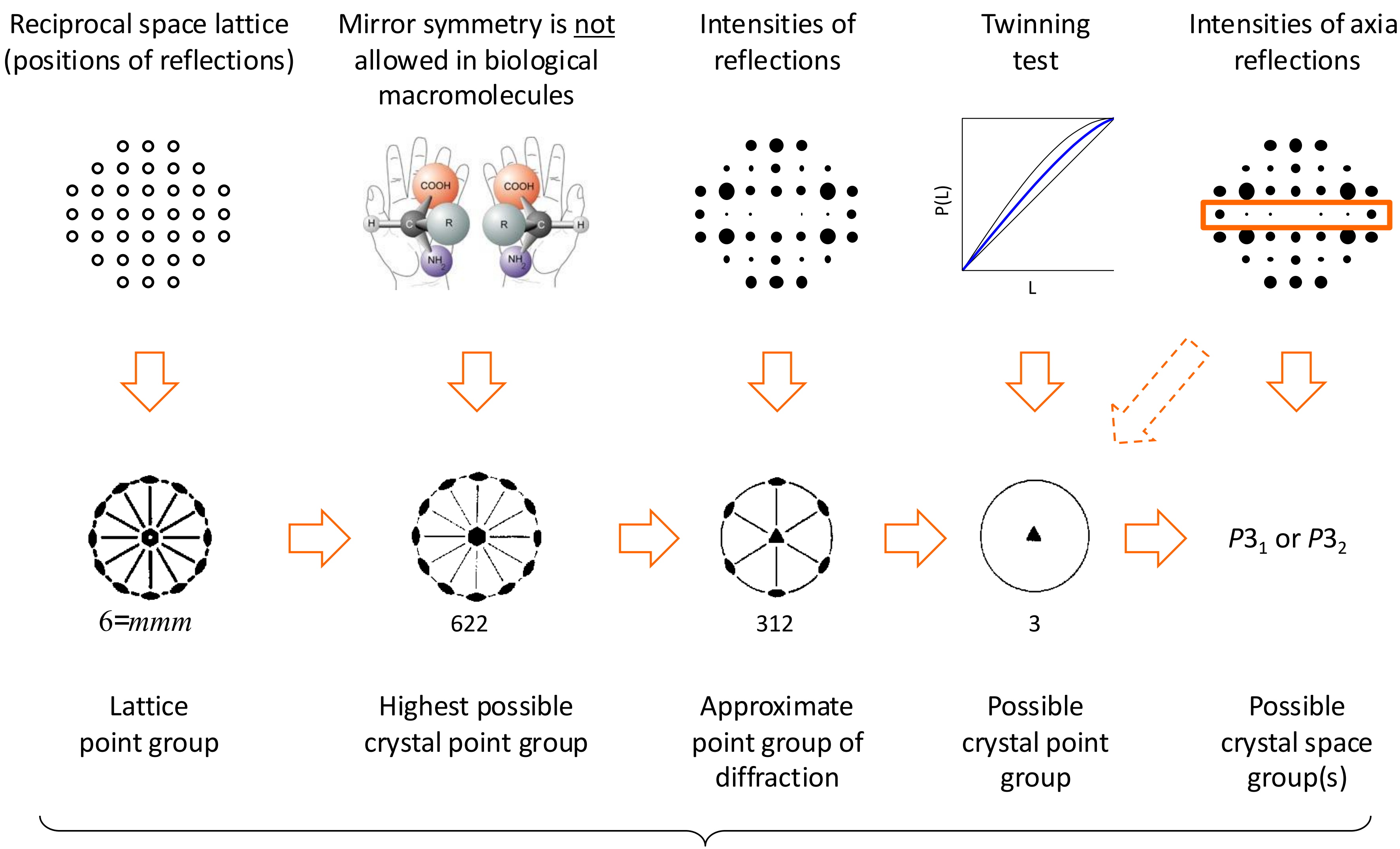
m m m



The eleven Laue point groups or crystal classes

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

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



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

End

(Short) Hermann-Mauguin symbol

$\boxed{P2_12_12_1}$

No. 19

(Extended) Hermann-Mauguin symbol

D_2^4

$\boxed{P2_12_12_1}$

Crystal Class (point group)

$\boxed{222}$

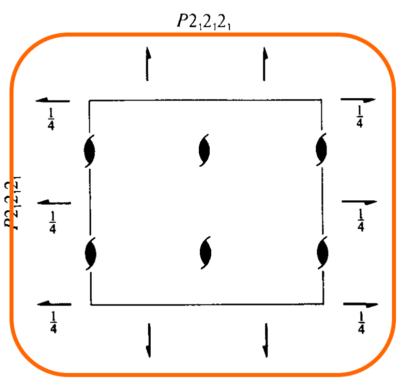
Crystal system

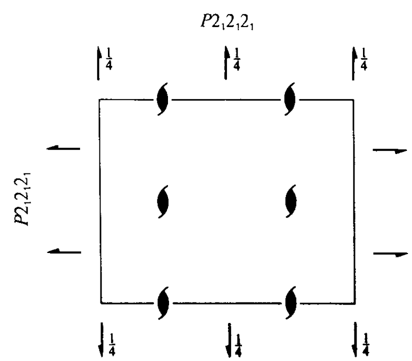
$\boxed{\text{Orthorhombic}}$

Patterson symmetry $\boxed{Pmmm}$

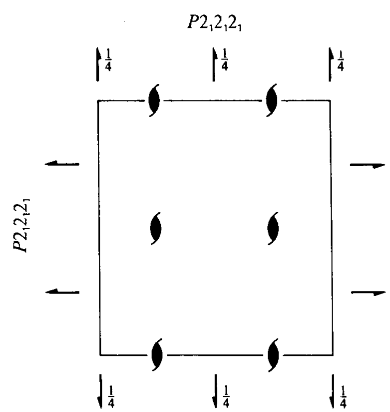
Patterson symmetry

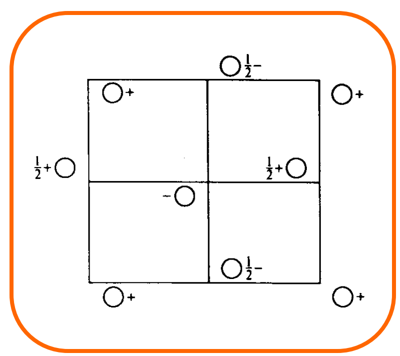
Location of symmetry elements





Two other projections are also shown for this space group





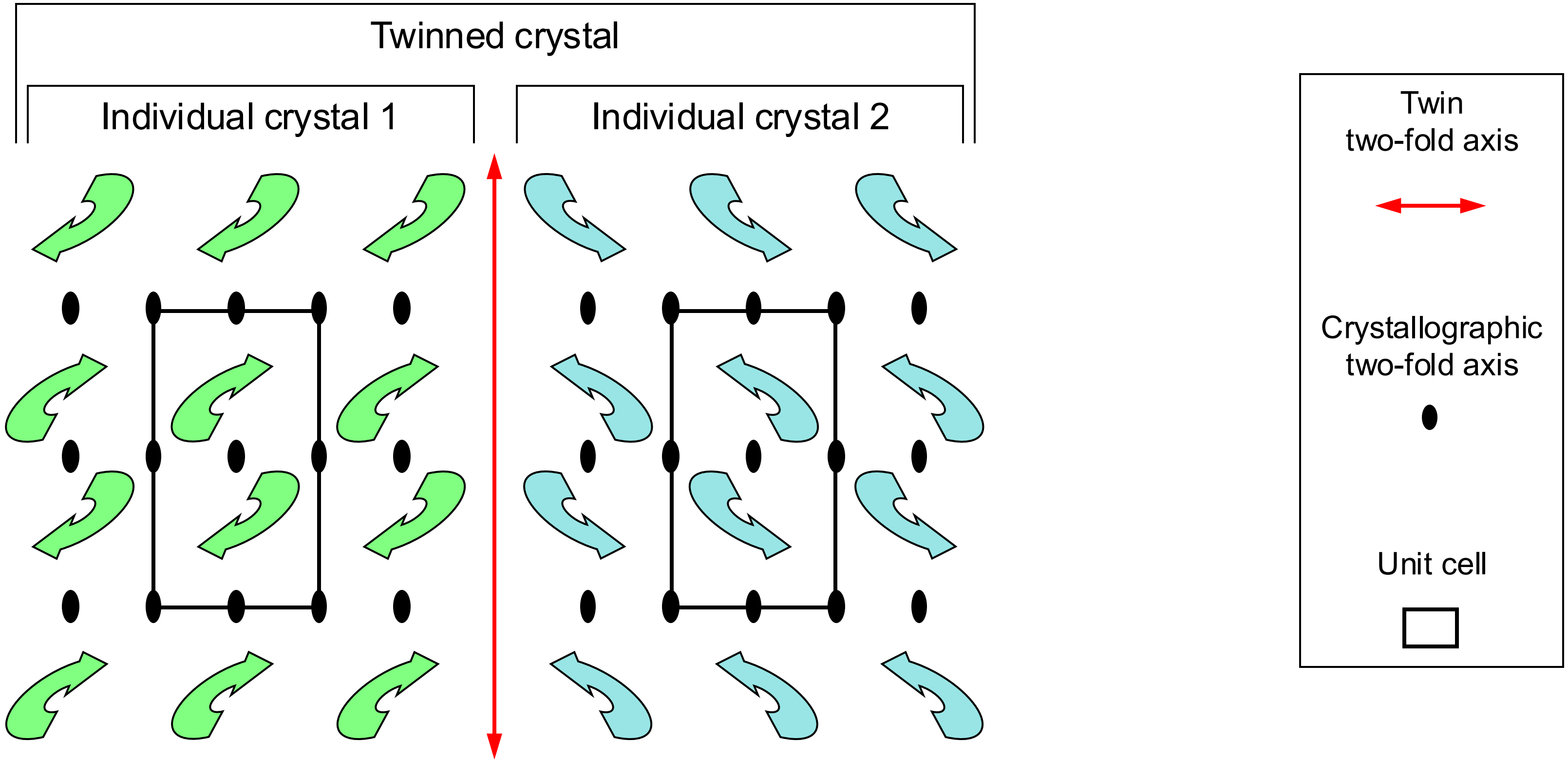
Set of equivalent points in general position.

We were looking at "molecular wallpaper" instead

Twinning by (pseudo)merohedry

lattice in orientation 1	=	lattice in orientation 2		
crystal in orientation 1	≠	crystal in orientation 2		
crystal in orientation 1	+	crystal in orientation 2	=	Twinned crystal

Example: P2, β = 90



Twinning by (pseudo)merohedry

lattice in orientation 1	=	lattice in orientation 2		
crystal in orientation 1	≠	crystal in orientation 2		
crystal in orientation 1	+	crystal in orientation 2	=	Twinned crystal

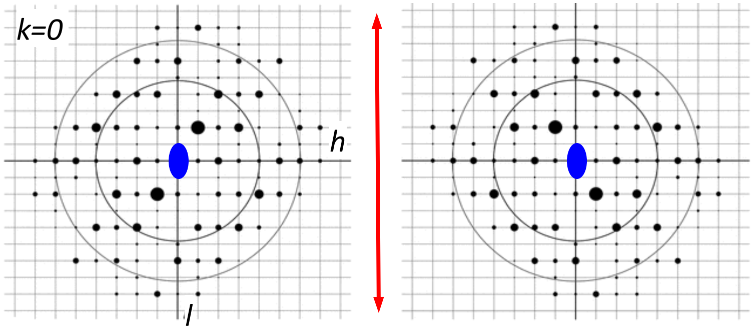
P121, β = 90

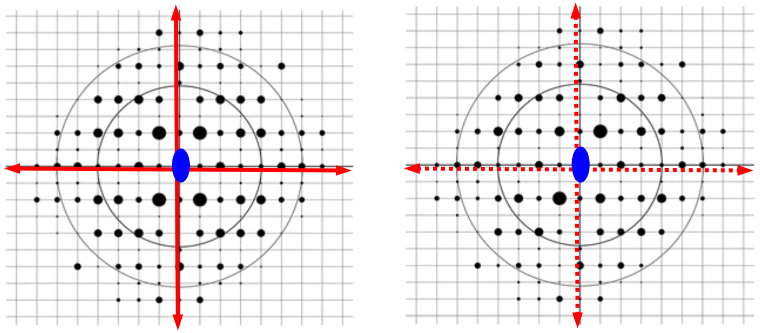
Perfect twin (individual crystals of equal sizes)

Partial twin (individual crystals of different sizes)

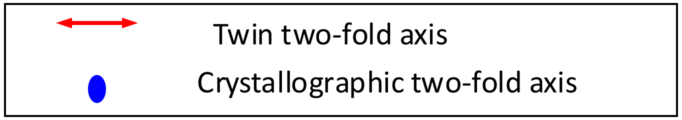
Intensities from individual crystal 1

Intensities from individual crystal 2





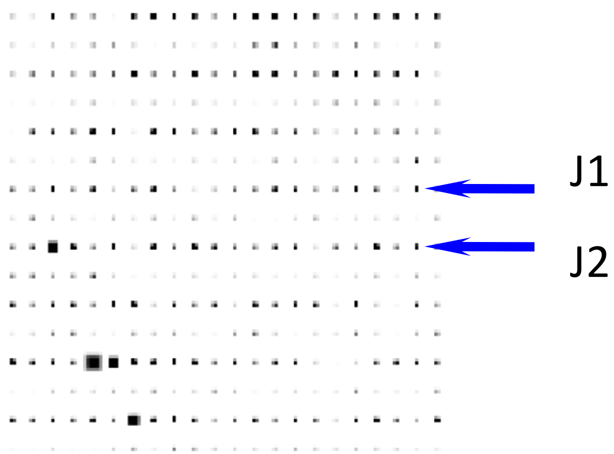
less weak reflections



Allows for twinning tests based on statistics of intensities

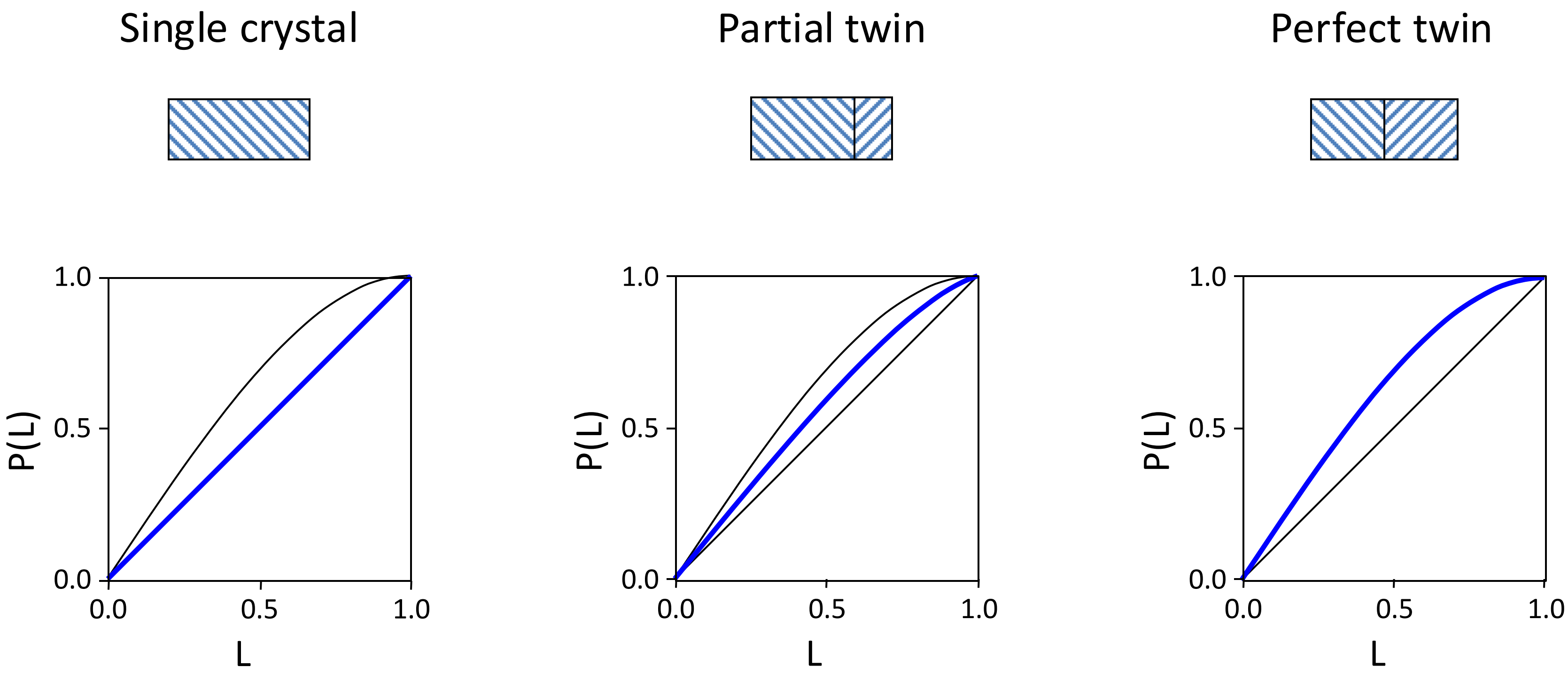
L-test

$$L = | J1 - J2 | / (J1 + J2)$$



L-test is designed to be suitable for most of cases
- with and without pseudo-translation
- isotropic and anisotropic data

Theoretical distribution of L



Purpose of twinning tests

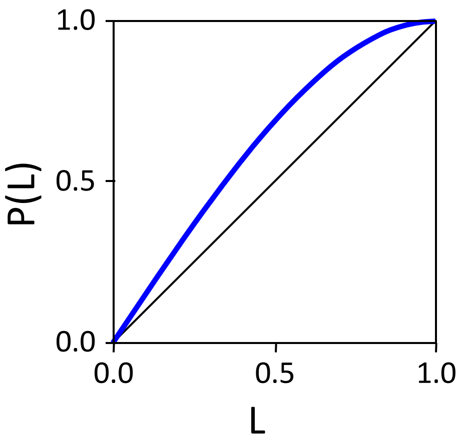
Twinning tests only indicate possible issues with crystal symmetry

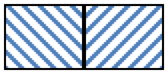
All the rest belongs to refinement

- twinning fraction estimation
- evaluation of R-factors
- “detwinning” for map calculation
- final decision on crystal symmetry

Example

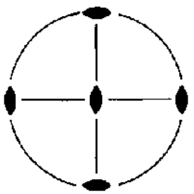
L-test



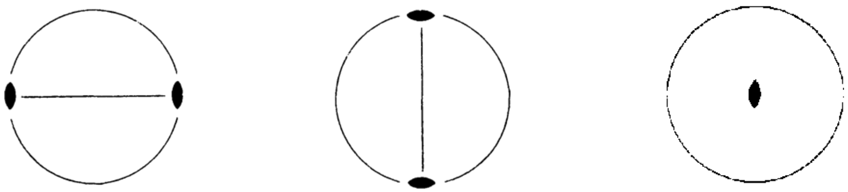


Perfect twin

Symmetry of diffraction* 222, lattice type P



Point group symmetry of the crystal:
a subgroup of 222 (one of the point groups 2):



Space groups to try by MR**:

P121	P211	P112
$P12_11$	$P2_111$	$P112_1$

A wake-up slide

Attached is a zipped directory with the sequence file (…) of the crystallised protein (pyruvate kinase from Methanosarcina thermophila), merged data used in refinement (…), and results of my last refinement (…).