Fundamentals. Crystal patterns and crystal structures. Lattices, their symmetry and related basic concepts

Didactic material for the MaThCryst schools

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Ideal vs. real crystal, perfect vs. imperfect crystal

Ideal crystal:

Perfect periodicity, no static (vacancies, dislocations, chemical heterogeneities, even the surface!) or dynamic (phonons) defects.

Real crystal:

A crystal whose structure differs from that of an ideal crystal for the presence of static or dynamic defects.

Perfect crystal:

A real crystal whose structure contains only equilibrium defects.

Imperfect crystal:

A real crystal whose structure contains also non-equilibrium defects (dislocations, chemical heterogeneities...).

What follows describes the structure of an ideal crystals (something that does not exist!), whereas ***a real crystal is rarely in thermodynamic equilibrium***.

What do you get from a (conventional) diffraction experiment?

Time and space averaged structure!

“**Time-averaged**” because the time span of a diffraction experiment is much larger that the time of an atomic vibration.

↓

The instantaneous position of an atom is replaced by the envelop (most often an ellipsoid) that describes the volume spanned by the atom during its vibration.

“**Space-averaged**” because a conventional diffraction experiment gives the average of the atomic position in the whole crystal volume, which corresponds to “the” position of the atom only if perfect periodicity is respected.

↓

Importance of studying the “ideal” crystal

Non-conventional experiments (time-resolved crystallography, nanocrystallography etc.) allow to go beyond the ideal crystal model, but also some information that are often neglected in a conventional experiment (diffuse scattering) can give precious insights on the real structure of the crystal under investigation.

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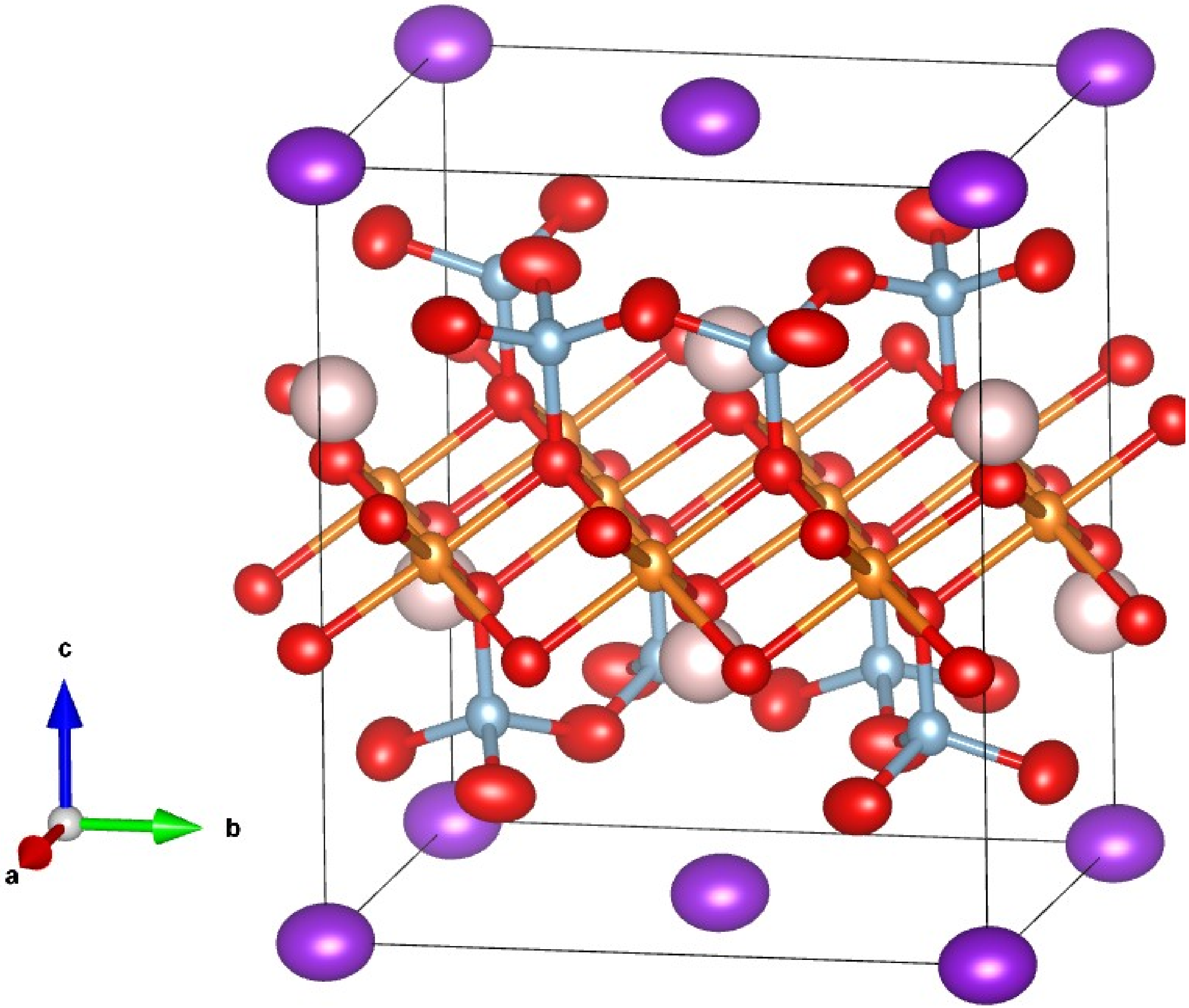
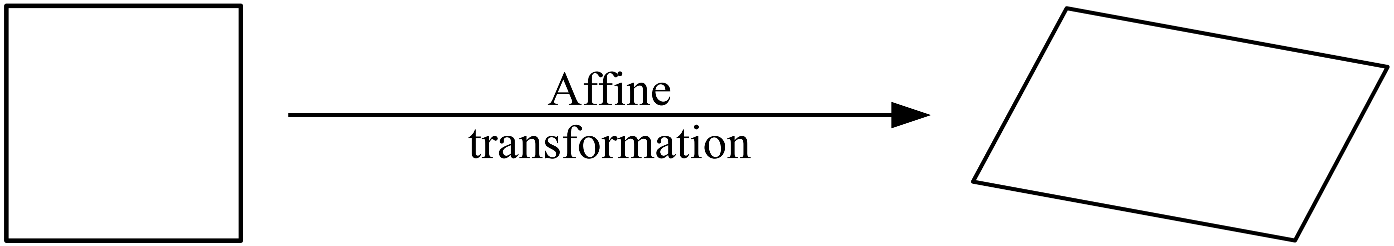
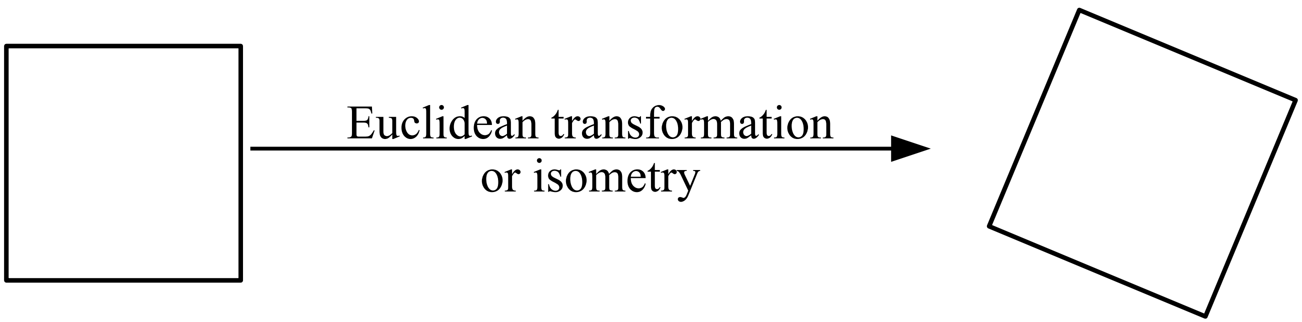
Space and time-averaged structure



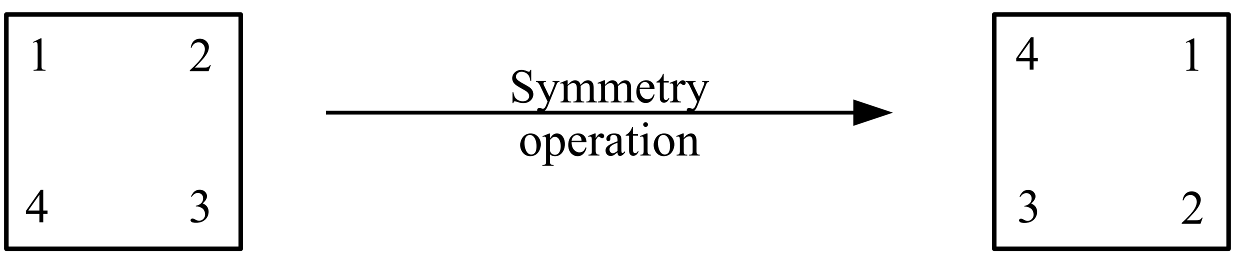
Transformations



An affine transformation is a deformation that sends corners to corners, parallel lines to parallel lines, mid-points of edges to mid-point of edges but does not preserves distances or angles.



An isometry is a special case of affine transformation which is not a deformation: the object on which it acts can change its orientation and position in space.



A symmetry operation is a special case of isometry: the object on which it acts can change its orientation and position in space only in such a way that its configuration (position, orientation) after the action cannot be distinguished from its configuration before the action.

Symmetry operations of a crystal pattern

- A crystal pattern is an idealized crystal structure which makes abstraction of the defects (including the surface!) and of the atomic nature of the structure.
- A crystal pattern is therefore infinite and perfect.
- A crystal pattern has both translational symmetry and point symmetry; these are described by its **space group**.
- We have to define the concepts of group and its declinations in crystallography.

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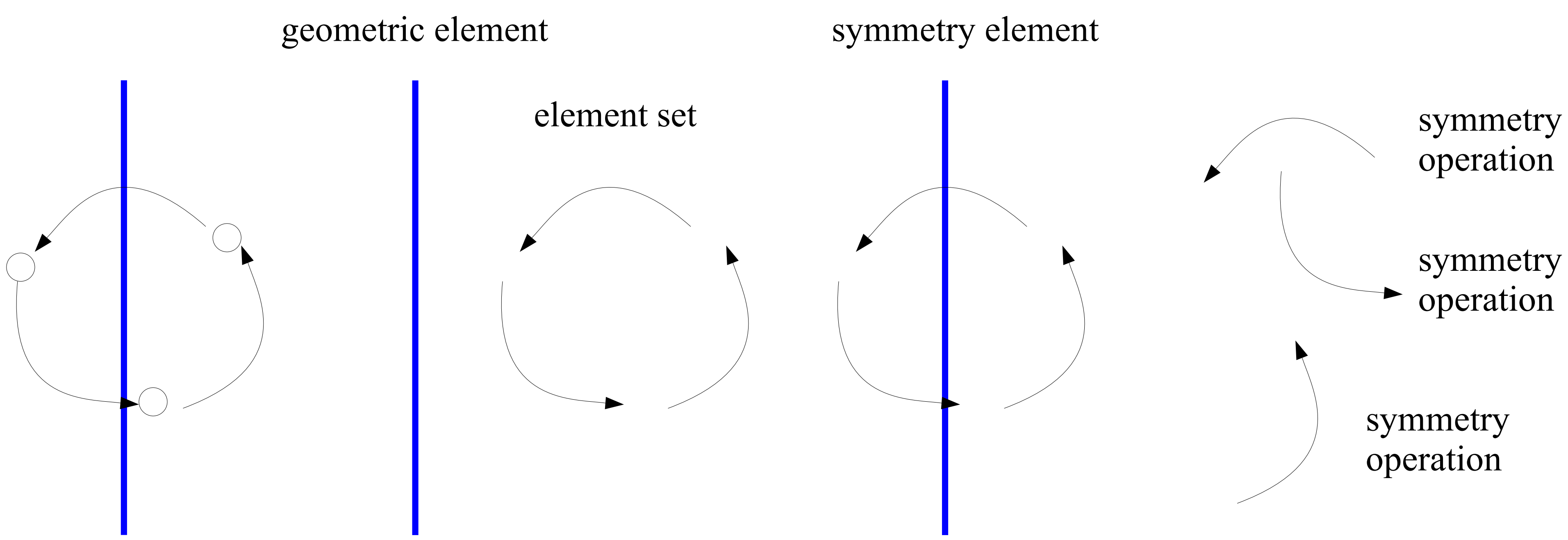
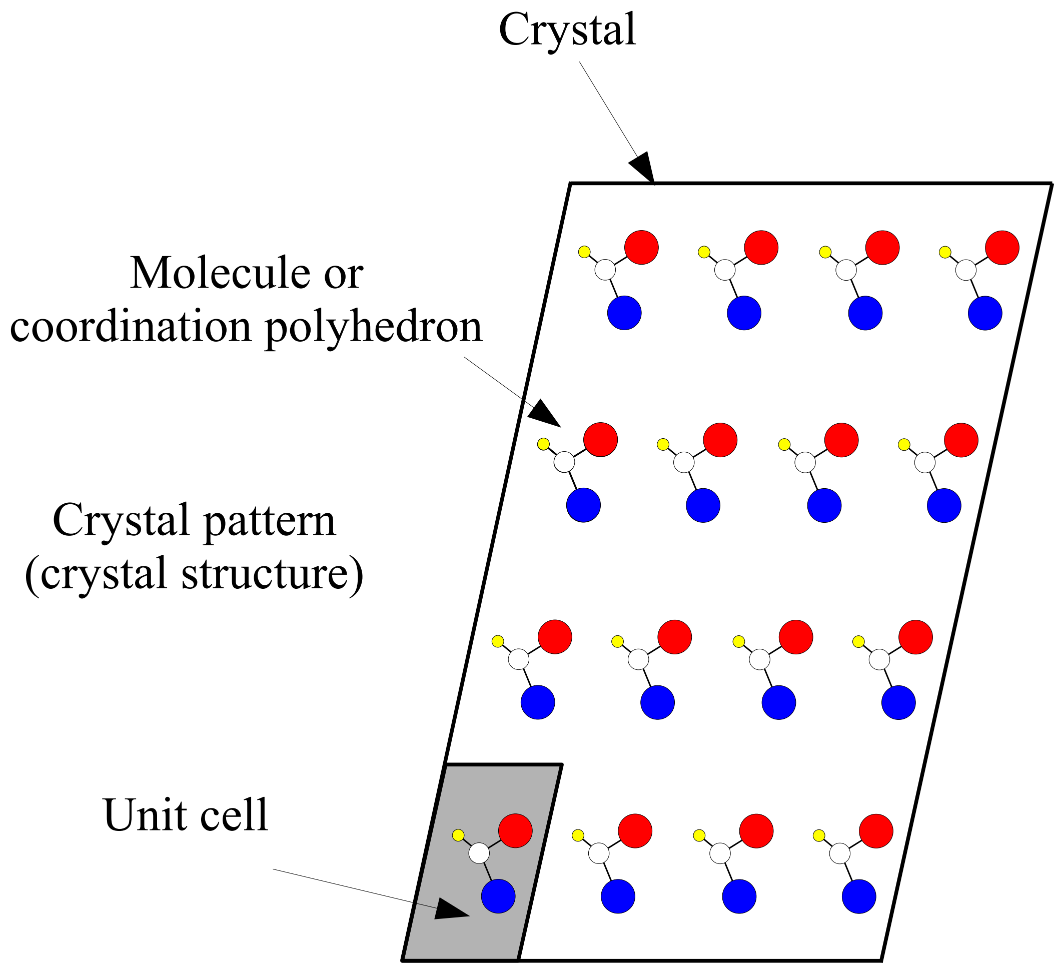
Elements and operations

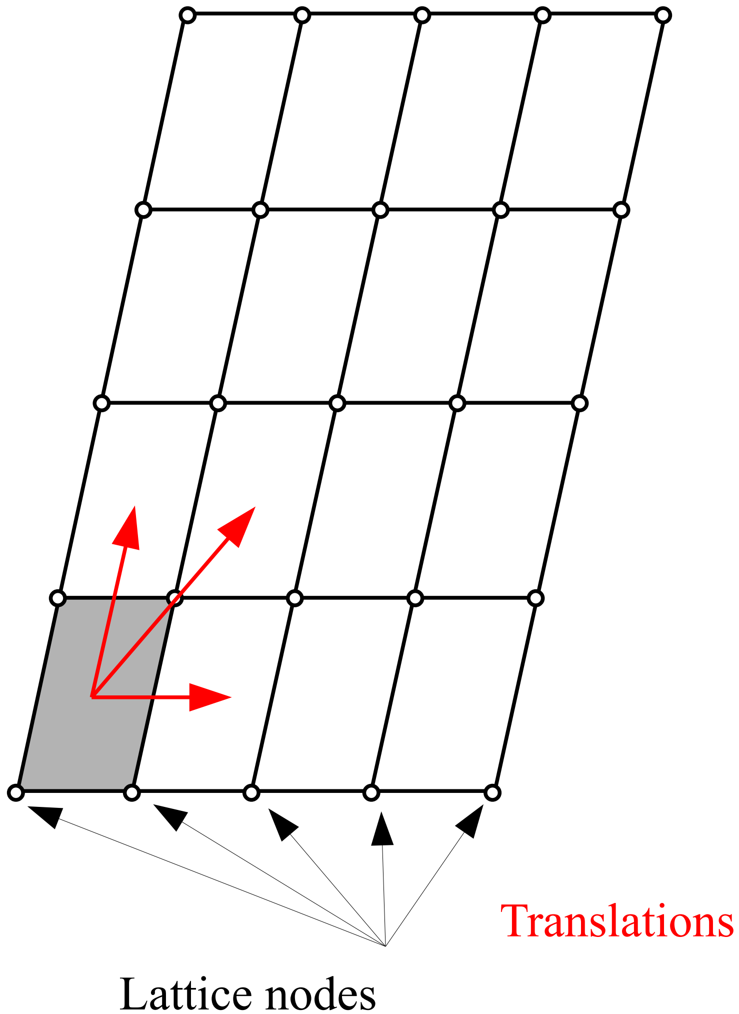
- **geometric element**: the point, line or plane left invariant by the symmetry operation.
- **symmetry element**: the geometric element defined above together with the set of operations (called **element set**) that leave in invariant.
- **symmetry operation**: an isometry that leave invariant the object to which it is applied.



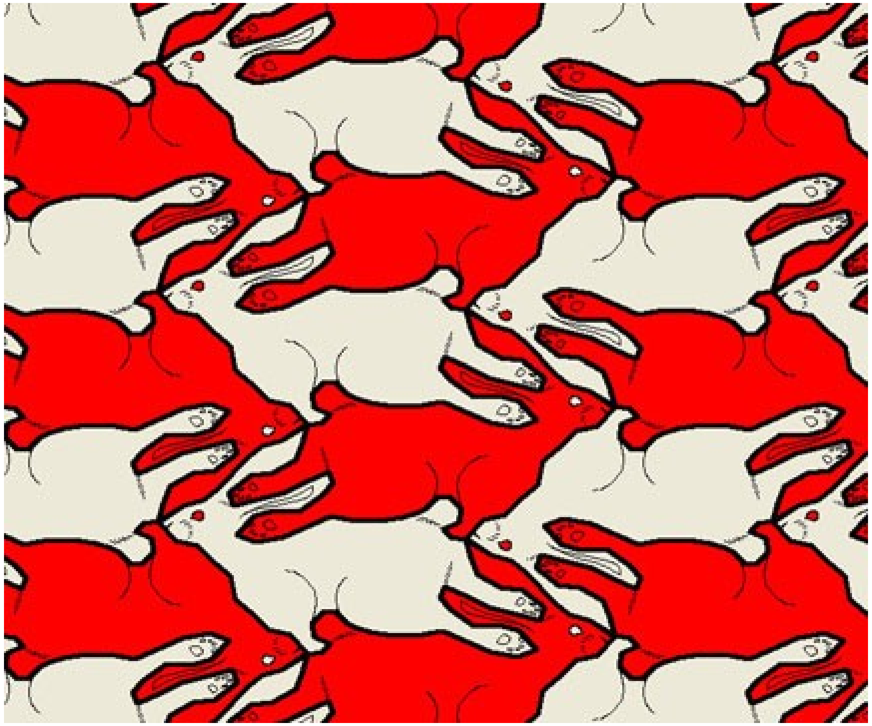
The operation that share a given geometric element differ by a lattice vector. The one characterized by the shortest vector is called **defining operation**.

Crystal structure/pattern vs. crystal lattice



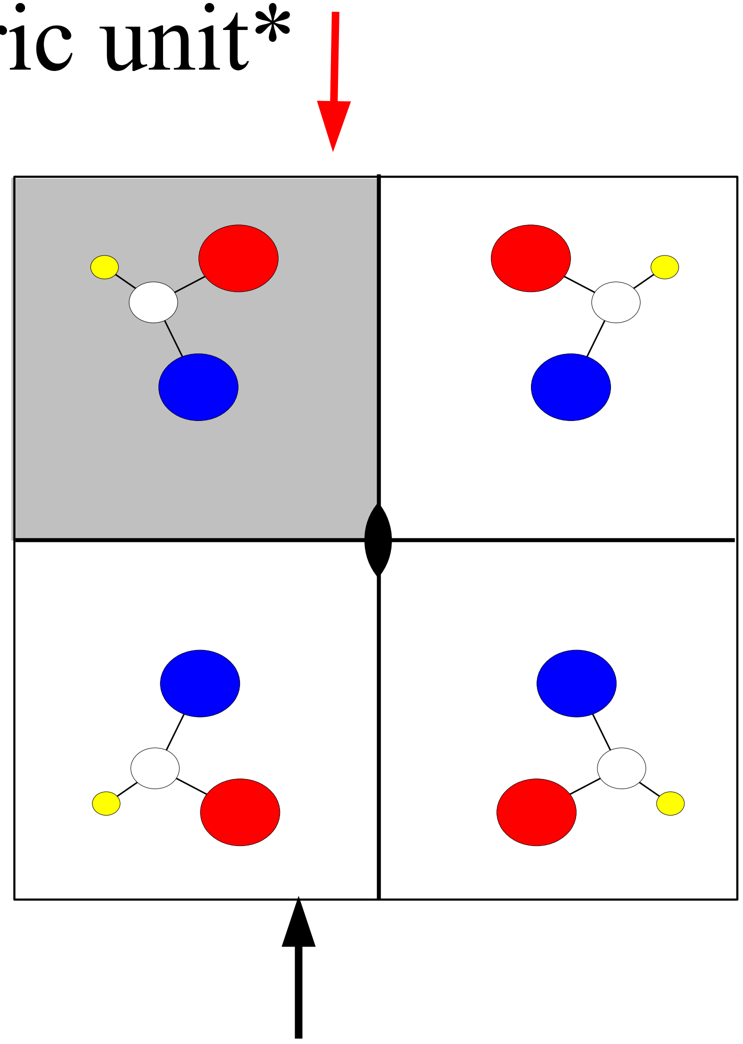


Example of crystal pattern which is not a crystal structure



The minimal unit you need to describe a crystal pattern

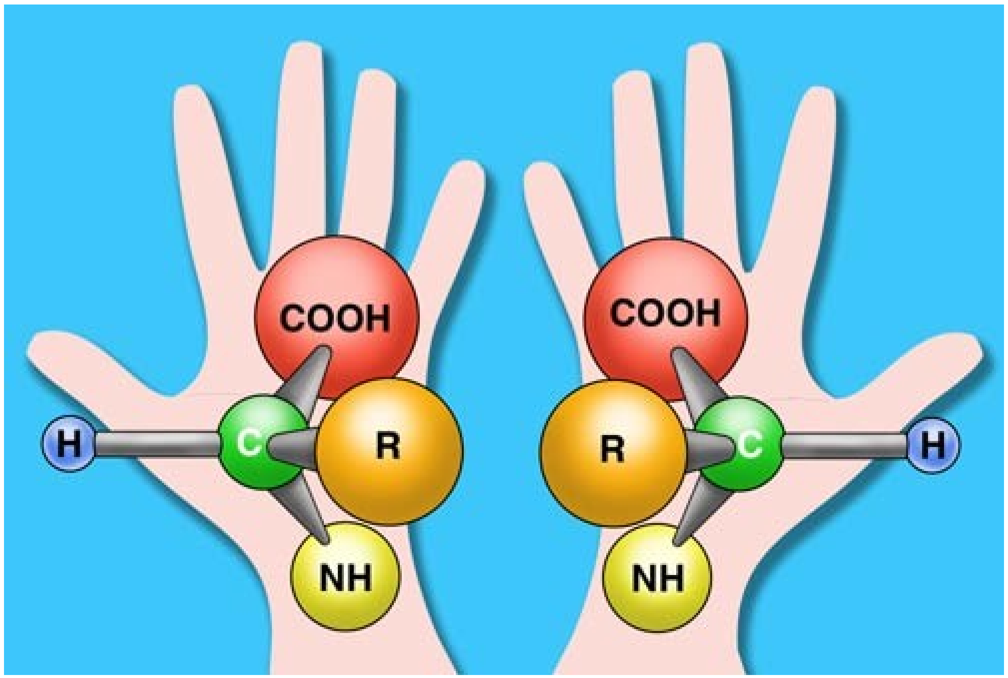
Asymmetric unit*

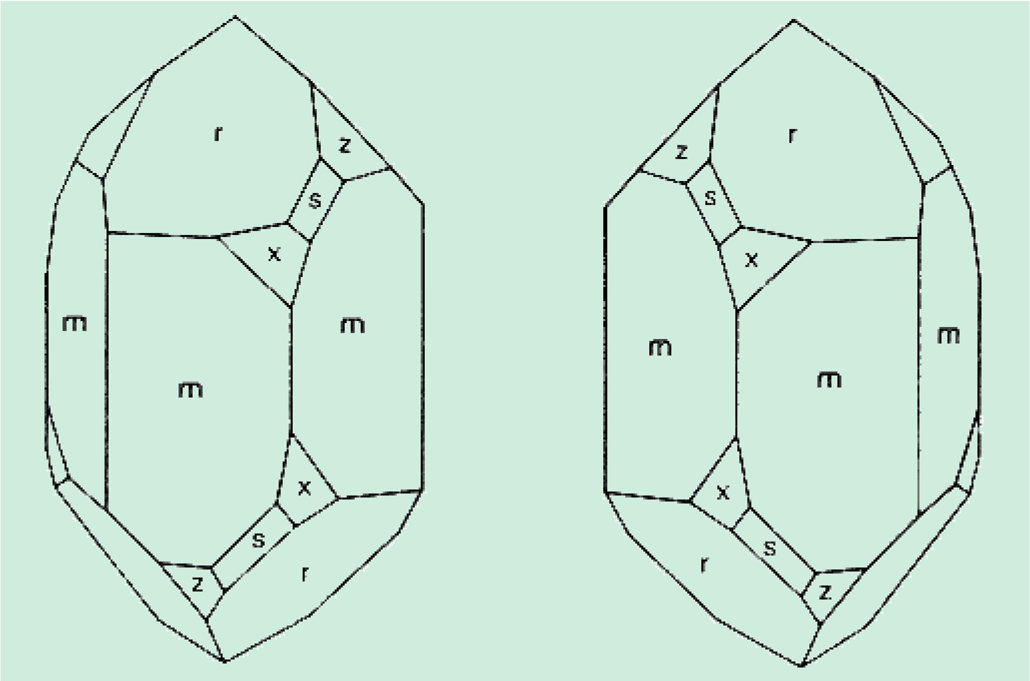


Unit cell

*In mathematics, it is called “fundamental region”

The concepts of chirality and handedness (the left-right difference)



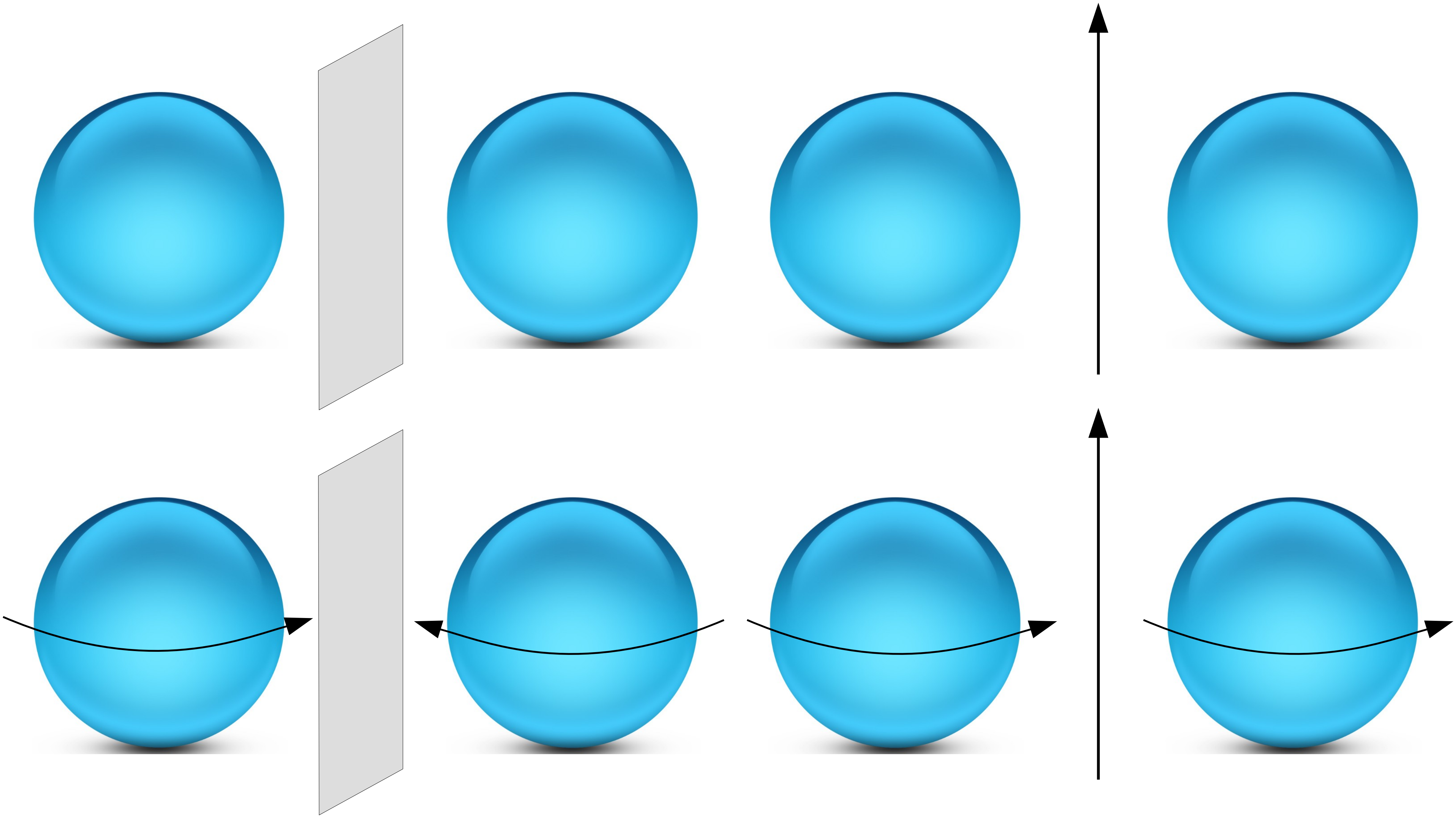


Symmetry operations are classified into **first kind** (keep the handedness) and **second kind** (change the handedness).
If the object on which the operation is applied is non-chiral, the effect of the operation on the handedness is not visible but the ***nature of the operation*** (first or second kind) is not affected!

The **determinant** of the matrix representation of a symmetry operation is **+1** (first kind) or **-1** (second kind)

Chirality: property of an object not being superimposable to its mirror image by a first-kind operation.
Handedness: one of the two configurations (left or right) of chiral object. Also known as **chirality sense**.

Handedness of the object and nature of the operation



Crystal structure, fractional atomic coordinates, crystallographic orbits, Wyckoff positions

Crystal structure: atomic distribution in space that complies with the order and periodicity of the crystal

Fractional atomic coordinates: atomic coordinates *x*,*y*,*z* within a unit cell with respect to the basis vectors **a**,**b**,**c**.

a,**b**,**c** (bold): basis vectors

a,*b*,*c* (italics): reference axes and cell parameters

x,*y*,*z* (italics): fractional atomic coordinates

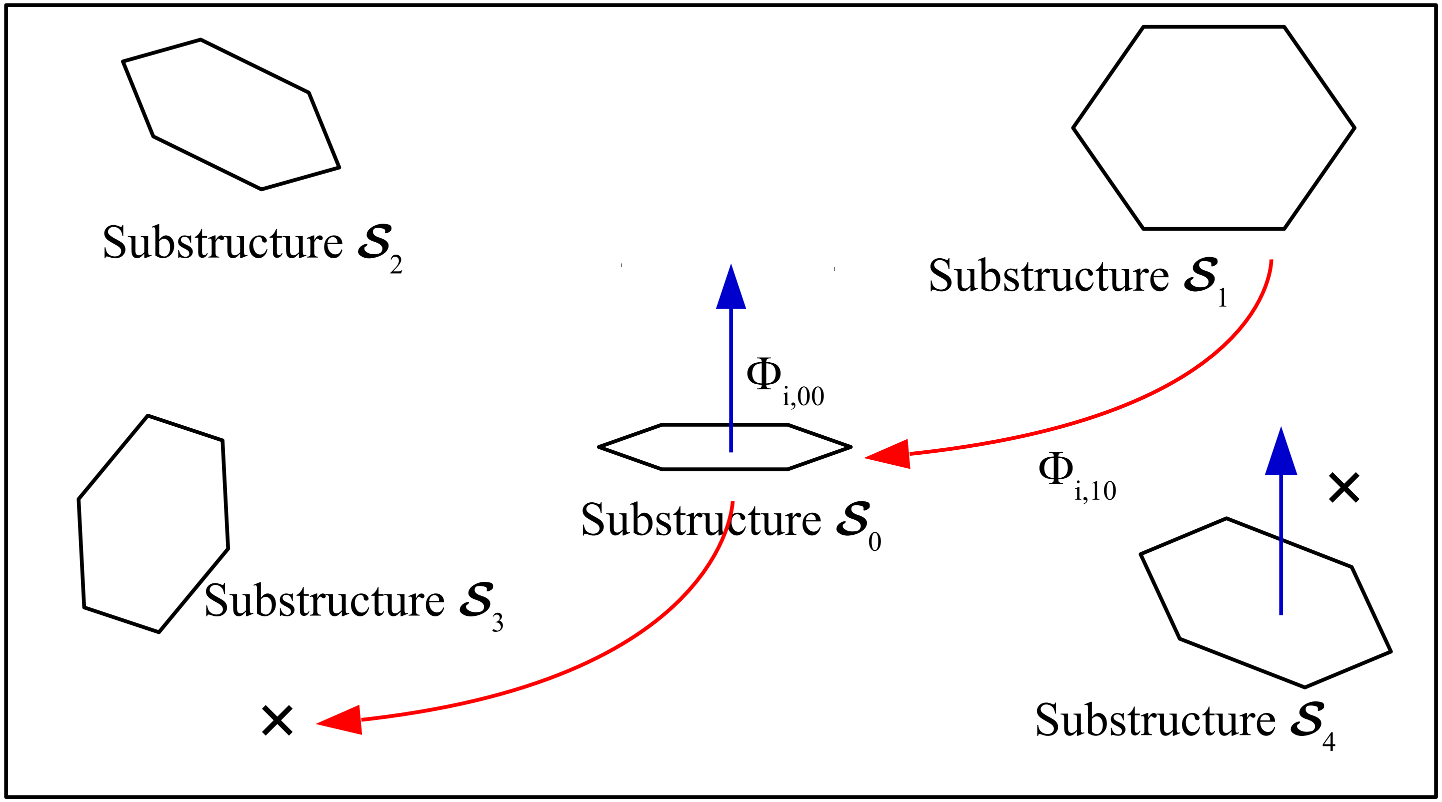
↓ Don't forget the translations!

crystallographic orbit: the infinite set of atoms obtained by applying all the symmetry operations of the space group to a given atom in the unit cell.

Wyckoff positions: classification of the crystallographic orbits on the basis of the symmetry of the atomic positions (site-symmetry group) (N to 1 mapping)*.

*More about this follows.

Global vs. local domain of action



Structure

Φ_{pp} local operations: act only on a specific substructure

Φ_{qp} partial operations: relate only a specific pair of substructures

Global (total) operations: that subset of local and partial operations that actually act on the whole structure

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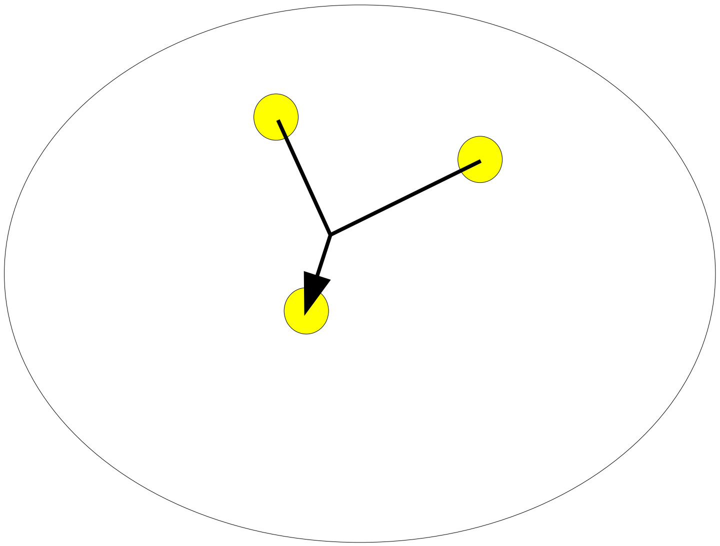
Binary operations acting on a set



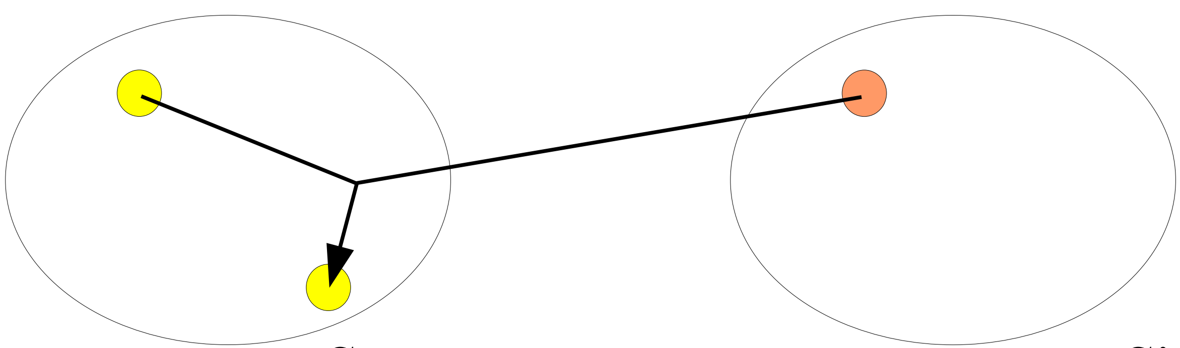
A set S

A binary operation ○

An "internal law of composition" S ○ S → S
(*closure property*)

We've got a "magma"

Note: An "external law of composition" acts on two disjoint sets S ○ S' → S



S S'

Possible properties associated to a magma

Associativity: $a \circ (b \circ c) = (a \circ b) \circ c$

Presence of identity (neutral element):
left identity $e \circ a = a$
right identity $a \circ e = a$

Presence of singular element:
left singular $s \circ a = s$
right singular $a \circ s = s$

Presence of the inverse (symmetric) element of each element:
left inverse: $a^{-1} \circ a = e$
right inverse: $a \circ a^{-1} = e$

Commutativity: $a \circ b = b \circ a$

Presence of a second binary operation: $a \in S \star b \in S = c \in S$

Algebraic structures

	globality	associativity	identity	inverse element
Magma	☑	×	×	×
Semigroup	☑	☑	×	×
Monoid	☑	☑	☑	×
Group	☑	☑	☑	☑
Semicategory	×	☑	×	×
Category	×	☑	☑	×
Groupoid	×	☑	☑	☑

The notion of symmetry group

A symmetry group $(G,\circ)$ is a set G whose elements are symmetry operations having the following features:

- the combination $\circ$ (*successive application*) of two symmetry operations g_i and g_j of the set G is still a symmetry operation g_k of the set G (closure property): $g_i \in G \circ g_j \in G \rightarrow g_k \in G$ $(g_i g_j = g_k)$
- the binary operation is associative: $g_i(g_j g_k) = (g_i g_j)g_k$
- the set G includes the identity (left and right identical): $eg_i = g_i e$
- for each element of the set G (each symmetry operation) the inverse element (inverse symmetry operation) is in the set G: $g_i^{-1}g_i = g_i g_i^{-1} = e$

In the following we will normally speak of a **group G**: it is a shortened expression for **group $(G,\circ)$** where $\circ$ is the "successive application" of symmetry operations $g \in G$. Rigorously speaking, G is not a group but just a **set**!

Abelian and cyclic groups

Commutativity is **NOT** included in the group properties (closure, associativity, presence of identity and of the inverse of each element).

A group which includes the **commutativity** property is called **Abelian**.

A special case of Abelian groups: cyclic groups

A **cyclic group** is a special Abelian group in which all elements of the group are generated from a single element (the generator).

$$\mathrm{G} = \{g, g^2, g^3, \ldots, g^n = \mathrm{e}\}$$

The notion of "order"

Order of a group element: the smallest n such that $g^n = e$.

If $n = 2$, then $g^{-1} = g$ and the element is known as an **involution**.

Order of a group: the number of elements of the group (finite or infinite)

If $n = \infty$ the group is infinite

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Homomorphism

Let G and H be two sets, and * and # two binary operations acting on G and H respectively.

The mapping f : G → H that satisfies the relation $f(u * v) = f(u) \# f(v)$ is called a **homomorphism**.

- If G contains the neutral element 1_G, then H too contains a neutral element 1_H and the homomorphism f maps them: $1_G \rightarrow 1_H$
- If G contains the inverse of each element g, then H too contains the inverse of each element h, and the homomorphism f maps the respective elements: $f(u^{-1}) = u'^{-1} = f(u)^{-1}$.

$f(u) = u'$

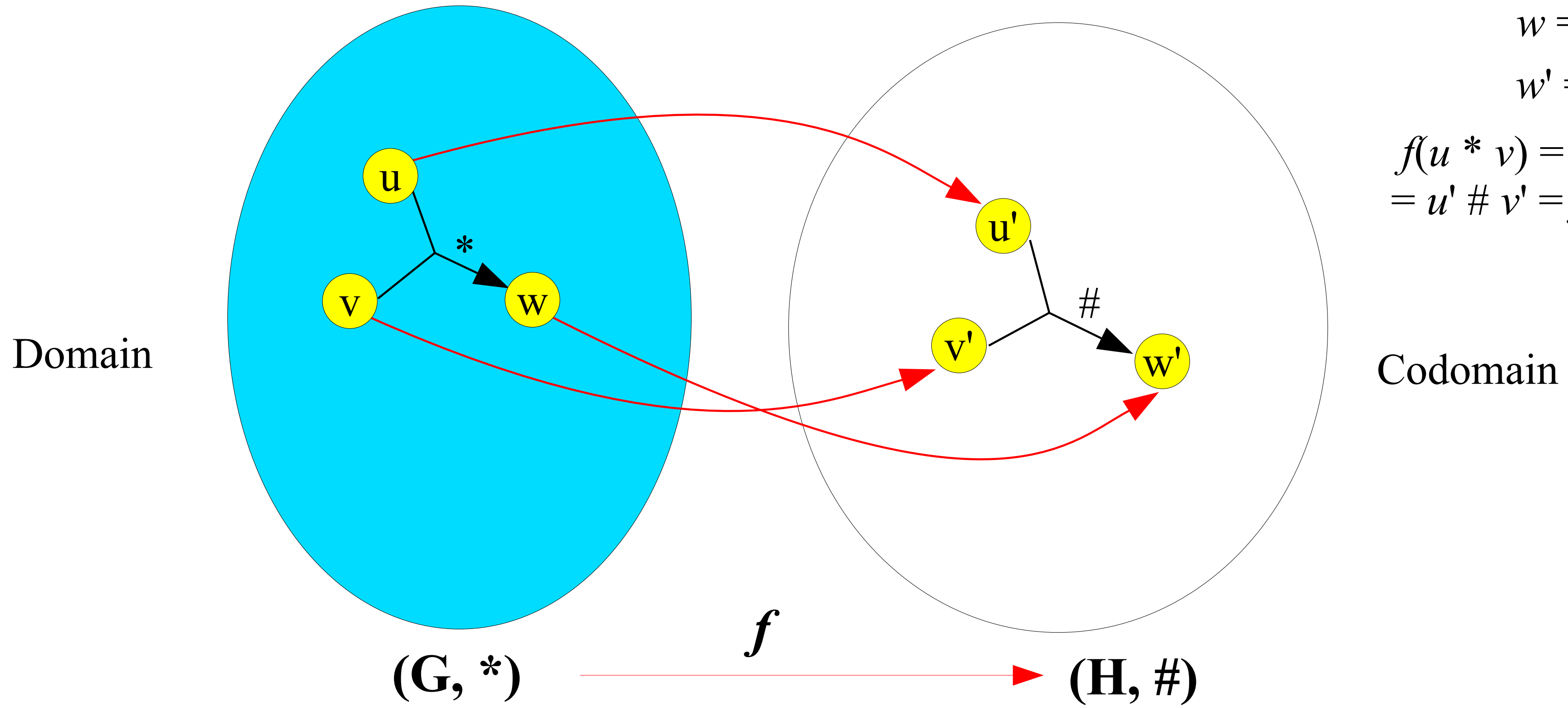
$f(v) = v'$

$f(w) = w'$

$w = u*v$

$w' = u'\#v'$

$f(u * v) = f(w) = w'$
$= u' \# v' = f(u) \# f(v)$



If H ⊂ G, the homomorphism takes the name of **endomorphism**

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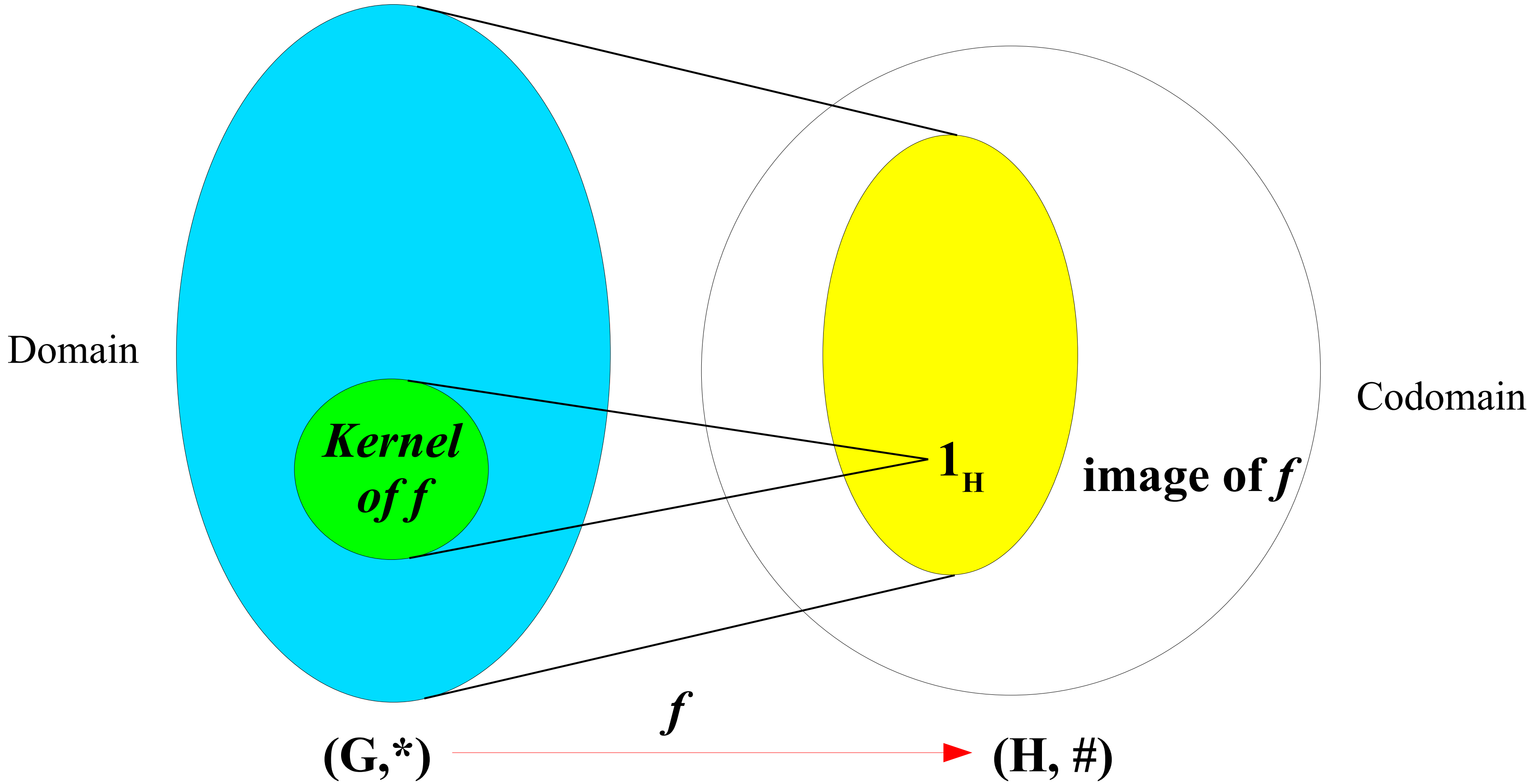
Kernel and image

The **kernel** of the homomorphism f : G → H is the subset of elements of G that is mapped by f on to neutral element of H.

$$\ker f = \{g \in G : f(g) = 1_H\}$$

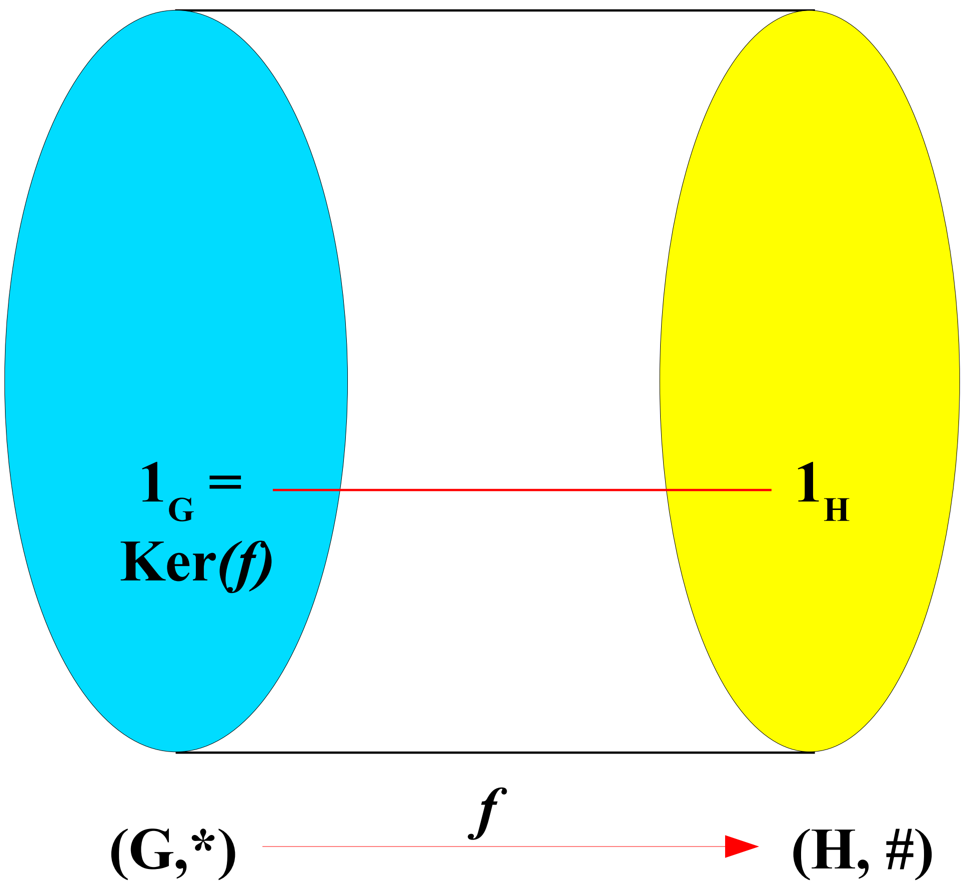
The **image** of the homomorphism f : G → H is the set of elements of G that are mapped by f on H. The image may coincide with the codomain or be a subset of it.



Isomorphism

A 1:1 mapping f : G → H is called an isomorphism. For an isomorphism Ker(f) = 1.

We are especially interested in **isomorphic groups**, which have the same structure but differ only for the labelling of the elements.



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Dimensions of the space and periodicity of the pattern

G^n_m n-dimensional space, m-dimensional periodicity

m = 0:**point groups**；n = m：**space groups**；0 < m < n: **subperiodic groups**

n	m	No. of types of groups	Name
1	0	2	1-dimensional **point groups**
	1	2	Line groups： **1-dimensional space groups**
2	0	10	2-dimensional **point groups**
	1	7	**Frieze groups**
	2	17	Plane groups, wallpaper groups: **2-dimensional space groups**
3	0	32	3-dimensional **point-groups**
	1	75	**Rod groups**
	2	80	**Layer groups**
	3	230	(3-dimensional) **Space groups**

Symmetry group of the crystal

Space group: shows the symmetry of the crystal structure and is obtained as intersection of eigensymmetries that build up the structure.

$$G = \cap_i E_i$$

Translation group: the group containing only the translations of the crystal structure。It is a normal subgroup of the space group G.

$$T \triangleleft G \rightarrow \forall t_j \in T, g_i \in G \; : g_i t_j g_i^{-1} = t_j$$

Point group: shows the morphological symmetry of the crystal as well as the symmetry of its physical properties. It is isomorphic to the factor group of the space group and its translation subgroup.

$$P \approx G/T$$

Some of the definitions will follow

Bravais lattices

- Bravais lattices are sets of (zero-dimensional) points (nodes).
- The lattice **nodes** are (quite obviously…) different from **atoms**. **Warning**: In the literature, this difference is often overlooked!
- The space group of a Bravais lattice is a **Bravais group (B)**.
- The subgroup T of B which contains, apart from the identity, only the translations of B, is the translation subgroup.
- The subgroup H of B obtained by removing all the translations from B is isomorphic to the point group P of the lattice.

B $=\{(\mathbf{W},\mathbf{w})\}$

Projection: B → T $= \{(\mathbf{I},\mathbf{w})\}$

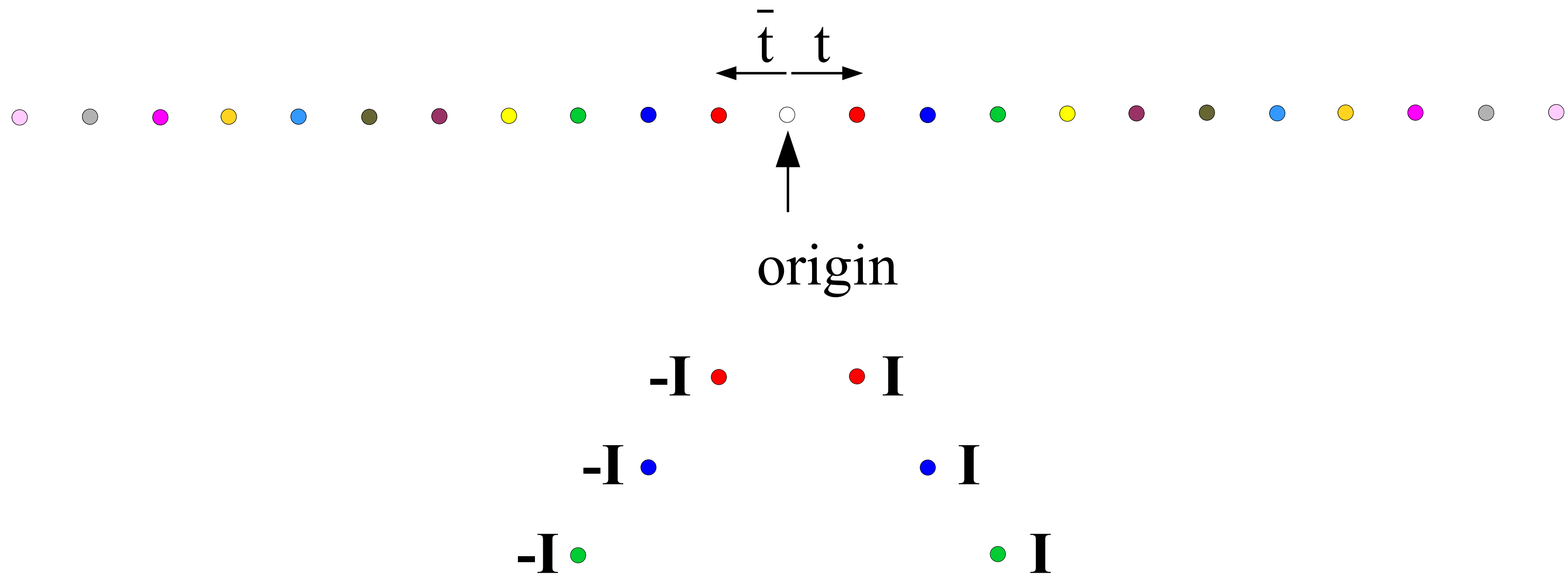
Endomorphism: B → H $= \{(\mathbf{W},\mathbf{0})\}$

Isomorphism: H → P $= \{\mathbf{W}\}$

The minimal point group of a Bravais lattice is built on $\{\mathbf{I},-\mathbf{I}\}$.

$\mathbf{W}$ = $n\times n$ matrix, $\mathbf{I}$ = $n\times n$ identity matrix、$\mathbf{w}$ = $n\times 1$ matrix, $\mathbf{0}$ = $n\times 1$ zero matrix

Bravais lattices



etc….

The minimal point group of a Bravais lattice is built on $\{\mathbf{I},\mathbf{-I}\}$.

1-dimensional space : $x \rightarrow \bar{x}$: **-I** = reflection (or inversion)

2-dimensional space : $xy \rightarrow \overline{xy}$: **-I** = rotation

3-dimensional space : $xyz \rightarrow \overline{xyz}$: **-I** = inversion

etc….

-I in E^n

$$\begin{bmatrix} \bar{1} & & & & \\ & \bar{1} & & & \\ & & \bar{1} & & \\ & & & \dots & \\ & & & & \bar{1} \end{bmatrix} \begin{bmatrix} x \\ y \\ z \\ \dots \\ w \end{bmatrix} \longrightarrow \begin{bmatrix} -x \\ -y \\ -z \\ \dots \\ -w \end{bmatrix}$$

$$\det(-\mathbf{I}_n) = (-1)^n$$

→ Odd-dimensional space: -1
Second kind operation

→ Even-dimensional space: +1
First kind operation

The inversion does not exist in even-dimensional spaces

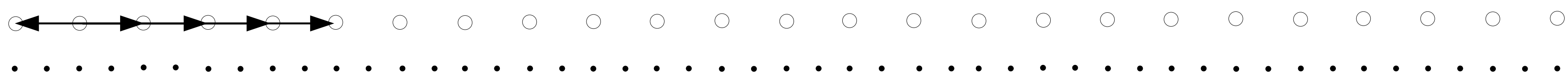
One-dimensional lattices

Symmetry operations

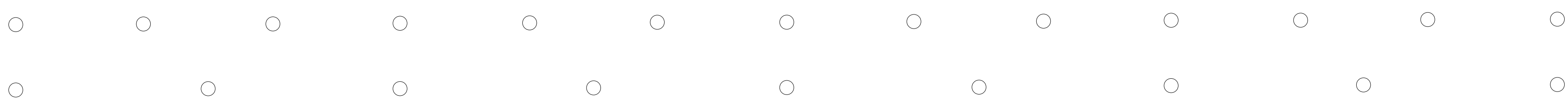
Identity

Translations

Reflections



How many 1D lattices are there? **Infinite!**



etc. etc.

How many ***types of*** 1D lattice are there? **One**

$\mathbf{I} = 1$, $-\mathbf{I} = m \Rightarrow$ point group of a Bravais lattice: $m = \{1,m\}$

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The world in two dimensions

E^2 : the two-dimensional Euclidean space

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Symmetry operations in E^2

Operations that leave invariant all the space (**2D**): the identity
Operations that leave invariant one direction of the space (**1D**): reflections
Operations that leave invariant one point of the space (**0D**): rotations
Operations that do not leave invariant any point of the space: translations

The subspace left invariant (if any) by the symmetry operation has dimensions from 0 to N (= 2 here)

Two independent directions in E^2 $\Rightarrow$ two axes (a, b) and one interaxial angle (γ)

$\mathbf{I} = 1$, $-\mathbf{I} = 2$ $\Rightarrow$ Minimal point group of a Bravais lattice: $2 = \{1,2\}$

Symmetry elements in E^2

First kind operations

Graphic symbol	Hermann-Mauguin symbol	Meaning
⬮	**2**	2-fold rotation point
▲	**3**	3-fold rotation point
◆	**4**	4-fold rotation point
⬢	**6**	6-fold rotation point

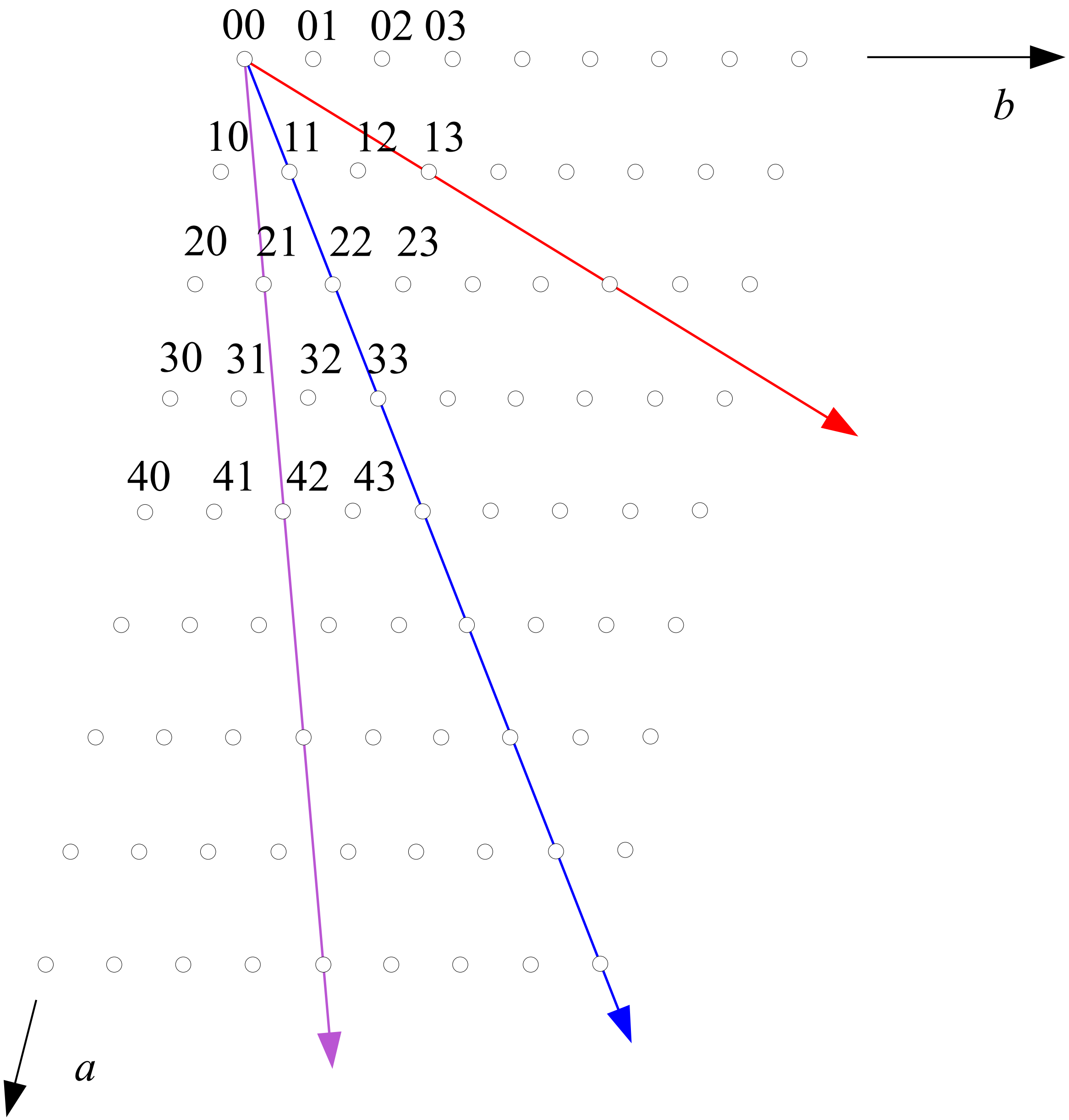
Second kind operation

Graphic symbol	Hermann-Mauguin symbol	Meaning
│	***m***	Reflection line (mirror)

Operations obtained as combination with a translation are introduced later

The orientation in space of a reflection line is always expressed with respect to the lattice direction to which it is perpendicular

Lattice node coordinates *uv*, lattice direction indices [*uv*]



a axis? [10]

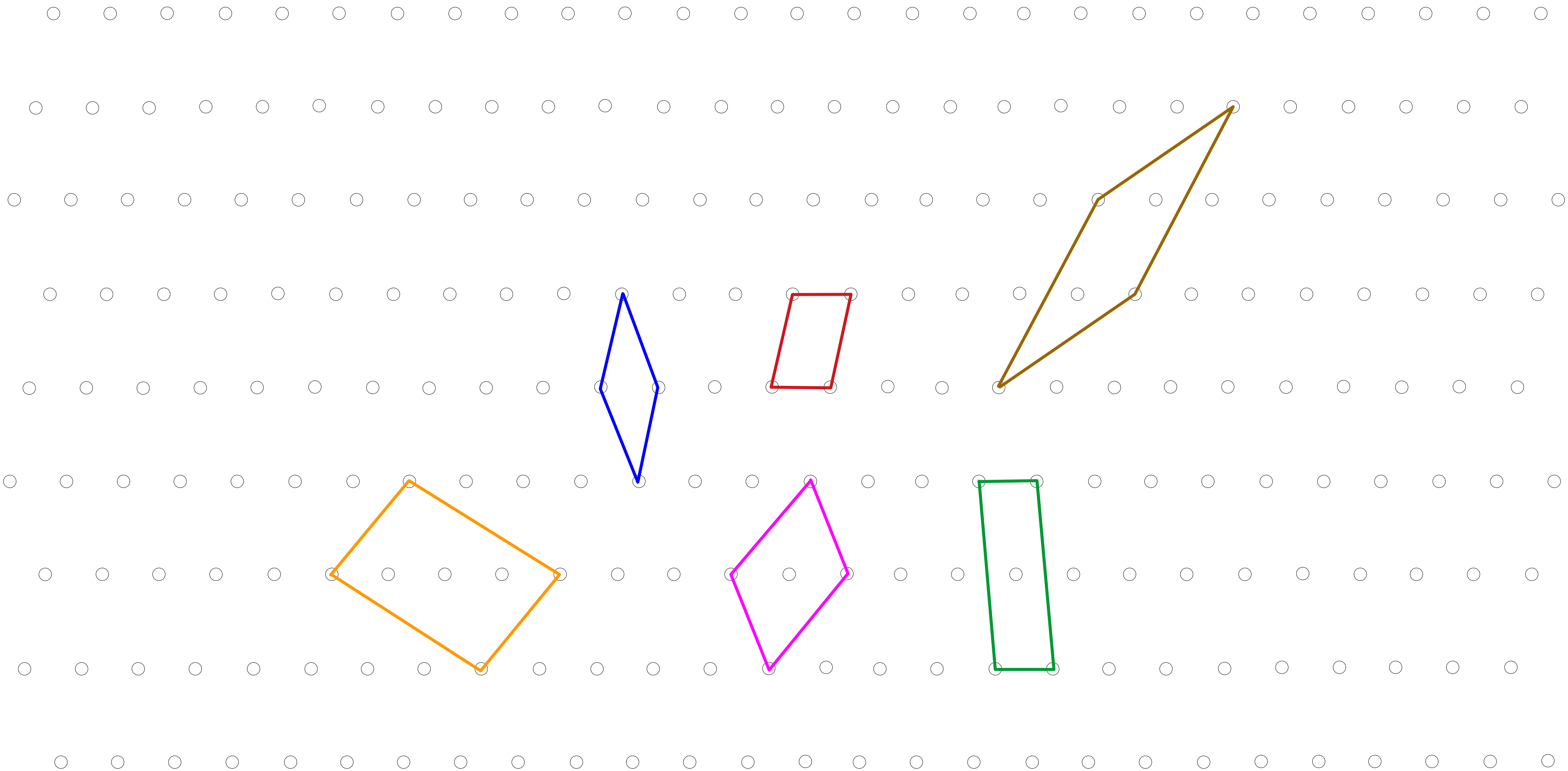
b axis? [01]

(blue line) [11]

(red line) [13]

~~[42]~~ direction ? [21]

Choice of the unit cell



$t(1,0)$, $t(0,1)$

$t(1,0)$, $t(0,1)$, $t(\tfrac{1}{2},\tfrac{1}{2})$

$t(1,0)$, $t(0,1)$, $t(\tfrac{2}{3},\tfrac{1}{3})$, $t(\tfrac{1}{3},\tfrac{2}{3})$

$t(1,0)$, $t(0,1)$, $t(\tfrac{3}{4},\tfrac{1}{4})$, $t(\tfrac{1}{2},\tfrac{1}{2})$, $t(\tfrac{1}{4},\tfrac{3}{4})$

Change of reference

$\begin{pmatrix} 1 & \bar{1} \\ 0 & 1 \end{pmatrix}$

Determ.: 1

$\begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}$

Determ.: 1

$\begin{pmatrix} 2 & 0 \\ \bar{1} & 1 \end{pmatrix}$

Determ.: 2

$\begin{pmatrix} 1/2 & 0 \\ 1/2 & 1 \end{pmatrix}$

Determ.: ½

$\begin{pmatrix} 1 & \bar{1} \\ 1 & 1 \end{pmatrix}$

Determ.: 2

$\begin{pmatrix} 1/2 & 1/2 \\ \bar{1}/2 & 1/2 \end{pmatrix}$

Determ.: ½

$\begin{pmatrix} 2 & 0 \\ 1 & 1 \end{pmatrix}$

Determ.: 2

$\begin{pmatrix} 1/2 & 0 \\ \bar{1}/2 & 1 \end{pmatrix}$

Determ.: ½

$\begin{pmatrix} 1 & 1 \\ \bar{1} & 1 \end{pmatrix}$

Determ.: 2

$\begin{pmatrix} 1/2 & \bar{1}/2 \\ 1/2 & 1/2 \end{pmatrix}$

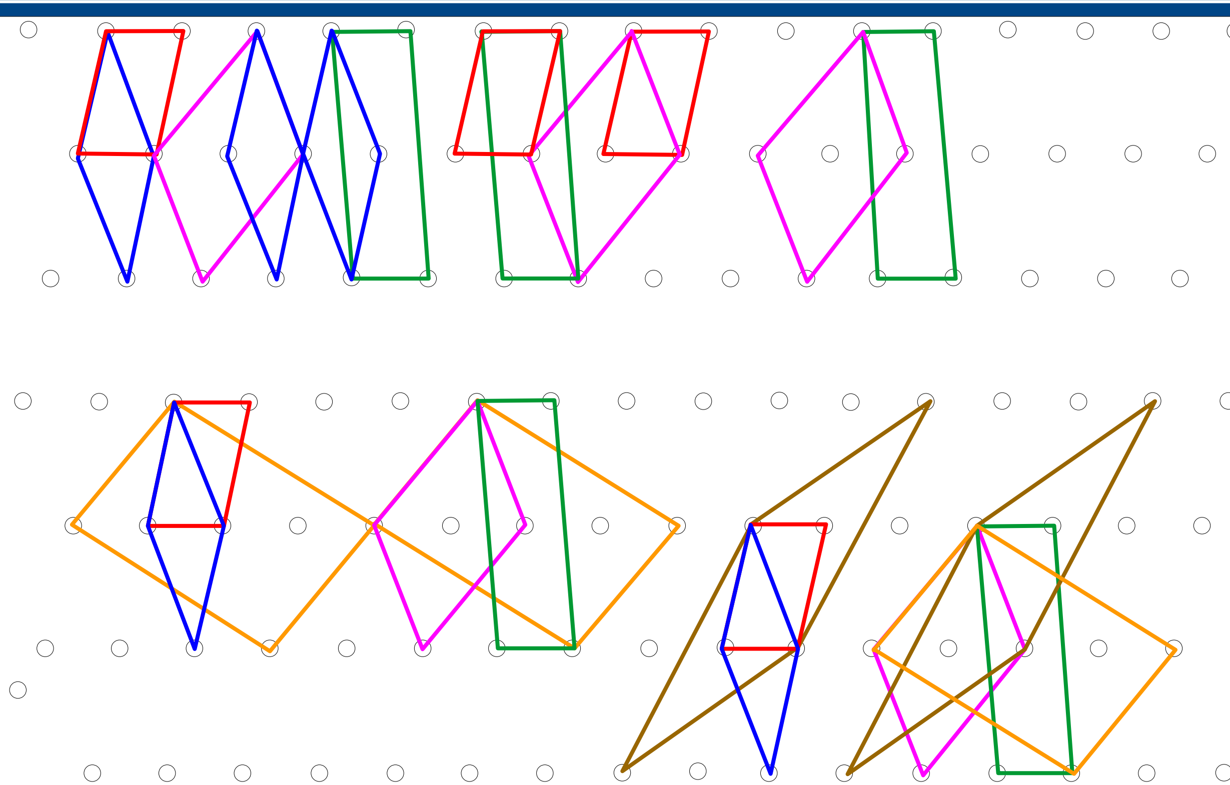
Determ.: ½

$\begin{pmatrix} 1/2 & 1/2 \\ \bar{3}/2 & 1/2 \end{pmatrix}$

Determ.: 1

$\begin{pmatrix} 1/2 & \bar{1}/2 \\ 3/2 & 1/2 \end{pmatrix}$

Determ.: 1



$\begin{pmatrix} 1 & \bar{1}/2 \\ \bar{2} & 5/2 \end{pmatrix}$

Determ.: 1.5

$\begin{pmatrix} 5/3 & 1/3 \\ 4/3 & 2/3 \end{pmatrix}$

Determ.: ⅔

$\begin{pmatrix} 3/2 & \bar{3}/2 \\ 1/2 & 1/2 \end{pmatrix}$

Determ.: 1.5

$\begin{pmatrix} 1/3 & 1 \\ \bar{1}/3 & 1 \end{pmatrix}$

Determ.: ⅔

$\begin{pmatrix} 7/4 & \bar{5}/4 \\ 1/4 & 1/4 \end{pmatrix}$

Determ.: ¾

$\begin{pmatrix} 1/3 & 5/3 \\ \bar{1}/3 & 7/3 \end{pmatrix}$

Determ.: 4/3

$\begin{pmatrix} 2 & \bar{2} \\ \bar{1} & 3 \end{pmatrix}$

Determ.: 4

$\begin{pmatrix} 3/4 & 1/2 \\ 1/4 & 1/2 \end{pmatrix}$

Determ.: ¼

$\begin{pmatrix} 1/2 & 1/2 \\ \bar{3}/2 & 5/2 \end{pmatrix}$

Determ.: 2

$\begin{pmatrix} 5/4 & \bar{1}/4 \\ 3/4 & 1/4 \end{pmatrix}$

Determ.: ½

$\begin{pmatrix} 3 & \bar{3} \\ \bar{1} & 2 \end{pmatrix}$

Determ.: 3

$\begin{pmatrix} 2/3 & 1 \\ 1/3 & 1 \end{pmatrix}$

Determ.: ⅓

$\begin{pmatrix} 1 & 1 \\ \bar{1} & 3 \end{pmatrix}$

Determ.: 4

$\begin{pmatrix} 3/4 & \bar{1}/4 \\ 1/4 & 1/4 \end{pmatrix}$

Determ.: ½

$\begin{pmatrix} 1 & \bar{1} \\ 0 & 2 \end{pmatrix}$

Determ.: 2

$\begin{pmatrix} 1 & 1/2 \\ 0 & 1/2 \end{pmatrix}$

Determ.: ½

$\begin{pmatrix} 2 & \bar{1} \\ \bar{1} & 2 \end{pmatrix}$

Determ.: 3

$\begin{pmatrix} 2/3 & 1/3 \\ 1/3 & 2/3 \end{pmatrix}$

Determ.: ⅓

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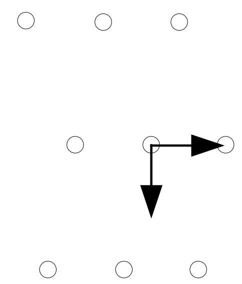
Change of the unit cell (cont.)

t(1,0), t(0,1) : **primitive** (*p*) unit cell

t(1,0), t(0,1), t(½,½) : **centred** (*c*) unit cell



Cartesian (orthonormal) cell:
unsuitable (in general)

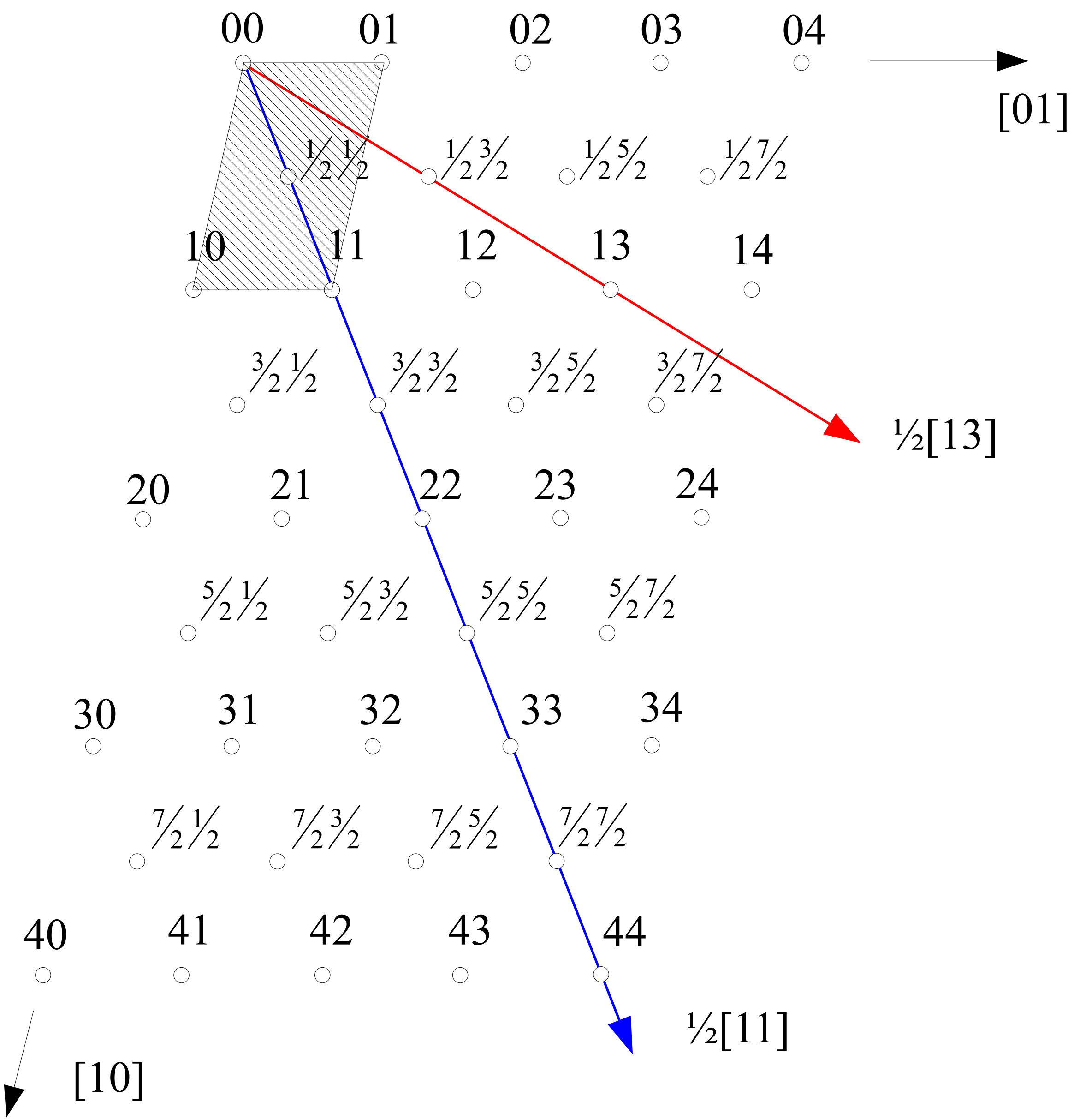
Conventional unit cell

1. Edges of the cell are parallel to the symmetry directions of the lattice (if any);
2. If more than one unit cell satisfies the above condition, the smallest one is the conventional cell.

Reduced cell (Lagrange-Gauss reduction)

1. Basis vectors correspond to the shortest lattice translation vectors;
2. $||\mathbf{a}|| \leq ||\mathbf{b}||$, $||\mathbf{b}|| \leq ||\mathbf{b}+q\mathbf{a}||$, q any integer. For q = ±1, this condition means that the sides of the unit cell are not longer than its diagonals.

Lattice node coordinates *uv*, lattice direction indices [*uv*]



Exercise:
Find the lattice symmetry and ***then*** choose a suitable unit cell

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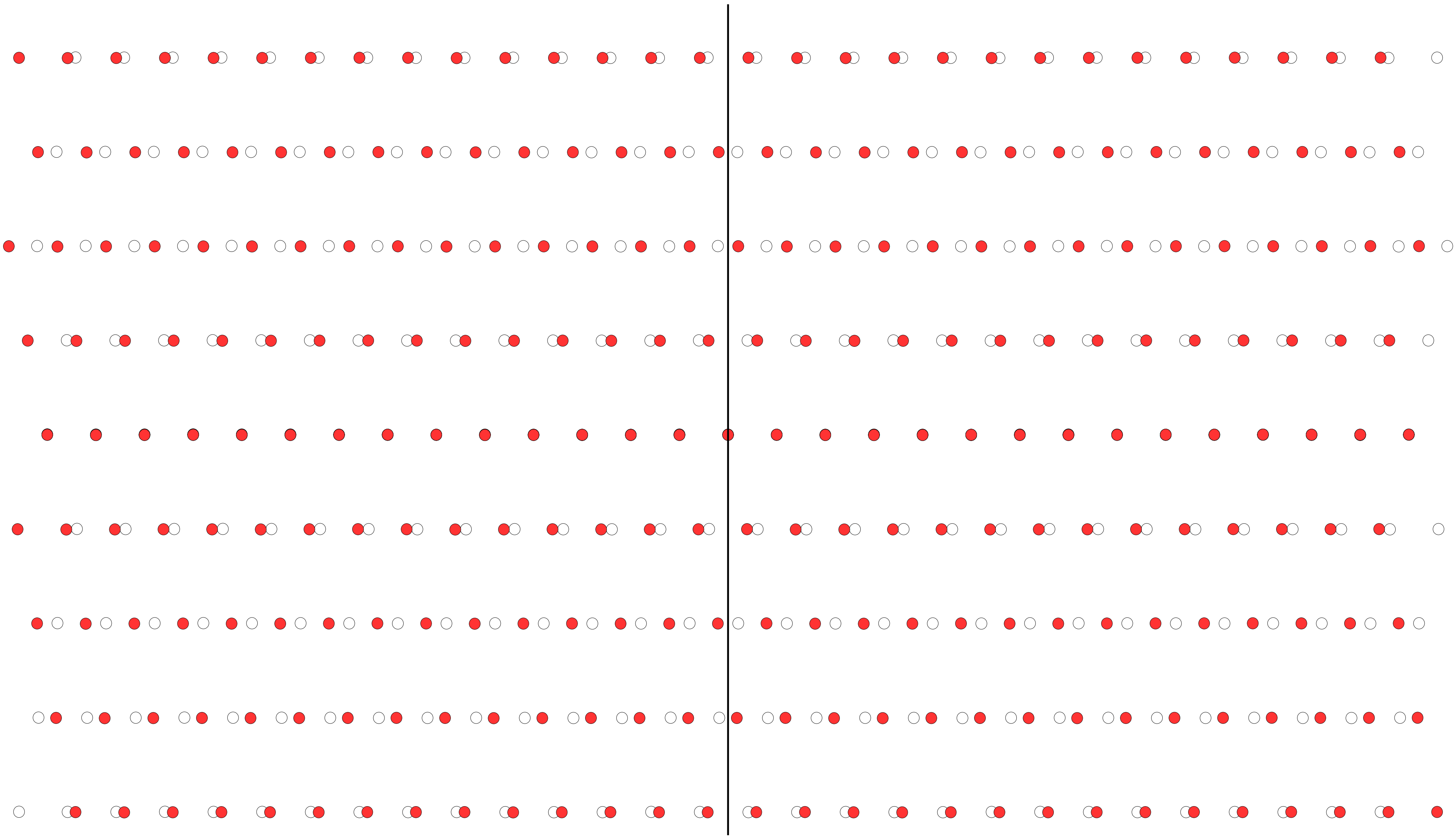

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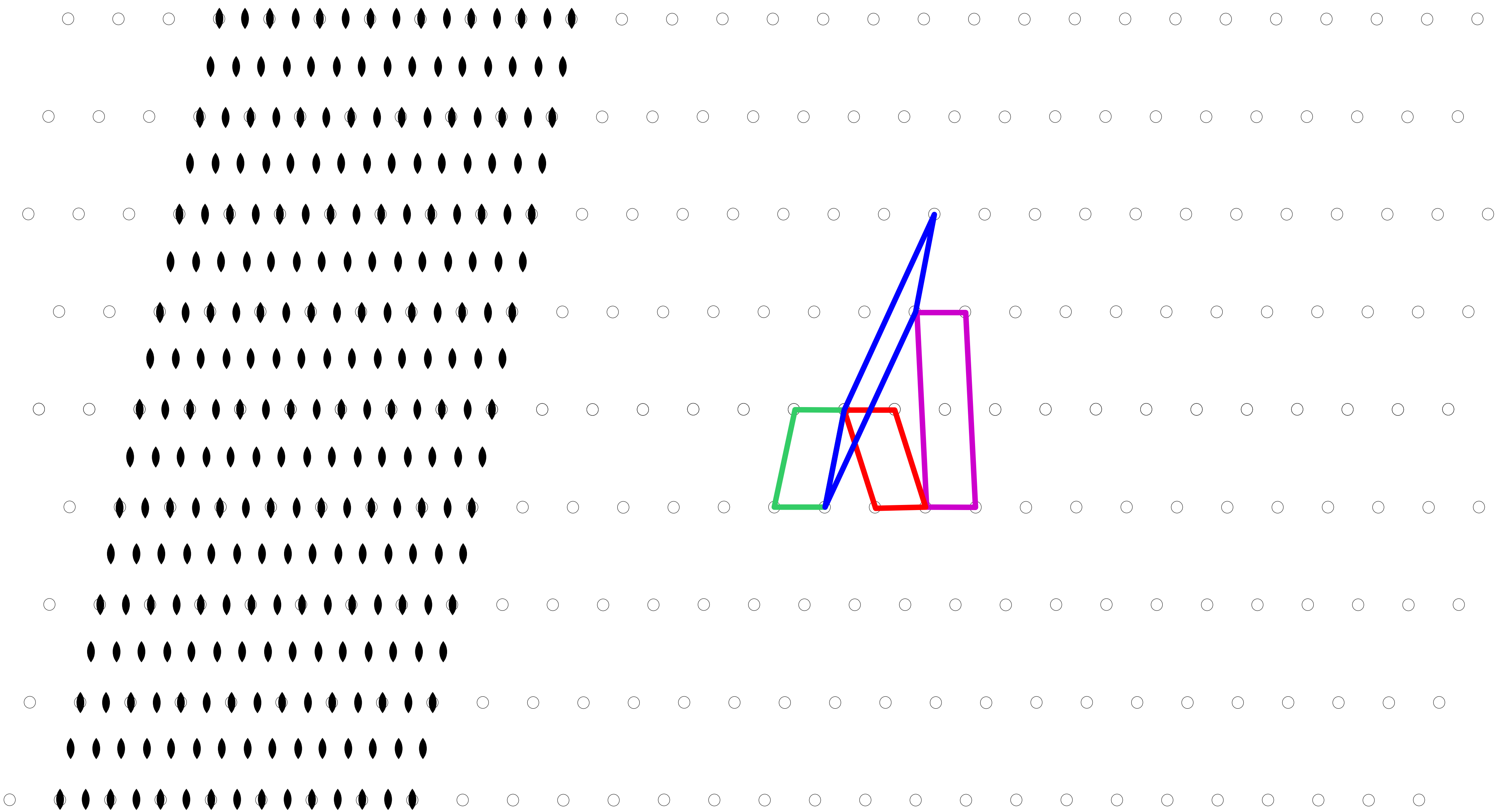
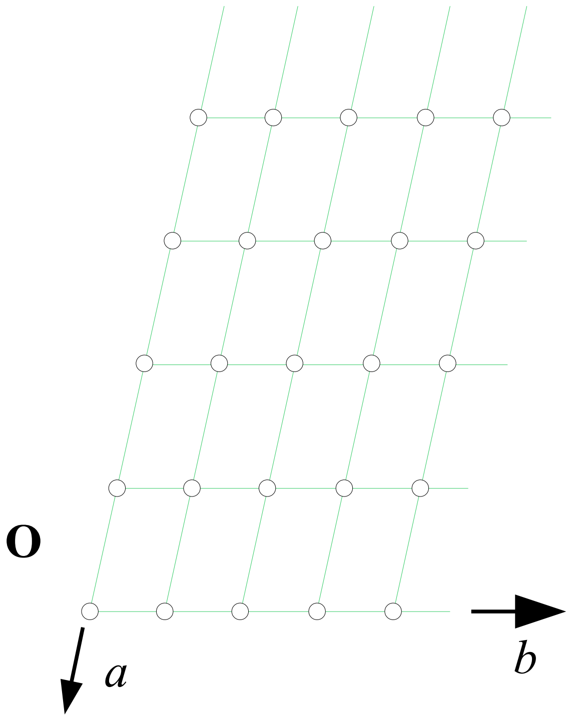
Exercise:
Find the lattice symmetry and ***then*** choose a suitable unit cell



Exercise:
Find the lattice symmetry and *then* choose a suitable unit cell



no symmetry direction for this lattice
point group of the lattice: 2 = {**I**, **-I**}
no symmetry restriction on the cell parameters:
a; b; γ

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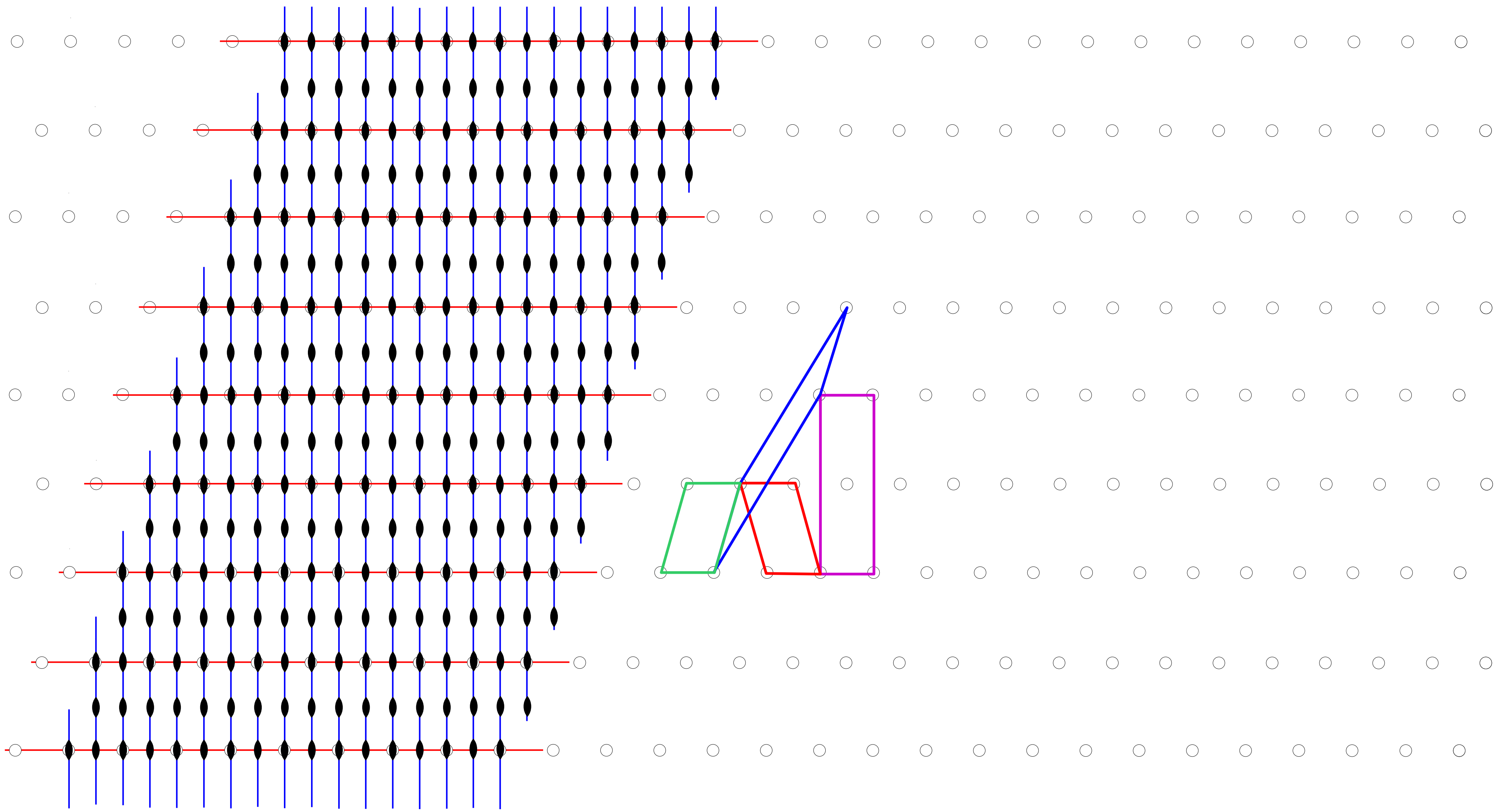
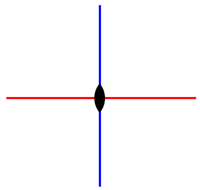
Exercise:
Find the lattice symmetry and ***then*** choose a suitable unit cell

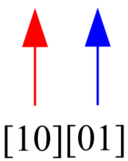


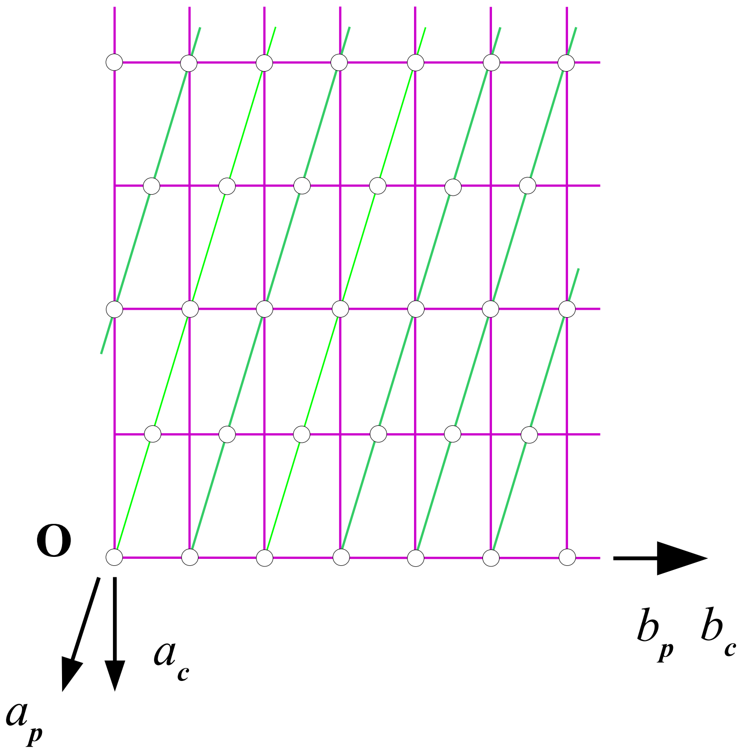
Exercise:
Find the lattice symmetry and ***then*** choose a suitable unit cell

two symmetry directions for this lattice, that are taken as axes *a* and *b*

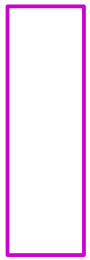


point group of the lattice: 2 *m* *m*

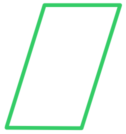




symmetry restriction on the cell parameters:
a; b; $\gamma = 90^{\circ}$



Conventional unit cell



Primitive unit cell

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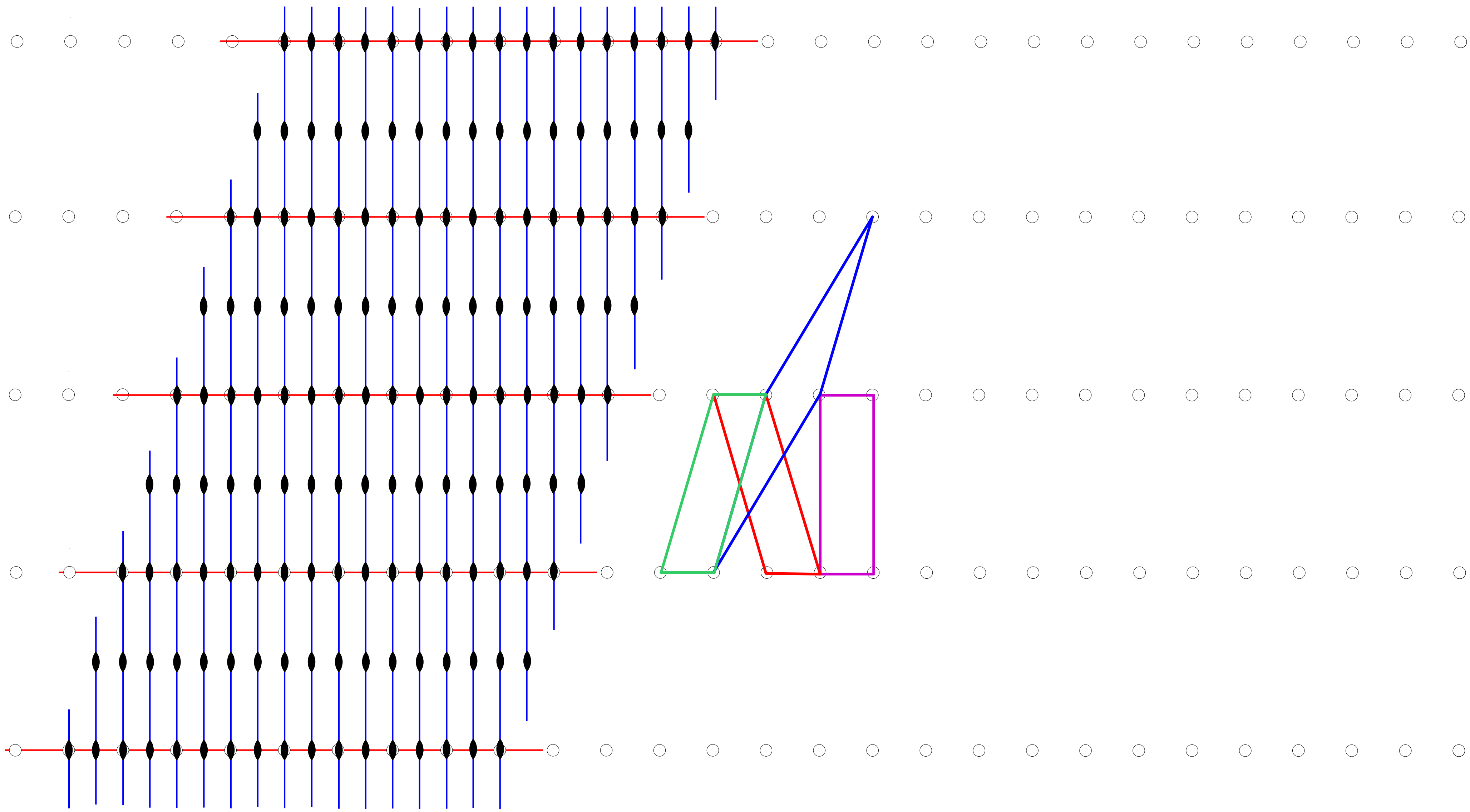
Exercise:
Find the lattice symmetry and ***then*** choose a suitable unit cell



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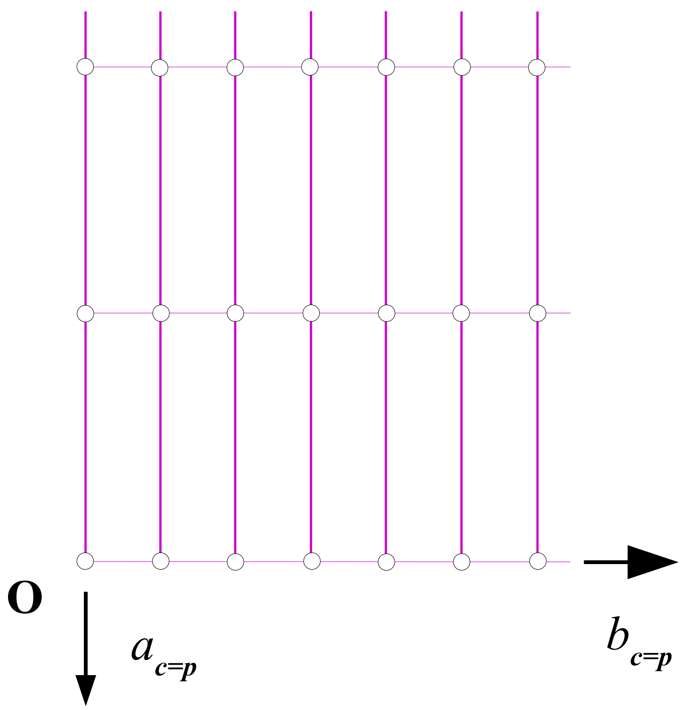
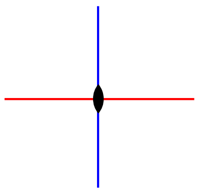
Exercise:
Find the lattice symmetry and ***then*** choose a suitable unit cell



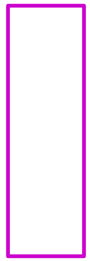
two symmetry directions for this lattice, that are taken as axes *a* and *b*



point group of the lattice: 2 *m* *m*

[10][01]

symmetry restriction on the cell parameters:
a; *b*; $\gamma = 90^\circ$



Conventional (primitive) unit cell

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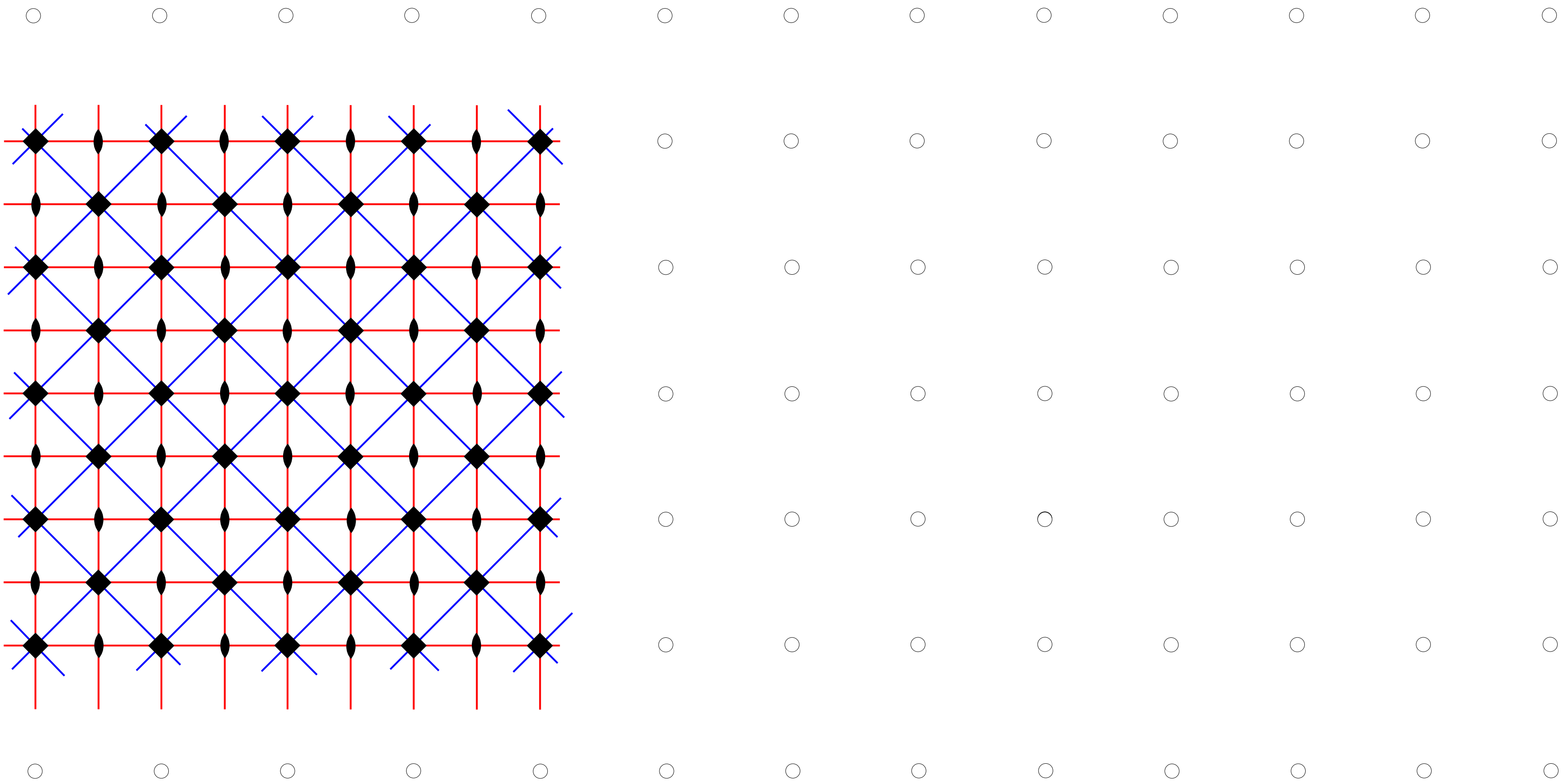
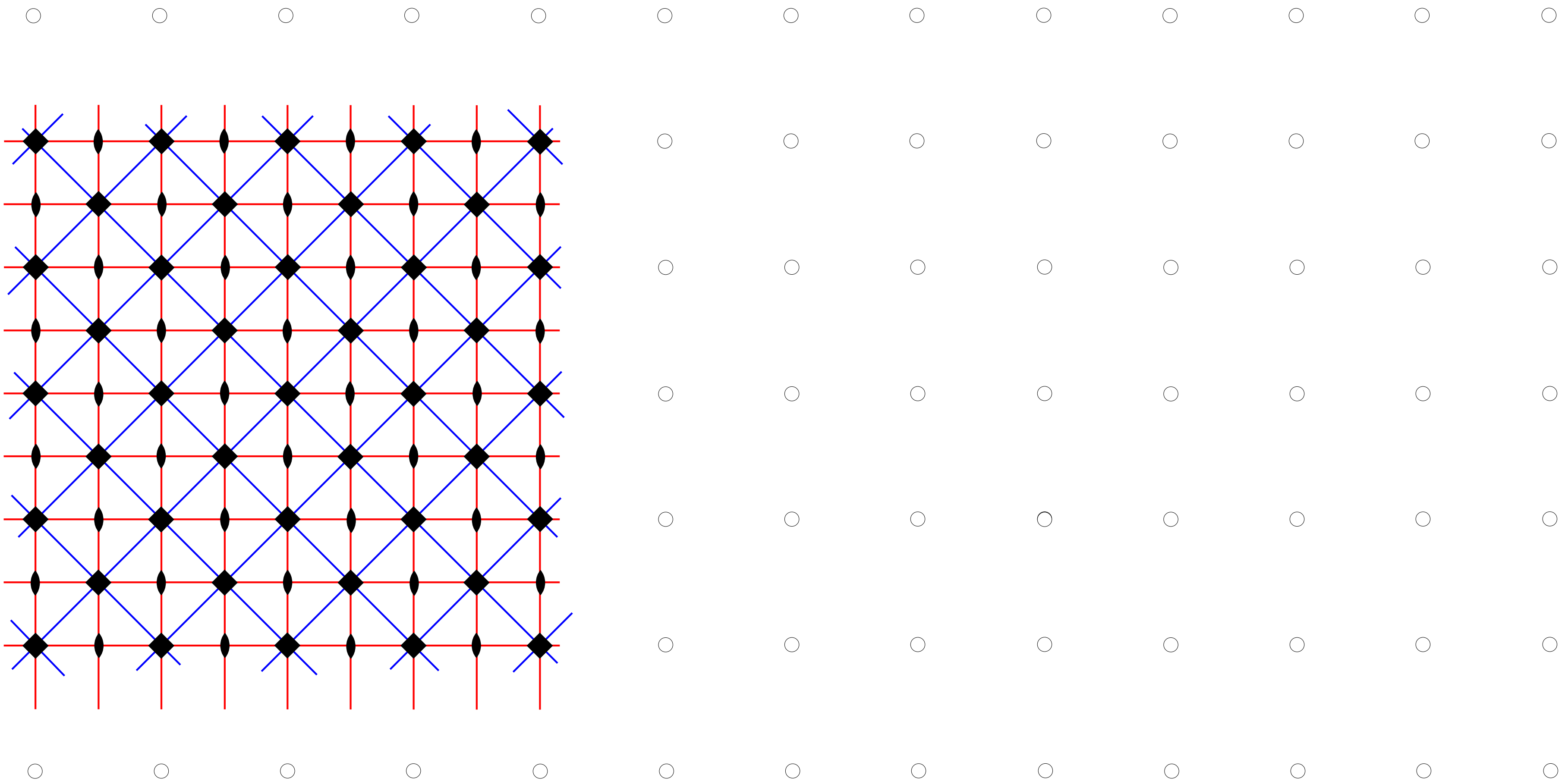
Exercise:
Find the lattice symmetry and ***then*** choose a suitable unit cell

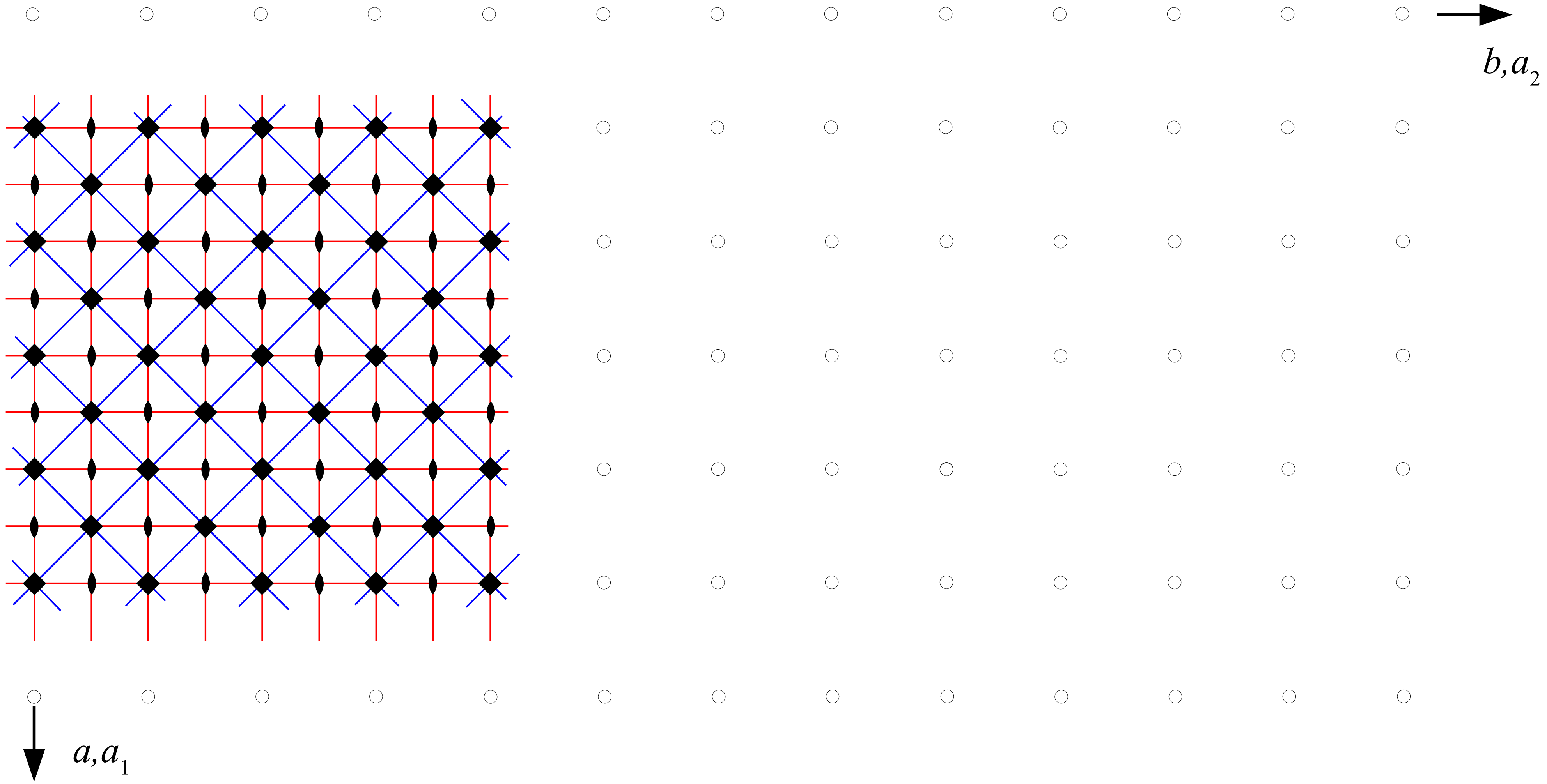


Exercise:
Find the lattice symmetry and ***then*** choose a suitable unit cell



This lattice has four symmetry directions. Those corresponding to the shortest period are taken as axes a_1 and a_2.

Exercise:
Find the lattice symmetry and *then* choose a suitable unit cell



This lattice has four symmetry directions. Those corresponding to the shortest period are taken as axes a_1 and a_2.

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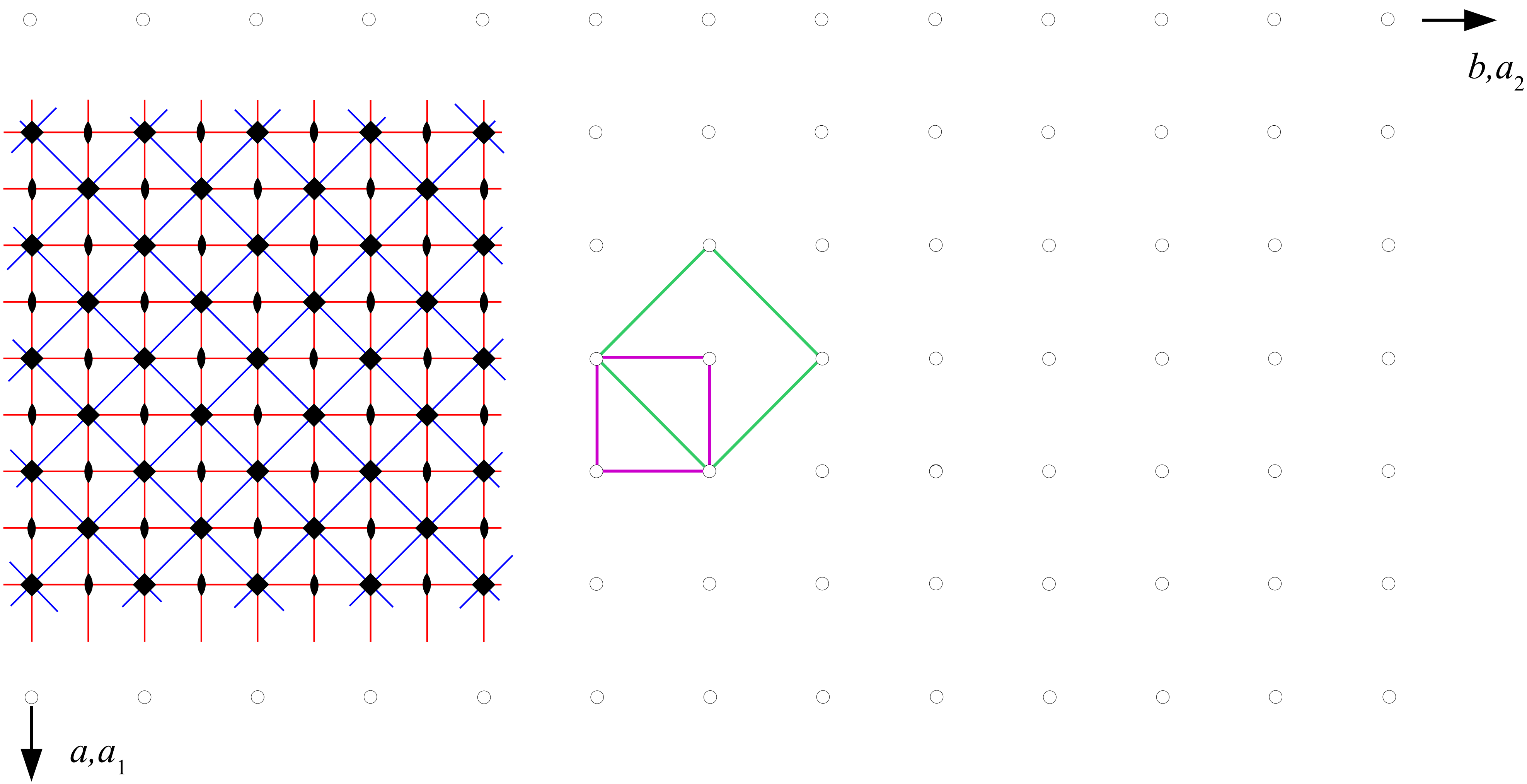
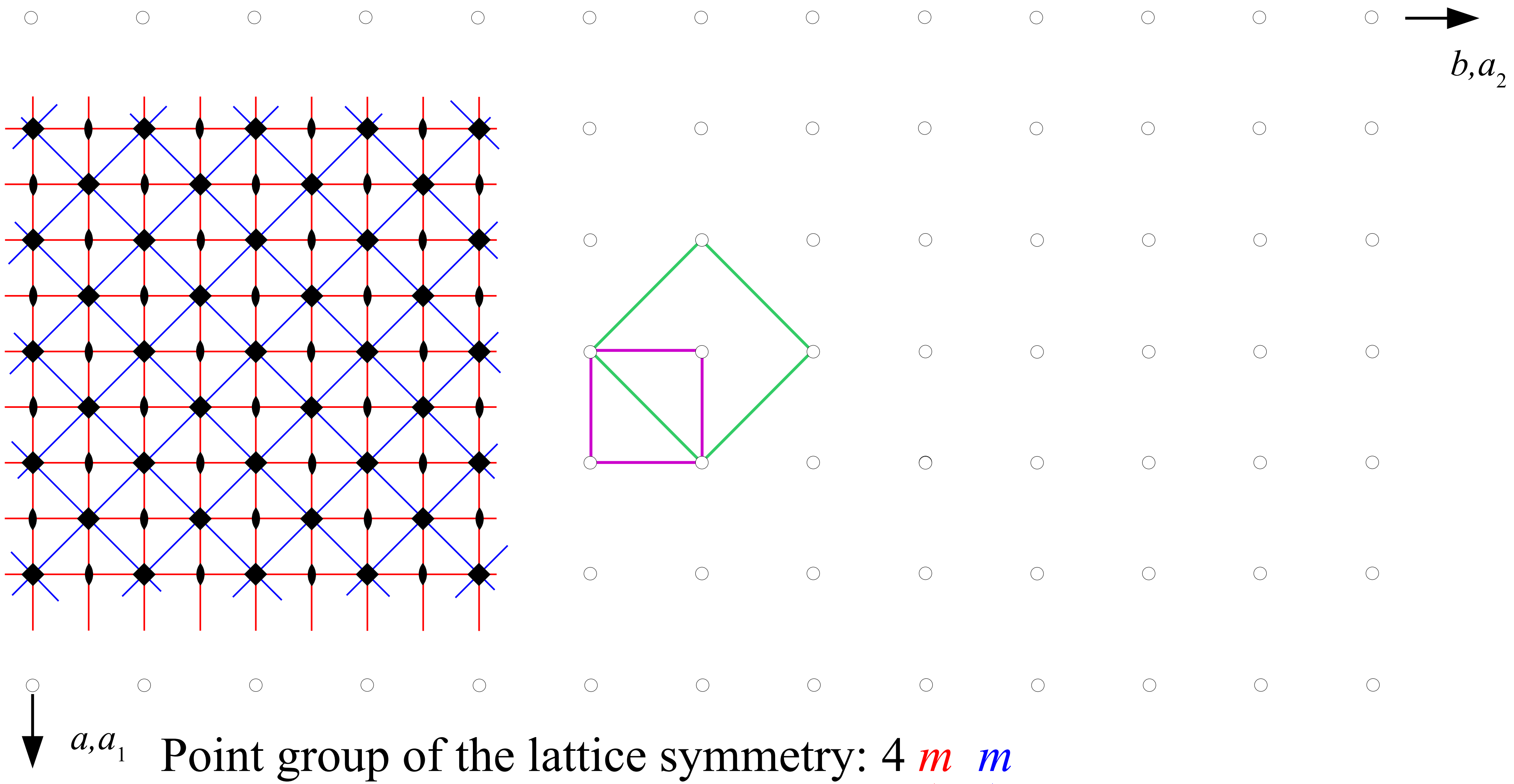
Exercise:
Find the lattice symmetry and *then* choose a suitable unit cell



This lattice has four symmetry directions. Those corresponding to the shortest period are taken as axes a_1 and a_2.

Exercise:
Find the lattice symmetry and *then* choose a suitable unit cell



Point group of the lattice symmetry: 4 *m* *m*

⟨10⟩ ⟨1$\bar{1}$⟩

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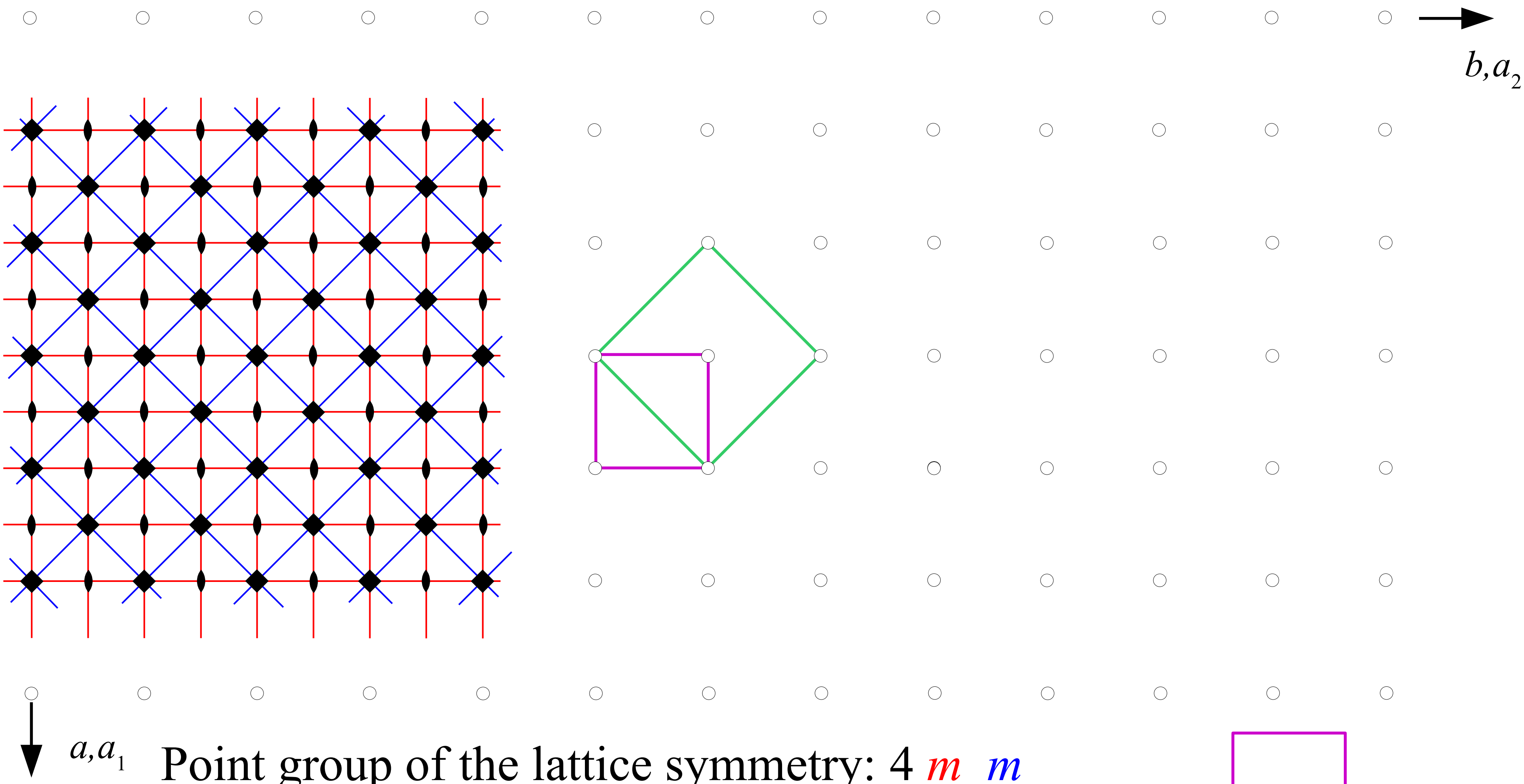
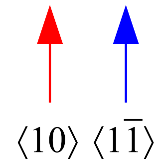
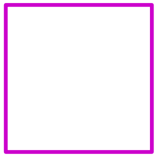
Exercise:
Find the lattice symmetry and ***then*** choose a suitable unit cell



Point group of the lattice symmetry: 4 *m* *m*





p cell (conventional)

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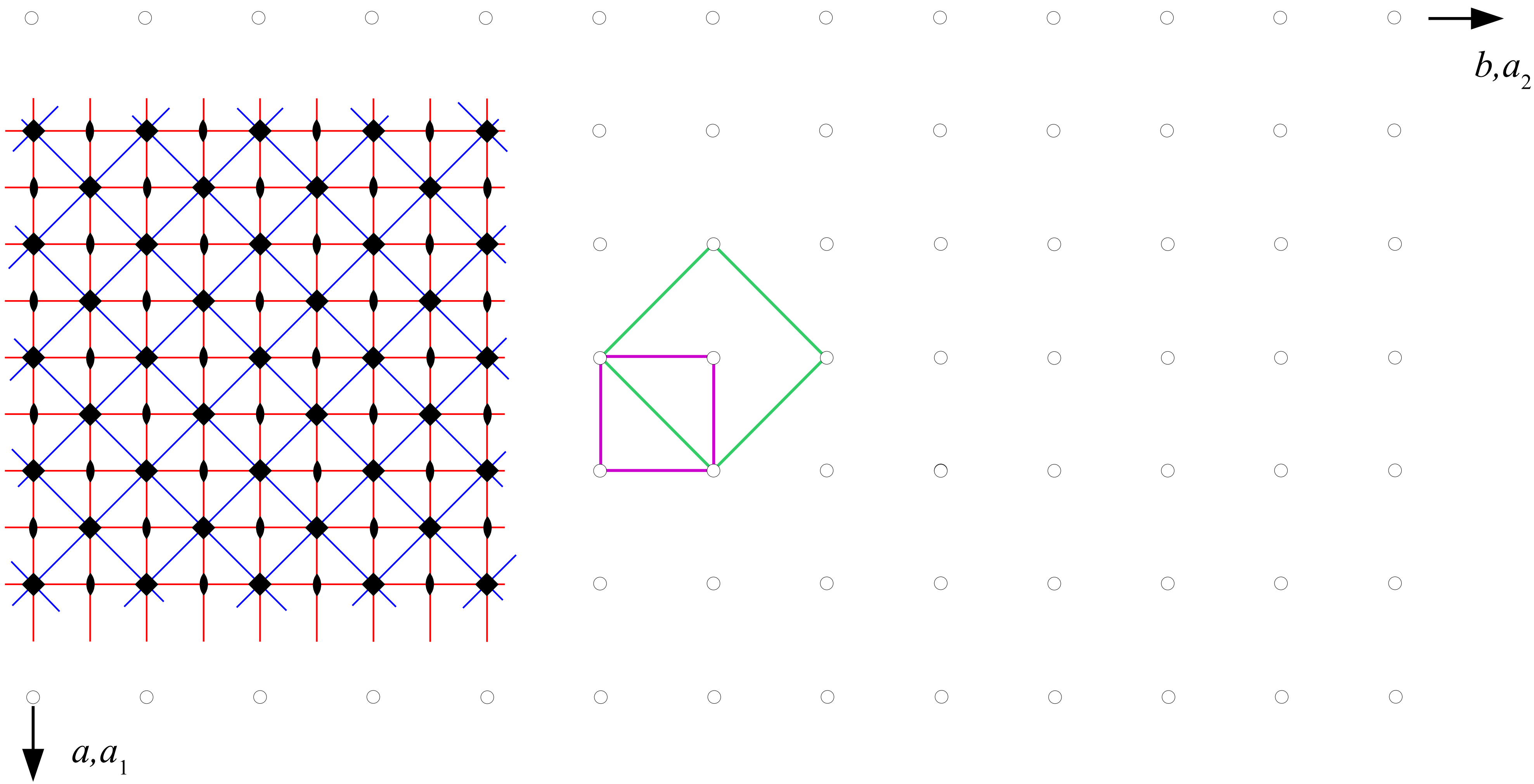
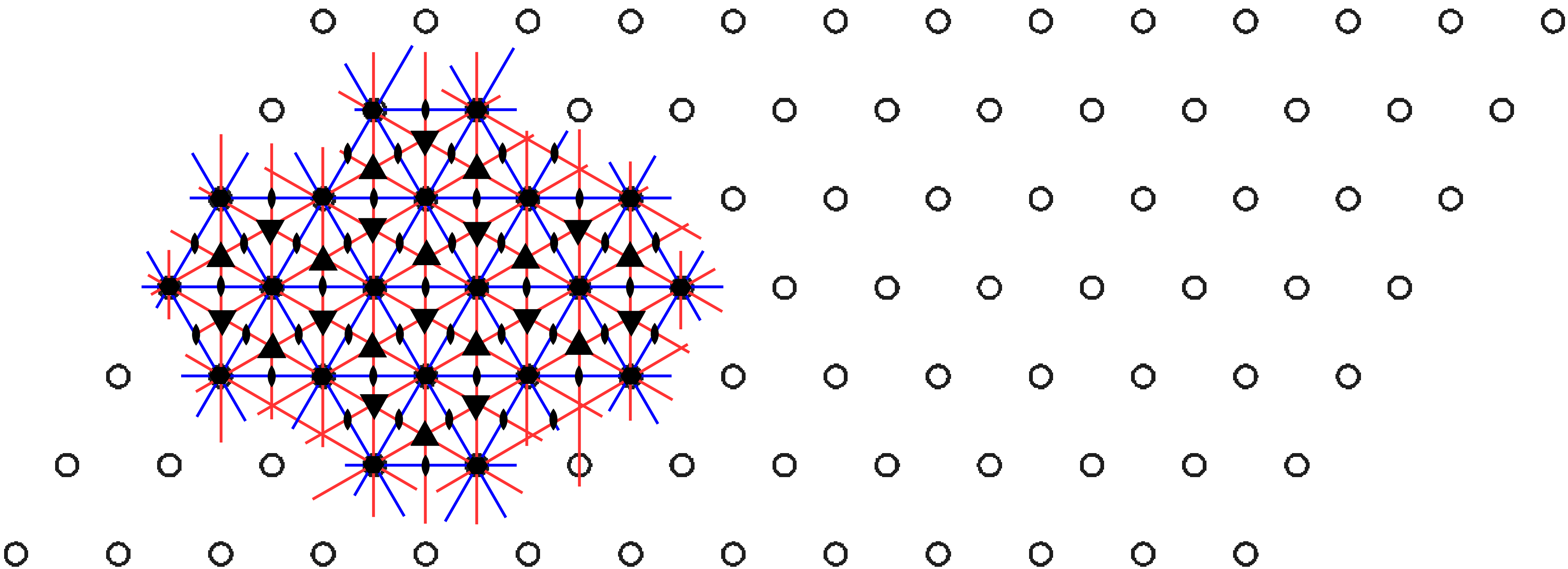
Exercise:
Find the lattice symmetry and ***then*** choose a suitable unit cell



Restrictions on cell parameters: $a = b$; $\gamma = 90°$

Exercise:
Find the lattice symmetry and ***then*** choose a suitable unit cell



This lattice has six symmetry directions. Two among the three corresponding to the shortest period are taken as axes a_1 et a_2.

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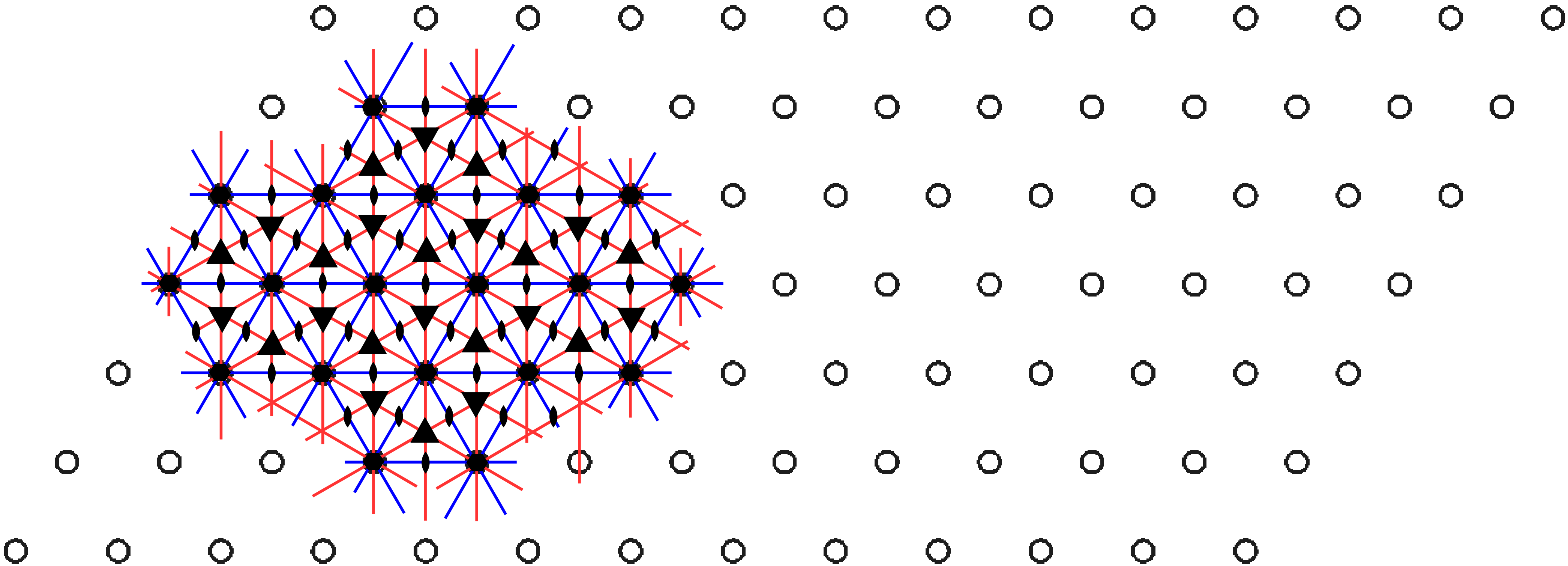
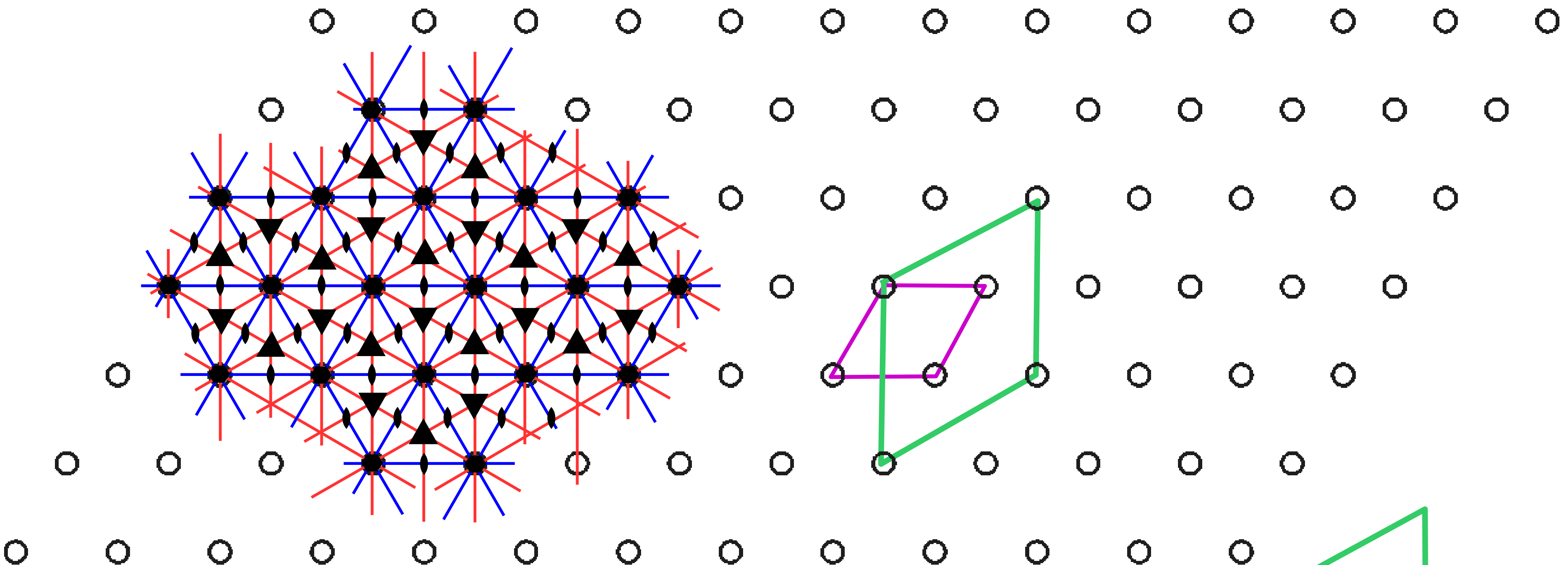
Exercise:
Find the lattice symmetry and ***then*** choose a suitable unit cell



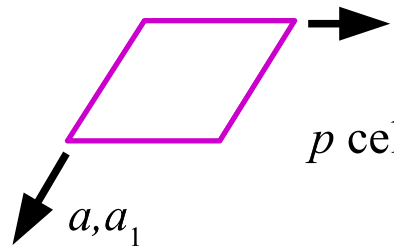
Exercise:
Find the lattice symmetry and *then* choose a suitable unit cell



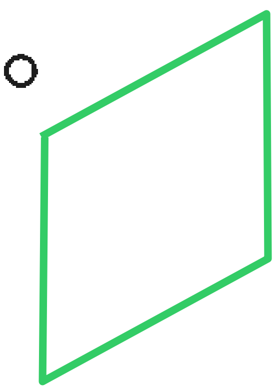
Point group of the lattice:

6 m m

⟨10⟩ ⟨1$\bar{1}$⟩



p cell (conventional)



h cell (triple)

Restrictions on the cell parameters: $a = b$; $\gamma = 120°$

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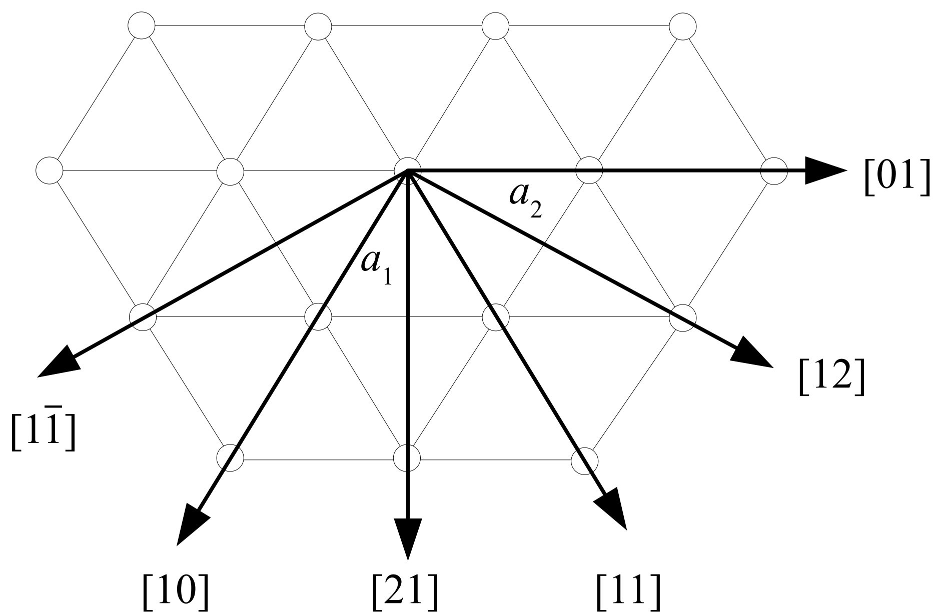
Direction indices [*uv*] in the hexagonal lattice of E^2



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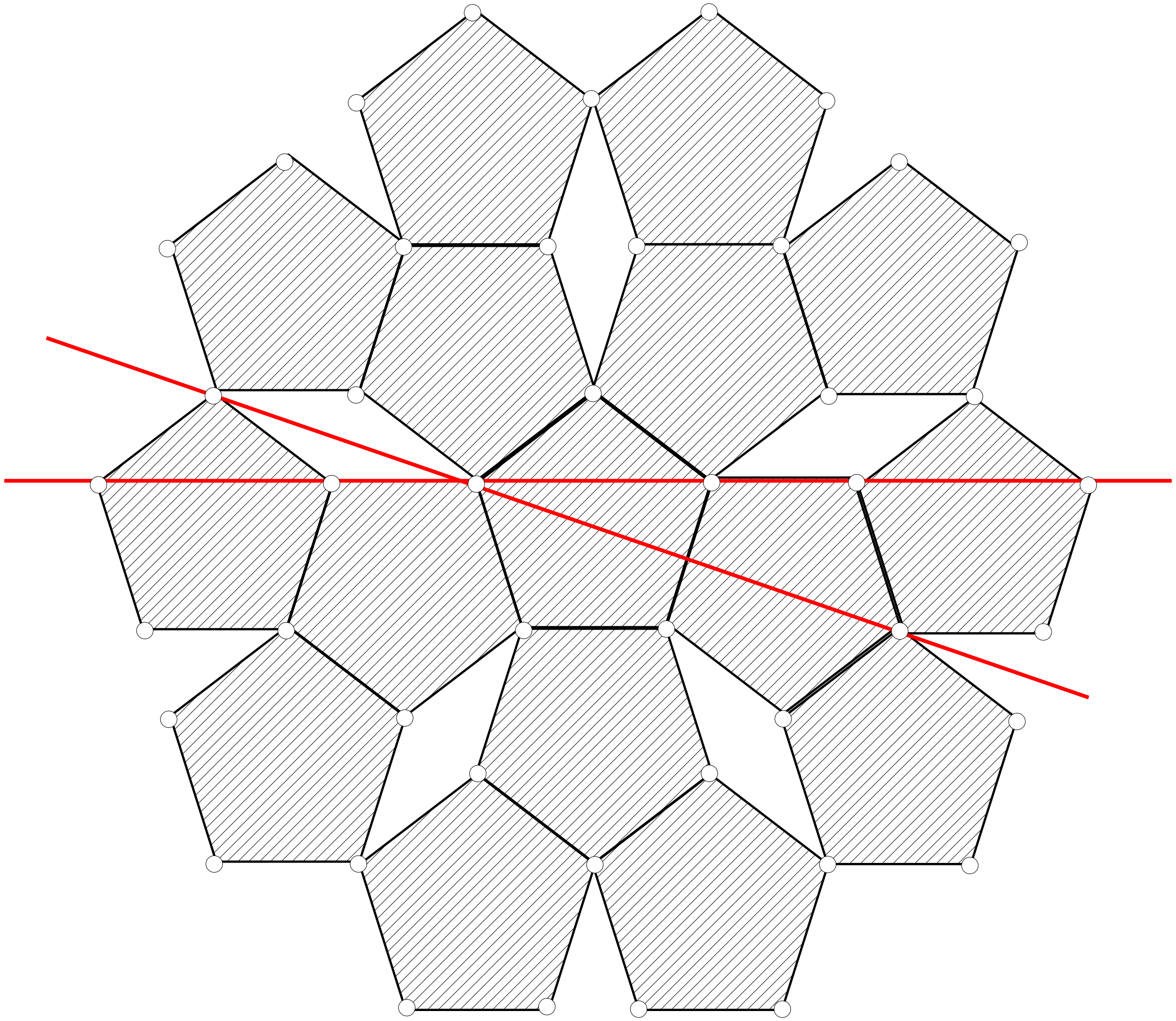
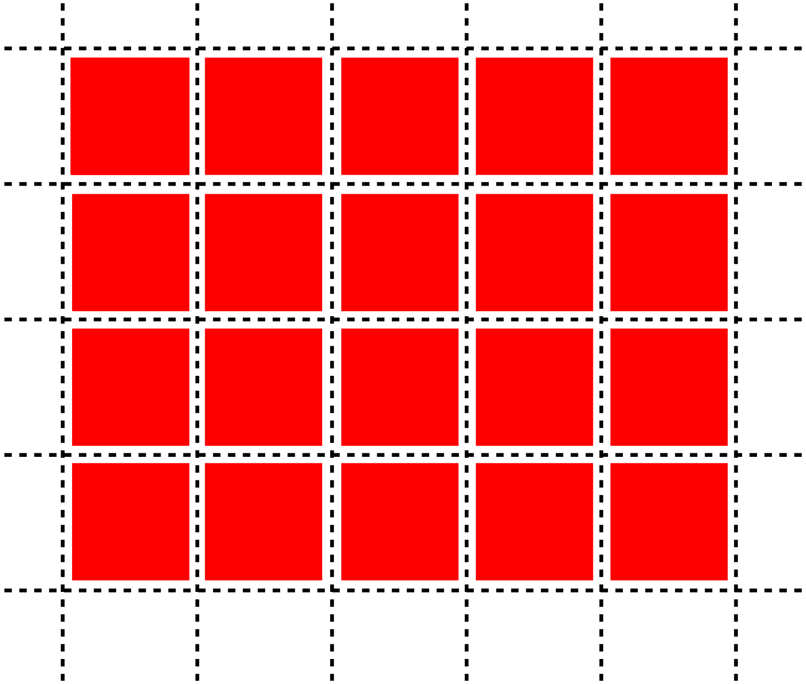
Why not 5, then?



Crystal patterns in 2D

The concept of holohedry



Lattice

« Object » (content of the unit cell)

Pattern

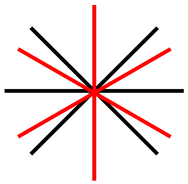
Symmetry of the lattice : S_L = 4*mm*

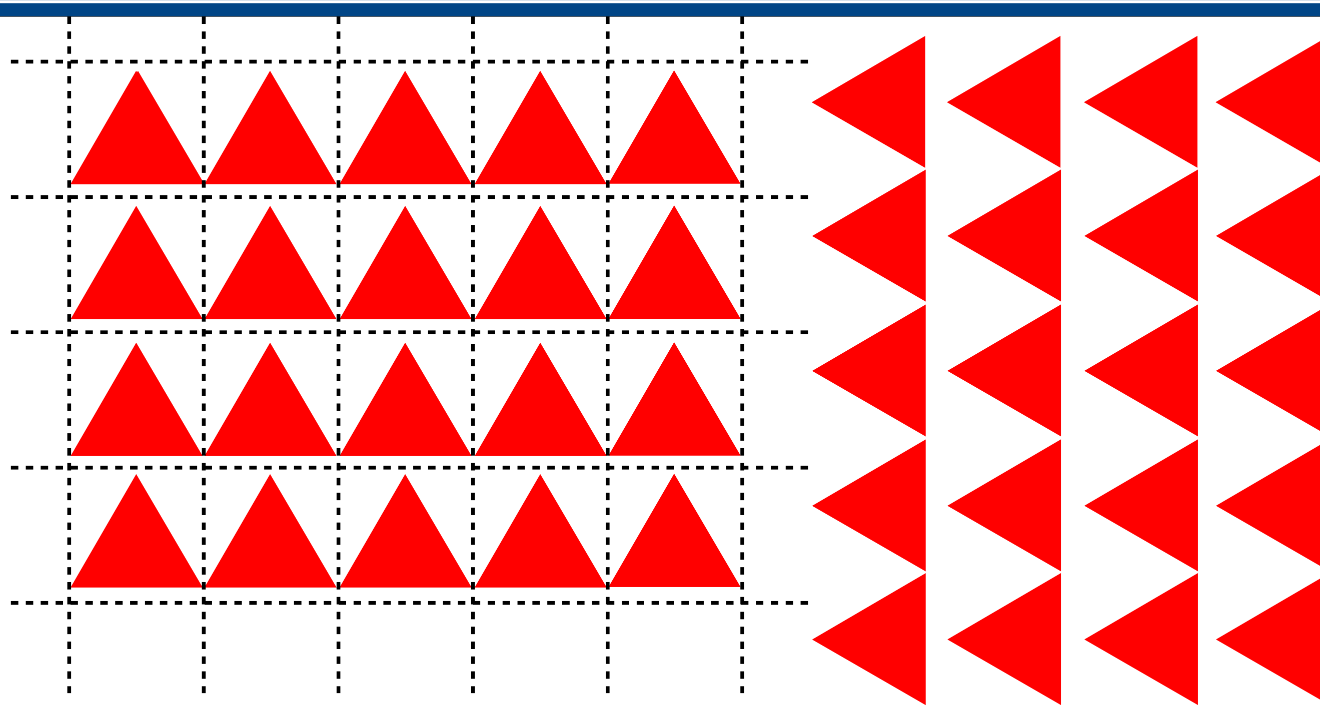
Symmetry of the object : S_o = 4*mm*

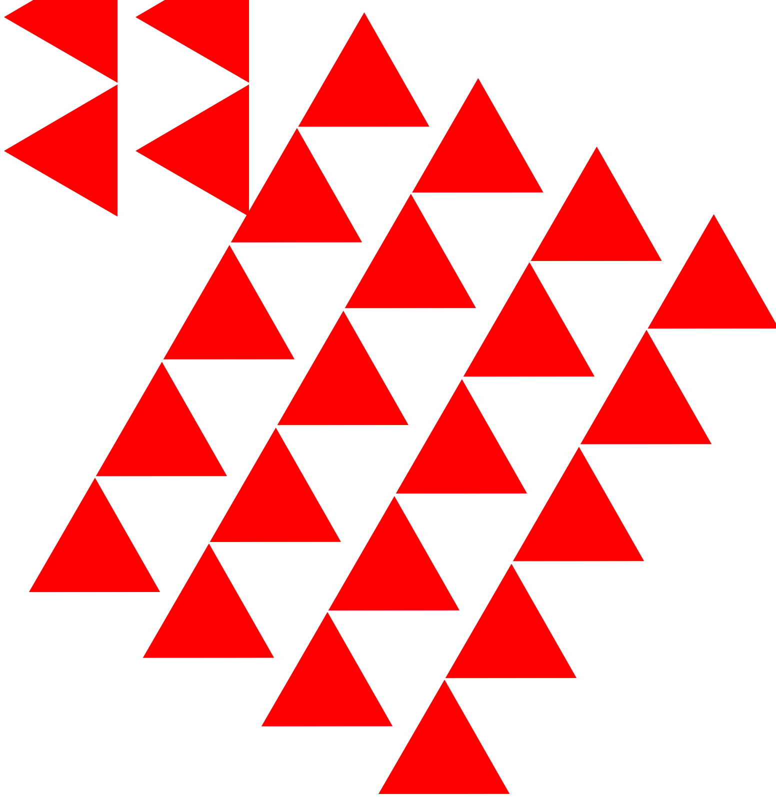
Symmetry of the pattern : S_p = 4*mm*

$S_p = S_L$: holohedry

The concept of holohedry







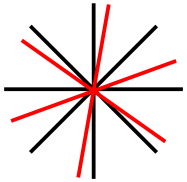
Symmetry of the lattice: $S_L = 4mm$

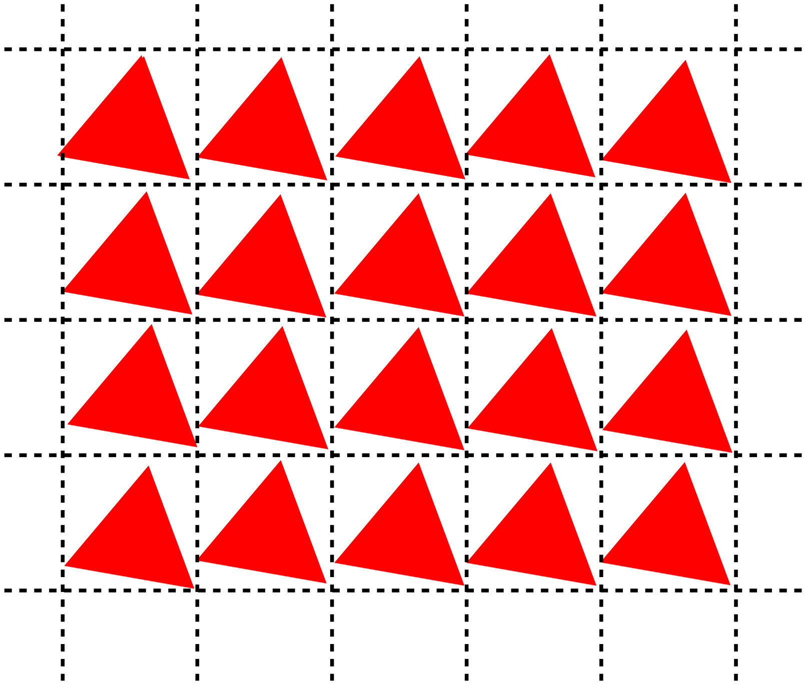
Symmetry of the object: $S_o = 3m$

Symmetry of the pattern : $S_p = m = 4mm \cap 3m$

$S_p < S_L$: merohedry

The concept of holohedry





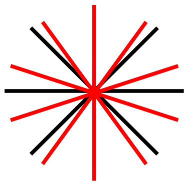
Symmetry of the lattice: $S_L = 4mm$

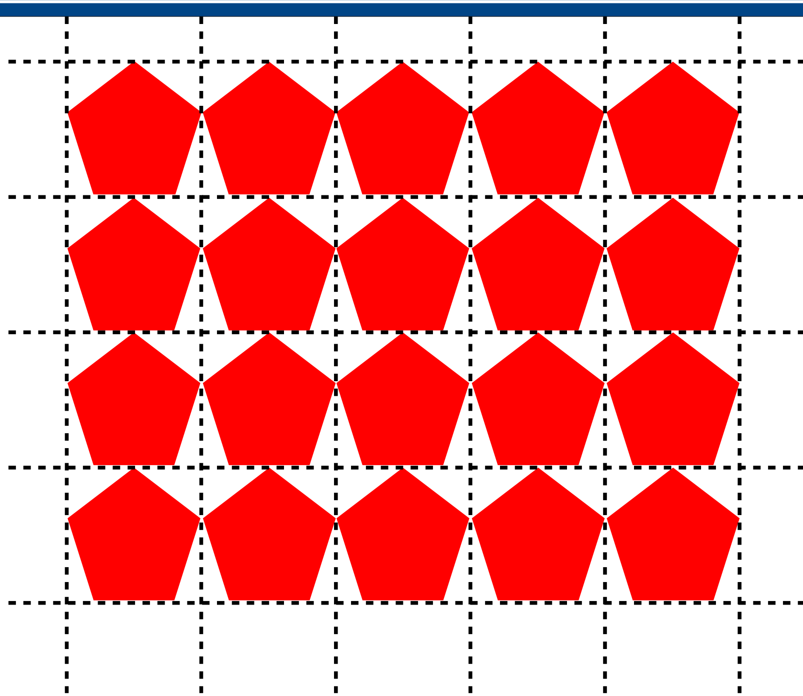
Symmetry of the object: $S_o = 3m$

Symmetry of the pattern : $S_p = 1 = 4mm \cap 3m$

$S_P < S_L$: merohedry

The concept of holohedry





The crystallographic restriction (n = 1, 2, 3, 4, 6) applies to the lattice and to the pattern, but not to the content of the unit cell!

Symmetry of the lattice : $S_L = 4mm$

Symmetry of the object : $S_o = 5m$

Symmetry of the pattern : $S_p = m = 4mm \cap 5m$

$S_p < S_L$: merohedry

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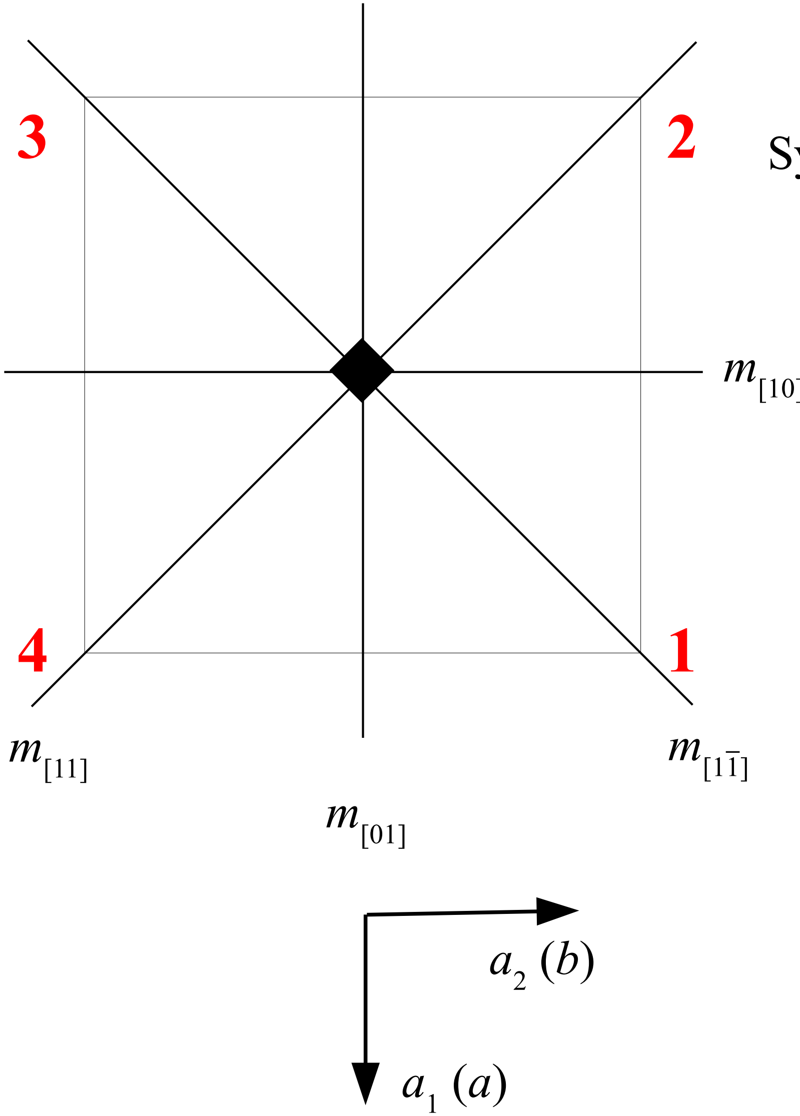
The notion of subgroup

Exercise: find the elements, the operations and the symmetry group of a square in E^2



Geometric elements: one point (centre of the square),
four lines ([10], [01], [11], [$1\bar{1}$])

Symmetry elements: one fourfold rotation point: 4
four reflection lines: $m_{[10]}$, $m_{[01]}$, $m_{[11]}$, $m_{[1\bar{1}]}$

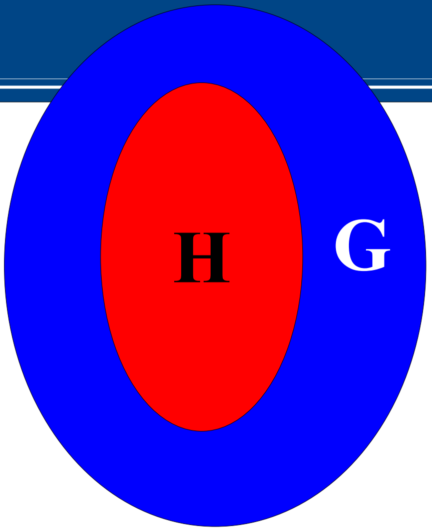
Symmetry operations:
Four rotations (4^1, $4^2 = 2$, $4^3 = 4^{-1}$, $4^4 = 1$)
Four reflections ($m_{[10]}$, $m_{[01]}$, $m_{[11]}$, $m_{[1\bar{1}]}$)

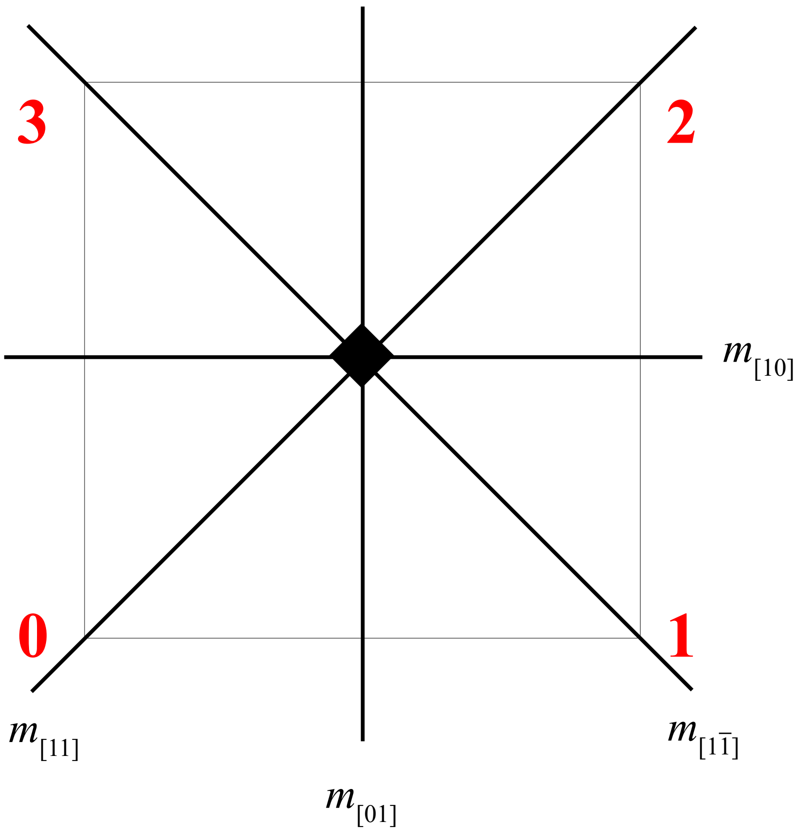
Check that these operations do form a group

- Isometries are always associative
- The identity belong to the set (it corresponds to 4^4 and m^2)
- The inverse of each operation belongs to the set ($1^{-1}=1$; $m^{-1} = m$; $2^{-1} = 2$, $4^{-1} = 4^3$)
- To check the closure, let us build the multiplication (Cayley) table.

Subgroups

From the group (G,○) we select a subset of elements forming a subset H. If the (H,○) is a group under the same binary operation ○ as (G,○), then (H,○) is a subgroup of (G,○).





	1	2	4^1	4^3	$m_{[10]}$	$m_{[01]}$	$m_{[11]}$	$m_{[1\bar{1}]}$
1	1	2	4^1	4^3	$m_{[10]}$	$m_{[01]}$	$m_{[11]}$	$m_{[1\bar{1}]}$
2	2	1	4^3	4^1	$m_{[01]}$	$m_{[10]}$	$m_{[1\bar{1}]}$	$m_{[11]}$
4^1	4^1	4^3	2	1	$m_{[11]}$	$m_{[1\bar{1}]}$	$m_{[01]}$	$m_{[10]}$
4^3	4^3	4^1	1	2	$m_{[1\bar{1}]}$	$m_{[11]}$	$m_{[10]}$	$m_{[01]}$
$m_{[10]}$	$m_{[10]}$	$m_{[01]}$	$m_{[1\bar{1}]}$	$m_{[11]}$	1	2	4^3	4^1
$m_{[01]}$	$m_{[01]}$	$m_{[10]}$	$m_{[11]}$	$m_{[1\bar{1}]}$	2	1	4^1	4^3
$m_{[11]}$	$m_{[11]}$	$m_{[1\bar{1}]}$	$m_{[10]}$	$m_{[01]}$	4^1	4^3	1	2
$m_{[1\bar{1}]}$	$m_{[1\bar{1}]}$	$m_{[11]}$	$m_{[01]}$	$m_{[10]}$	4^3	4^1	2	1

Multiplication table of the group（G,○）

Multiplication table of the subgroup (H,○)

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Order and index of a subgroup

group G, order |G|

$H \subset G$

group H, order |H|

|H| is a divisor of |G| (Lagrange's theorem)

The ratio $i_G(H) = |G|/|H|$ is called the **index of H in G**

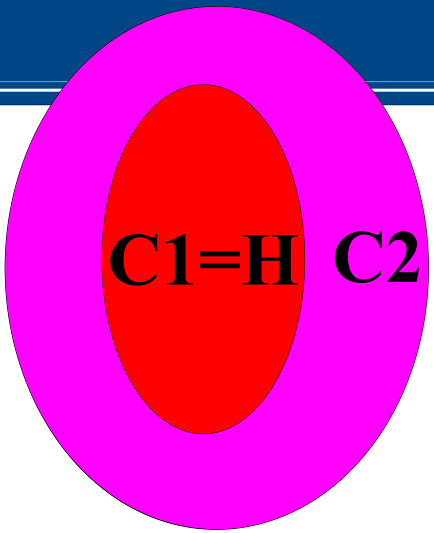
$i_G(H) = 2$: hemihedry

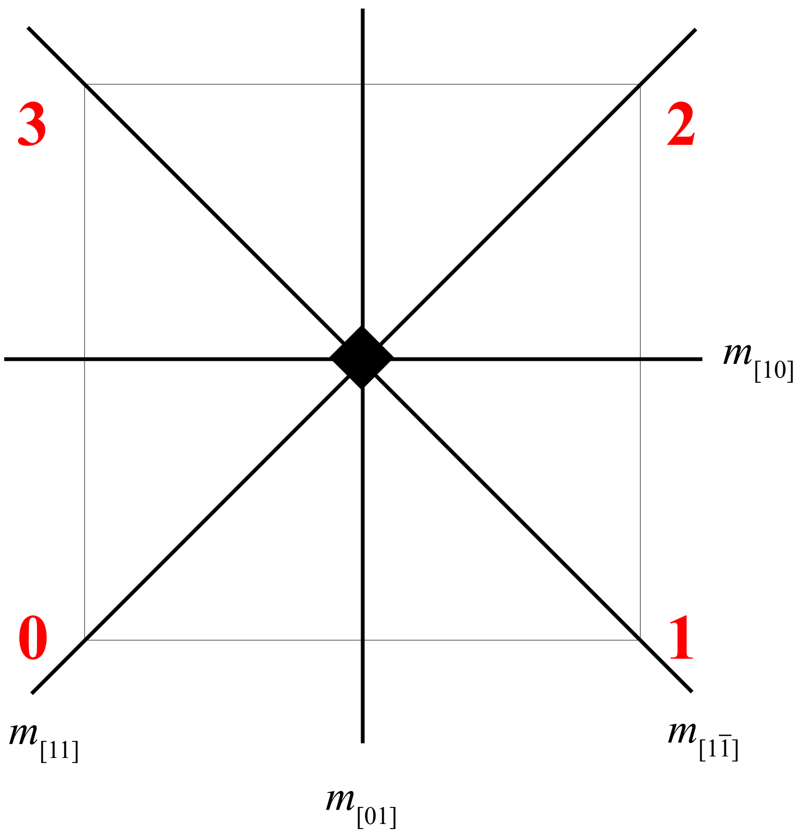
$i_G(H) = 4$: tetartohedry

$i_G(H) = 8$ ： ogdohedry （3-dimensional space）

Cosets

By decomposing (G,○) with respect to (H,○) we get i = |G|/|H| cosets. Each coset has the same number of elements |H| as the subgroup, which is called the **length of the coset**.



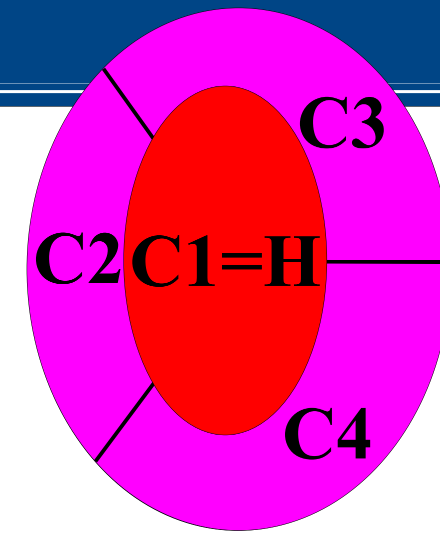


	1	2	4^1	4^3	$m_{[10]}$	$m_{[01]}$	$m_{[11]}$	$m_{[1\bar{1}]}$
1	1	2	4^1	4^3	$m_{[10]}$	$m_{[01]}$	$m_{[11]}$	$m_{[1\bar{1}]}$
2	2	1	4^3	4^1	$m_{[01]}$	$m_{[10]}$	$m_{[1\bar{1}]}$	$m_{[11]}$
4^1	4^1	4^3	2	1	$m_{[11]}$	$m_{[1\bar{1}]}$	$m_{[01]}$	$m_{[10]}$
4^3	4^3	4^1	1	2	$m_{[1\bar{1}]}$	$m_{[11]}$	$m_{[10]}$	$m_{[01]}$
$m_{[10]}$	$m_{[10]}$	$m_{[01]}$	$m_{[1\bar{1}]}$	$m_{[11]}$	1	2	4^3	4^1
$m_{[01]}$	$m_{[01]}$	$m_{[10]}$	$m_{[11]}$	$m_{[1\bar{1}]}$	2	1	4^1	4^3
$m_{[11]}$	$m_{[11]}$	$m_{[1\bar{1}]}$	$m_{[10]}$	$m_{[01]}$	4^1	4^3	1	2
$m_{[1\bar{1}]}$	$m_{[1\bar{1}]}$	$m_{[11]}$	$m_{[01]}$	$m_{[10]}$	4^3	4^1	2	1

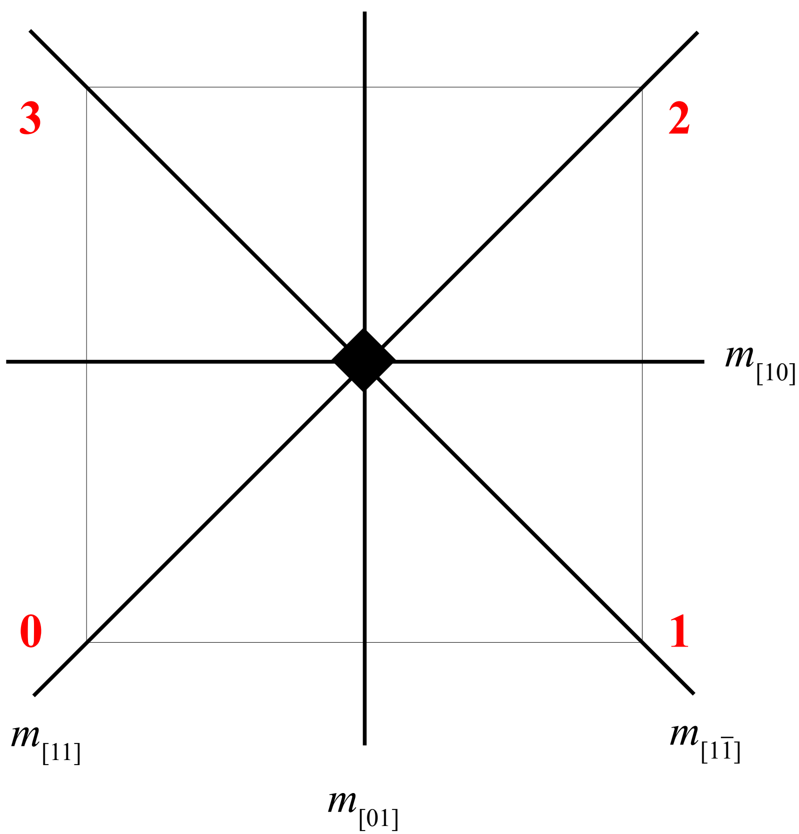
Group **Subgroup = 1st coset**

2nd coset

Cosets



By decomposing (G,○) with respect to (H,○) we get i = |G|/|H| cosets. Each coset has the same number of elements |H| as the subgroup, which is called the **length of the coset**.



	1	2	4^1	4^3	$m_{[10]}$	$m_{[01]}$	$m_{[11]}$	$m_{[1\bar{1}]}$
1	1	2	4^1	4^3	$m_{[10]}$	$m_{[01]}$	$m_{[11]}$	$m_{[1\bar{1}]}$
2	2	1	4^3	4^1	$m_{[01]}$	$m_{[10]}$	$m_{[1\bar{1}]}$	$m_{[11]}$
4^1	4^1	4^3	2	1	$m_{[11]}$	$m_{[1\bar{1}]}$	$m_{[01]}$	$m_{[10]}$
4^3	4^3	4^1	1	2	$m_{[1\bar{1}]}$	$m_{[11]}$	$m_{[10]}$	$m_{[01]}$
$m_{[10]}$	$m_{[10]}$	$m_{[01]}$	$m_{[1\bar{1}]}$	$m_{[11]}$	1	2	4^3	4^1
$m_{[01]}$	$m_{[01]}$	$m_{[10]}$	$m_{[11]}$	$m_{[1\bar{1}]}$	2	1	4^1	4^3
$m_{[11]}$	$m_{[11]}$	$m_{[1\bar{1}]}$	$m_{[10]}$	$m_{[01]}$	4^1	4^3	1	2
$m_{[1\bar{1}]}$	$m_{[1\bar{1}]}$	$m_{[11]}$	$m_{[01]}$	$m_{[10]}$	4^3	4^1	2	1

Group **Subgroup = 1st coset**

2nd, 3rd, 4th coset

Desymmetrization of the square

Order	Index	
8	1	$4mm = \{1, 4^1, 2, 4^3, m_{[10]}, m_{[01]}, m_{[11]}, m_{[1\bar{1}]}\}$
4	2	$\{1, 4^1, 2, 4^3\} = 4$ $\{1, 2, m_{[10]}, m_{[01]}, \} = 2mm.$ $\{1, 2, m_{[11]}, m_{[1\bar{1}]}\} = 2.mm$
2	4	$\{1, 2\} = 2$ $\{1, m_{[10]}\} = .m.$ $\{m_{[01]}\} = .m.$ $\{1, m_{[11]}\} = ..m$ $\{1, m_{[1\bar{1}]}\} = ..m$
1	8	$\{1\} = 1$

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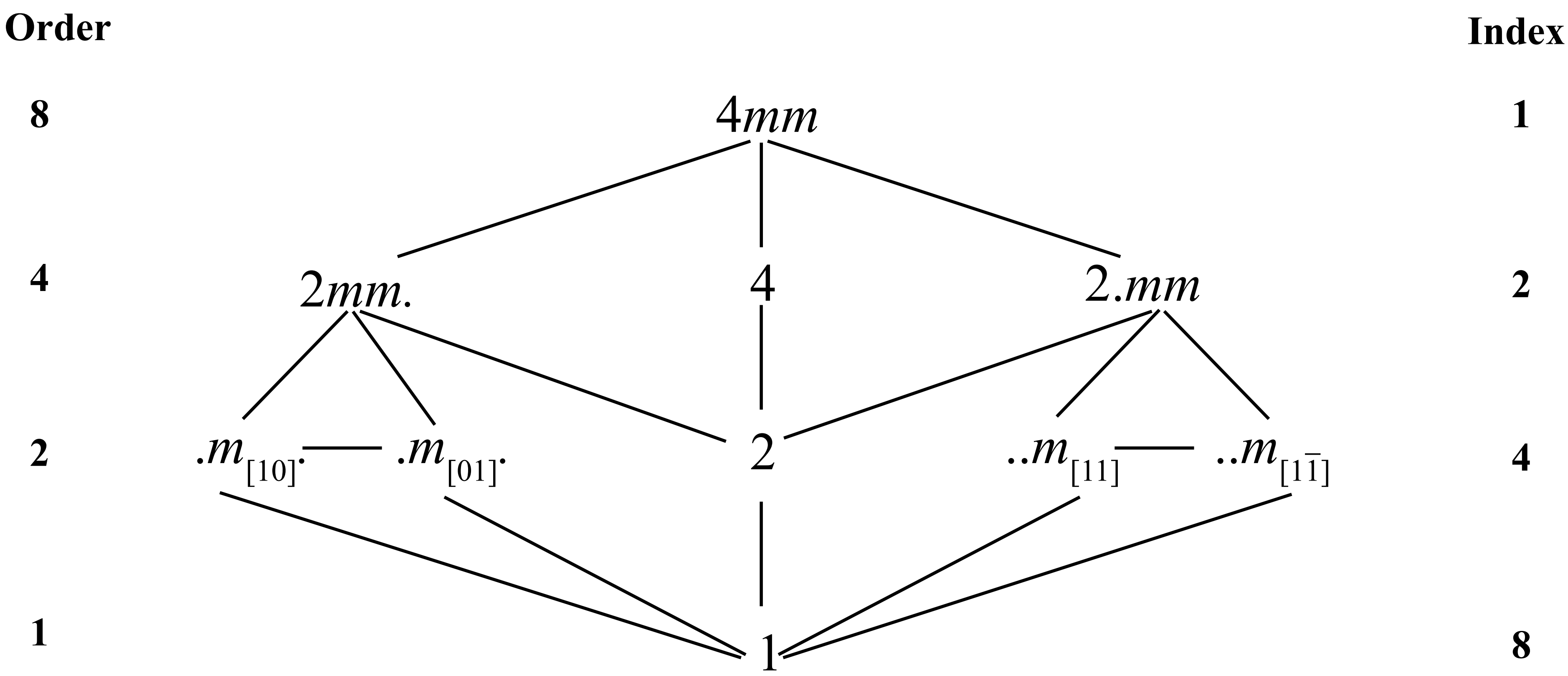
Desymmetrization of the square



Cosets
Conjugacy classes
Conjugate subgroups
Normal or invariant subgroups

Left and right cosets

$G = H \cup_i C_i = H \cup_i g_i H,\ g_i \notin (H, C_{j<i})$ Left coset

$G = 4mm = \{1, 4^1, 4^2 = 2, 4^3 = 4^{-1}, m_{[10]}, m_{[01]}, m_{[11]}, m_{[1\bar{1}]}\}$

$H = 2mm.$

$4mm = \{2mm.\} \cup g \notin \{2mm.\} = \{1, 2, m_{[10]}, m_{[01]}\} \cup \{4^1, 4^3, m_{[11]}, m_{[1\bar{1}]}\}$

$H = 2.mm$

$4mm = \{2.mm\} \cup g \notin \{2.mm\} = \{1, 2, m_{[11]}, m_{[1\bar{1}]}\} \cup \{4^1, 4^3, m_{[10]}, m_{[01]}\}$

$H = 4$

$4mm = \{4\} \cup g \notin \{4\} = \{1, 4^1, 2, 4^3\} \cup \{m_{[10]}, m_{[01]}, m_{[11]}, m_{[1\bar{1}]}\}$

Etc. etc.

$G = H \cup_i C_i = H \cup_i H g_i,\ g_i \notin (H, C_{j<i})$ Right coset

Usually, $g_i H \neq H g_i$

If $g_i H = H g_i$, $\forall i$, then H is called a **normal (invariant) subgroup**.

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Decomposition of 4*mm* with respect to 2 and $m_{[10]}$

$$4mm = \{1,2\} \cup 4^1\{1,2\} \cup m_{[10]}\{1,2\} \cup m_{[11]}\{1,2\} =$$

$$\{1,2\} \cup \{4^1,4^3\} \cup \{m_{[10]},m_{[01]}\} \cup \{m_{[11]},m_{[1\bar{1}]}\}$$

$$4mm = \{1,2\} \cup \{1,2\}4^1 \cup \{1,2\}m_{[10]} \cup \{1,2\}m_{[11]} =$$

$$\{1,2\} \cup \{4^1,4^3\} \cup \{m_{[10]},m_{[01]}\} \cup \{m_{[11]},m_{[1\bar{1}]}\}$$

$=$ Normal subgroup

$$4mm = \{1,m_{[10]}\} \cup 4^1\{1,m_{[10]}\} \cup 4^3\{1,m_{[10]}\} \cup 2\{1,m_{[10]}\} =$$

$$\{1,m_{[10]}\} \cup \{4^1,m_{[11]}\} \cup \{4^3,m_{[1\bar{1}]}\} \cup \{2,m_{[01]}\}$$

$$4mm = \{1,m_{[10]}\} \cup \{1,m_{[10]}\}4^1 \cup \{1,m_{[10]}\}4^3 \cup \{1,m_{[10]}\}2 =$$

$$\{1,m_{[10]}\} \cup \{4^1,m_{[1\bar{1}]}\} \cup \{4^3,m_{[11]}\} \cup \{2,m_{[01]}\}$$

$\neq$

Conjugate and normal subgroups

$H \subset G$

$gh_ig^{-1} = h_j$; $h_i \in H, \forall g \in G$: **conjugate elements**

↓

Conjugation is a similarity transformation: "do the same thing somewhere else"

$gh_i = h_jg$; $h_i \in H, \forall g \in G$

If $h_i = h_j, \forall g \in G$, h_i is a **self-conjugate element**

The set of conjugate elements form a class $\cup_i g_ihg_i^{-1} = Cl(h)$ **conjugacy class**

$$\mathbf{Cl(h) = \{ h' \in G \mid \exists\, g \in G : h' = ghg^{-1} \}}$$

Next consider not one element h but the whole subgroup H

$\cup_i g_iHg_i^{-1} = \{H, H', H'' \cdots\}$ are **conjugate subgroups** of G

If $H' = H'' = \cdots = H$ ($g_iH = Hg_i, \forall g \in G$), H is a **normal or invariant subgroup** of G: $\mathbf{H \triangleleft G}$.

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Conjugacy classes of 4*mm*

$\cup_i g_i h g_i^{-1}$ = Cl(h): conjugacy class

h = 1 $\cup_i g_i 1 g_i^{-1} = \cup_i g_i g_i^{-1} = \{1\}$

h = 2 $\cup_i g_i 2 g_i^{-1} = \{2\}$

h = 4^1 $\cup_i g_i 4^1 g_i^{-1} = \{4^1, 4^3\}$

h = $m_{[10]}$ $\cup_i g_i m_{[10]} g_i^{-1} = \{m_{[10]}, m_{[01]}\}$

h = $m_{[11]}$ $\cup_i g_i m_{[11]} g_i^{-1} = \{m_{[11]}, m_{[1\bar{1}]}\}$

$$4mm = \{1\}, \{2\}, \{4^1, 4^3\}, \{m_{[10]}, m_{[01]}\}, \{m_{[11]}, m_{[1\bar{1}]}\}$$

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When we apply an isometry…
The object is transformed directly($O \rightarrow O'$)
The symmetry group of the object is transformed by conjugation

$hO = O, h \in H$ $\quad$ $h'O' = O', h' \in H'$ $\quad$ $gO = O', g \notin H, H'$

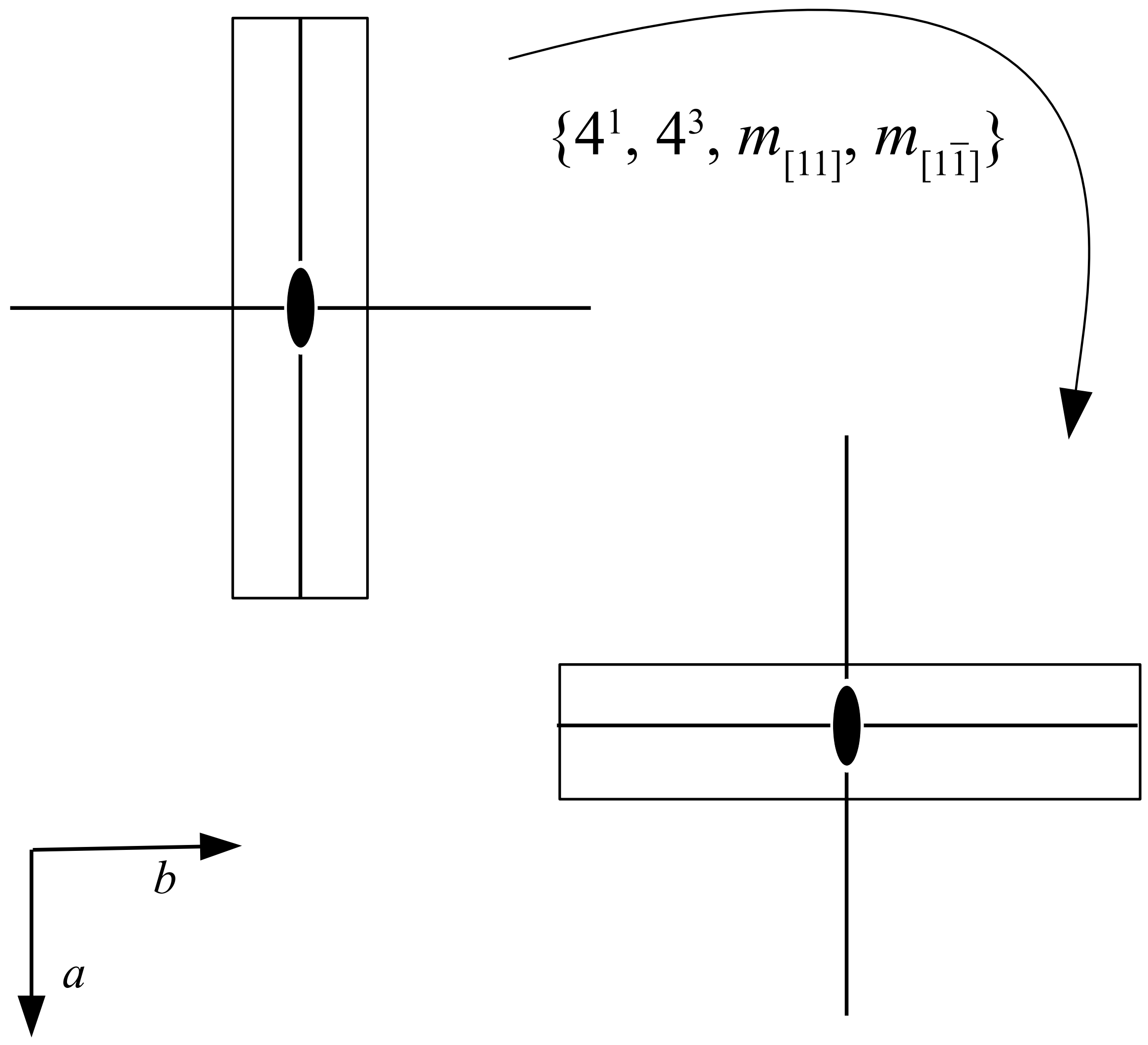
$$H' = gHg^{-1}$$

Effects of the operations in a coset

$H = 2mm. = \{1, 2, m_{[10]}, m_{[01]}\}$

$gHg^{-1} = H \Rightarrow H = 2mm. \lhd G = 4mm$

Normal subgroup



$gHg^{-1} = 2mm.$

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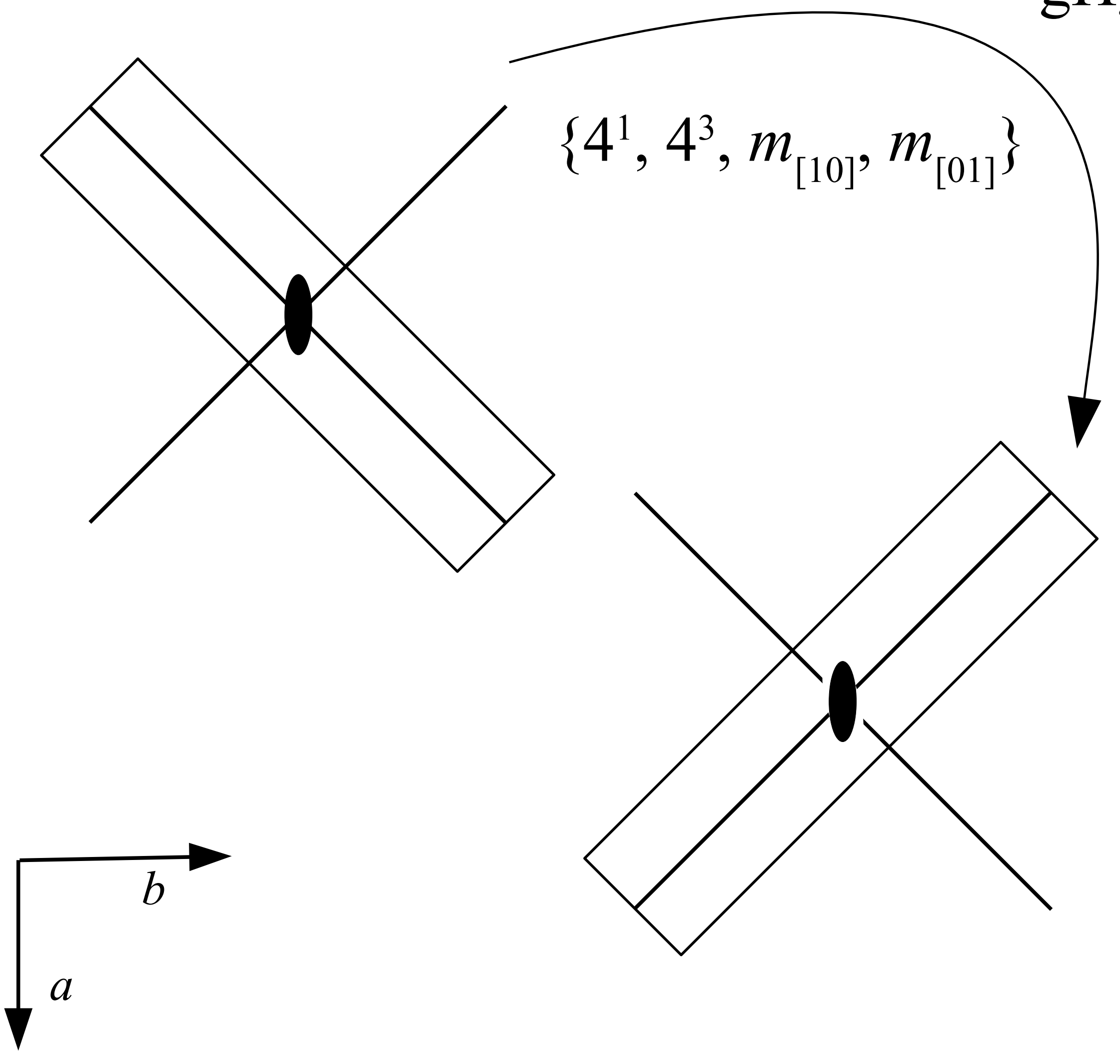
Effects of the operations in a coset

$H = 2.mm = \{1, 2, m_{[11]}, m_{[1\bar{1}]}\}$

$gHg^{-1} = H \Rightarrow H = 2.mm \triangleleft G = 4mm$

Normal subgroup



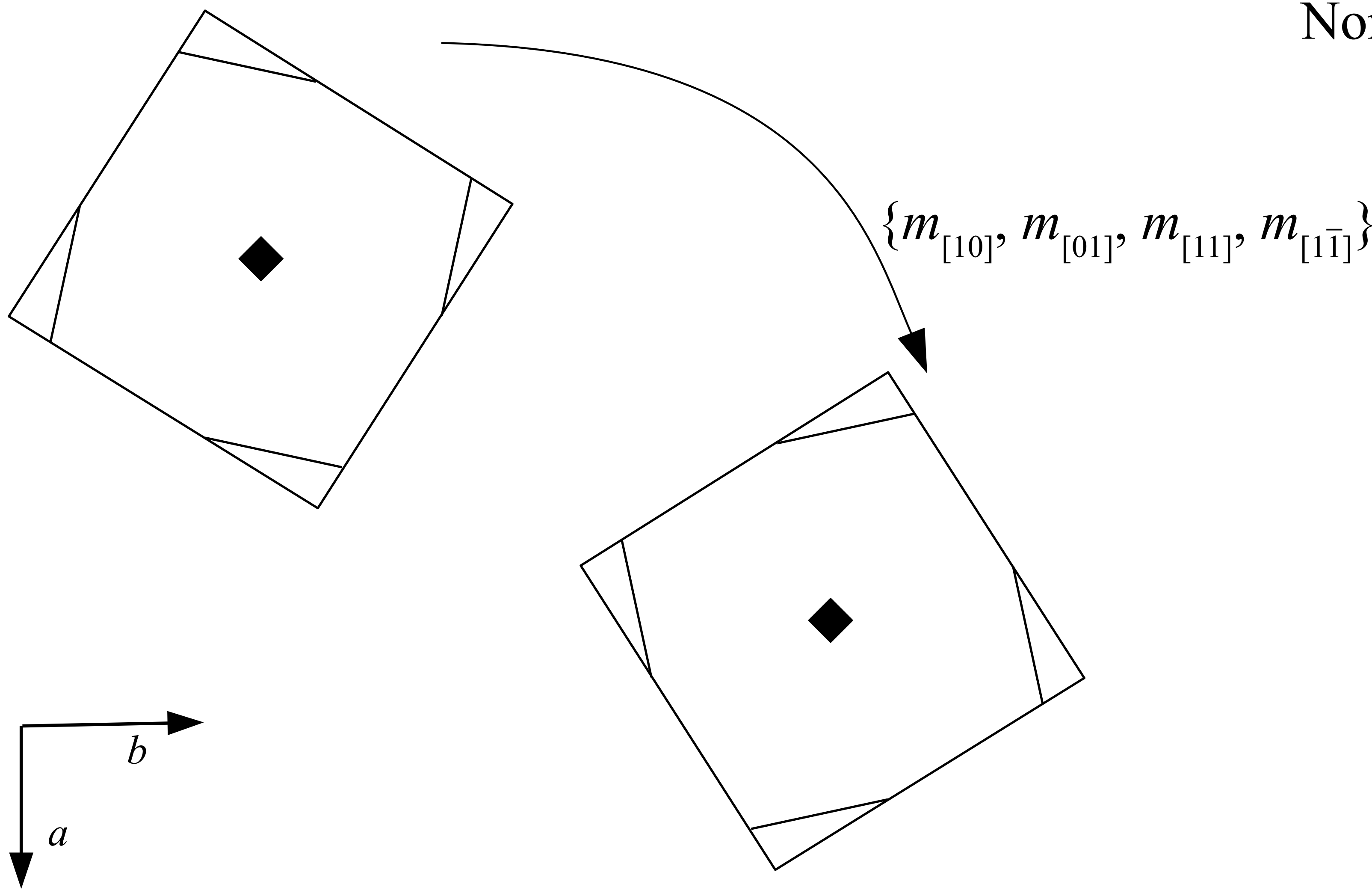
$gHg^{-1} = 2.mm$

Effects of the operations in a coset

$H = 4 = \{1, 4, 2, 4^3\}$

$gHg^{-1} = H \Rightarrow H = 4 \triangleleft G = 4mm$

Normal subgroup



$gHg^{-1} = 4$

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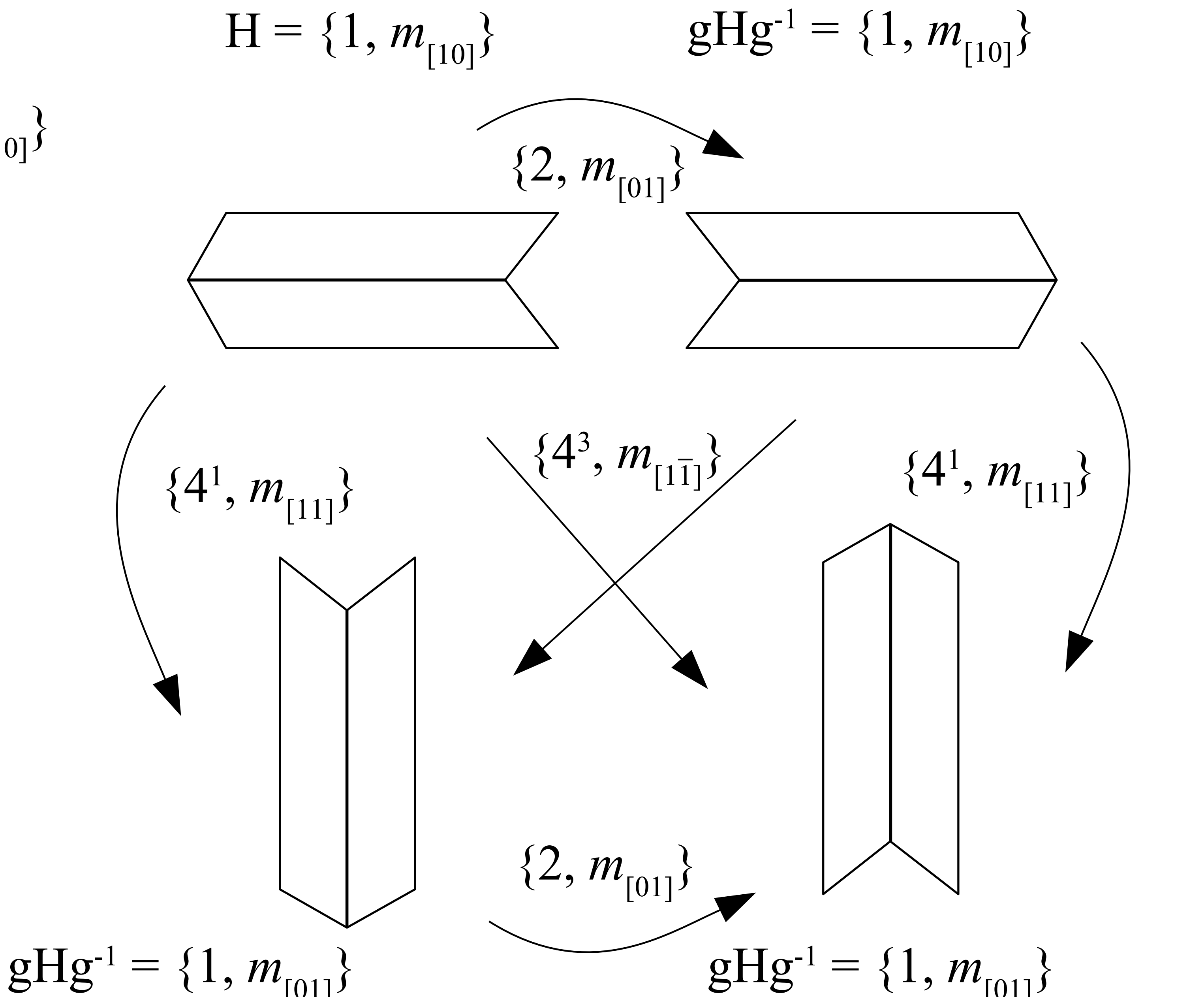
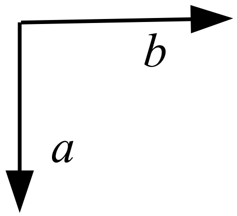
Effects of the operations in a coset

$g\{1,m_{[01]}\}g^{-1} = \{1,m_{[10]}\}$

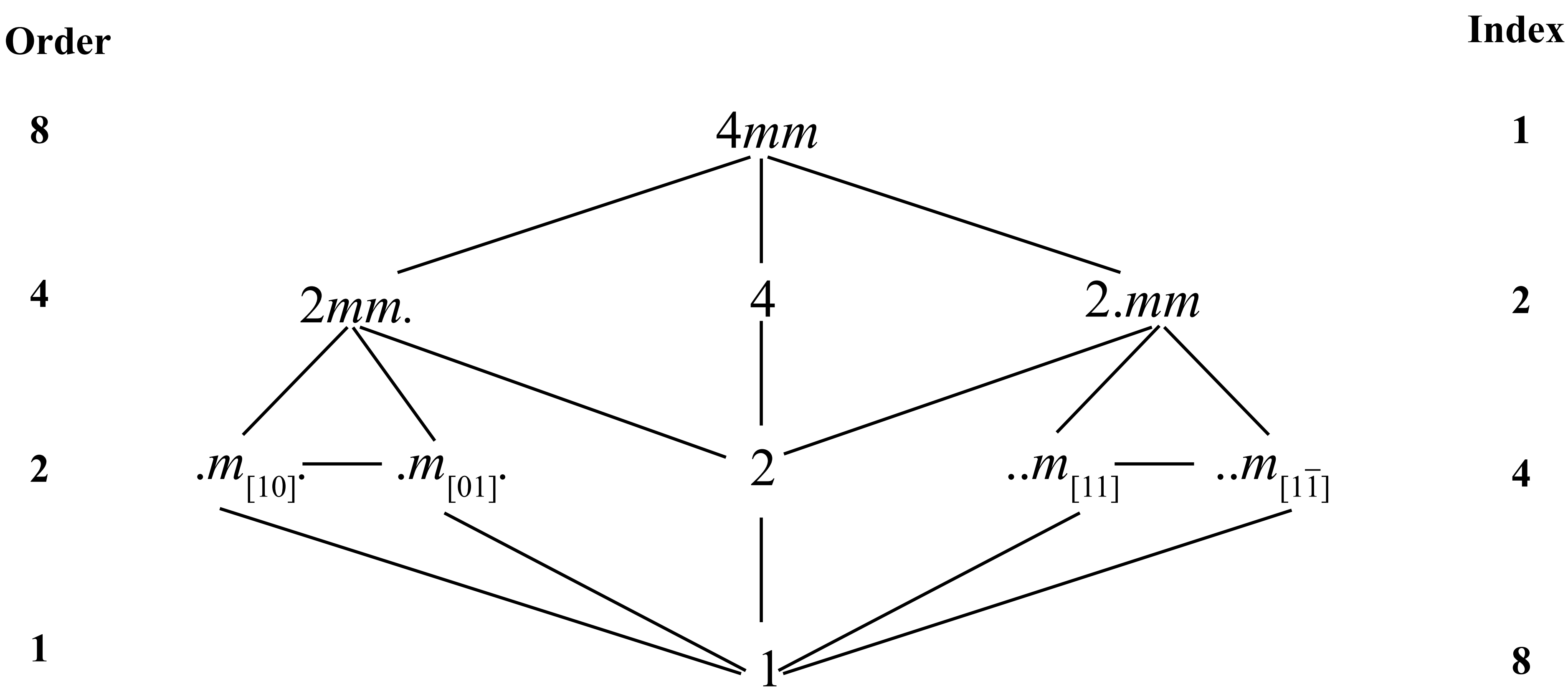
$\Rightarrow .m. \subset G = 4mm$

onjugate subgroups





Desymmetrization of the square

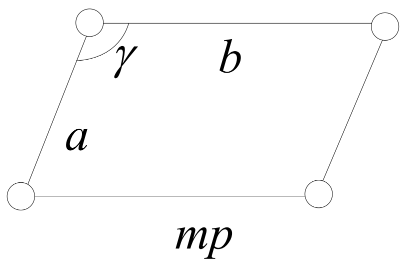


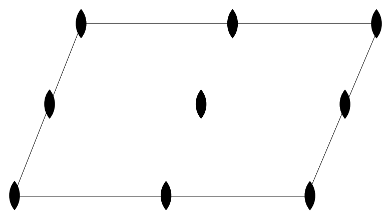
Extra-simple exercise

Show that a subgroup of index 2 is always normal

Holohedries and merohedries in the two-dimensional space

Monoclinic (oblique) lattice





Holohedry 2 : {1,2}

Merohedry 1 : {1}

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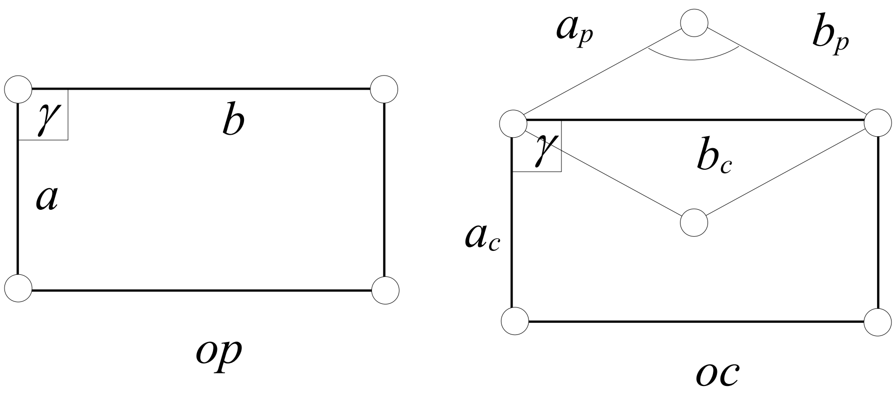
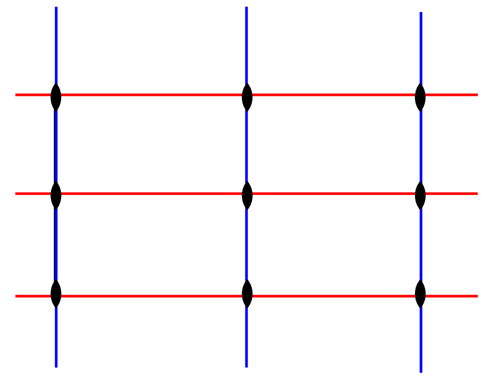
Orthorhombic (rectangular) lattice

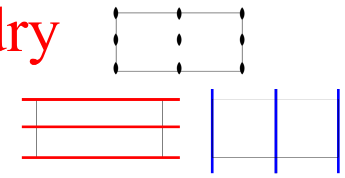




Holohedry $2mm$: $\{1,2,m_{[10]},m_{[01]}\}$

Merohedries

2 : $\{1,2\}$ → Monoclinic holohedry
m : $\{1,m_{[10]}\}$, $\{1,m_{[01]}\}$
1 : $\{1\}$ → Monoclinic merohedry



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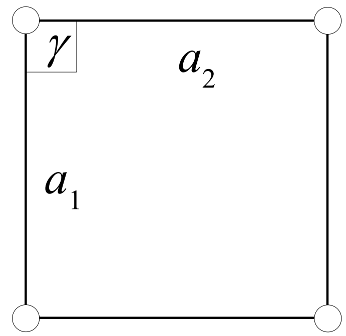
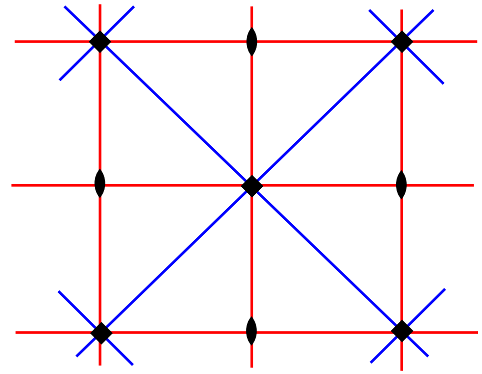
Tetragonal (square) lattice

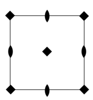


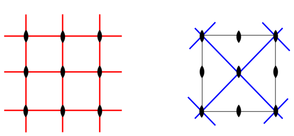
tp



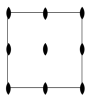
Holohedry $4mm$: $\{1, 4^1, 4^2 = 2, 4^3 = 4^{-1}, m_{[10]}, m_{[01]}, m_{[11]}, m_{[1\bar{1}]}\}$

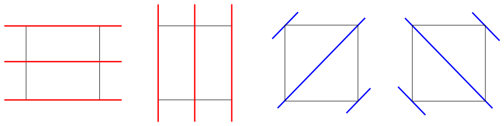
Merohedries

4 : $\{1, 4^1, 4^2, 4^3\}$ 

$2mm$: $\{1, 2, m_{[10]}, m_{[01]}\}$, $\{1, 2, m_{[11]}, m_{[1\bar{1}]}\}$ 

→ Orthorhombic holohedry

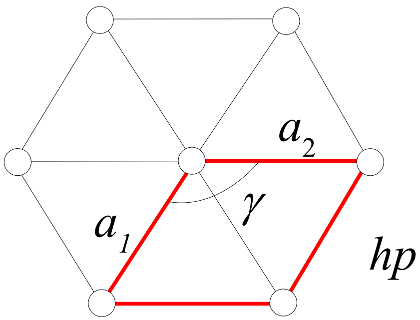
2 : $\{1, 2\}$ → Monoclinic holohedry 

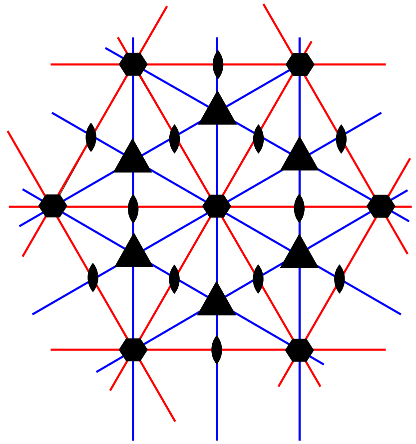
m : $\{1, m_{[10]}\}$, $\{1, m_{[01]}\}$, $\{1, m_{[11]}\}$, $\{1, m_{[\bar{1}1]}\}$ 

→ Orthorhombic merohedry

1 : $\{1\}$ → Monoclinic merohedry

Hexagonal lattice

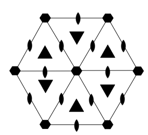


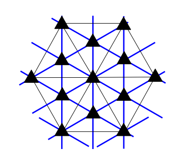
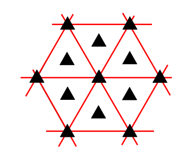


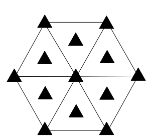
Holohedry

$6mm$: $\{1, 6^1, 6^2 = 3, 6^3 = 2, 6^4 = 3^{-1}, 6^5 = 6^{-1}, m_{[10]}, m_{[01]}, m_{[11]}, m_{[1\bar{1}]}, m_{[12]}, m_{[21]}\}$

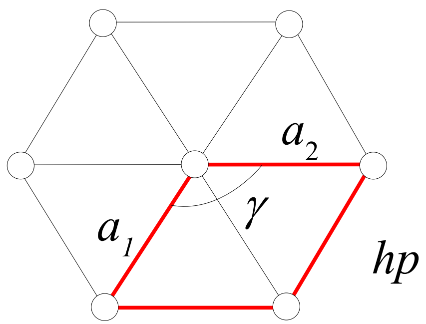
Merohedries (1)

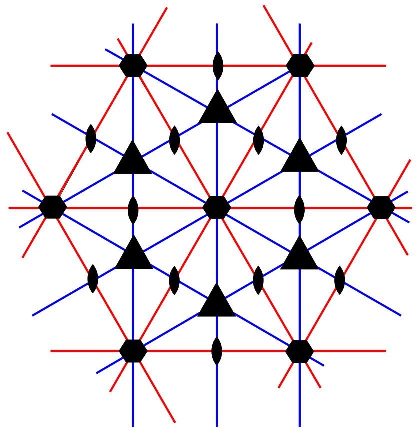
6 : $\{1, 6^1, 6^2, 6^3, 6^4, 6^5\}$ 

$3m$: $\{1, 3^1, 3^2, m_{[10]}, m_{[01]}, m_{[11]}\}$, $\{1, 3^1, 3^2, m_{[1\bar{1}]}, m_{[12]}, m_{[21]}\}$  

3 : $\{1, 3, 3^{-1}\}$ 

Hexagonal lattice





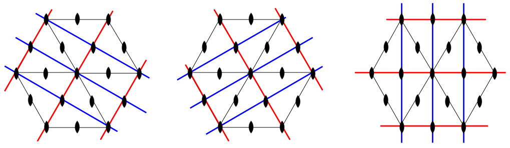
Holohedry

$6mm$: $\{1, 6^1, 6^2 = 3, 6^3 = 2, 6^4 = 3^{-1}, 6^5 = 6^{-1}, m_{[10]}, m_{[01]}, m_{[11]}, m_{[1\bar{1}]}, m_{[12]}, m_{[21]}\}$

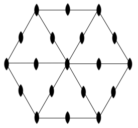
Merohedries (2)

$2mm$: $\{1, 2, m_{[10]}, m_{[12]}\}$, $\{1, 2, m_{[01]}, m_{[\overline{21}]}\}$, $\{1, 2, m_{[11]}, m_{[\bar{1}1]}\}$

→ Orthorhombic holohedry

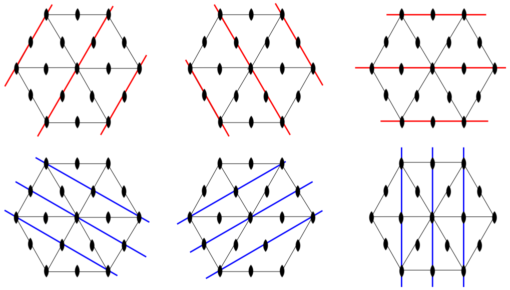


2 : {1,2} → Monoclinic merohedry



m : $\{1,m_{[10]}\}$, $\{1,m_{[01]}\}$, $\{1,m_{[11]}\}$, $\{1,m_{[1\bar{1}]}\}$, $\{1,m_{[12]}\}$, $\{1,m_{[21]}\}$

→ Orthorhombic merohedry



1 : {1}→ Monoclinic merohedry

Holohedry 2 : $\{1,2\}$ Conjugacy classes $\{1\}$, $\{2\}$

Subgroup 1 : $\{1\}$

Holohedry $2mm$: $\{1,2,m_{[10]},m_{[01]}\}$

Conjugacy classes $\{1\}$, $\{2\}$, $\{m_{[10]}\}$, $\{m_{[01]}\}$

Subgroups 2 : $\{1,2\}$, m : $\{1,m_{[10]}\}$, $\{1,m_{[01]}\}$, 1 : $\{1\}$

Holohedry $4mm$: $\{1,\ 4^1,\ 4^2 = 2,\ 4^3 = 4^{-1},\ m_{[10]},\ m_{[01]},\ m_{[11]},\ m_{[1\bar{1}]}\}$

Conjugacy classes $\{1\}$, $\{2\}$, $\{4^1, 4^3\}$, $\{m_{[10]}, m_{[01]}\}$, $\{m_{[11]}, m_{[1\bar{1}]}\}$

Subgroups 4 : $\{1, 4^1, 4^2, 4^3\}$, $2mm$: $\{1, 2, m_{[10]}, m_{[01]}\}$, $\{1, 2, m_{[11]}, m_{[1\bar{1}]}\}$,

2 : $\{1, 2\}$, m : $\{1,m_{[10]}\}$, $\{1,m_{[01]}\}$, $\{1,m_{[11]}\}$, $\{1,m_{[\bar{1}1]}\}$, 1 : $\{1\}$

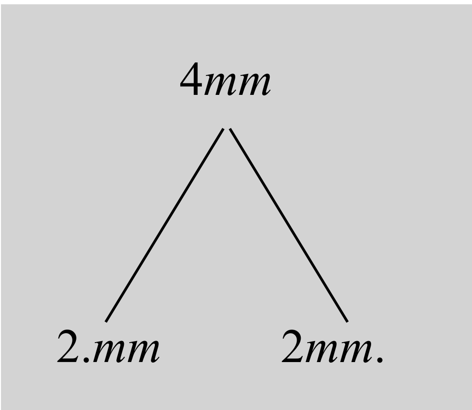
Holohedry $6mm$: $\{1,\ 6^1,\ 6^2 = 3,\ 6^3 = 2,\ 6^4 = 3^{-1},\ 6^5 = 6^{-1},\ m_{[10]},\ m_{[01]},\ m_{[11]},\ m_{[1\bar{1}]},\ m_{[12]},\ m_{[21]}\}$

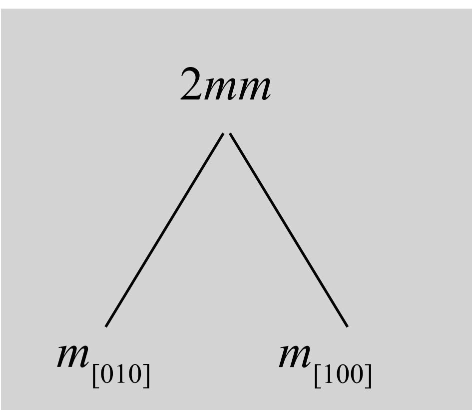
Conjugacy classes:

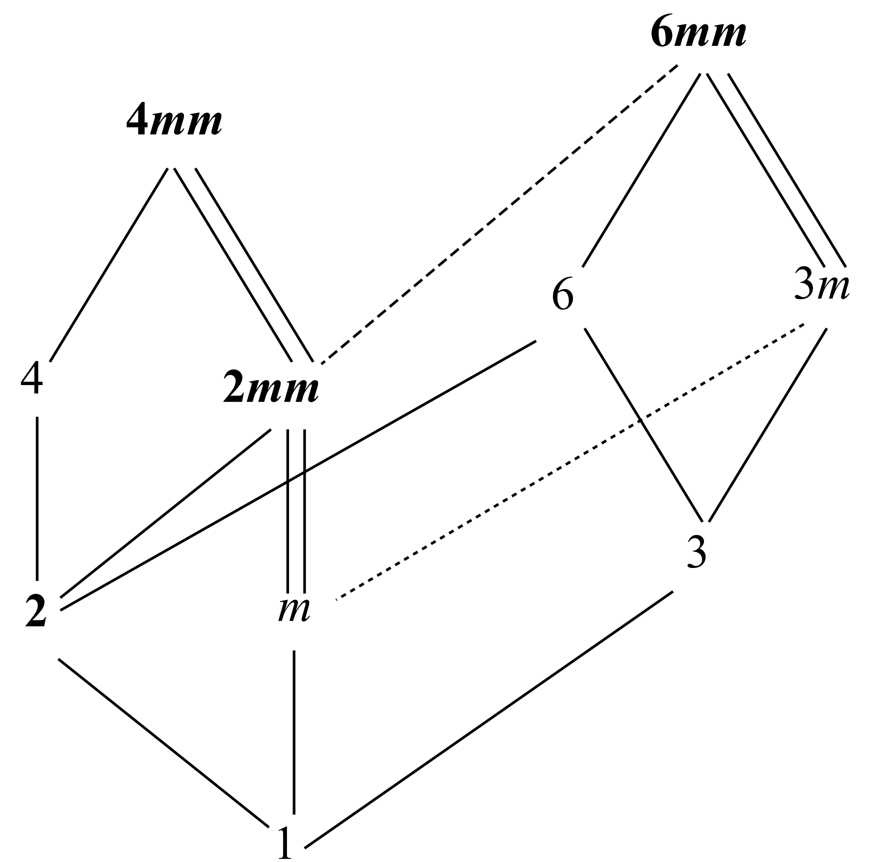
$\{1\}$, $\{2\}$, $\{3^1, 3^2\}$, $\{6^1, 6^5\}$, $\{m_{[10]}, m_{[01]}, m_{[11]}, \}$, $\{m_{[1\bar{1}]}, m_{[12]}, m_{[21]}\}$

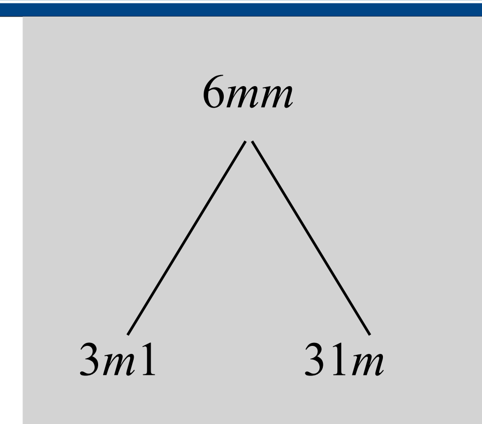
Subgroups 6 : $\{1, 6^1, 6^2, 6^3, 6^4, 6^5\}$, $3m$: $\{1, 3^1, 3^2, m_{[10]}, m_{[01]}, m_{[11]}\}$, $\{1, 3^1, 3^2, m_{[1\bar{1}]}, m_{[12]}, m_{[21]}\}$, 3 : $\{1, 3, 3^{-1}\}$, $2mm$: $\{1, 2, m_{[10]}, m_{[12]}\}$, $\{1, 2, m_{[01]}, m_{[\overline{21}]}\}$, $\{1, 2, m_{[11]}, m_{[\bar{1}1]}\}$, 2 : $\{1,2\}$, m : $\{1,m_{[10]}\}$, $\{1,m_{[01]}\}$, $\{1,m_{[11]}\}$, $\{1,m_{[1\bar{1}]}\}$, $\{1,m_{[12]}\}$, $\{1,m_{[21]}\}$, 1 : $\{1\}$

Tree of group-subgroups in E^2









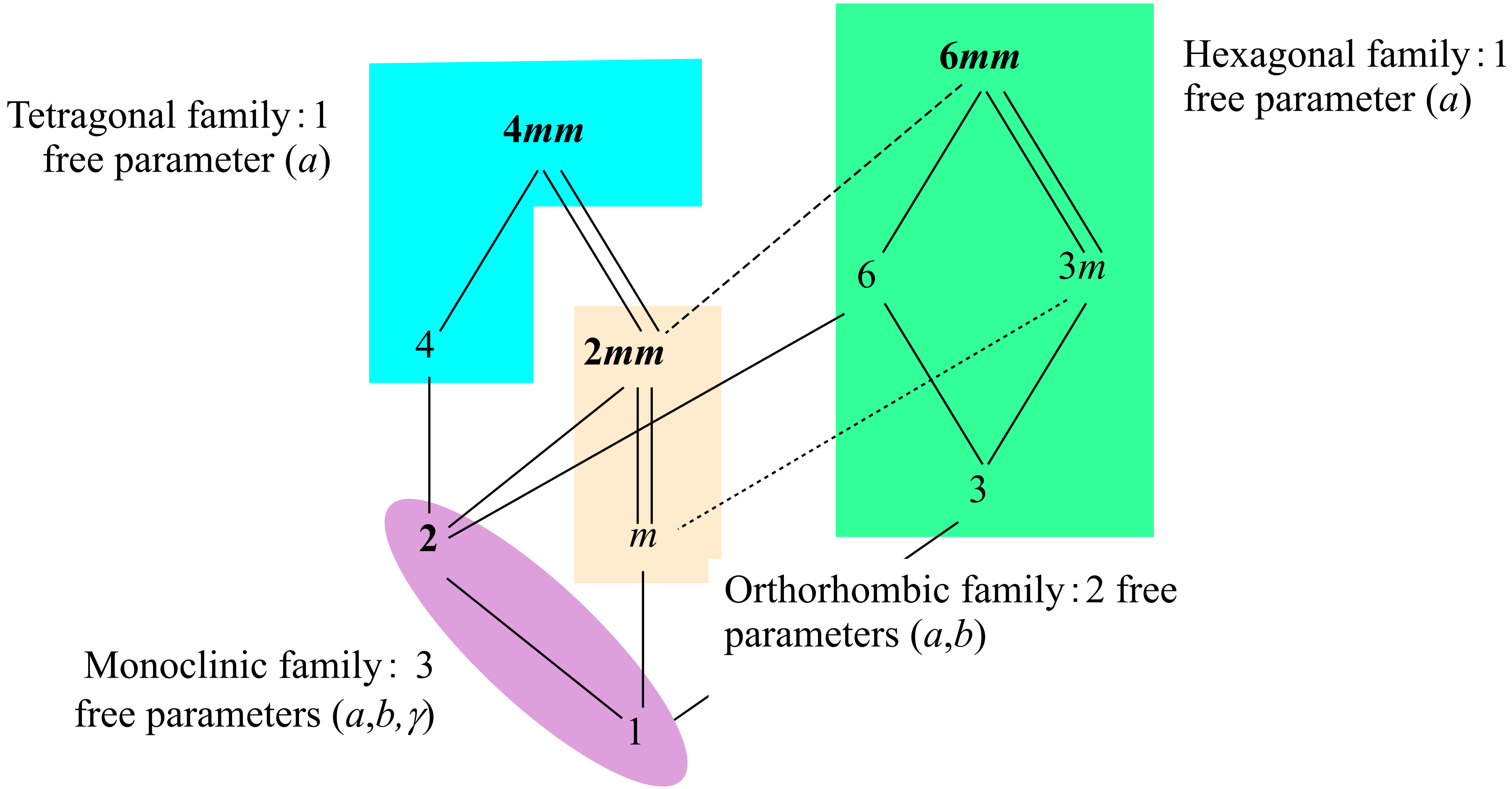
Tree of maximal group-subgroups (in bold the holohedries)

———————— Normal subgroup

.... Conjugate subgroups

Crystal families

Point-group types that satisfy the following criteria belong to the same crystal family:
1.they correspond to the same holohedry;
2.they are in group-subgroup relation;
3.the types of Bravais lattice on which they act have the same number of free parameters.



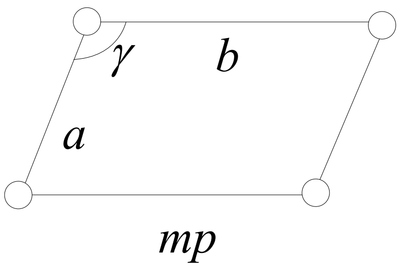
Conventional cell parameters and symmetry directions in the four crystal families of E^2

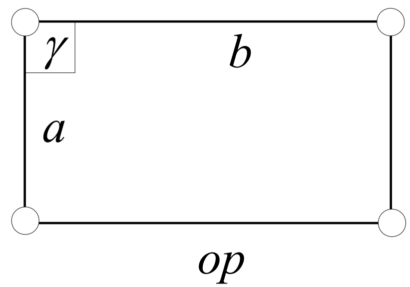
monoclinic
point group 2
(minimal point group)
No restriction
on a, b, γ
No symmetry direction

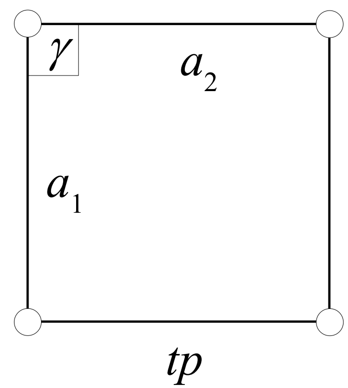
orthorhombic
point group $2mm$
No restriction
on a, b ;
$\gamma = 90°$
[10] and [01]

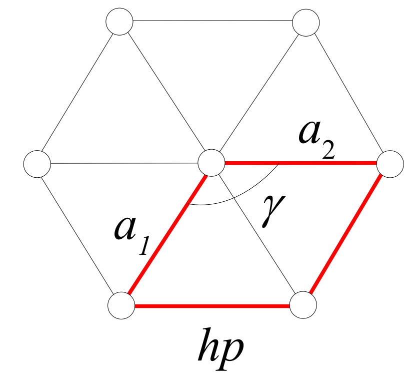
tetragonal
point group $4mm$
$a = b$; $\gamma = 90°$
$\langle 10 \rangle$ ([10] and [$0\bar{1}$])
$\langle 1\bar{1} \rangle$ ([11] and [$1\bar{1}$])

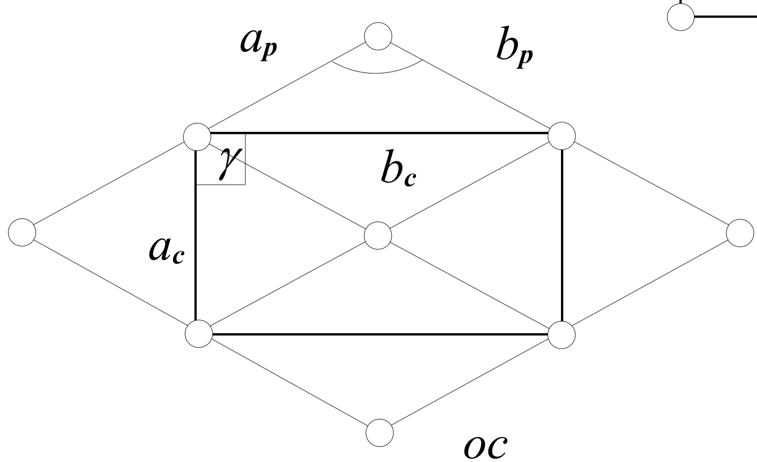
hexagonal
point group $6mm$
$a = b$; $\gamma = 120°$
$\langle 10 \rangle$ ([10], [01] and [$\bar{1}\bar{1}$])
$\langle 1\bar{1} \rangle$ ([21], [12] and [$1\bar{1}$])











Crystal families: ***m***onoclinic, ***o***rthorhombic, ***t***etragonal, ***h***exagonal
Type of lattice*: ***p***rimitive, ***c***entred

*Lattice whose conventional unit cell is primitive or centred

Kettle S.F.A, Norrby L.J., *J. Chem. Ed*. **70**(12), 1993, 959-963

Crystal systems

Point-group types that act on the same types of Bravais lattices belong to the same crystal system.

Type of group	*mp*	*op*	*oc*	*tp*	*hp*	Crystal system
2, 1	☑	☑	☑	☑	☑	monoclinic
2*mm*, *m*		☑	☑	☑	☑	orthorhombic
4*mm*, 4				☑		tetragonal
6*mm*, 6, 3*m*, 3					☑	hexagonal
No. of free parameters	3	2	2	1	1	

Lattice systems

Point-group types that correspond to the same lattice symmetry belong to the same lattice system.

6*mm*, 6, 3*m*, 3 : hexagonal lattice system

4*mm*, 4 : tetragonal lattice system

2*mm*, *m* : orthorhombic lattice system

2, 1 : monoclinic lattice system

The world in three dimensions

E^3 : the three-dimensional Euclidean space

Symmetry operations in E^3

Operations that leave invariant all the space (**3D**): the identity
Operations that leave invariant a plane (**2D**): the reflections
Operations that leave invariant one direction of the space (**1D**): the rotations
Operations that leave invariant one point of the space (**0D**): the roto-inversions
Operations that do not leave invariant any point of the space : the translations

The subspace left invariant (if any) by the symmetry operation has dimensions from 0 to N (= 3 here)

Three independent directions in $E^3 \Rightarrow$ three axes (a, b, c) and three interaxial angles (α, β, γ)

$\mathbf{I} = 1$, $-\mathbf{I} = \bar{1} \Rightarrow$ Minimal point group of a Bravais lattice: $\bar{1} = \{1, \bar{1}\}$

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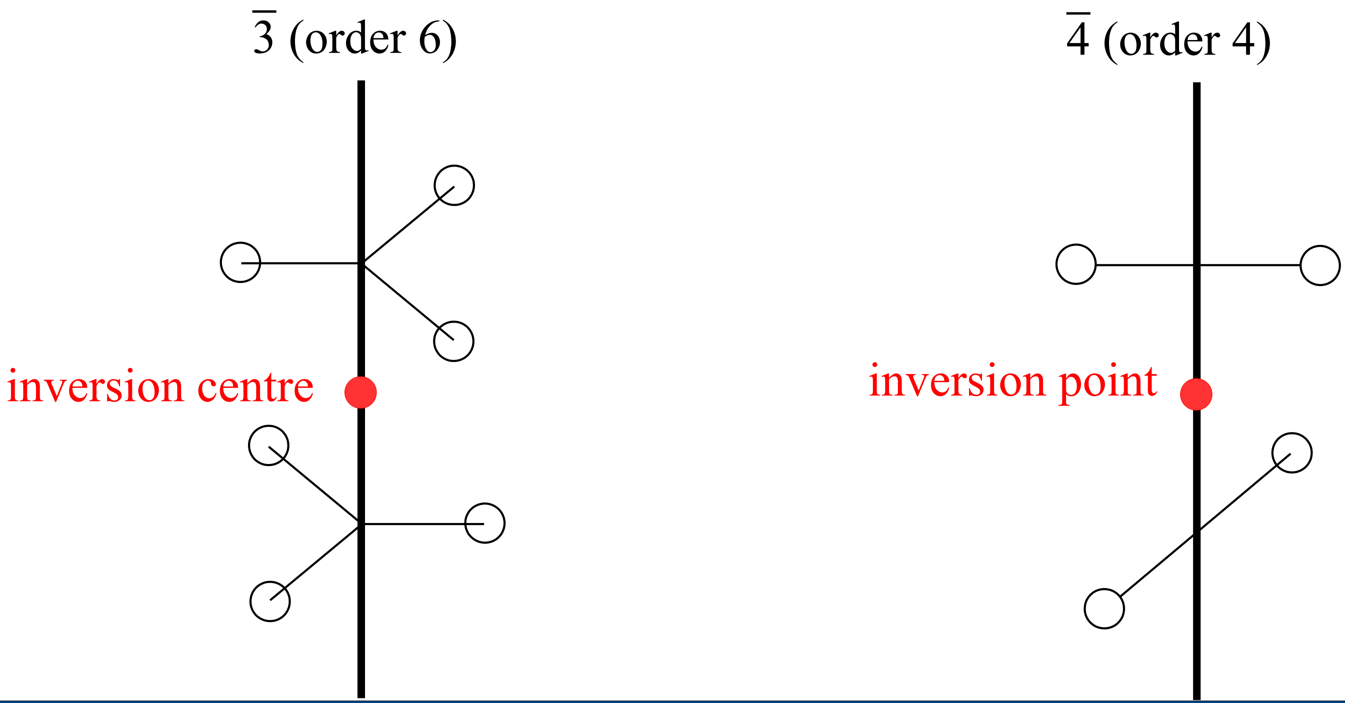
Inversion centre vs. inversion point

Rotoinversion: $\bar{n}$

On a mono-dimensional element (axis) a zero-dimensional element (point) exists:

- if n is odd, the inversion operation exists as an independent operation and the corresponding element is called an inversion **centre**;
- if n is even, the inversion operation does not exist as an independent operation and the corresponding element is an inversion **point**.



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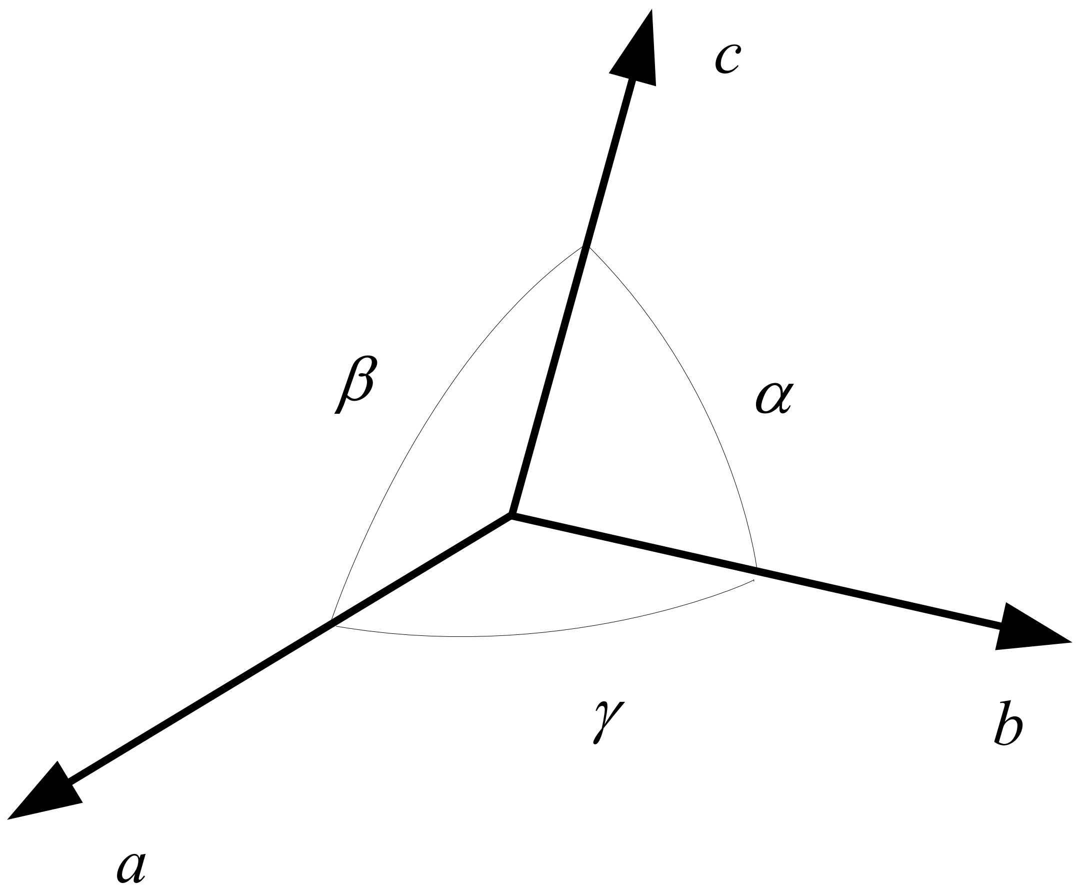
Labelling of axes and angles in E^3



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Graphic symbols for symmetry elements

n-fold rotation axis

2 2-fold rotation axis

3 3-fold rotation axis

4 4-fold rotation axis

6 6-fold rotation axis

n-fold rotoinversion axis

$\bar{1}$ one-fold rotoinversion axis (inversion centre)

$\bar{3}$ three-fold rotoinversion axis

$\bar{4}$ four-fold rotoinversion axis

$\bar{6}$ (3/*m*) six-fold rotoinversion axis

n-fold rotation axis and mirror plane perpendicular to it

2/*m*

4/*m*

6/*m*

two-fold rotoinversion axis is a mirror plane

First-kind operations

Second-kind operations

Operations including translations are introduced later

The orientation of a mirror plane is indicated by the vector normal to it

The orientation of a mirror plane is indicated by the vector normal to it

An isometry of the second kind, f_{II}, can always be expressed as $\bar{1}f_I$

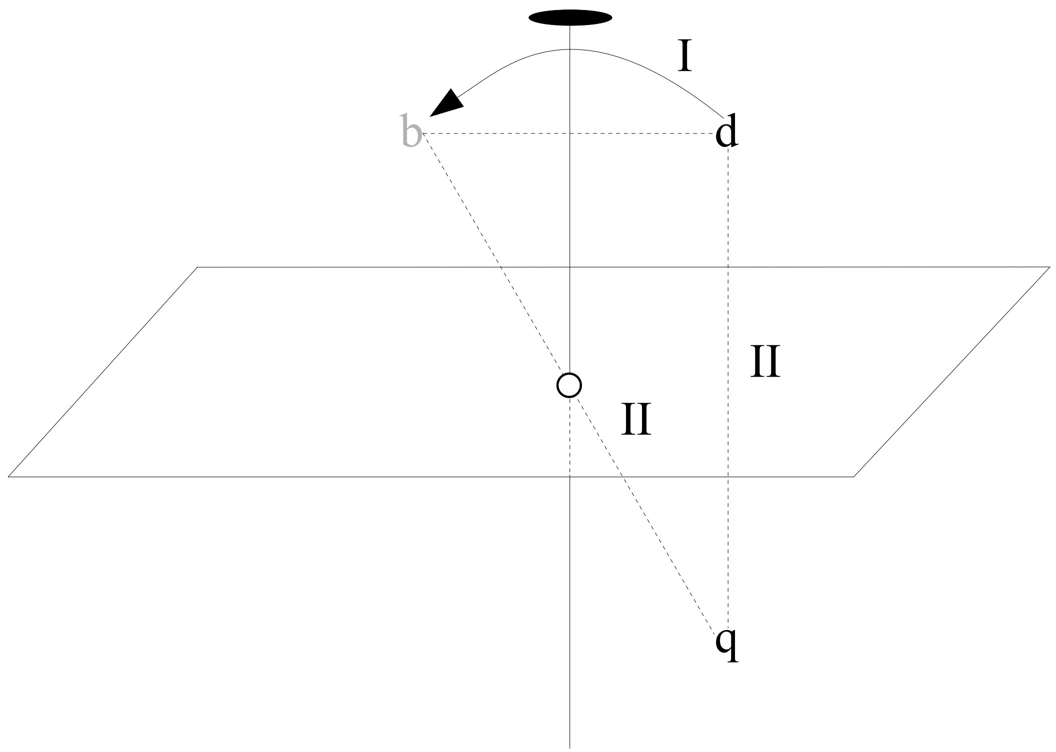
$$f_{II}\begin{bmatrix}x\\y\\z\end{bmatrix}=\begin{bmatrix}x'\\y'\\z'\end{bmatrix} \quad f_{II}\left(\bar{1}\,\bar{1}\right)\begin{bmatrix}x\\y\\z\end{bmatrix}=\begin{bmatrix}x'\\y'\\z'\end{bmatrix} \xrightarrow{\text{Associativity}} \left(f_{II}\,\bar{1}\right)\bar{1}\begin{bmatrix}x\\y\\z\end{bmatrix}=\begin{bmatrix}x'\\y'\\z'\end{bmatrix}$$

$$f_I\,\bar{1}\begin{bmatrix}x\\y\\z\end{bmatrix}=\begin{bmatrix}x'\\y'\\z'\end{bmatrix} \xrightarrow{\text{Commutativity}} \bar{1}\,f_I\begin{bmatrix}x\\y\\z\end{bmatrix}=\begin{bmatrix}x'\\y'\\z'\end{bmatrix}$$

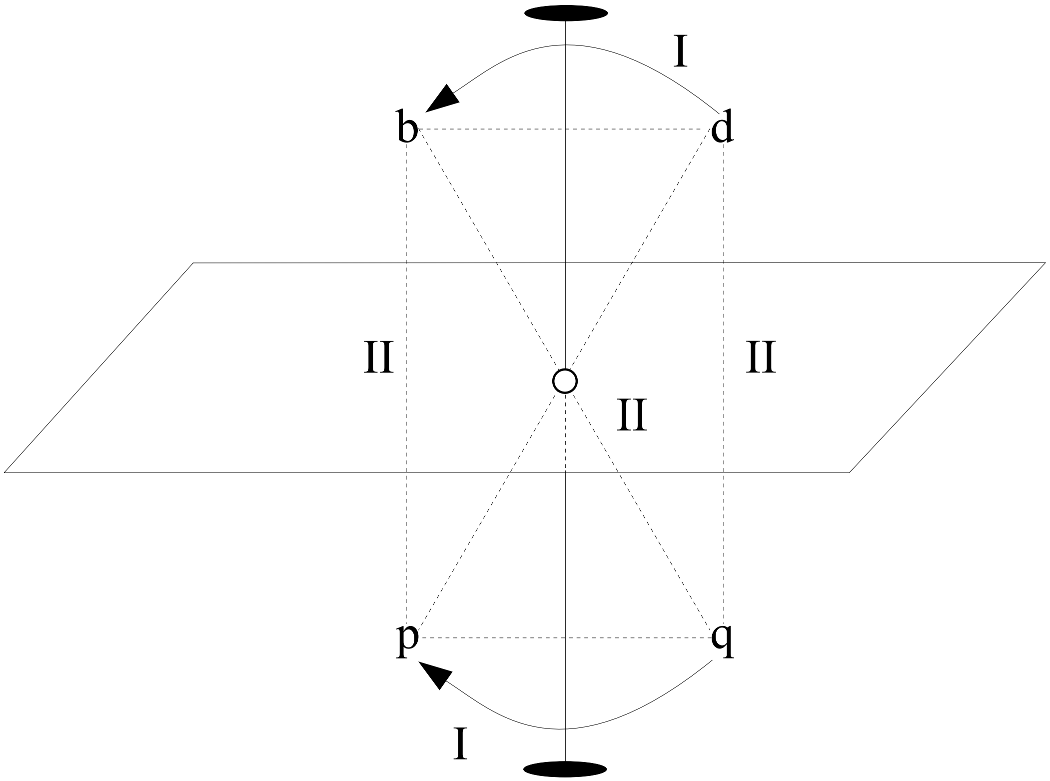
$$\bar{1}=\begin{bmatrix}\bar{1}&&\\&\bar{1}&\\&&\bar{1}\end{bmatrix}$$

If f_{II} is a symmetry operation of a given object, and if that object is not centrosymmetric, f_I is not a symmetry operation of the object.

Equivalence of $\bar{2}$ and m



Combination of 2 and $\bar{1}$ gives *m*



Applies to even-fold rotations as well, because they all "contain" a twofold rotation

$4^2 = 2; 6^3 = 2$

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Choice of the unit cell

t(1,0,0), t(0,1,0), t(0,0,1) : **Primitive cell** (*P*)

t(1,0,0), t(0,1,0), t(0,0,1), t(0,½,½): *A*

t(1,0,0), t(0,1,0), t(0,0,1), t(½,0,½): *B*

t(1,0,0), t(0,1,0), t(0,0,1), t(½,½,0): *C*

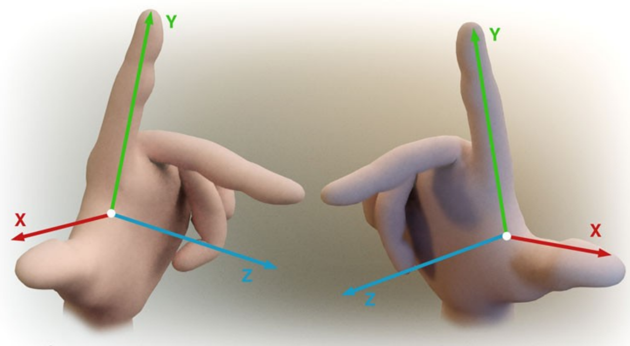
t(1,0,0), t(0,1,0), t(0,0,1), t(½,½,½): *I*

t(1,0,0), t(0,1,0), t(0,0,1), t(½,½,0), t(½,0,½), t(0,½,½): *F*

t(1,0,0), t(0,1,0), t(0,0,1), t(⅔,⅓,0), t(⅓,⅔,0): *H*

t(1,0,0), t(0,1,0), t(0,0,1), t(⅔,⅓,⅓), t(⅓,⅔,⅔): *R*

t(1,0,0), t(0,1,0), t(0,0,1), t(⅓,⅓,⅓), t(⅔,⅔,⅔): *D*



Conventional unit cell

1. the basis vectors **a**, **b**, **c** form a right-handed reference;
2. edges of the cell are parallel to the symmetry directions of the lattice (if any);
3. if more than one unit cell satisfies the above condition, the smallest one is the conventional cell.

Reduced cell

1. the basis vectors **a**, **b**, **c** form a right-handed reference;
2. its faces are two-dimensional reduced unit cells and its edges are not longer than its diagonals; concretely:
   a. basis vectors correspond to the shortest lattice translation vectors;
   b. the angles between pairs of basis vectors are either all acute (type I reduced cell) or non-acute (type II reduced cell).

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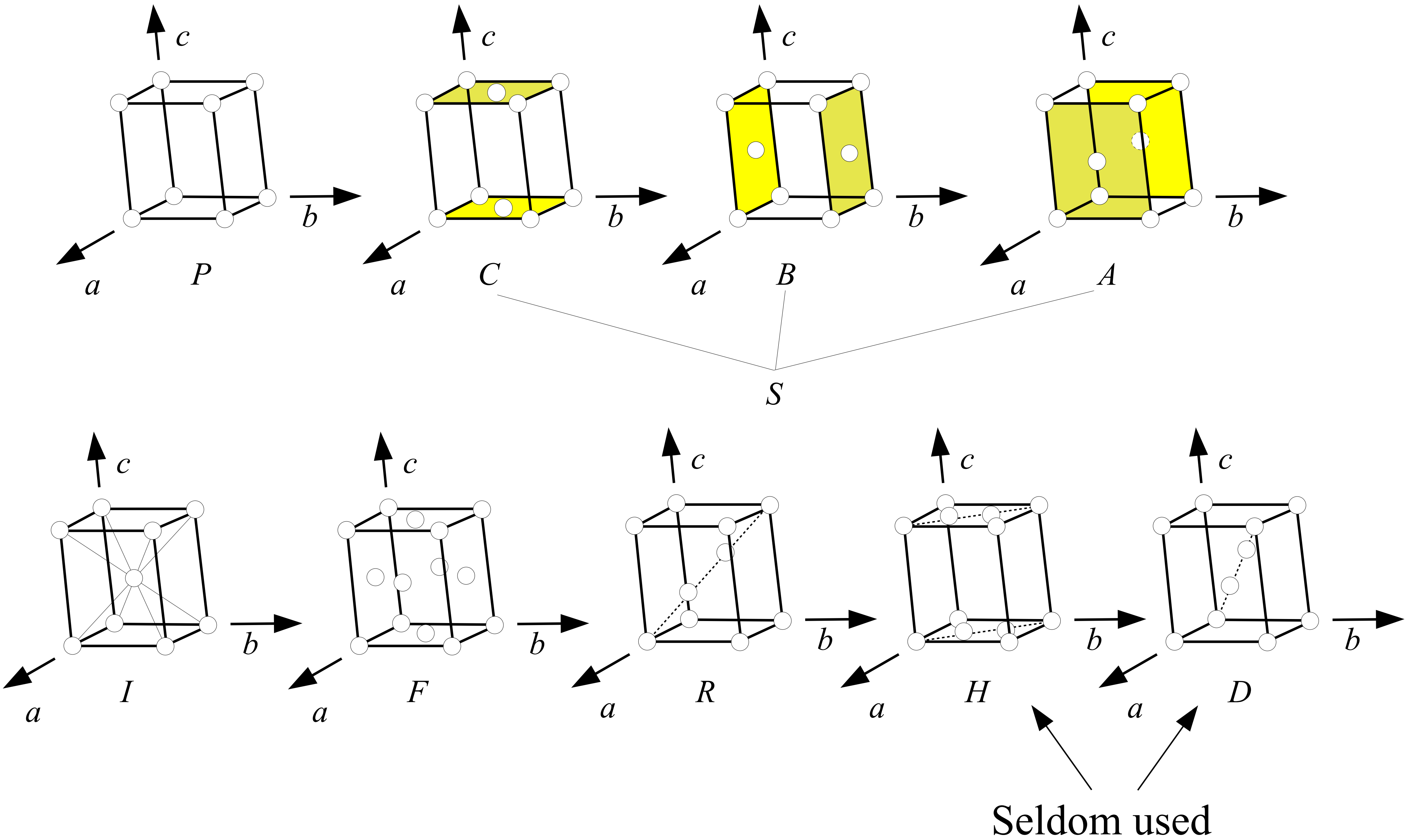
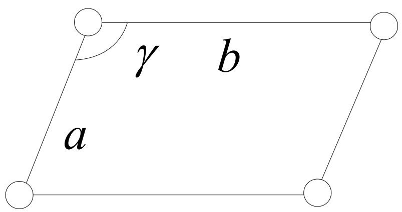
Types of unit cells that bring a letter in E^3



Crystal families and types of lattices in E^3: the triclinic (*a*northic) family



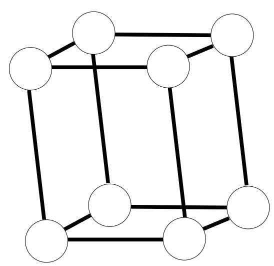
mp

+ a third direction inclined on the plane

2D ⟶ 3D

$2 \longrightarrow 1 \otimes \bar{1} = \bar{1}$

triclinic crystal family (***a***northic)



aP

- One symmetry element: the inversion centre
- No symmetry direction
- The conventional unit cell is not defined – no reason to choose *a priori* a centred cell
- Point group of the lattice: $\bar{1}$
- No restriction on a, b, c, α, β, γ

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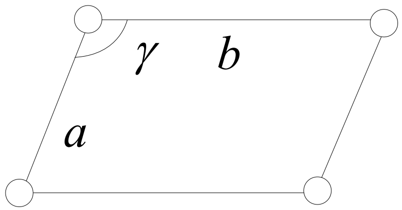
Crystal families and types of lattices in E^3: the ***m***onoclinic family

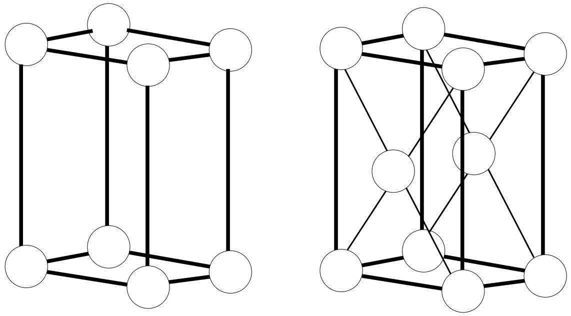


mp

+ a third direction perpendicular to the plane

2D ⟶ 3D

$2 \longrightarrow 2 \otimes \bar{1} = 2/m$

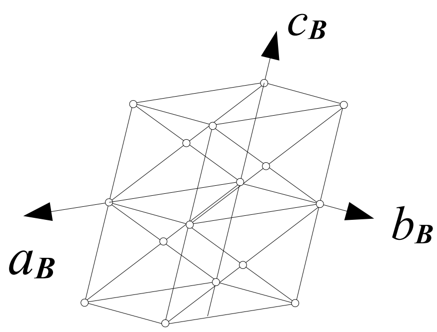


mP   *mS*

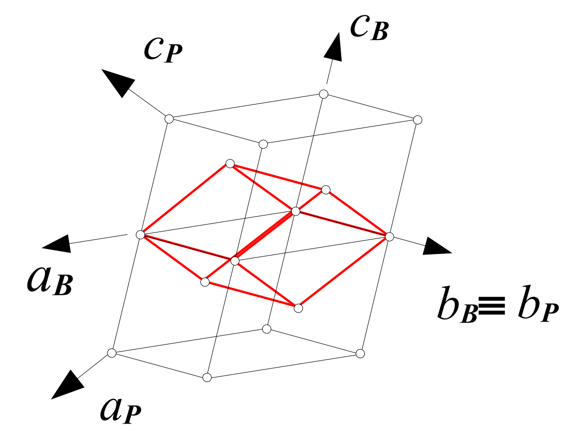
monoclinic crystal family

- One symmetry direction (***usually*** taken as the *b* axis).
- The conventional unit cell has two right angles (α and γ)
- Point group of the lattice: $2/m$
- Two independent types of unit cell respect these conditions

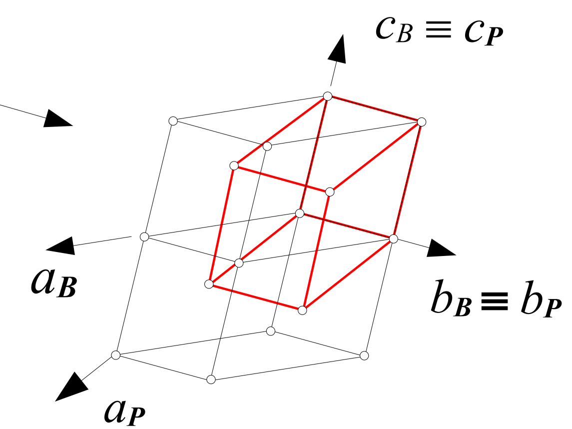
A lattice of type *mP* is equivalent to *mB*



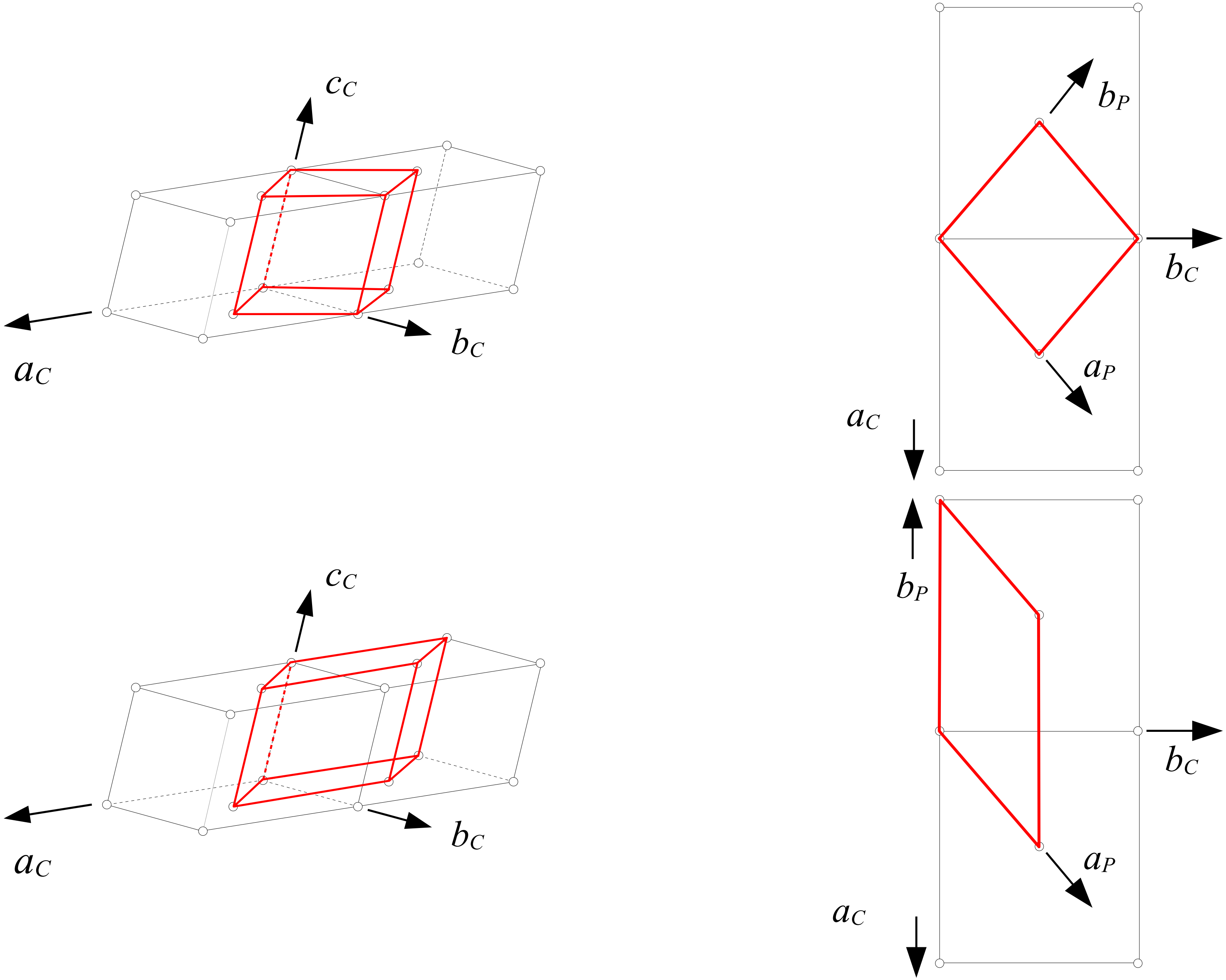
$\mathbf{a}_P = (\mathbf{a}_B - \mathbf{c}_B)/2$; $\mathbf{c}_P = (\mathbf{a}_B + \mathbf{c}_B)/2$



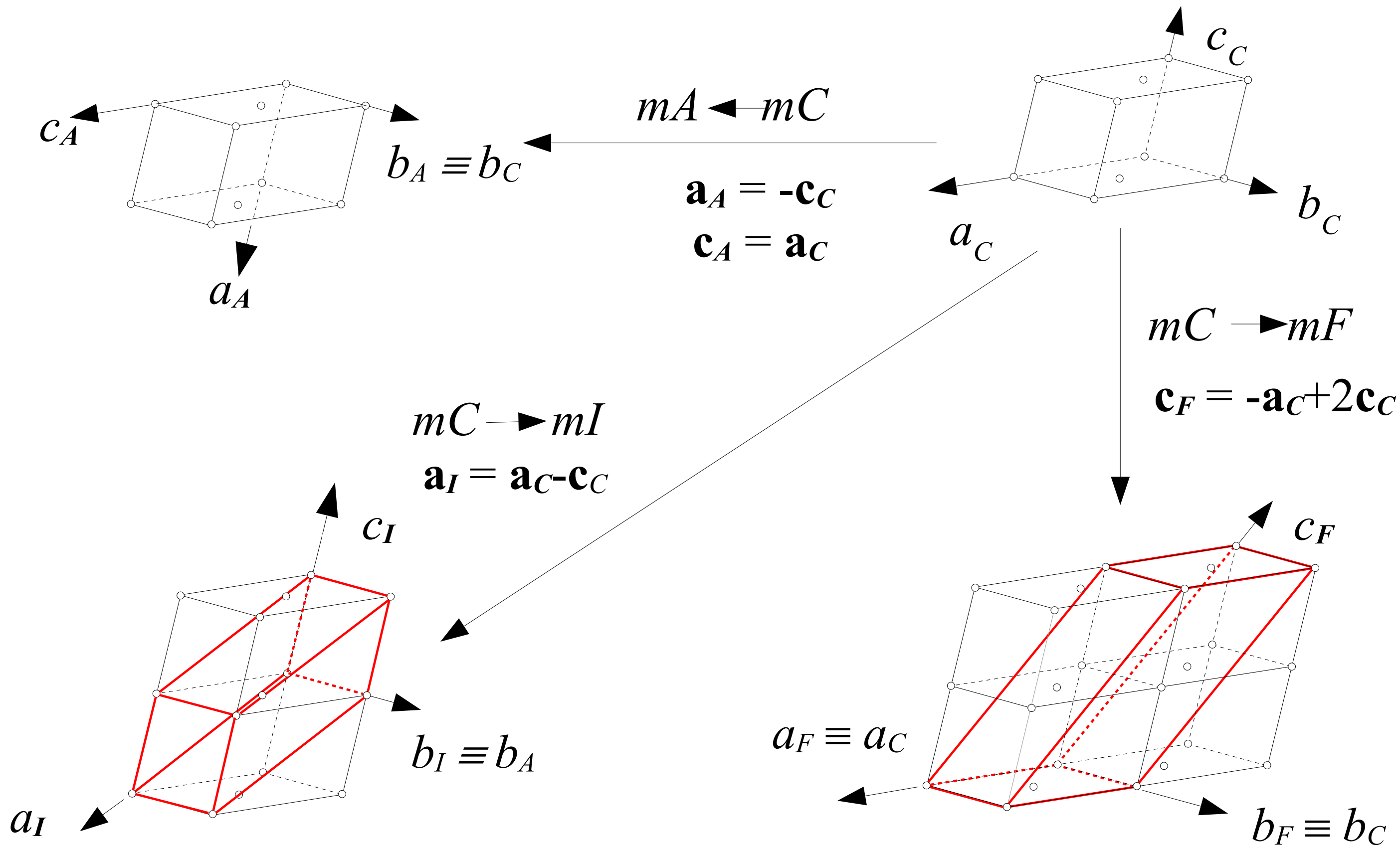
$\mathbf{a}_P = (\mathbf{a}_B - \mathbf{c}_B)/2$



A lattice of type *mP* is NOT equivalent to *mC*



Lattices of type *mC*, *mA*, *mI* and *mF* are all equivalent



Three monoclinic settings

b-unique

β unrestricted by symmetry

$mB = mP$
$mA = mC = mI = mF$

c-unique

γ unrestricted by symmetry

$mC = mP$
$mA = mB = mI = mF$

a-unique

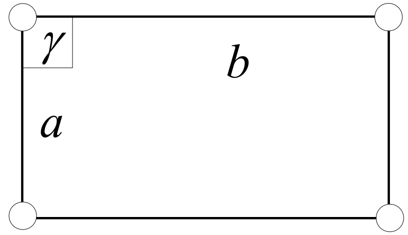
α unrestricted by symmetry

$mA = mP$
$mB = mC = mI = mF$

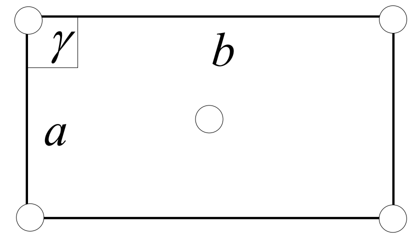
The symbol of a monoclinic space group will change depending on which setting and what type of unit cell you choose, leading to up to **21** possible symbols for a monoclinic space group (the “monoclinic monster”).

http://dx.doi.org/10.1107/S2053273316009293

Crystal families and types of lattices in E^3: the ***o***rthorhombic family



op



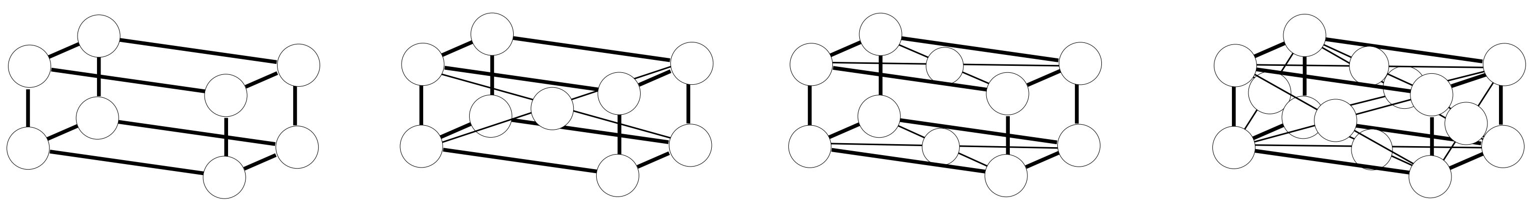
oc

+ a third direction perpendicular to the plane

orthorhombic crystal family

2D → 3D

$2mm \longrightarrow 2mm \otimes \bar{1} = 2/m2/m2/m$



oP *oI* *oS* *oF*

- Three symmetry directions (axes *a*, *b*, *c*)
- The conventional unit cell has three right angles (α, β, γ)
- Point group of the lattice: $2/m\ 2/m\ 2/m$
- Four types of cell respect these conditions
- The unit cell with one pair of faces centred can be equivalently described as *A*, *B* or *C* by a permutation of the (collective symbol : *S*)

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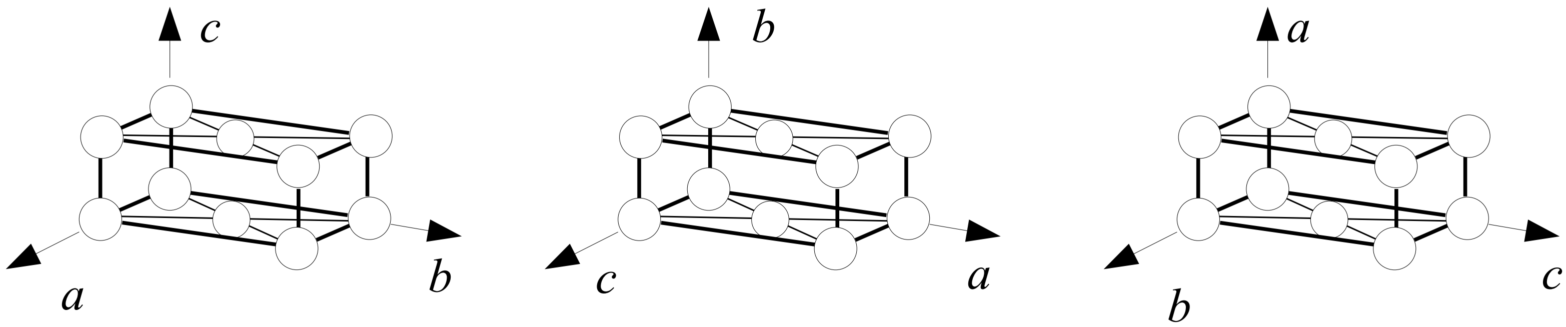
Three possible setting for the *oS* type of lattice in E^3



oC ***oB*** ***oA***

oS

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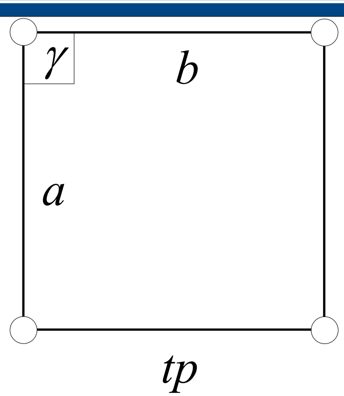
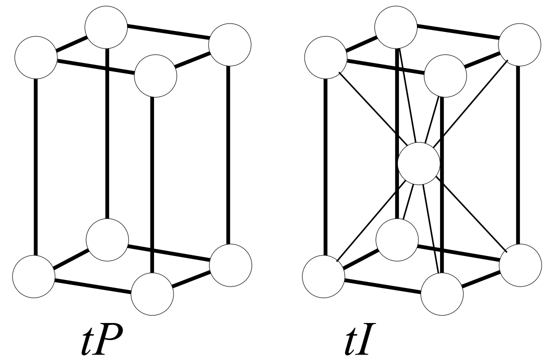
Crystal families and types of lattices in E^3: the *t*etragonal family





2D → 3D

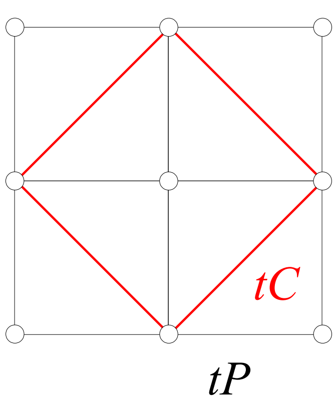
$4mm \rightarrow 4mm \otimes \bar{1}$

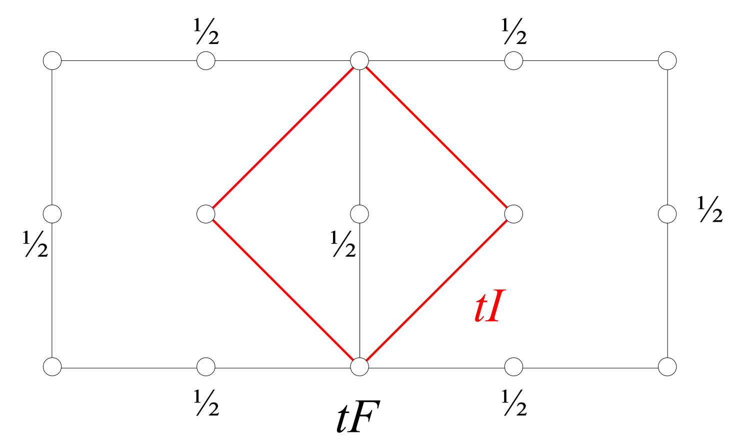
$= 4/m2/m2/m$

+ a third direction perpendicular to the plane

***t*etragonal crystal family**

- Five symmetry directions (*c*, *a*&*b*, the two diagonals in the *a*-*b* plane)
- Point group of the lattice: $4/m\ 2/m\ 2/m$
- The conventional cell has three right angles and two identical edges
- Two independent types of unit cell respect these conditions: *tP* (equivalent to *tC*) and *tI* (equivalent to *tF*)





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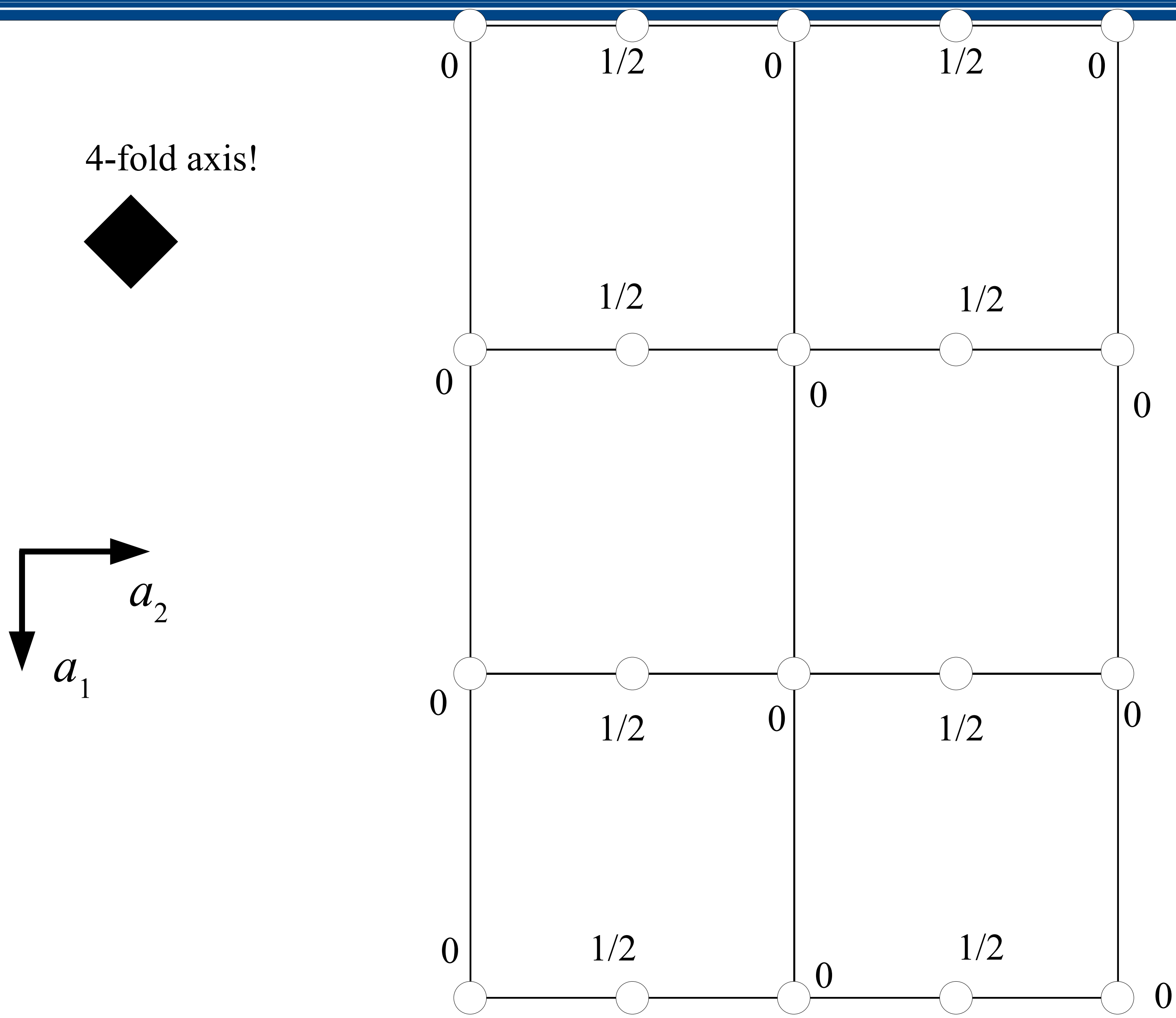
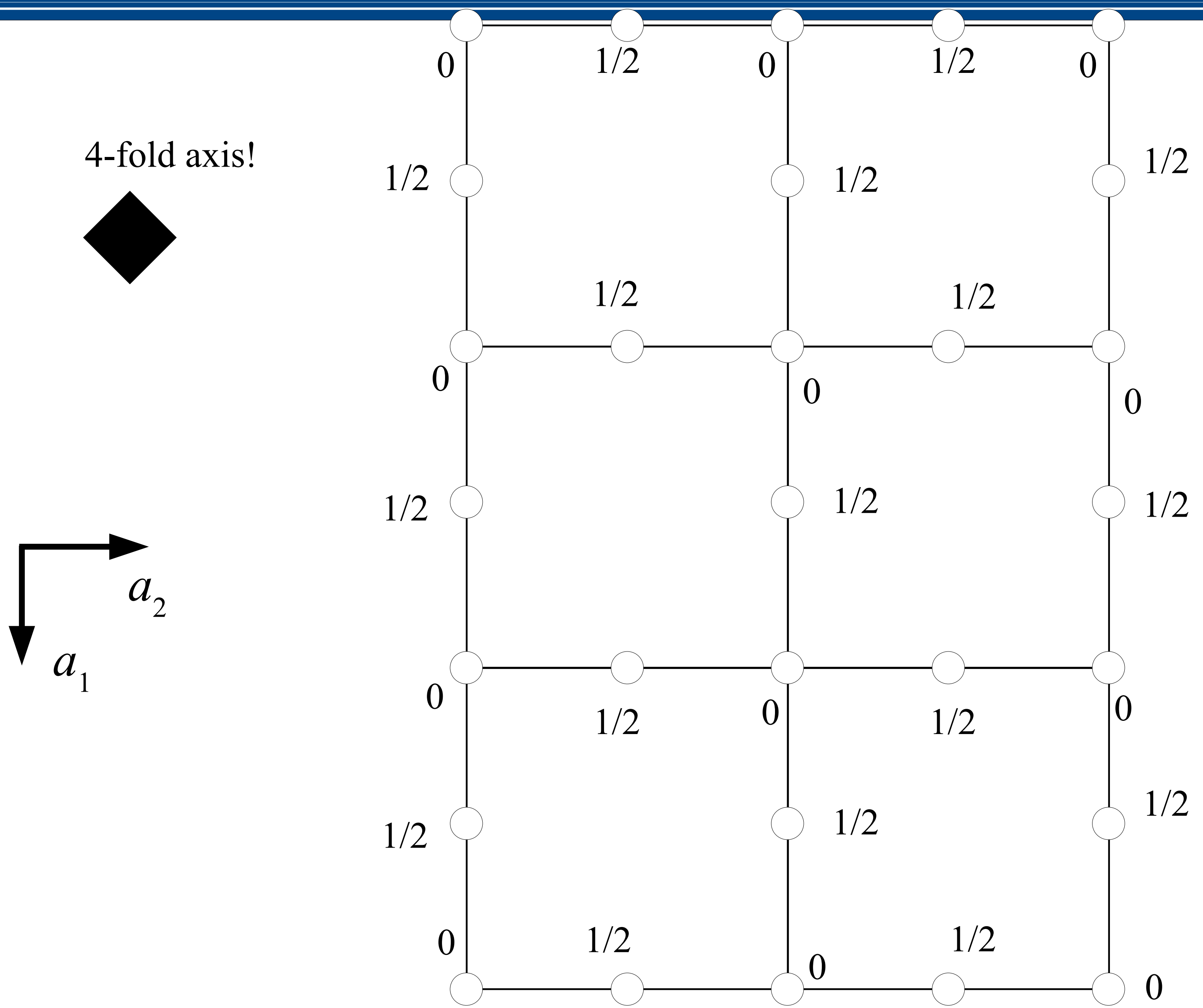
Why unit cells of type *tA* et *tB* cannot exist?

4-fold axis!



Why unit cells of type *tA* et *tB* cannot exist?



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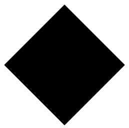
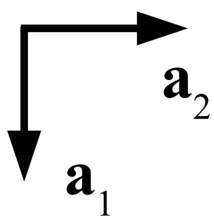
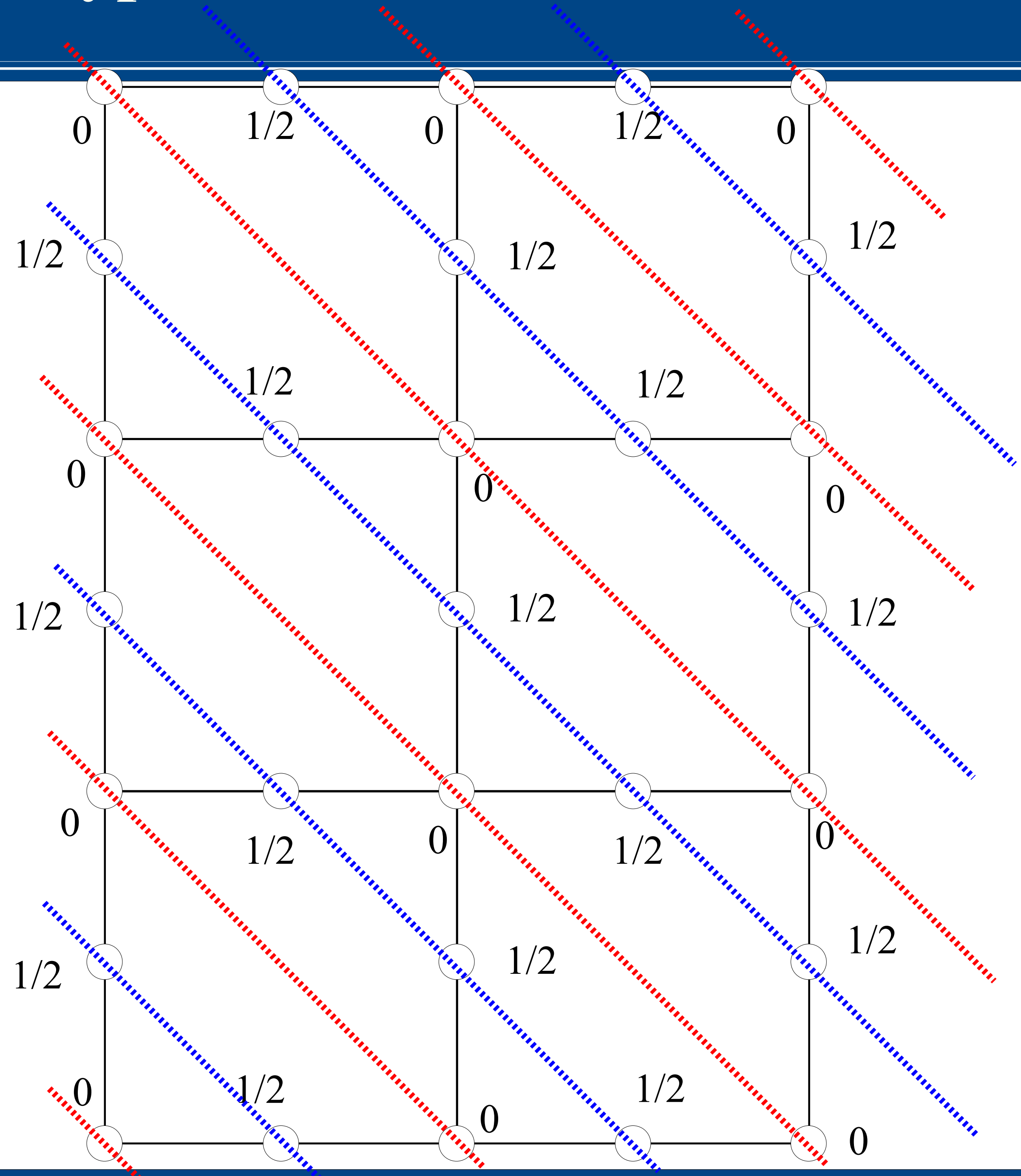
Why unit cells of type *tA* et *tB* cannot exist?

4-fold axis!

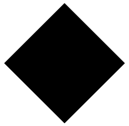


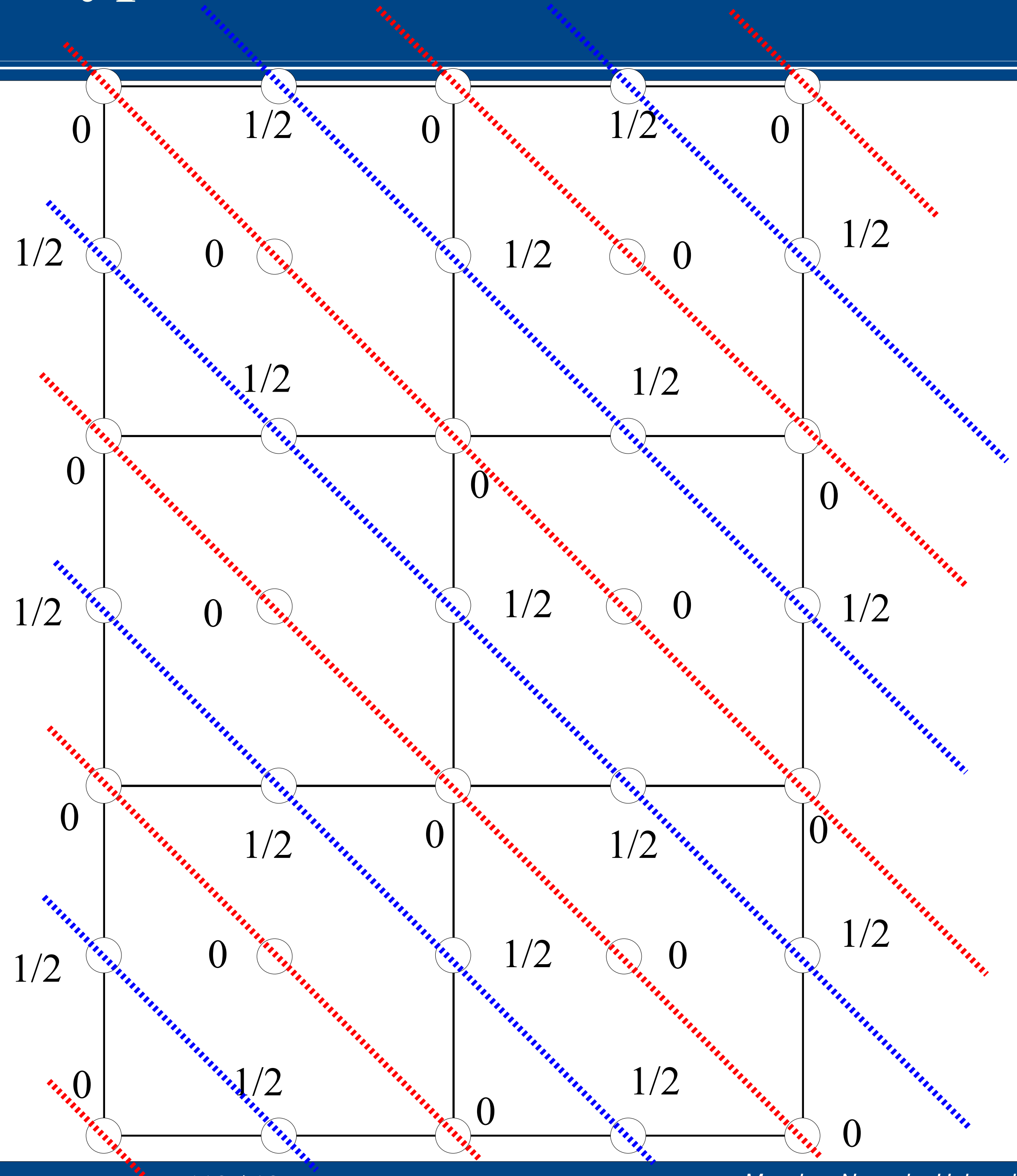


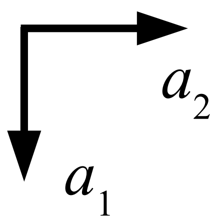


Why unit cells of type *tA* et *tB* cannot exist?

4-fold axis!







tF!

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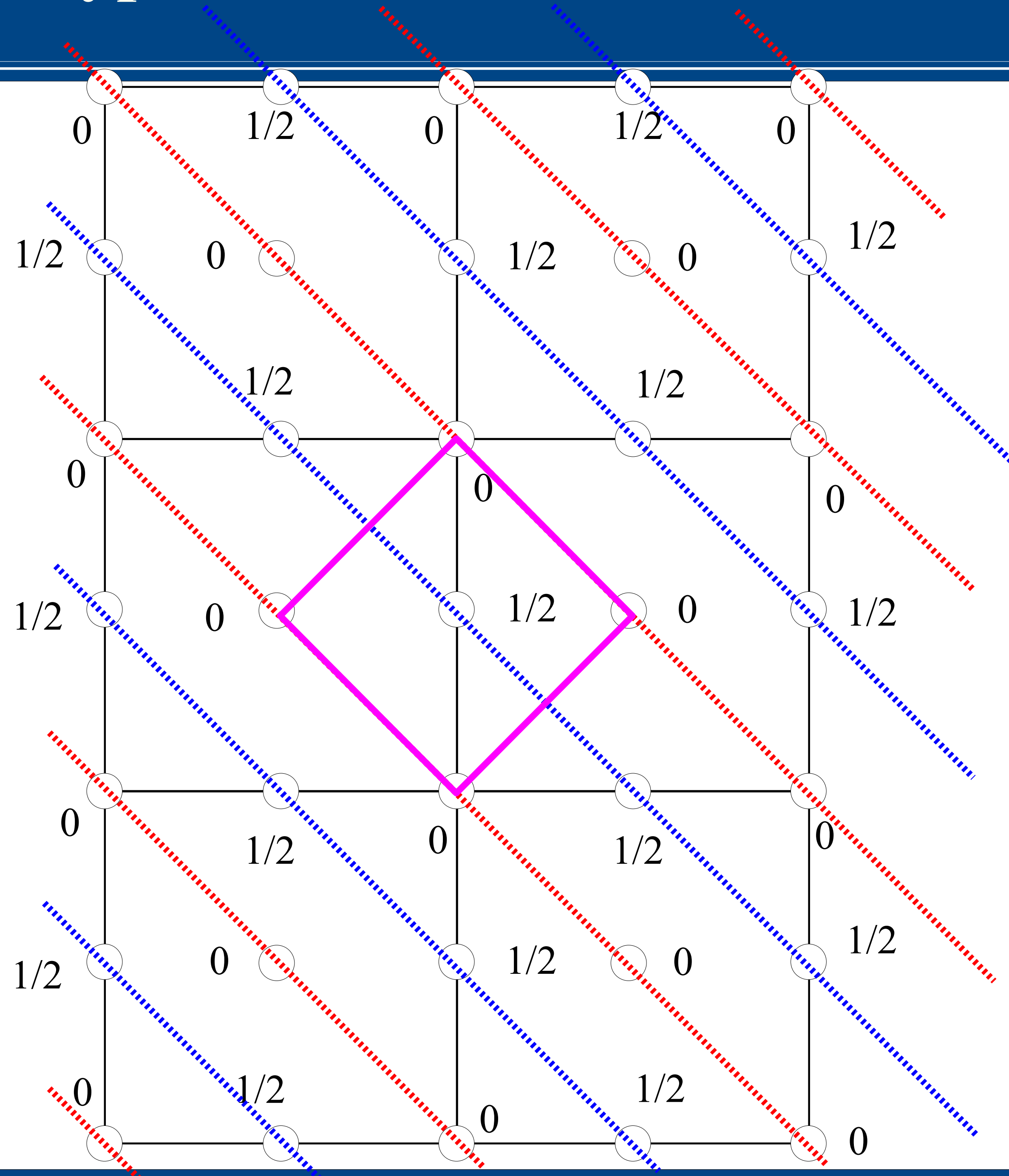
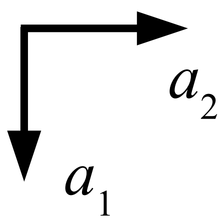
Why unit cells of type *tA* et *tB* cannot exist?

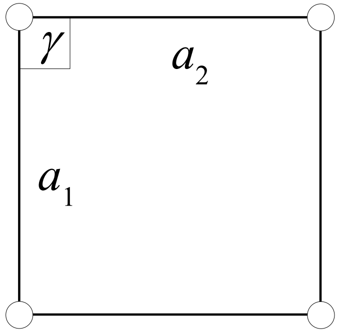
4-fold axis!





tF! → ***tI!***

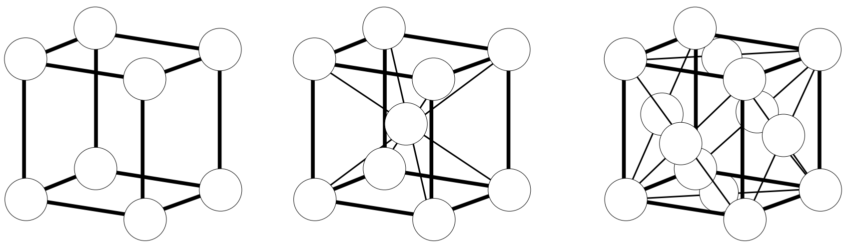
Crystal families and types of lattices in E^3: the <u>***c***</u>ubic family



tp

+ a third direction perpendicular to the plane AND $c = a = b$

cubic crystal family



cP *cI* *cF*

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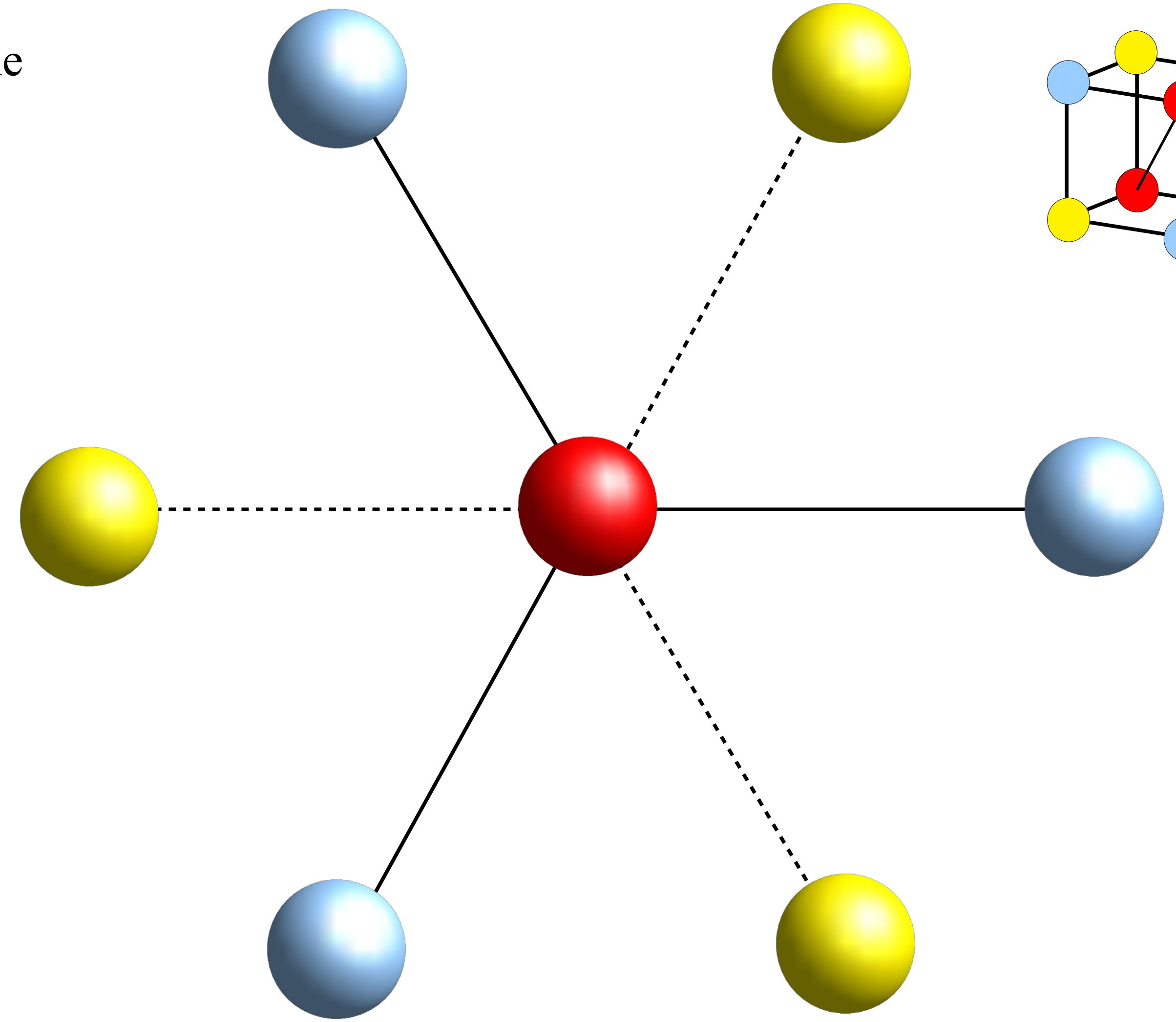
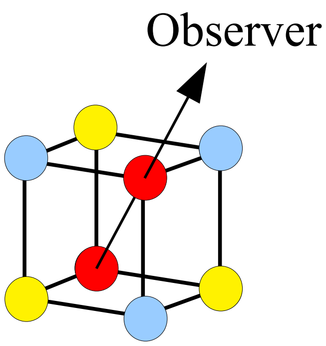
Three-fold rotoinversion along the ⟨111⟩ direction

First and fourth plane from the observer

Second plane from the observer

Third plane from the observer





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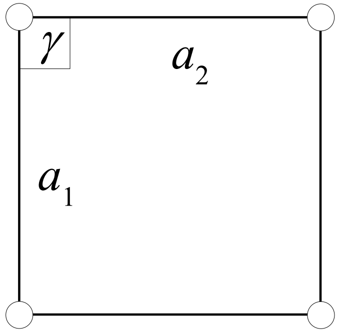
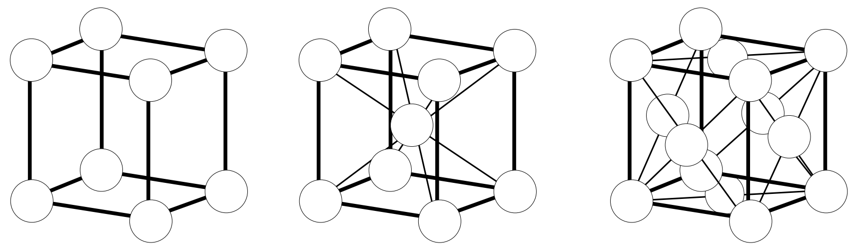
Crystal families and types of lattices in E^3: the *c*ubic family



tp

+ a third direction perpendicular to the plane AND $c = a = b$



cP *cI* *cF*

cubic crystal family

2D ⟶ 3D

$4mm \longrightarrow 4mm \otimes \bar{3} = 4/m\bar{3}2/m$

- Thirteen symmetry directions (the 3 axes; the 4 body diagonals ; the six face diagonals)
- Point group of the lattice: $4/m\ \bar{3}\ 2/m$
- The conventional unit cell has three right angles and three identical edges
- Three types of unit cell respect these conditions : c*P*, *cI* et *cF*

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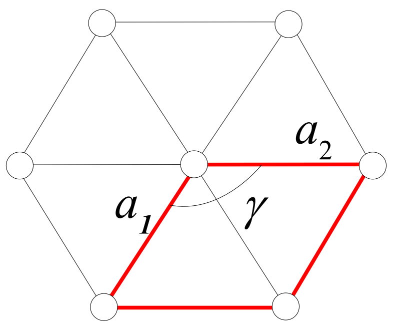
Crystal families and types of lattices in E^3: the *h*exagonal family



hp

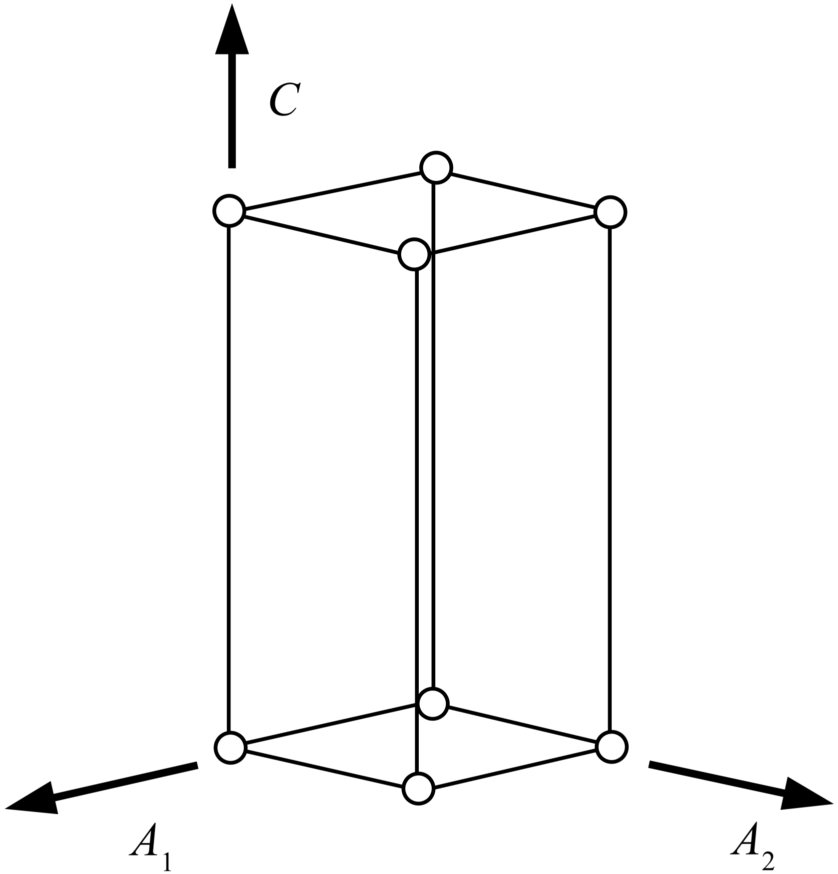
+ a third direction perpendicular to the plane

2D ⟶ 3D

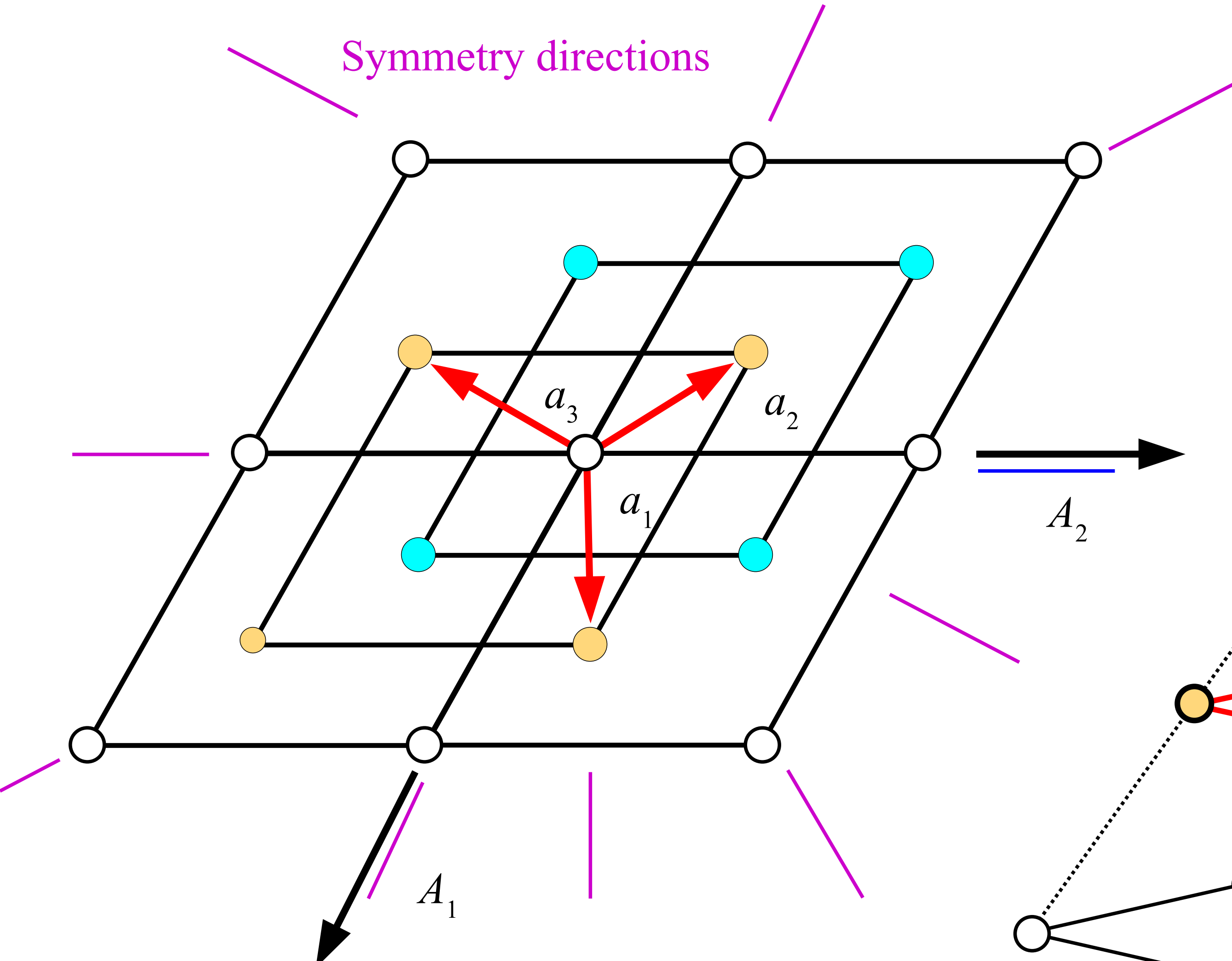
$6mm \longrightarrow 6mm \otimes \bar{1} = 6/m2/m2/m$

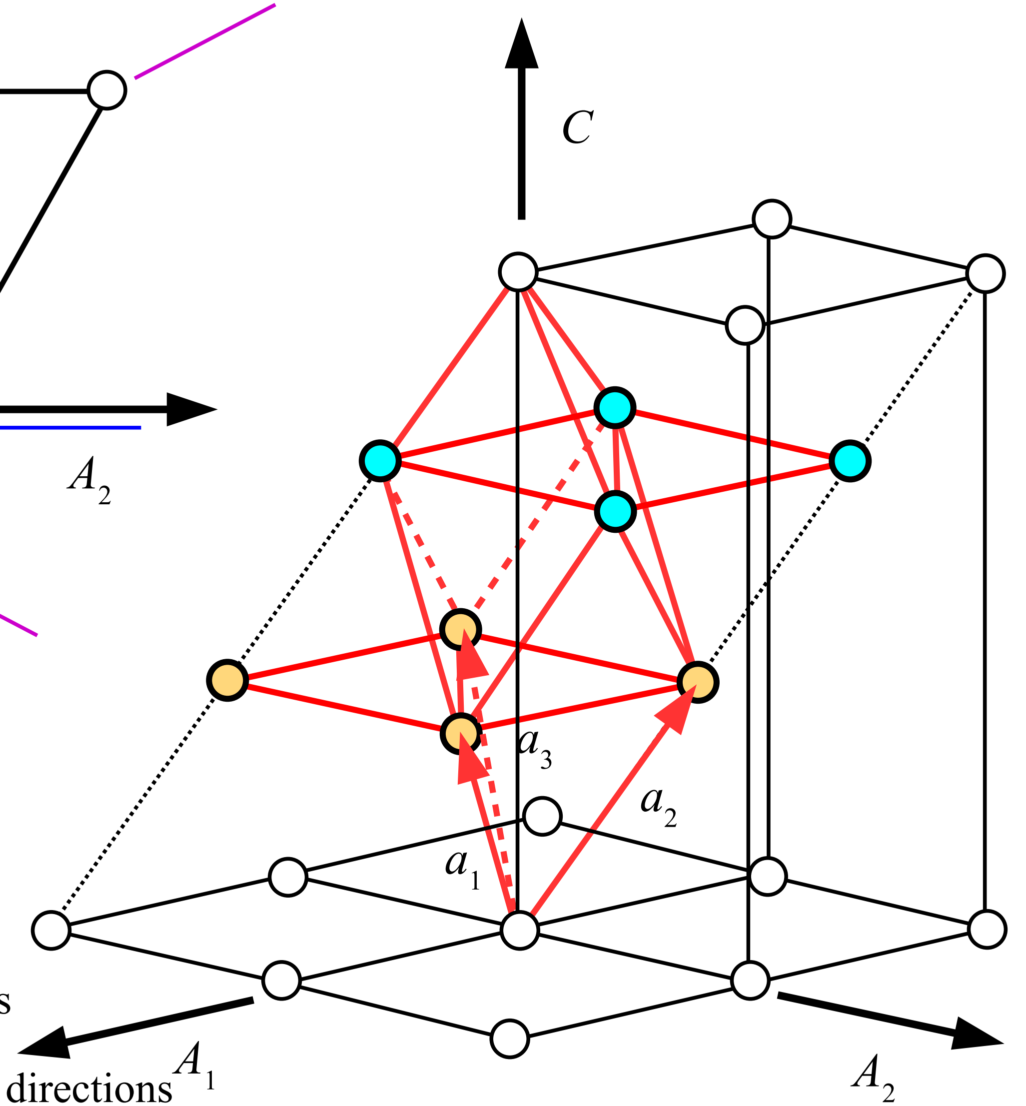
***h*exagonal crystal family**

+ a new type of unit cell!



Peculiarity of the *h*exagonal crystal family in E^3



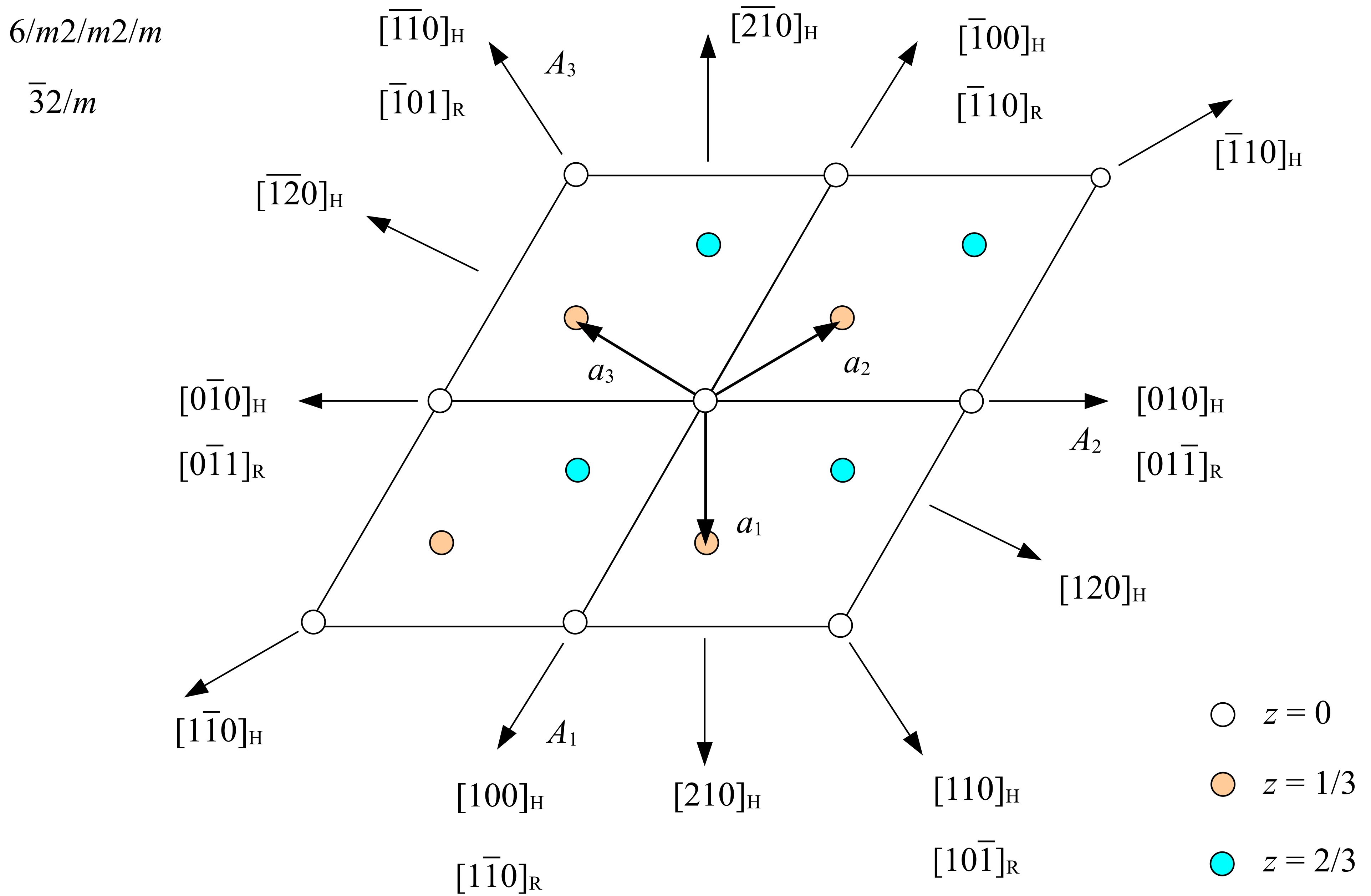


A_1, A_2, C hexagonal axes parallel to the symmetry directions

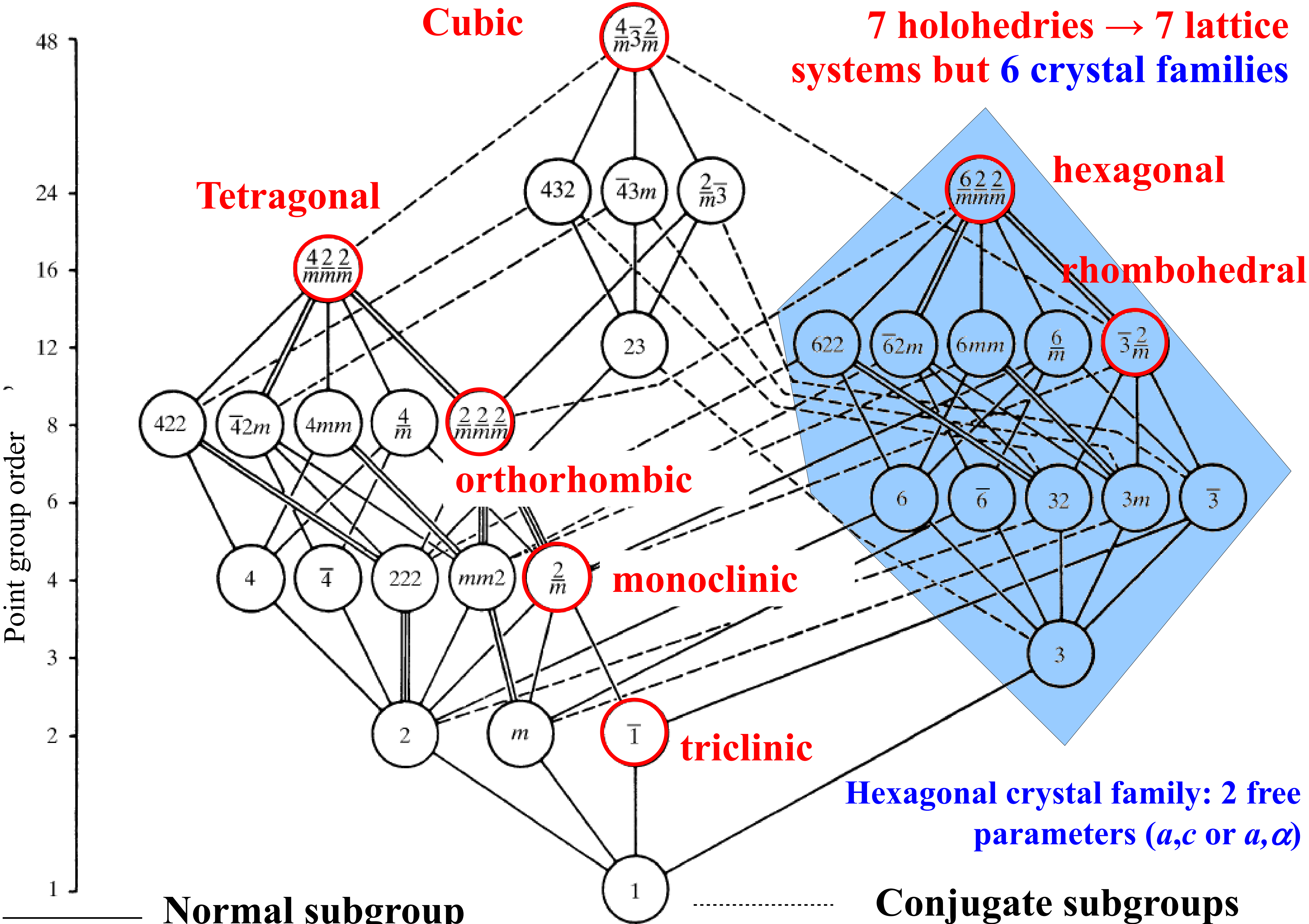
a_1, a_2, a_3 rhombohedral axes **NOT** parallel to the symmetry directions

Two types of lattice with different symmetry in the hexagonal crystal family

Symmetry difference between *hP* and *hR* types of lattice



7 holohedries → 7 lattice systems but 6 crystal families

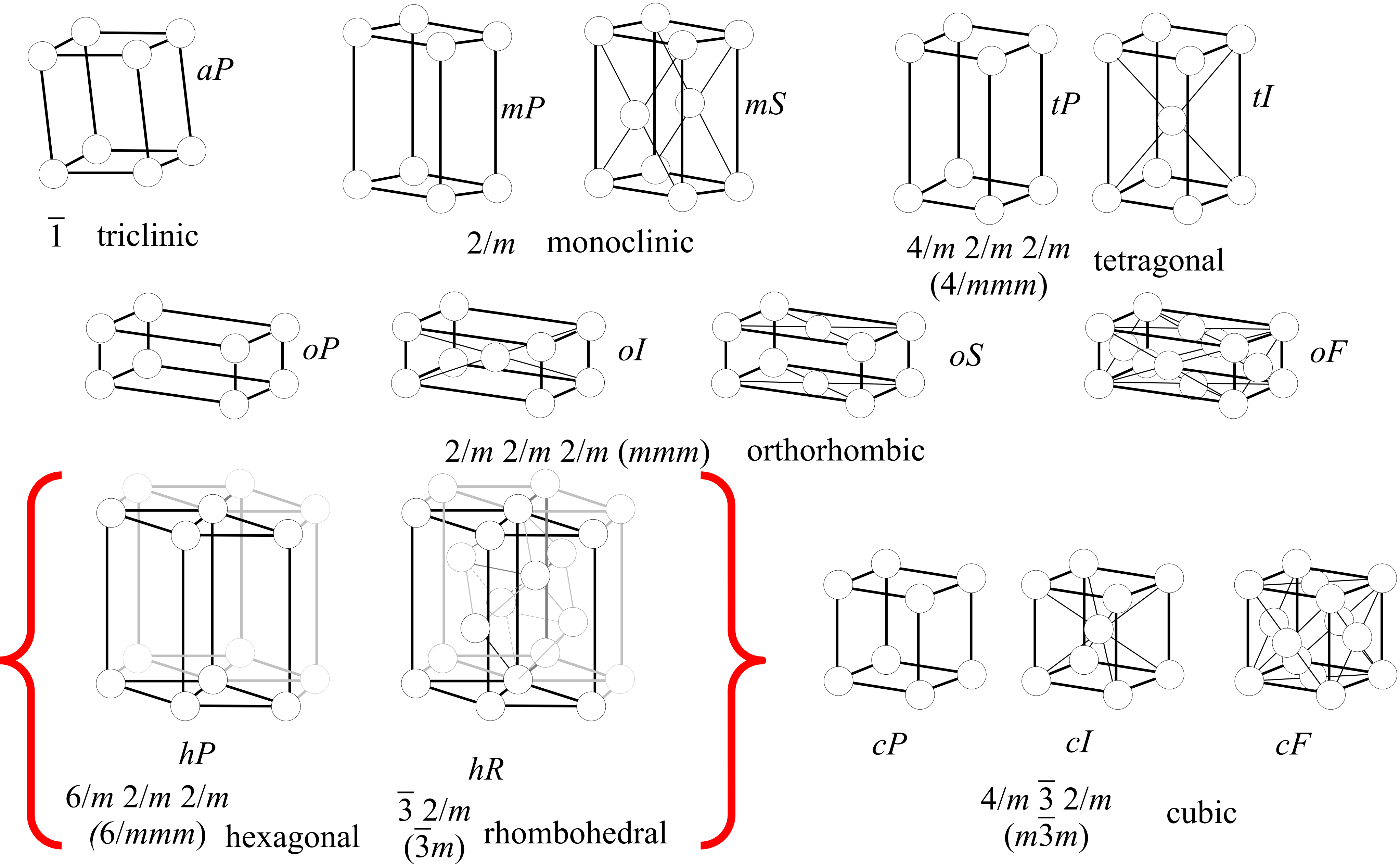


Hexagonal crystal family: 2 free parameters (a,c or a,α)

Normal subgroup

Conjugate subgroups

Lattice systems: classification based on the symmetry of the lattices



Crystal systems: morphological (macroscopic) and physical symmetry

Type of group (in bold the holohedries)	*aP*	*mP*	*mS*	*oP*	*oS*	*oI*	*oF*	*tP*	*tI*	*hR*	*hP*	*cP*	*cI*	*cF*	Crystal system
1, $\mathbf{\bar{1}}$	☑	☑	☑	☑	☑	☑	☑	☑	☑	☑	☑	☑	☑	☑	triclinic
2, m, $\mathbf{2/m}$		☑	☑	☑	☑	☑	☑	☑	☑	☑	☑	☑	☑	☑	monoclinic
222, $mm2$, $\mathbf{2/m2/m2/m}$				☑	☑	☑	☑	☑	☑		☑	☑	☑	☑	orthorhombic
4, $\bar{4}$, 422, $\bar{4}2m$, $4/m$, $4mm$, $\mathbf{4/m2/m2/m}$								☑	☑			☑	☑	☑	tetragonal
3, $\bar{3}$, $3m$, 32, $\mathbf{\bar{3}2/m}$										☑	☑	☑	☑	☑	trigonal
6, $\bar{6}$, 622, $\bar{6}2m$, $6/m$, $6mm$, $\mathbf{6/m2/m2/m}$											☑				hexagonal
23, $m\bar{3}$, 432, $\bar{4}3m$, $\mathbf{4/m\bar{3}2/m}$												☑	☑	☑	cubic
No. of free parameters	6	4	4	3	3	3	3	2	2	2	2	2	2	1	

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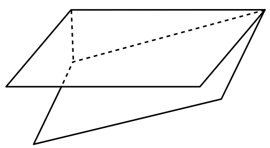
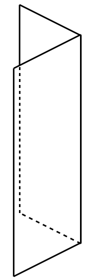
Crystal systems: morphological (macroscopic) and physical symmetry



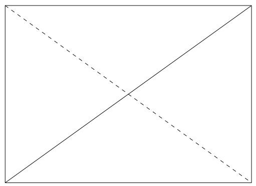
A_1
1 or $\bar{1}$

triclinic



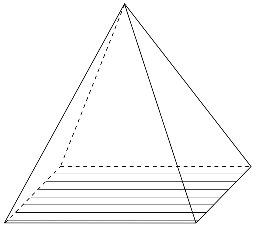
A_2
2 or *m* or 2/*m*

monoclinic



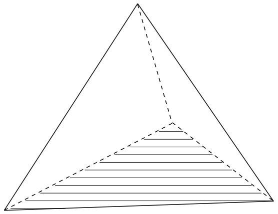
$3\times A_2$
Three twofold elements

orthorhombic



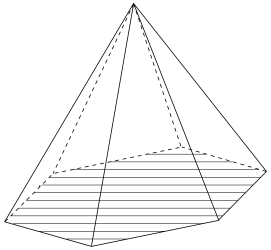
A_4

tetragonal



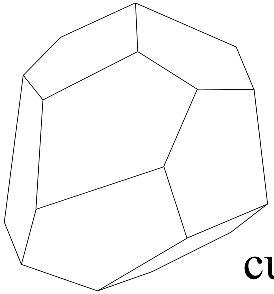
A_3

trigonal



A_6

hexagonal



$4\times A_3$

cubic

$A_n = n$ or $\bar{n}$

Crystal families, crystal systems, lattice systems and types of Bravais lattices in E^3

6 crystal families	**conventional unit cell**	**7 crystal systems** (morphological symmetry)	**7 lattice systems** (lattice symmetry)	**14 types of Bravais lattices**(**)
a = *a*nortic* (triclinic, asynmetric, tetartoprismac...)	no restriction on a ; b ; c, α , β , γ	triclinic	triclinic	*aP*
m = *m*onoclinic (clinorhombic, monosymmetric, binary, hemiprismatic, monoclinohedral, ...)	no restriction on a ; b ; c ; β. $\alpha = \gamma = 90°$	monoclinic	monoclinic	*mP* (*mB*)
				mS (*mC, mA, mI, mF*)
o = *o*rthorhombic (rhombic, trimetric, terbinary, prismatic, anisometric,...)	no restriction on a ; b ; c. $\alpha = \beta = \gamma = 90°$	orthorhombic	orthorhombic	*oP*
				oS (*oC, oA, oB*)
				oI
				oF
t = *t*etragonal (quadratic, dimetric, monodimetric, quaternary...)	$a = b$; $\alpha = \beta = \gamma = 90°$ no restriction on c	tetragonal	tetragonal	*tP* (*tC*)
				tI (*tF*)
h = *h*exagonal (senaiey, monotrimetric...)	$a = b$; $\alpha = \beta = 90°$, $\gamma = 120°$ no restriction on c	trigonal (ternary...) (***)	rhombohedral	*hR*
		hexagonal	hexagonal	*hP*
c = *c*ubic (isometric, monometric, triquaternary, regular, tesseral, tessural...)	$a = b = c$ $\alpha = \beta = \gamma = 90°$	cubic	cubic	*cP* *cI* *cF*

(*) Synonyms within parentheses.
(**) S = one pair of faces centred. Within parentheses the types of lattices that are equivalent (axial setting change – see the monoclinic example).
(***) Crystals of the trigonal crystal system may have a rhombohedral or hexagonal lattice

Interpretation of the Hermann-Mauguin symbol of a point group

In the three-dimensional space, the Hermann-Mauguin symbol of a space group contains up to three placeholders. A symbol in each of the three positions shows the symmetry element along the corresponding lattice direction.

First position	Second position	Third position

Only **1**or $\bar{\mathbf{1}}$: **triclinic** crystal system

Only one two-fold rotation or rotoinversion (*m*):
monoclinic crystal system

Three two-fold rotation or rotoinversions (*m*):
orthorhombic crystal system

4or $\bar{\mathbf{4}}$ in the first position, without 3 and $\bar{3}$ in the second position : **tetragonal**系crystal system

3or $\bar{\mathbf{3}}$ in the <u>first</u> position : **trigonal** crystal system

6 or $\bar{\mathbf{6}}$ in the first position : **hexagonal** crystal system

3or $\bar{\mathbf{3}}$ in the <u>second</u> position (with or without 4 or $\bar{4}$ in the first position) : **cubic** crystal system

Symmetry directions of the lattices in the three-dimensional space (directions in the same box are equivalents by symmetry)

Lattice system	Symmetry restrictions on the parameters of the conventional cell		First symmetry direction	Second symmetry direction	Third symmetry direction
triclinic	No restriction on any parameter		———	———	———
monoclinic (b-unique)	$\alpha = \gamma = 90^\circ$ No restriction on a; b; c; β		[010]	———	———
orthorhombic	$\alpha = \beta = \gamma = 90^\circ$ No restriction on a; b; c		[100]	[010]	[001]
tetragonal	$a = b$; $\alpha = \beta = \gamma = 90^\circ$ No restriction on c		[001]	[100] [010] $\equiv \langle 100 \rangle$	[110] $[1\bar{1}0] \equiv \langle 1\bar{1}0 \rangle$
rhombohedral	rhombohedral axes	$a = b = c$ $\alpha = \beta = \gamma$	[111]	$[1\bar{1}0]$ $[01\bar{1}]$ $[\bar{1}01]$ $\equiv \langle \bar{1}10 \rangle$	———
	hexagonal axes	$a = b$; $\alpha = \beta = 90^\circ$; $\gamma = 120^\circ$ No restriction on c	[001]	[100] [010] $[\bar{1}\bar{1}0]$ $\equiv \langle 100 \rangle$	———
hexagonal	$a = b$; $\alpha = \beta = 90^\circ$; $\gamma = 120^\circ$ No restriction on c		[001]	[100] [010] $[\bar{1}\bar{1}0]$ $\equiv \langle 100 \rangle$	$[1\bar{1}0]$ [120] $[\bar{2}\bar{1}0]$ $\equiv \langle 1\bar{1}0 \rangle$
cubic	$a = b = c$ $\alpha = \beta = \gamma = 90^\circ$		[001] [100] [010] $\equiv \langle 001 \rangle$	[111] $[1\bar{1}\bar{1}]$ $[\bar{1}1\bar{1}]$ $[\bar{1}\bar{1}1]$ $\equiv \langle 111 \rangle$	[110] $[1\bar{1}0]$ [011] $[01\bar{1}]$ [101] $[\bar{1}01]$ $\equiv \langle 110 \rangle$

Symmetry restrictions on cell parameters (conventional cell)

Restrictions incorrectly given in many textbooks

Triclinic family:
none

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

Monoclinic family
$\alpha = \gamma = 90°$

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

For the crystal structure, too restrictive

Orthorhombic family
$\alpha = \beta = \gamma = 90°$

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

For the crystal lattice (geometric concept), insufficient

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

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

Hexagonal family
Hexagonal axes: $a = b$; $\alpha = \beta = 90°$; $\gamma = 120°$
Rhombohedral axes: $a = b = c$; $\alpha = \beta = \gamma$

$a = b \neq c$; $\alpha = \beta = 90°$; $\gamma = 120°$
$a = b = c$; $\alpha = \beta = \gamma \neq 90°$

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

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

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Bravais type	Centring mode of the cell (**a**, **b**, **c**)	Conditions
cP	P	$a = b = c$, $\alpha = \beta = \gamma = 90°$
cI	I	$a = b = c$, $\alpha = \beta = \gamma = 90°$
cF	F	$a = b = c$, $\alpha = \beta = \gamma = 90°$
tP	P	$a = b \neq c$, $\alpha = \beta = \gamma = 90°$
tI	I	$c/\sqrt{2} \neq a = b \neq c$, * $\alpha = \beta = \gamma = 90°$
oP	P	$a < b < c$, † $\alpha = \beta = \gamma = 90°$
oI	I	$a < b < c$, $\alpha = \beta = \gamma = 90°$
oF	F	$a < b < c$, $\alpha = \beta = \gamma = 90°$
oC	C	$a < b \neq a\sqrt{3}$, ‡ $\alpha = \beta = \gamma = 90°$
hP	P	$a = b$, $\alpha = \beta = 90°,\ \gamma = 120°$
hR	P	$a = b = c$, $\alpha = \beta = \gamma$, $\alpha \neq 60°,\ \alpha \neq 90°,\ \alpha \neq \omega$§
mP	P	$-2c\cos\beta < a < c$, ¶ $\alpha = \gamma = 90° < \beta$
mI	I	$-c\cos\beta < a < c$, ** $\alpha = \gamma = 90° < \beta$, (9.3.4.2) but not $a^2 + b^2 = c^2$, $a^2 + ac\cos\beta = b^2$, †† (9.3.4.3) nor $a^2 + b^2 = c^2$, $b^2 + ac\cos\beta = a^2$, ‡‡ (9.3.4.4) nor $c^2 + 3b^2 = 9a^2$, $c = -3a\cos\beta$, §§ (9.3.4.5) nor $a^2 + 3b^2 = 9c^2$, $a = -3c\cos\beta$¶¶ (9.3.4.6)

Note: All remaining cases are covered by Bravais type aP.

Why insufficient for the crystal lattice?

A simple example: mP

if $\beta = 90°$ the lattice is oP (obviously)

Let us suppose $\cos\beta = -a/2c$