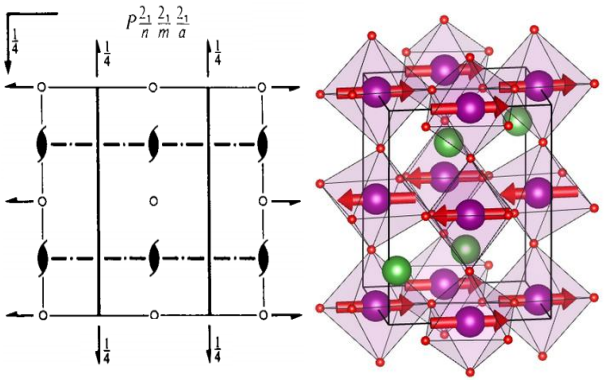
GDR MEETICC

Matériaux, Etats ElecTroniques, Interaction et Couplages non Conventionnels



Winter school

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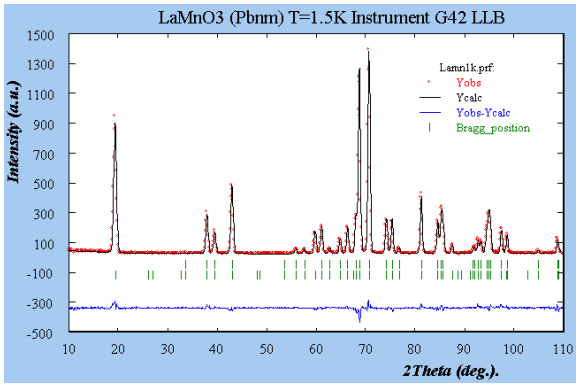
Banyuls-sur-Mer, France



CRYSTALLOGRAPHIC and MAGNETIC STRUCTURES from NEUTRON DIFFRACTION: the POWER of SYMMETRIES (Lecture I)

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Global outline *(Lectures I, II, and III)*

I- Crystallographic structures

Point Group Symmetry: *from the elementary point symmetries to the 32 point groups*

Translation Symmetry: *lattice, motif, unit cell, directions and net planes, twins*

Space group symmetry: *glide planes and screw axes, the 230 space groups, the ITC*

II- Magnetic structures

Description in terms of propagation vector: *the various orderings, examples*

Description in terms of symmetry:

- **Magnetic point groups**: *time reversal, the 122 magnetic point groups*
- **Magnetic lattices:** *translations and anti-translations, the 36 magnetic lattices*
- **Magnetic space groups** = Shubnikov groups

III- Determination of nucl. and mag. structures from neutron diffraction

Nuclear and magnetic neutron diffraction: *structure factors, extinction rules*

Examples in powder neutron diffraction

Examples in single-crystal neutron diffraction

Crystallography: *introduction*

The word crystal comes from Greek (*krustallas*) and means “solidified by the cold”.

Crystallography = science of crystals

→ external shape, internal structure, crystal growth, and physical properties.

Objective: determine the atomic positions in the unit cell.
Mean: diffraction techniques (X-rays, neutrons, electrons)

Curie's principle : The symmetry of a cause is always preserved in its effects

Existence or not of some phenomena, symmetries of the possible ones

Examples: existence or not of ferroelectricity
relations between the various components of the stress tensor
…

Crystallography: *introduction*

Crystallography → Link between structure and physical properties

1- Translation symmetry

Periodicity of the physical properties: **Solid state physics**

- *Phonons, magnons, ...*
- *Diffraction*

2- Point (group) symmetry

Anisotropy of the physical properties: **macroscopic physics**

→ reflects the point symmetry of crystals

- *External shape of crystals (natural faces)*
- *Electric conductivity, optical, mechanical, magnetic, …. properties*

To describe crystals: geometrical aspects, symmetries, atomic positions, …
Direct space

To determine the crystal structure: diffraction
Reciprocal space

Crystallography: *Outline*

1. Point group symmetry

Elementary point symmetry operations
Crystallographic point groups: definition, international notation
Examples of point groups
The 32 crystallographic point groups and 11 Laue classes

2. Translation symmetry

Lattice and motif, Unit cell
The orientation symmetries of lattices:
the 6 conventional cells, 7 crystal systems and 14 Bravais lattices
Lattice directions and net planes

3. Space group symmetry

Glide planes and screw axes
The 230 space groups
The International Tables for Crystallography

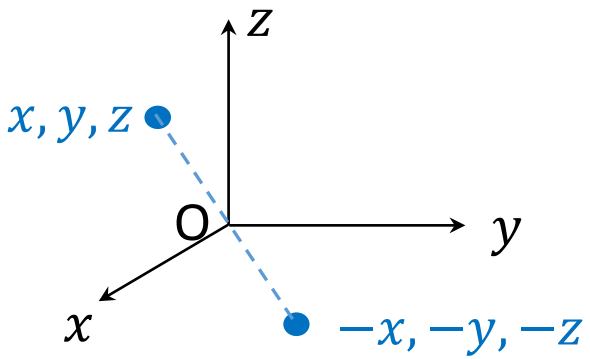
1. Point Group Symmetry: *Elementary point symmetries*

At the macroscopic & atomic (to within a translation) scales, ∃ point symmetries, named **point symmetries**, that keep at least one point fixed, the origin.

Inversion (through a point)

→ *centrosymmetric crystal*

$\bar{1}$



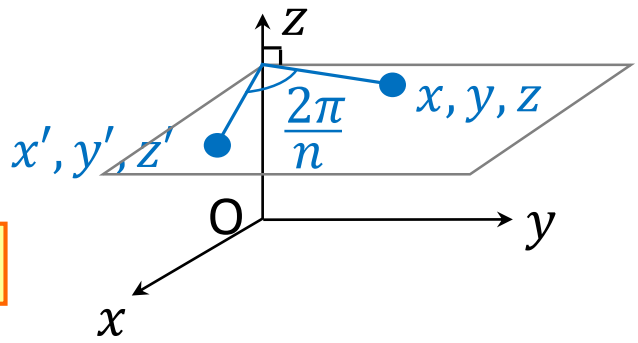
$$\alpha(\bar{1}) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

Det = -1

Rotation (around an axis)

Rotation of order n = rotation by $\frac{2\pi}{n}$

1, 2, 3, ...



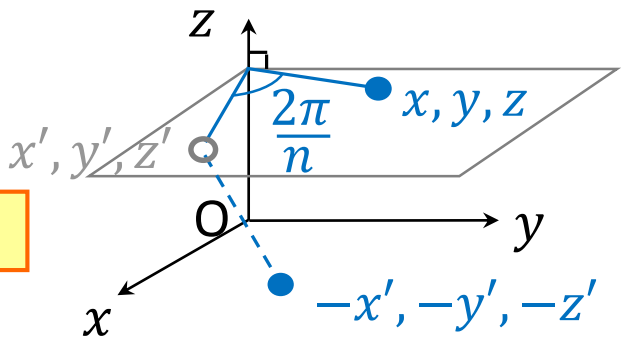
$$\alpha(n) = \begin{pmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Det = +1

1. Point Group Symmetry: *Elementary point symmetries*

Rotoinversion

(around an axis and through a point)

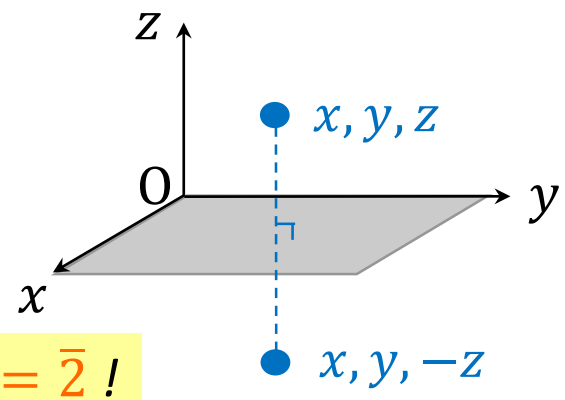


$\bar{1}, \bar{2}, \bar{3}, \ldots$

$$\alpha(n) = \begin{pmatrix} -\cos\phi & \sin\phi & 0 \\ -\sin\phi & -\cos\phi & 0 \\ 0 & 0 & -1 \end{pmatrix}$$ Det = -1

Reflection

(through a mirror plane)



m

NB : $m = \bar{2}$ *!*

$$\alpha(m) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$ Det = -1

Rotations compatible with the translation symmetry = those of orders 1, 2, 3, 4, 6

→ 10 elementary operations: point groups $1, 2, 3, 4, 6,$ $\bar{1}, \bar{2} = m, \bar{3}, \bar{4}, \bar{6}$

Proper (Det = 1) Improper (Det = -1)

1. Point Group Symmetry: *Definition of a group*

The point symmetry operations form a group

A **group** $(G,\times)$ of order n is a set of distinct elements $g_1, g_2, \ldots, g_n$ equipped with an operation (**group multiplication** $\times$) that combines any two elements to form a third element and that satisfies the four axioms:

Closure: $g_i \times g_j \in G$

Identity: $\exists!\, e$ such that $g \times e = e \times g = g$ → 1 (does nothing)

Invertibility: each element g has a unique inverse g^{-1} such that: $g \times g^{-1} = g^{-1} \times g = e$

inverse of n: $-n$ (rotate in the other way)

Associativity: $(g_i \times g_j) \times g_k = g_i \times (g_j \times g_k)$

For point symmetry operations:

$\times$ ↔ apply successively 2 symmetry operations

1. Point Group Symmetry: *How to obtain and name all point groups?*

How to obtain all crystallographic point groups (= crystal classes) ?

Combine the 10 elementary symmetry operations, with the following constraints:

- all symmetry elements go through a common point,
- compatibility with the translation symmetry

⇒ constraints between the orientations of the various symmetry axes / planes

Notation of the point groups – *International (Hermann-Mauguin) symbol*

Symmetry operations along 1, 2 or 3 directions (primary, secondary, tertiary), ordered with decreasing or equal degree of symmetry
(except for 2 cubic point groups)

Examples :

$4/m$

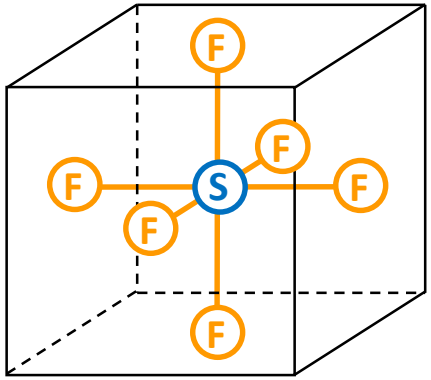
$\frac{4}{m}\,\frac{2}{m}\,\frac{2}{m}$ (= $4/mmm$)

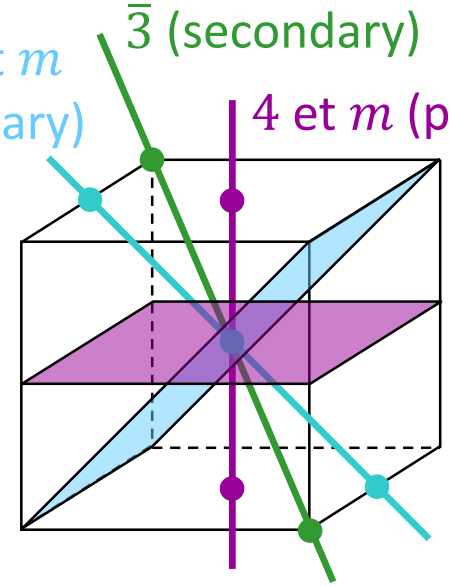
The direction of a rotation is given by its axis
The direction of a mirror is given by its normal
'n/m' = axis n and normal to mirror m along same direction
(*i.e.* plane of the mirror $\perp$ to axis n)

There exists another notation: ***Schoenflies symbol*** → widely used in spectroscopy

1. Point Group Symmetry: *Elementary point symmetries*

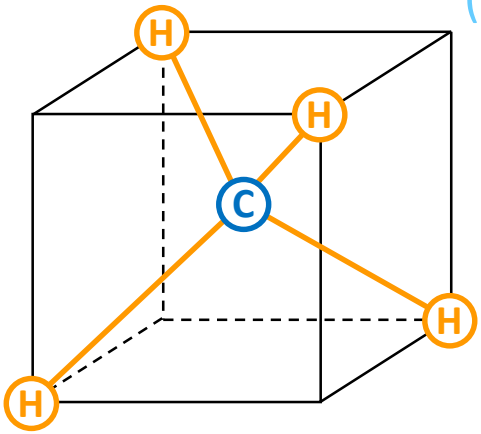
SF_6 molecule

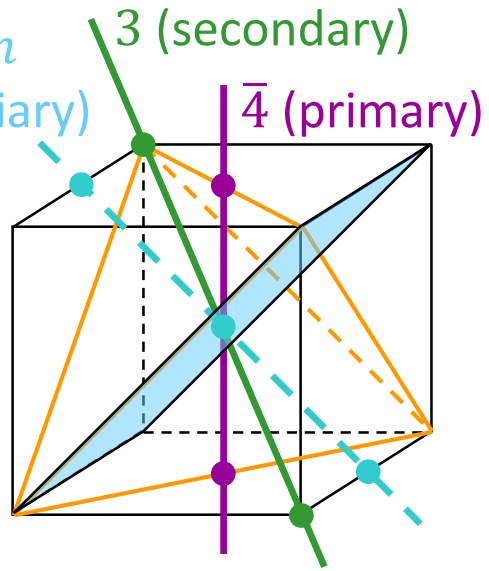




→ Point group: $\boxed{\frac{4}{m}\bar{3}\frac{2}{m}}$ (= $m\bar{3}m$)

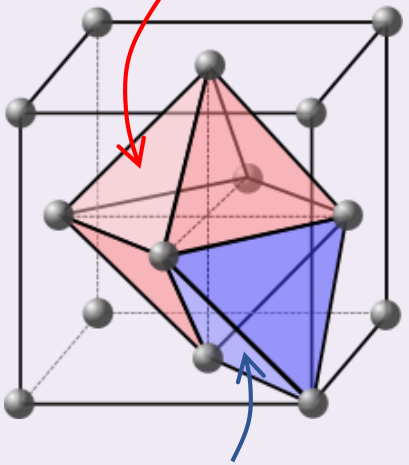
CH_4 molecule





→ Point group: $\boxed{\bar{4}3m}$

Octahedral site : $m\bar{3}m$ symmetry



Tetrahedral site : $\bar{4}3m$ symmetry

1. Point Group Symmetry: *Elementary point symmetries*

Order of the point symmetry along the: primary direction	secondary direction	tertiary direction	Point groups (short symbols) and Laue classes
–	–	–	$1, \bar{1}$
2	–	–	$2, m, 2/m$
2	2	2	$222, 2mm, mmm$
3	–	–	$3, \bar{3}$
3	2	–	$32, 3m, \bar{3}m$
4	–	–	$4, \bar{4}, 4/m$
4	2	2	$422, 4mm, \bar{4}2m, 4/mmm$
6	–	–	$6, \bar{6}, 6/m$
6	2	2	$622, 6mm, \bar{6}2m, 6/mmm$
2	3	–	$23, m\bar{3}$
4	3	2	$432, \bar{4}3m, m\bar{3}m$

1. Point Group Symmetry: *Elementary point symmetries*

- Example: **dielectric properties**

They can only be found for particular crystal symmetries

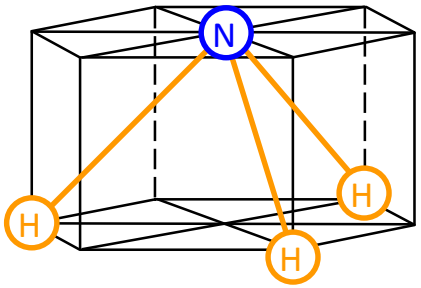
Piezoelectricity → point groups that do not possess inversion

Ferroelectricity and **pyroelectricity**

→ piezolectric point groups (i.e. non centrosymmetric)
with a unique polar axis ($\vec{p} \parallel n$-axis and contained in the plane of the mirror):

$1, 2, m, 2mm, 3, 3m, 4, 4mm, 6, 6mm$
polar groups

NH_3



Point group: $3m$
→ ∃ dipolar moment ($p = 1.46$ Debye)

2. Translation Symmetry: *Lattice and motif*

At the atomic scale, ∃ translation vectors $\vec{T}$ that put the crystallographic structure in coincidence with itself.

$$\vec{T} = u\vec{a} + v\vec{b} + w\vec{c} \text{ with } u, v, w \text{ integers}$$ (positive or negative)

$\vec{a}, \vec{b}$, and $\vec{c}$ are called the basis vectors
(non-coplanar elementary translation vectors defining a right-handed system).
The volume they define is called the unit cell.

Crystal = Lattice + Motif

The set of extremities of the $\vec{T}$ vectors define an abstract network of points (= nodes): the **lattice**.

At each lattice node, one associates a group of atoms: the **motif**.

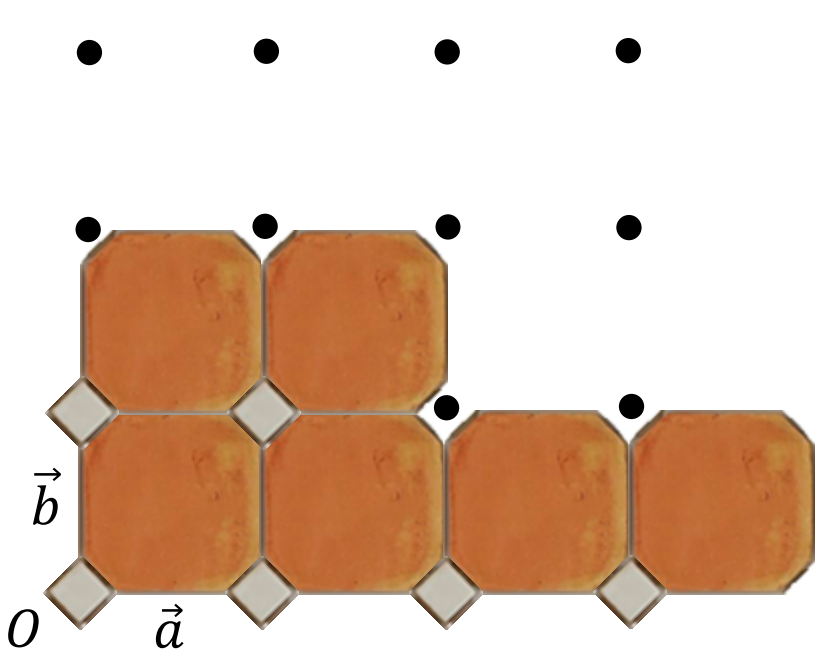
The knowledge of the lattice (basis vectors $\vec{a}, \vec{b}, \vec{c}$) and of the motif (nature and positions x, y, z of the atoms in the cell) completely characterizes the crystalline structure.

N.B. : $\vec{r} = x\vec{a} + y\vec{b} + z\vec{c}$ $(|x|, |y|, |z| < 1)$

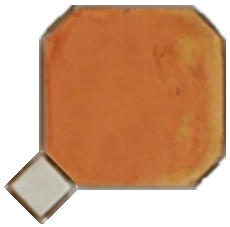
2. Translation Symmetry: *Lattice and motif*

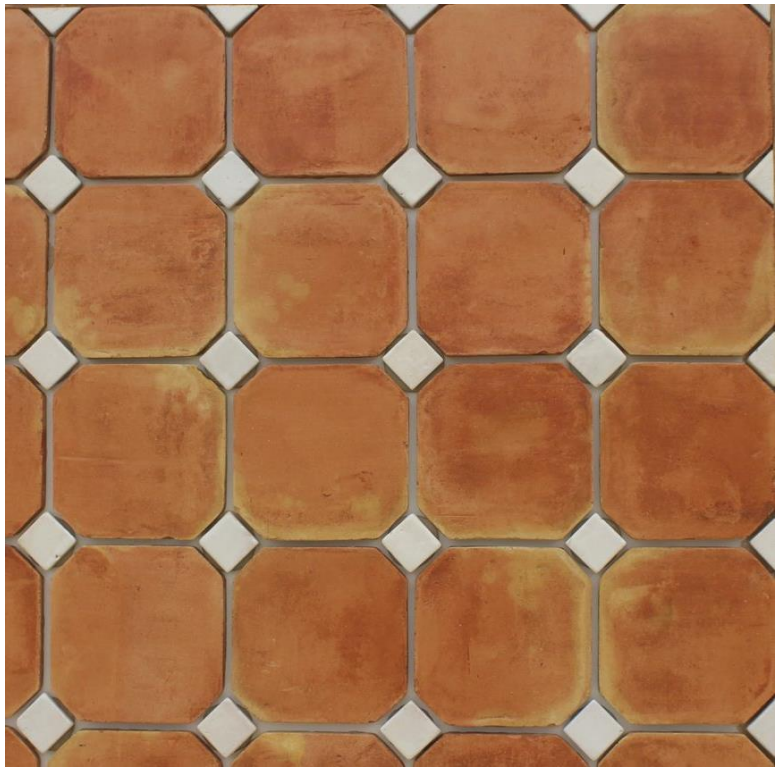
Example 1 : terracotta floor tiles (2D)

Lattice



Motif



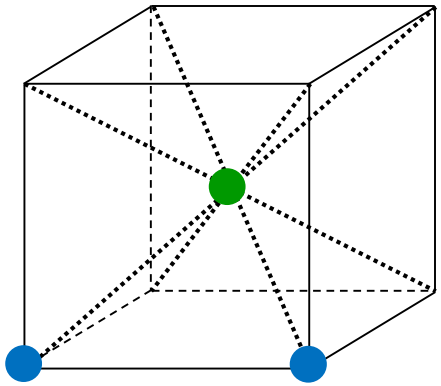


2. Translation Symmetry: *Lattice and motif*

Example 2 : CsCl single-crystal (3D)

Unit cell:

cubic
primitive

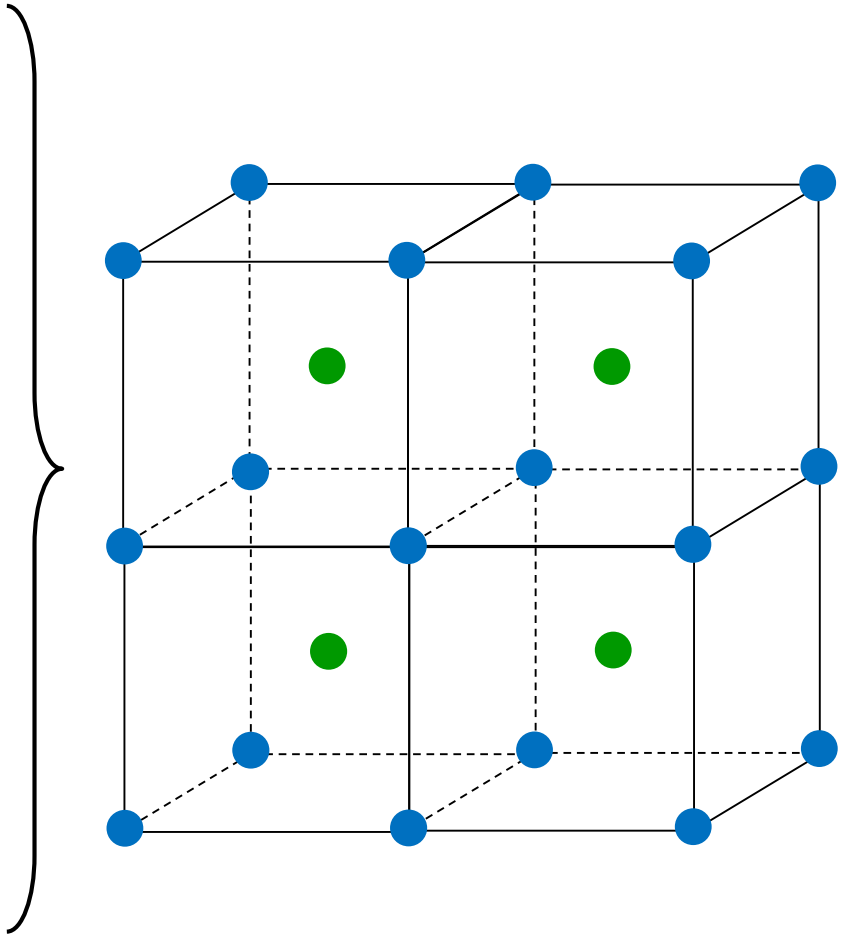


Motif:

Cs^+ on the corner
Cl^- at the center

Cl^-

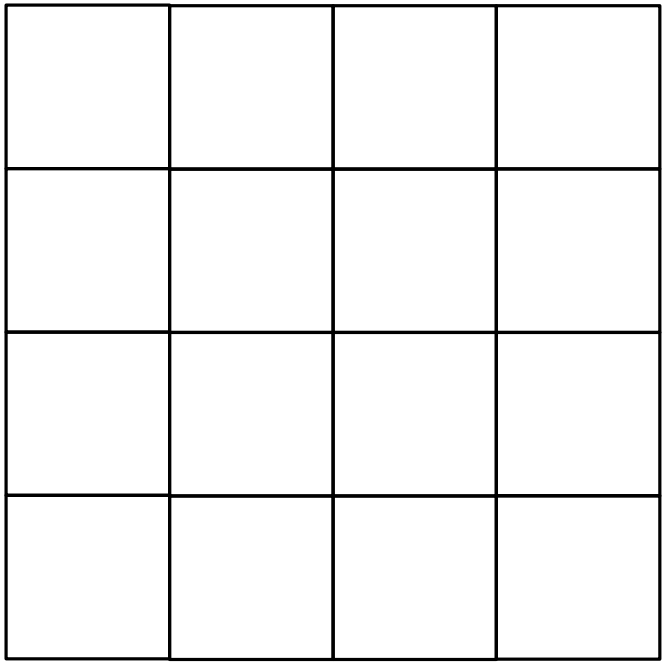
Cs^+

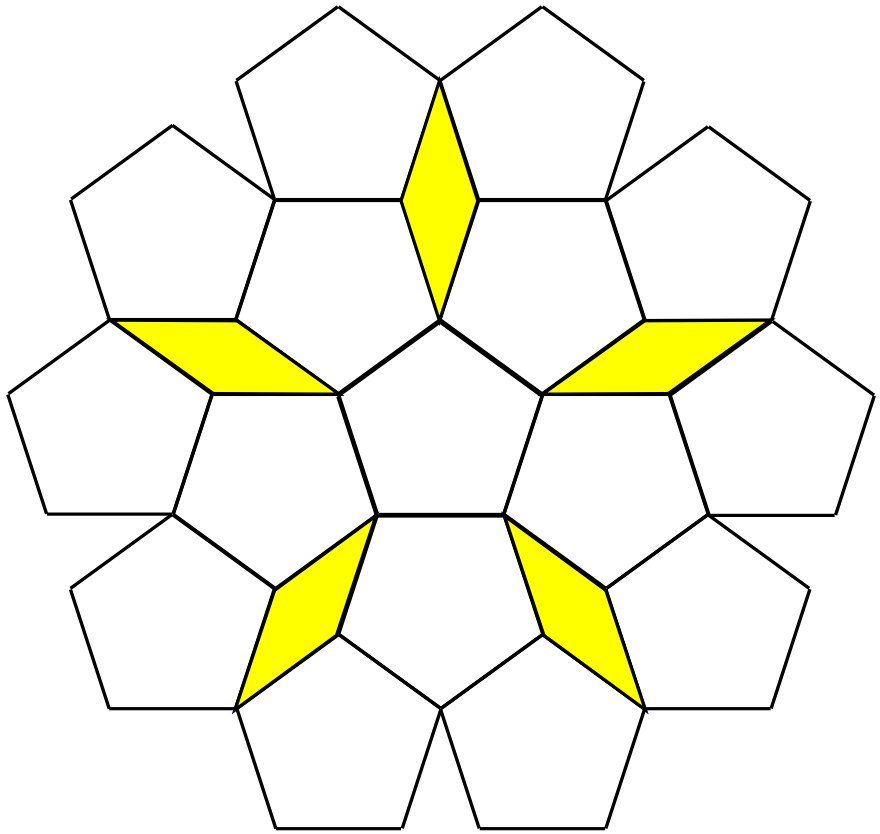


2. Translation Symmetry: *Unit cell*

The unit cell allows to pave the space with no empty space nor overlap, by applying the lattice translations.

Examples at 2D:

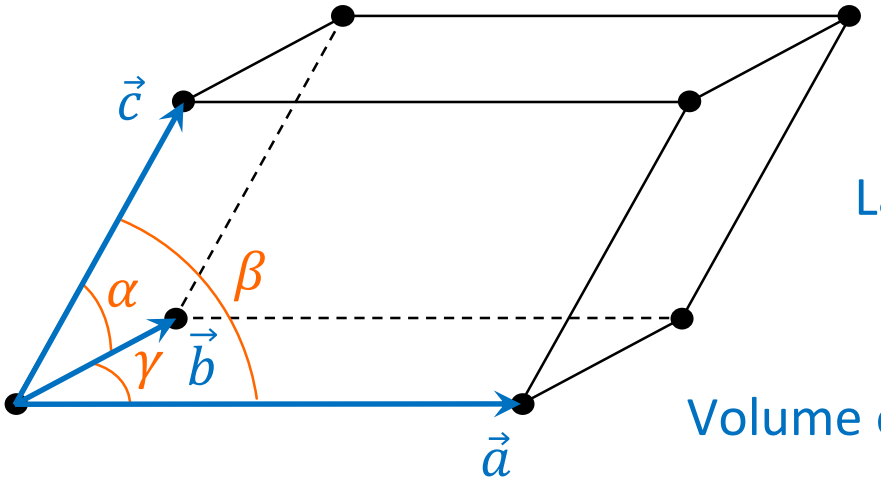




Rotation of **order 4** : compatible with translation symmetry.

Rotation of **order 5** : not compatible with translation symmetry → ***quasicrystals***

2. Translation Symmetry: *Unit cell*



Lattice parameters:

Lengths	Angles
a	$\alpha = (\vec{b}, \vec{c})$
b	$\beta = (\vec{c}, \vec{a})$
c	$\gamma = (\vec{a}, \vec{b})$

Volume of the unit cell: $V = (\vec{a}, \vec{b}, \vec{c}) = (\vec{a} \wedge \vec{b}).\vec{c}$

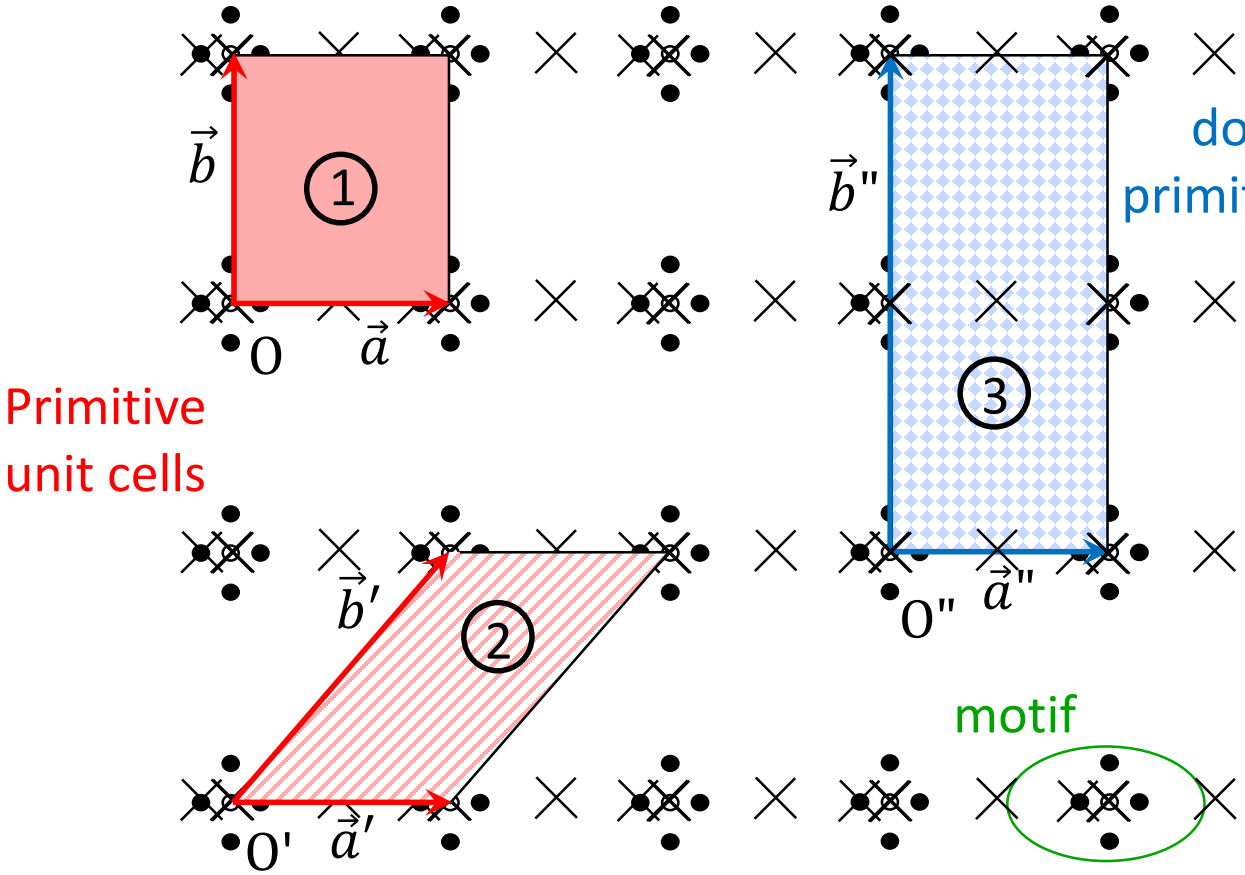
- Multiplicity m of a unit cell: Number of lattice nodes (and thus of motifs) per unit cell

How to count the number of lattice nodes per unit cell?
→ each lattice node counts for $1/n$, with n = number of unit cells to which it belongs

- Primitive unit cell: $m = 1$
  For a given lattice, all primitive unit cells have the same volume V

- Centered unit cell: $m = 2, 3$ or 4 (doubly, triply … primitive) → Volume : $V_m = m\,V$
  → **used only when more symmetrical than any primitive cell of the lattice**

2. Translation Symmetry: *Unit cell*



doubly primitive cell

Primitive unit cells

Best choice?

1

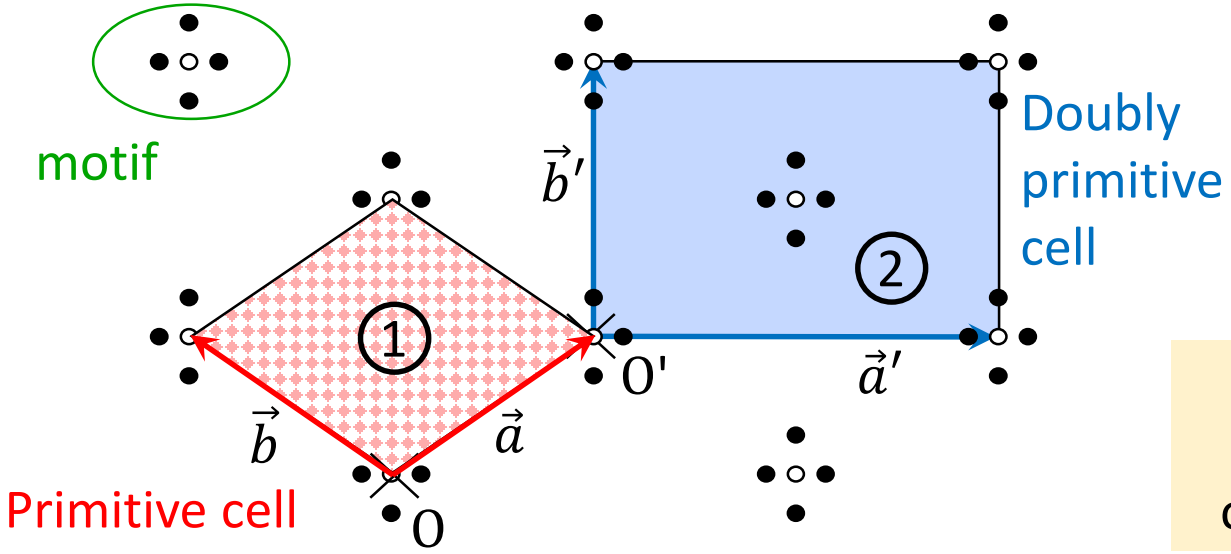
primitive unit cell

reflects the lattice symmetry

Primitive cells: 4 lattice nodes (on corners) $\in$ 4 cells $\rightarrow m = 4 \times 1/4 = 1$

Doubly primitive cell: 4 nodes (on corners) $\in$ 4 cells $\rightarrow 4 \times 1/4 = 1$
+ 2 nodes (on edges) $\in$ 2 cells $\rightarrow 2 \times 1/2 = 1$ $\Big\}\ m = 2$

2. Translation Symmetry: *Unit cell*



Cell (1) is primitive but does not reflect the $\perp^{ty}$

⇨ **Best choice**: (2)

Conventional unit cell
(basis vectors ‖ directions of symmetry of the lattice)

N.B.: For a primitive cell, the translation vectors $\vec{T}$ are defined by:

$\vec{T} = u\vec{a} + v\vec{b} + w\vec{c}$ with u, v, w integers.

For a non primitive cell of multiplicity m, one must add $(m-1)$ translation vectors such as: $\vec{T} = u'\vec{a} + v'\vec{b} + w'\vec{c}$ with u', v', w' integers or fractionals

half integers

Ex.: For unit cell (2) $(m = 2)$:

$$\begin{cases} \vec{T}_1 = u\vec{a}' + v\vec{b}' \\ \vec{T}_2 = \vec{T}_1 + \frac{1}{2}(\vec{a}' + \vec{b}') = \left(u + \frac{1}{2}\right)\vec{a}' + \left(v + \frac{1}{2}\right)\vec{b}' \end{cases}$$

2. Translation Symmetry: *The 6 conventional cells and 7 crystal systems*

Translation and orientation (point) symmetries:

The crystals can be classified into 6 conventional cells and 7 crystal systems each of them having a characteristic orientation symmetry

The 6 conventional cells are, by increasing degree of symmetry:

				Number of parameters
a	triclinic	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma$	6
m	monoclinic	$a \neq b \neq c$	$\alpha = \gamma = 90°,\ \beta > 90°$	4
o	orthorhombic	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90°$	3
t	tetragonal or quadratic	$a = b \neq c$	$\alpha = \beta = \gamma = 90°$	2
h	hexagonal **	$a = b \neq c$	$\alpha = \beta = 90°,\ \gamma = 120°$ *	2
c	cubic	$a = b = c$	$\alpha = \beta = \gamma = 90°$	1

* $\gamma = 120°$ *and not 60° (for the hexagonal reciprocal lattice:* $\gamma^* = 60°$*)*

** *The hexagonal conventional cell splits in two crystal systems:*
trigonal (axis 3) and hexagonal (axis 6); the 5 other ones are the same.

2. Translation Symmetry: *Crystal system vs point group*

Crystal system	Point groups and Laue classes	Primary direction	Secondary direction	Tertiary direction
triclinic	$1, \bar{1}$	–	–	–
monoclinic	$2, m, 2/m$	$\vec{b}$ (ou $\vec{c}$)	–	–
orthorhombic	$222, 2mm, mmm$	$\vec{a}$	$\vec{b}$	$\vec{c}$

2. Translation Symmetry: *Crystal system vs point group*

Crystal system	Point groups and Laue classes	Primary direction	Secondary direction	Tertiary direction
triclinic	$1, \bar{1}$	–	–	–
monoclinic	$2, m, 2/m$	$\vec{b}$ (ou $\vec{c}$)	–	–
orthorhombic	$222, 2mm, mmm$	$\vec{a}$	$\vec{b}$	$\vec{c}$
trigonal	$3, \bar{3}$ $32, 3m, \bar{3}m$	$\vec{c}$	$\vec{a}, \vec{b}, -\vec{a}-\vec{b}$	–
tetragonal or quadratic	$4, \bar{4}, 4/m$ $422, 4mm, \bar{4}2m, 4/mmm$	$\vec{c}$	$\vec{a}, \vec{b}$	$\vec{a}+\vec{b}, \vec{a}-\vec{b}$
hexagonal	$6, \bar{6}, 6/m$ $622, 6mm, \bar{6}2m, 6/mmm$	$\vec{c}$	$\vec{a}, \vec{b}, -\vec{a}-\vec{b}$	$2\vec{a}+\vec{b}$, …

2. Translation Symmetry: *Crystal system vs point group*

Crystal system	Point groups and Laue classes	Primary direction	Secondary direction	Tertiary direction
triclinic	$1, \bar{1}$	–	–	–
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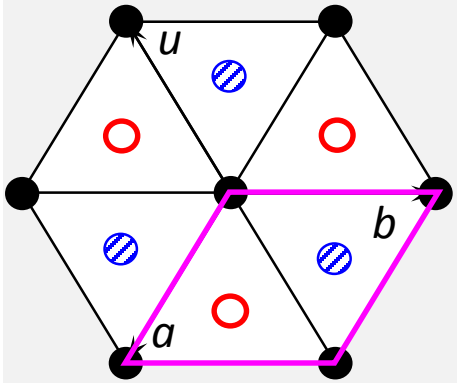
orthorhombic	$222, 2mm, mmm$	$\vec{a}$	$\vec{b}$	$\vec{c}$
trigonal	$3, \bar{3}$ $32, 3m, \bar{3}m$	$\vec{c}$	$\vec{a}, \vec{b}, -\vec{a}-\vec{b}$	–
tetragonal or quadratic	$4, \bar{4}, 4/m$ $422, 4mm, \bar{4}2m, 4/mmm$	$\vec{c}$	$\vec{a}, \vec{b}$	$\vec{a}+\vec{b}, \vec{a}-\vec{b}$
hexagonal	$6, \bar{6}, 6/m$ $622, 6mm, \bar{6}2m, 6/mmm$	$\vec{c}$	$\vec{a}, \vec{b}, -\vec{a}-\vec{b}$	$2\vec{a}+\vec{b}$, …
cubic	$23, m\bar{3}$ $432, \bar{4}3m, m\bar{3}m$	$\vec{a}, \vec{b}, \vec{c}$	$\vec{a}+\vec{b}+\vec{c}$, …	$\vec{a}+\vec{b}$, …

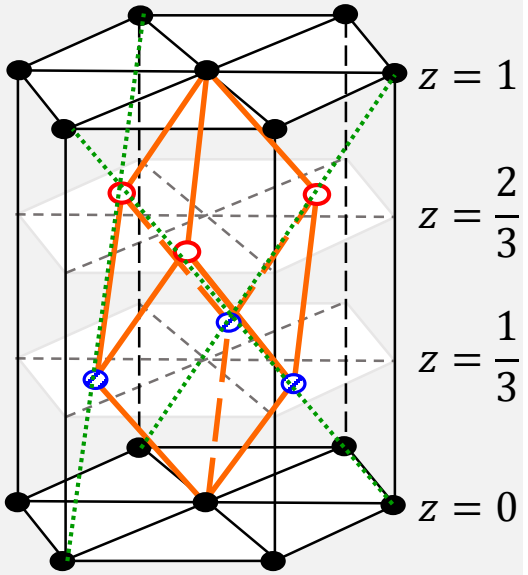
2. Translation Symmetry: *The 14 Bravais lattices*

- 6 primitive lattices (one for each of the 6 conventional cells),
- 8 non primitive ones, by adding nodes in the former cells, provided no symmetry element is lost & the centered cell is more symmetric than any primitive cell.

Symbole	Lattice mode	m
P	primitive	1
I	body centered	2
F	all face centered	4
A, B, C	A-, B-, C-face centered: $(\vec{b},\vec{c}), (\vec{a},\vec{c}), (\vec{a},\vec{b})$ respectively	2
R	rhombohedrally centered: additional lattice nodes at 1/3 and 2/3 of the long diagonal of the h cell (→ trigonal system)	3

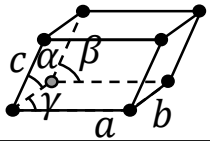
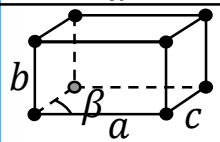
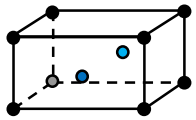
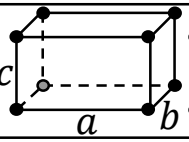
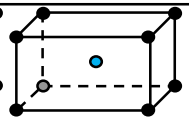
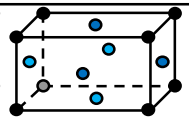
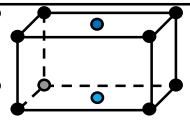
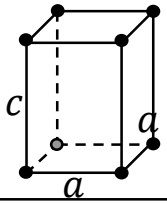
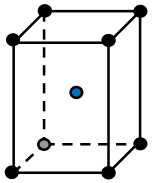
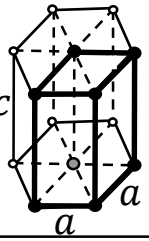
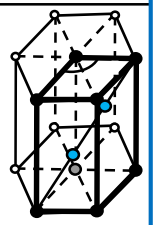
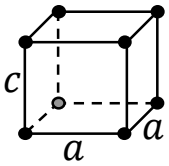
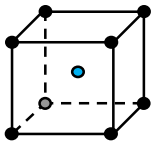
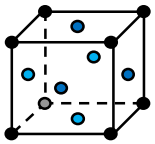
N.B.: the primitive cell of the hR cell is a rhombohedral cell
$(a = b = c, \alpha = \beta = \gamma \neq 90°)$





nodes at $z = 0$ and 1
nodes at $z = 1/3$
nodes at $z = 2/3$

2. Translation Symmetry: *The 14 Bravais lattices*

Conventional cell	Lattice mode P	I	F	C	R
triclinic					
monoclinic					
orthorhombic					
tetragonal					
hexagonal					
cubic					

Reminder:
For centered cells,
∃ additional lattice translations.

Example: I lattice

$$\begin{cases} \vec{T} = u\vec{a} + v\vec{b} + w\vec{c} \\ \vec{T}' = \vec{T} + \frac{1}{2}(\vec{a} + \vec{b} + \vec{c}) \end{cases}$$

with u, v, w integers

2. Translation Symmetry: *Example – the diamond structure*

Si (diamond structure): cubic F lattice, motif = atoms at $(0,0,0)$ and $\left(\frac{1}{4},\frac{1}{4},\frac{1}{4}\right)$

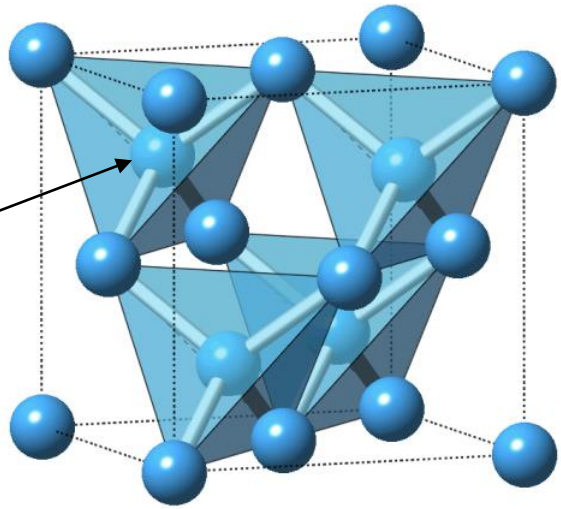
F lattice $(m = 4) \rightarrow$ lattice translations:

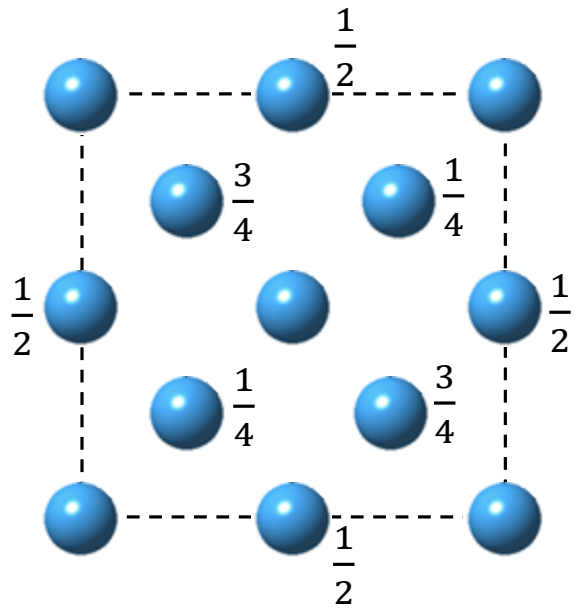
$$\vec{T}_1 = u\vec{a} + v\vec{b} + w\vec{c}, \vec{T}_2 = \vec{T}_1 + \frac{1}{2}(\vec{a}+\vec{b}), \vec{T}_3 = \vec{T}_1 + \frac{1}{2}(\vec{b}+\vec{c}), \vec{T}_4 = \vec{T}_1 + \frac{1}{2}(\vec{a}+\vec{c})$$

$\rightarrow 4 \times 2 = 8$ Si atoms per unit cell with coordinates:

$(0,0,0)$, $\left(\frac{1}{2},\frac{1}{2},0\right)$, $\left(0,\frac{1}{2},\frac{1}{2}\right)$, $\left(\frac{1}{2},0,\frac{1}{2}\right)$, and $\left(\frac{1}{4},\frac{1}{4},\frac{1}{4}\right)$, $\left(\frac{3}{4},\frac{3}{4},\frac{1}{4}\right)$, $\left(\frac{1}{4},\frac{3}{4},\frac{3}{4}\right)$, $\left(\frac{3}{4},\frac{1}{4},\frac{3}{4}\right)$

Si on a tetrahedral site



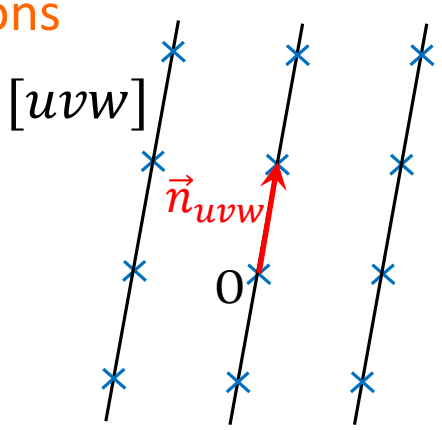


2. Translation Symmetry: *Lattice directions* $[uvw]$

- Family of **lattices directions**

One can group all lattice nodes into parallel equidistant directions

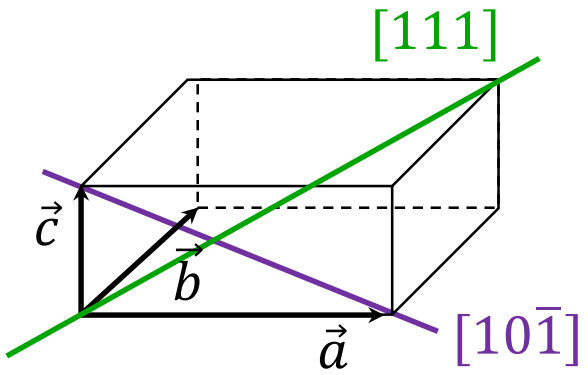
labelled $[uvw]$ along $\vec{n}_{uvw} = u\vec{a} + v\vec{b} + w\vec{c}$

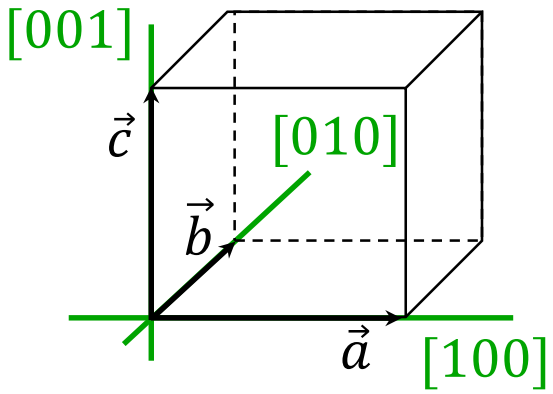


n_{uvw} (length of the direction vector): direction parameter
u, v, w (coprime integers): direction indices

A family of lattice directions contains all lattice points.

- Examples:





Cubic unit cell:

→ directions symmetrically equivalent are labeled $\langle 100 \rangle$

2. Translation Symmetry: *Net planes* (hkl)

- Family of **net planes**

One can group all lattice nodes into parallel equidistant net planes labelled (hkl) of equation: $\boxed{hx + ky + lz = m}$ with m integer (> 0 or < 0)

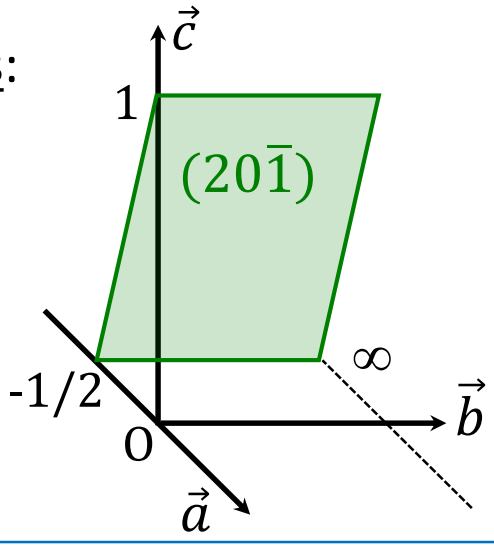
The plane the closest to the origin ($m = 1$) intercepts the $\vec{a}$ axis at $1/h$, the $\vec{b}$ axis at $1/k$, and the $\vec{c}$ axis at $1/l$.

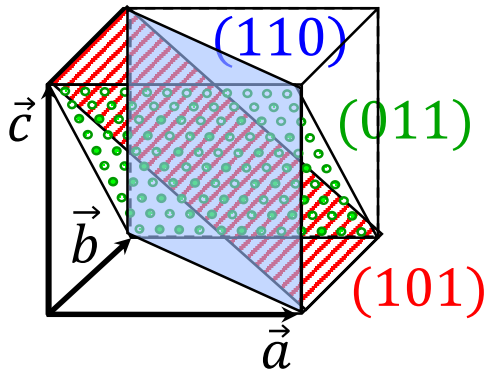
h, k, l (integers, which are coprime for a P lattice): Miller indices

d_{hkl} (distance between 2 consecutive planes): d-spacing

A family of net planes contains all lattice points.

- Examples:





Cubic unit cell:

→ planes symmetrically equivalent are labeled $\{110\}$

Symmetry relations between crystals: *twinned crystals*

Twinned crystal: association of identical single-crystals with different orientations, connected through a point group symmetry: reflection, rotation, or inversion.

Formation of twinned crystals

- Growth twins: occurs during the crystal growth;
- Annealing or Transformation twins: upon cooling (phase transition)
- Deformation or gliding twins: result of stress after the crystal has formed

Twinned pyrite crystal

Japanese twins of quartz

Symmetry relations between crystals: *phase transitions*

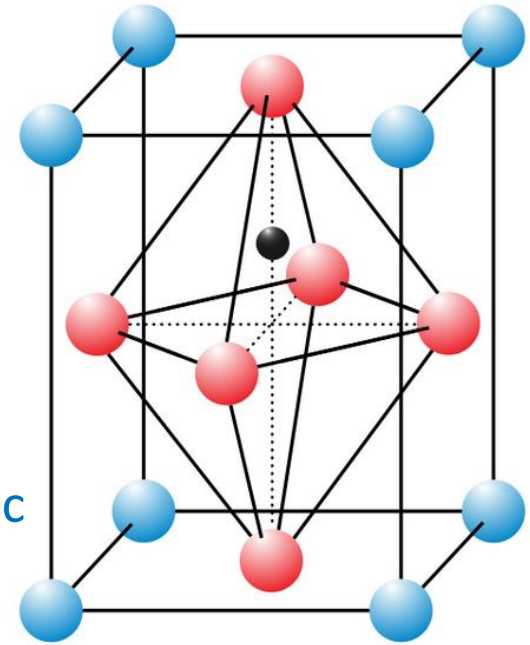
Example : $BaTiO_3$

$120°C$

T

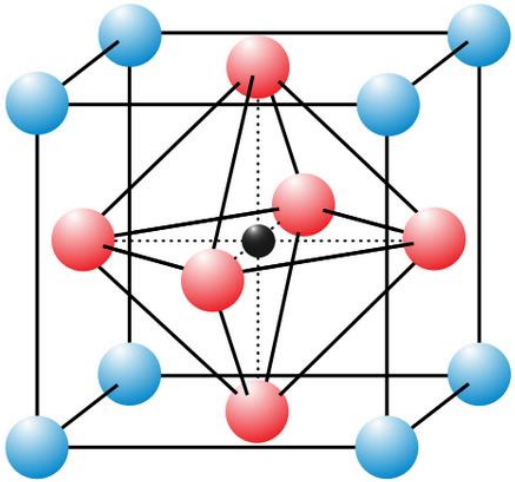
Tetragonal $(4mm)$
$a = 4.000$ Å
$c = 4.017$ Å

Cubic $(m\bar{3}m)$
$c = 4.007$ Å



$\vec{p}$

ferroelectric



paraelectric

With no external stress (pressure, electric field, …) :

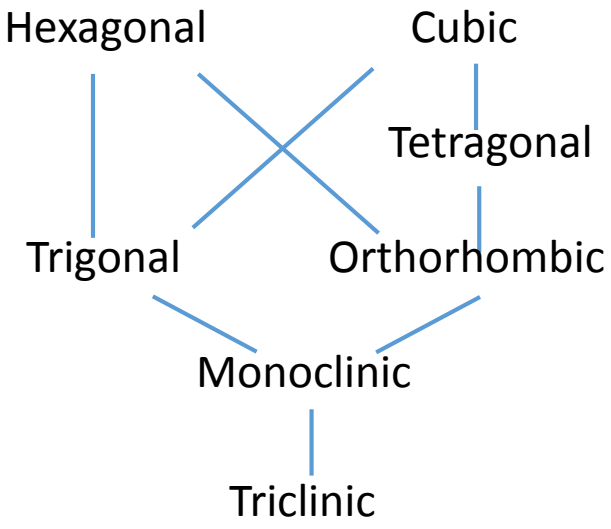
3 different twins with 2 domains at 180° each

Symmetry relations between crystals: *phase transitions*

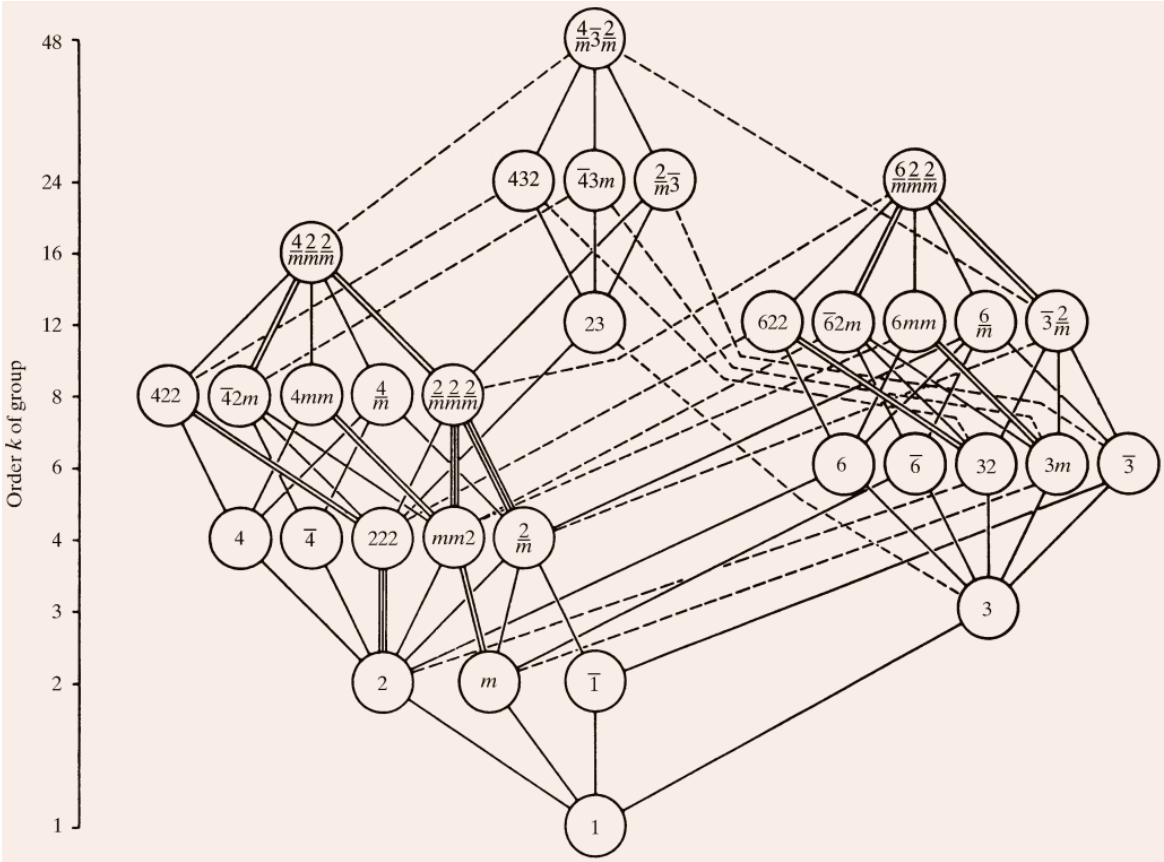
2nd order phase transition:

There exist a group / subgroup relation between the 2 phases

Example: cooling down → **symmetry lowers** (change of point group)



Relation between the 7 crystal systems



Group / subgroup relations between the 32 point groups
Source: ITC, volume A, page 796

3. Space group symmetry

Crystal = lattice + motif

translations $\vec{T}$

+

$\exists$ symmetries acting inside the motif
(symmetry planes and axes)

14 Bravais lattices

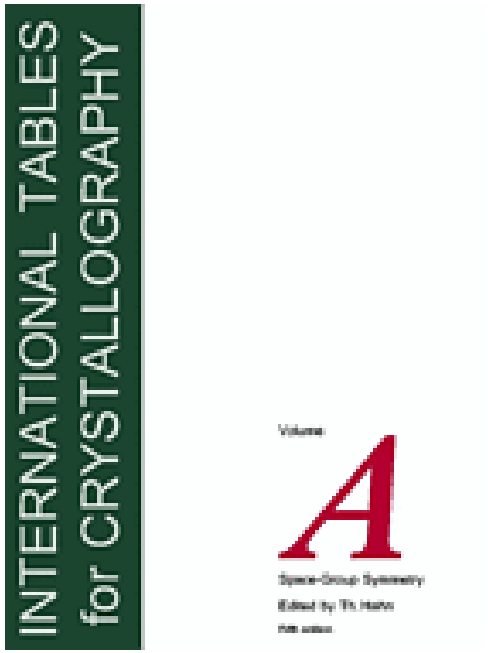
Point symmetries
(32 point groups)
combined or not with
a fractional translation

230 SPACE GROUPS

- Describe the symmetry of the internal structure of crystals
- Allow to classify all the crystals

- International Tables for Crystallography (ITC) (**https://it.iucr.org**)
- Bilbao Crystallographic Server (**http://www.cryst.ehu.es**)
- A Hypertext Book of Crystallographic Space Group Diagrams and Tables (**http://img.chem.ucl.ac.uk/sgp/mainmenu.htm**)

3. Space group symmetry



https://it.iucr.org/resources/

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INTERNATIONAL TABLES Resources

| A | A1 | B | C | D | E | F | G |

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International Tables for Crystallography Resources

The following resources are available as part of **International Tables Online**:

- Search for a crystallographic symmetry group

  Go to space group **No.** 1 (P 1) Go
- Symmetry database
- Retrieve scattering factors for electron diffraction
- Plot scattering factors for electron diffraction
- Retrieve scattering lengths for neutron diffraction
- Resources for Volume D (*Tenχar* and *GI*KoBo-1*)
- Superspace Group Finder
- CIF dictionaries
  - Core CIF Dictionary
  - Electron Density CIF Dictionary
  - Image CIF Dictionary
  - Macromolecular CIF Dictionary
  - Modulated Structures CIF Dictionary
  - Powder CIF Dictionary
  - Symmetry CIF Dictionary

3. Space group symmetry

www.cryst.ehu.es

bilbao crystallographic server

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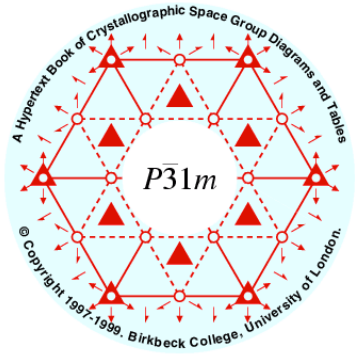
Space-group symmetry

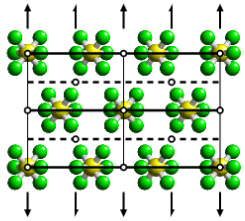
GENPOS	Generators and General Positions of Space Groups
WYCKPOS	Wyckoff Positions of Space Groups
HKLCOND	Reflection conditions of Space Groups
MAXSUB	Maximal Subgroups of Space Groups
SERIES	Series of Maximal Isomorphic Subgroups of Space Groups
WYCKSETS	Equivalent Sets of Wyckoff Positions
NORMALIZER	Normalizers of Space Groups
KVEC	The k-vector types and Brillouin zones of Space Groups
SYMMETRY OPERATIONS	Geometric interpretation of matrix column representations of symmetry operations
IDENTIFY GROUP	Identification of a Space Group from a set of generators in an arbitrary setting

img.chem.ucl.ac.uk/sgp/mainmenu.htm



A Hypertext Book of

Crystallographic Space Group Diagrams and Tables



CD-ROM Cover Picture

High-Resolution Space Group Diagrams and Tables
(1280 × 1024 pixel screens)

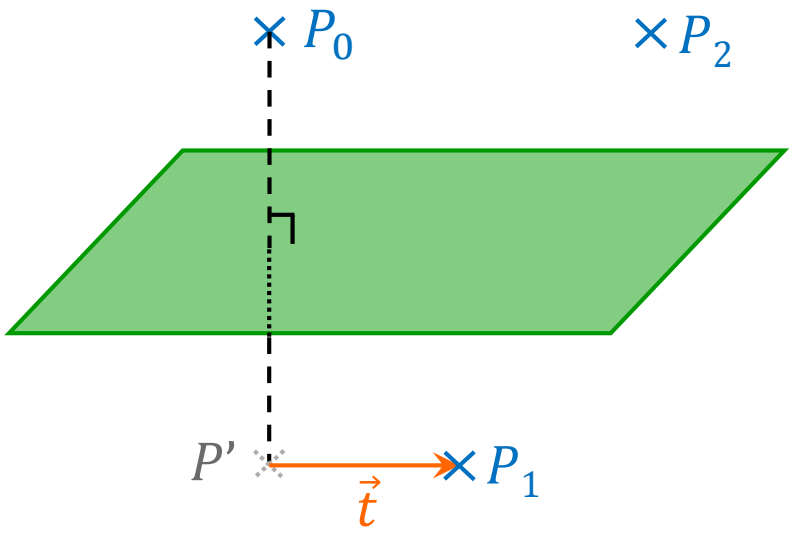
Medium-Resolution Space Group Diagrams and Tables
(1024 × 768 pixel screens)

3. Space group symmetry: *symmetry planes*

- Glide plane

Combination of a reflection (through a plane) and a fractional translation $\vec{t}$ ∥ plane

acting inside the unit cell



Example: **glide plane** $a \perp \vec{c}$ at $z = \frac{1}{4}$

$a \times a \rightarrow$ lattice translation

$$P_0P_2 = \vec{a} \rightarrow \boxed{\vec{t} = \frac{\vec{a}}{2}}$$

Seitz notation: $\{\alpha|\vec{t}_\alpha\} = \left\{m_z\middle|\frac{1}{2}, 0, \frac{1}{2}\right\}$

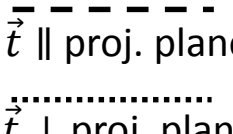
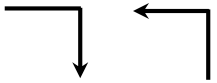
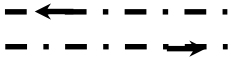
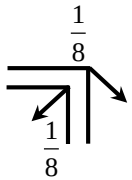
4 × 4 matrix:
$$\begin{pmatrix} 1 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1/2 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

α: point symmetry

$\vec{t}_\alpha$: translation embedding the glide translation + the position of α

3. Space group symmetry: *symmetry planes*

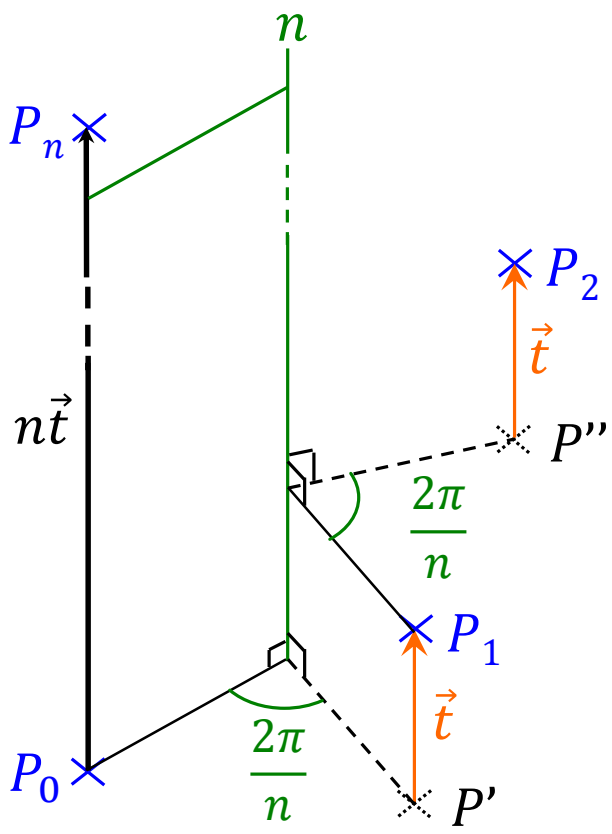
The various symmetry planes and their Hermann-Mauguin symbol

Printed symbol	Symmetry plane	Graphic symbol		Nature of the gliding (fractional translation $\vec{t}$)
		⊥ projection plane	∥ projection plane	
m	mirror			none
a, b, c	Axial glide plane			$a/2$, $b/2$, or $c/2$ respectively
e	Double glide plane			$a/2$ and $b/2$, $b/2$ and $c/2$, or $a/2$ et $c/2$; OR $(a \pm b)/2$ and $c/2$, etc … for t and c systems
n	Diagonal glide plane			$(a+b)/2$, $(b+c)/2$ or $(c+a)/2$; OR $(a+b+c)/2$ in some cases for t and c systems
d	Diamond glide plane			$(a+b)/4$, $(b+c)/4$ or $(c+a)/4$; OR $(a+b+c)/4$ in some cases for t and c systems

3. Space group symmetry: *symmetry axes*

- Screw axes

Combination of a rotation (around an axis *n*) and a fractional translation $\vec{t}$ ∥ axis



Example: screw axis n_p ∥ $\vec{c}$

$\underbrace{n_p \times \cdots \times n_p}_{n \text{ times}} \rightarrow$ lattice translation

$$\overrightarrow{P_0P_n} = n\vec{t} = p\vec{c}$$

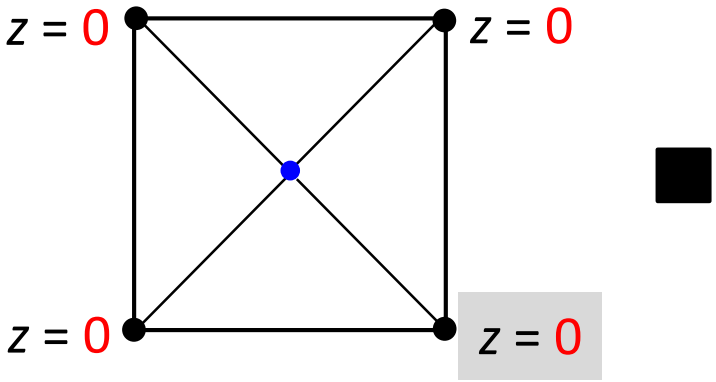
with $\begin{cases} n = 1,2,3,4, \text{or } 6 \\ p \text{ integer} < n \end{cases}$

$\rightarrow \boxed{\vec{t} = \frac{p}{n}\vec{c}}$ with $\boxed{p = 0,1,\ldots,n-1}$

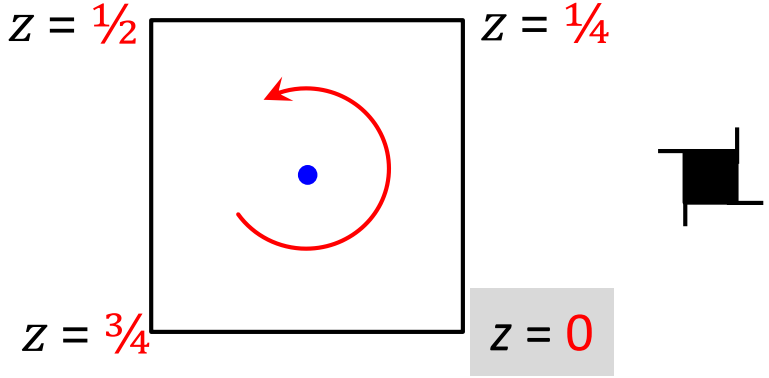
3. Space group symmetry: *symmetry axes*

Example: screw axes $4_p \parallel \vec{c}$

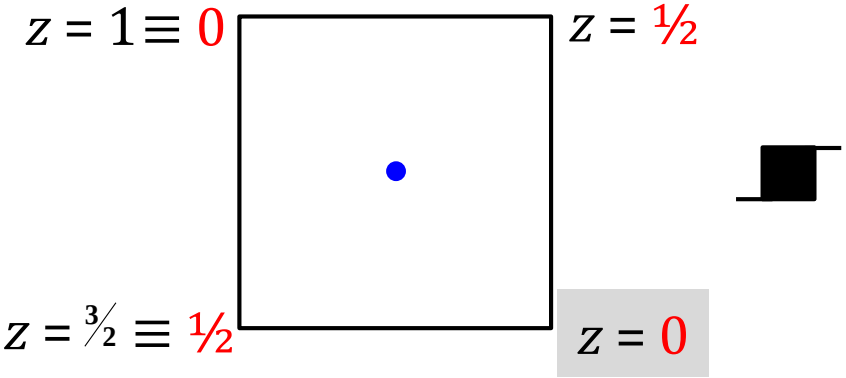
Axis 4: $\vec{t} = \vec{0}$



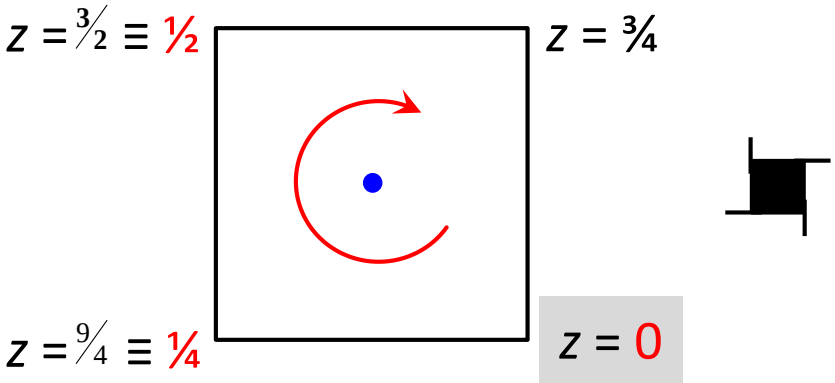
Axis 4_1: $\vec{t} = \frac{1}{4}\vec{c}$



Axis 4_2: $\vec{t} = \frac{1}{2}\vec{c}$

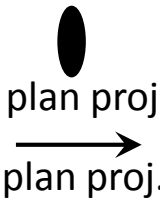
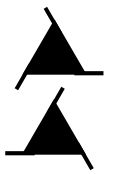


Axis 4_3: $\vec{t} = \frac{3}{4}\vec{c}$



3. Space group symmetry: *symmetry axes*

The various symmetry axes and their Hermann-Mauguin symbol *(projection plane ⊥ $\vec{c}$)*

Printed symbol	Symmetry axis	Graphic symbol	Gliding $\vec{t}$
1	Identity	none	none
$\bar{1}$	Inversion	o	none
2	2-fold rotation axis	 (⊥ plan proj.) (∥ plan proj.)	none
2_1	2-fold screw axis	 (⊥ plan proj.) (∥ plan proj.)	$c/2$ $a/2$ ou $b/2$
3	3-fold rotation axis	⊥ plan proj. 	none
3_1 3_2	2-fold screw axes		$c/3$ $2c/3$
$\bar{3}$	3-fold rotoinversion		none

Printed symbol	Symmetry axis	Graphic symbol	Gliding $\vec{t}$
4	4-fold rotat°		none
4_1 4_2 4_3	4-fold screw axes		$c/4$ $2c/4$ $3c/4$
$\bar{4}$	4-fold rotoinversion		none
6	6-fold rotat°		none
6_1 6_2 6_3 6_4 6_5	6-fold screw axes		$c/6$ $2c/6$ $3c/6$ $4c/6$ $5c/6$
$\bar{6}$	6-fold rotoinversion		none

3. Space group symmetry: *the 230 space groups*

- International notation (Hermann-Mauguin symbol) Ex. $P4_2/mmc$

1st letter : capital letter designing the lattice mode P, I, F, A (B or C), R

Following letters: nature of the symmetry elements

Symmetry axes (with n max and p min) and planes ($m > e > a > b > c > n > d$)

Along the primary, secondary, and tertiary directions: 3 non equivalent directions of symmetry (the same ones as point groups)

Conventional cell	Primary direction	Secondary direction	Tertiary direction
triclinic	A single symbol (1 or $\bar{1}$), thus no direction of symmetry		
monoclinic	A single direction of symmetry: b or c (order 2, unique axis)		
orthorhombic	a (order 2)	b (order 2)	c (order 2)
tetragonal	$[001]$ (order 4)	$<100>$, i.e. a and b (order 2)	$<110>$, i.e. $a \pm b$ (order 2)
hexagonal	c (order 6 or 3)	$<100>$, i.e. a, b, $[1\bar{1}0]$ (order 2)	$<210>$, i.e.$[210]$, $[\bar{1}20]$, $[1\bar{1}0]$ (order 2)
cubic	$<100>$ (order 4 or 2)	$<111>$ (order 3)	$<110>$ (order 2)

3. Space group symmetry: *the 230 space groups*

cryst. syst.	point group	space group No.	space group symbol
a	1	1	*P*1
	$\bar{1}$	2	$P\bar{1}$
m	2	3	*P*2
		4	$P2_1$
		5	*C*2
	m	6	*Pm*
		7	*Pc*
		8	*Cm*
		9	*Cc*
	2/*m*	10	*P*2/*m*
		11	$P2_1/m$
		12	*C*2/*m*
		13	*P*2/*c*
		14	$P2_1/c$
		15	*C*2/*c*
o	222	16	*P*222
		17	$P222_1$
		18	$P2_12_12$
		19	$P2_12_12_1$
		20	$C222_1$
		21	*C*222
		22	*F*222
		23	*I*222
		24	$I2_12_12_1$
	*mm*2	25	*Pmm*2
		26	$Pmc2_1$
		27	*Pcc*2
		28	*Pma*2
		29	$Pca2_1$
		30	*Pnc*2
		31	$Pmn2_1$
		32	$Pba2_1$
		33	$Pna2_1$
		34	*Pnn*2
		35	*Cmm*2
		36	$Cmc2_1$
		37	*Ccc*2
		38	*Amm*2
		39	*Aem*2
		40	*Ama*2
		41	*Aea*2
		42	*Fmm*2
		43	*Fdd*2
		44	*Imm*2
		45	*Iba*2
		46	*Ima*2
	mmm	47	*Pmmm*
		48	*Pnnn*
		49	*Pccm*
		50	*Pban*
		51	*Pmma*
		52	*Pnna*
		53	*Pmna*
		54	*Pcca*
		55	*Pbam*
		56	*Pccn*
		57	*Pbcm*
		58	*Pnnm*
		59	*Pmmn*
		60	*Pbcn*
		61	*Pbca*
		62	*Pnma*
		63	*Cmcm*
		64	*Cmce*
		65	*Cmmm*
		66	*Cccm*
		67	*Cmme*
		68	*Ccce*
		69	*Fmmm*
		70	*Fddd*
		71	*Immm*
		72	*Ibam*
		73	*Ibca*
		74	*Imma*
t	4	75	*P*4
		76	$P4_1$
		77	$P4_2$
		78	$P4_3$
		79	*I*4
		80	$I4_1$
	$\bar{4}$	81	$P\bar{4}$
		82	$I\bar{4}$
	4/*m*	83	*P*4/*m*
		84	$P4_2/m$
		85	*P*4/*n*
		86	$P4_2/n$
		87	*I*4/*m*
		88	$I4_1/a$
	422	89	*P*422
		90	$P42_12$
		91	$P4_122$
		92	$P4_12_12$
		93	$P4_222$
		94	$P4_22_12$
		95	$P4_322$
		96	$P4_32_12$
		97	*I*422
		98	$I4_122$
	4*mm*	99	*P*4*mm*
		100	*P*4*bm*
		101	$P4_2cm$
		102	$P4_2nm$
		103	*P*4*cc*
		104	*P*4*nc*
		105	$P4_2mc$
		106	$P4_2bc$
		107	*I*4*mm*
		108	*I*4*cm*
		190	$I4_1md$
		110	$I4_1cd$
	$\bar{4}2m$	111	$P\bar{4}2m$
		112	$P\bar{4}2c$
		113	$P\bar{4}2_1m$
		114	$P\bar{4}2_1c$
		115	$P\bar{4}m2$
		116	$P\bar{4}c2$
		117	$P\bar{4}b2$
		118	$P\bar{4}n2$
		119	$I\bar{4}m2$
		120	$I\bar{4}c2$
		121	$I\bar{4}2m$
		122	$I\bar{4}2d$
	4/*mmm*	123	*P*4/*mmm*
		124	*P*4/*mcc*
		125	*P*4/*nbm*
		126	*P*4/*nnc*
		127	*P*4/*mbm*
		128	*P*4/*mnc*
		129	*P*4/*nmm*
		130	*P*4/*nnc*
		131	$P4_2/mmc$
		132	$P4_2/mcm$
		133	$P4_2/nbc$
		134	$P4_2/nnm$
		135	$P4_2/mbc$
		136	$P4_2/mnm$
		137	$P4_2/nmc$
		138	$P4_2/ncm$
		139	*I*4/*mmm*
		140	*I*4/*mcm*
		141	$I4_1/amd$
		142	$I4_1/acd$
h	3	143	*P*3
		144	$P3_1$
		145	$P3_2$
		146	*R*3
	$\bar{3}$	147	$P\bar{3}$
		148	$R\bar{3}$
	32	149	*P*312
		150	*P*321
		151	$P3_112$
		152	$P3_121$
		153	$P3_212$
		154	$P3_221$
		155	*R*32
	3*m*	156	*P*3*m*1
		157	*P*31*m*
		158	*P*3*c*1
		159	*P*31*c*
		160	*R*3*m*
		161	*R*3*c*
	$\bar{3}m$	162	$P\bar{3}1m$
		163	$P\bar{3}1c$
		164	$P\bar{3}m1$
		165	$P\bar{3}c1$
		166	$R\bar{3}m$
		167	$R\bar{3}c$
h	6	168	*P*6
		169	$P6_1$
		170	$P6_5$
		171	$P6_2$
		172	$P6_4$
		173	$P6_3$
	$\bar{6}$	174	$P\bar{6}$
	6/*m*	175	*P*6/*m*
		176	$P6_3/m$
	622	177	*P*622
		178	$P6_122$
		179	$P6_522$
		180	$P6_222$
		181	$P6_422$
		182	$P6_322$
	6*mm*	183	*P*6*mm*
		184	*P*6*cc*
		185	$P6_3cm$
		186	$P6_3mc$
	$\bar{6}m2$	187	$P\bar{6}m2$
		188	$P\bar{6}c2$
		189	$P\bar{6}2m$
		190	$P\bar{6}2c$
	6/*mmm*	191	*P*6/*mmm*
		192	*P*6/*mcc*
		193	*P*6/*mcm*
		194	*P*6/*mmc*
c	23	195	*P*23
		196	*F*23
		197	*I*23
		198	$P2_13$
		199	$I2_13$
	*m*3	200	$Pm\bar{3}$
		201	$Pn\bar{3}$
		202	$Fm\bar{3}$
		203	$Fd\bar{3}$
		204	$Im\bar{3}$
		205	$Pa\bar{3}$
		206	$Ia\bar{3}$
	432	207	*P*432
		208	$P4_232$
		209	*F*432
		210	$F4_132$
		211	*I*432
		212	$P4_332$
		213	$P4_132$
		214	$I4_132$
	$\bar{4}3m$	215	$P\bar{4}3m$
		216	$F\bar{4}3m$
		217	$I\bar{4}3m$
		218	$P\bar{4}3n$
		219	$F\bar{4}3c$
		220	$I\bar{4}3d$
	$m\bar{3}m$	221	$Pm\bar{3}m$
		222	$Pn\bar{3}n$
		223	$Pm\bar{3}n$
		224	$Pn\bar{3}m$
		225	$Fm\bar{3}m$
		226	$Fm\bar{3}c$
		227	$Fd\bar{3}m$
		228	$Fd\bar{3}c$
		229	$Im\bar{3}m$
		230	$Ia\bar{3}d$

6 conventional cells

14 Bravais lattices (translation symmetry)

32 point groups

*Symmetry at the **macroscopic** scale*

230 space groups

*Symmetry at the **microscopic** scale*

3. Space group symmetry: *space group Pnma – ITC*

Non symmorphic SG
(∃ glide translations)

Diagrams of
symmetry operations

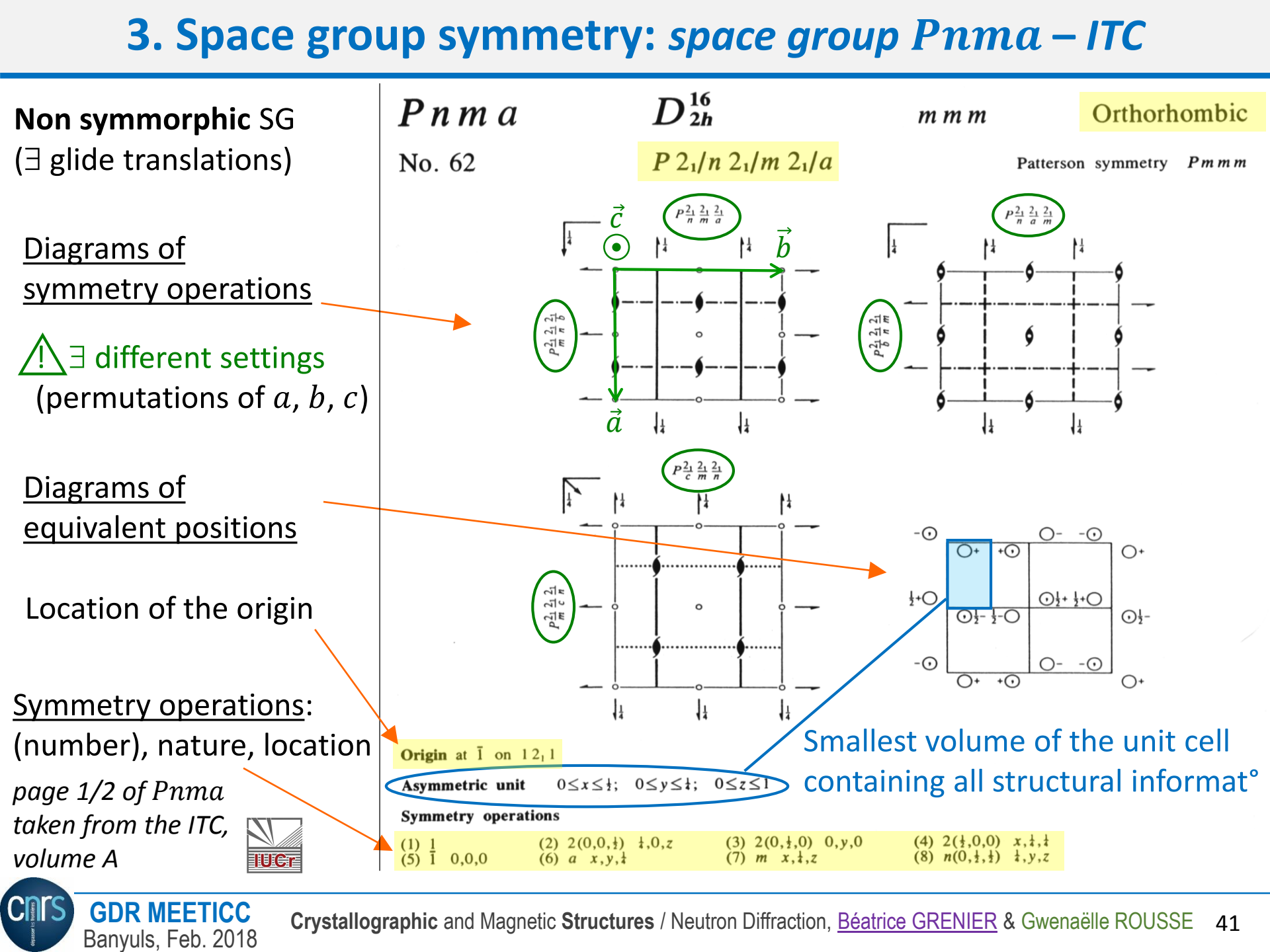
⚠ ∃ different settings
(permutations of a, b, c)

Diagrams of
equivalent positions

Location of the origin

Symmetry operations:
(number), nature, location

page 1/2 of Pnma taken from the ITC, volume A



Smallest volume of the unit cell containing all structural informat°

3. Space group symmetry: *space group Pnma – ITC*

Orthorhombic $P\,2_1/n\,2_1/m\,2_1/a$

Bravais lattice

Screw axis $2_1 \parallel \vec{a}$
Glide plane $n \perp \vec{a}$

Screw axis $2_1 \parallel \vec{c}$
Glide plane $a \perp \vec{c}$

Screw axis $2_1 \parallel \vec{b}$
Mirror plane $m \perp \vec{b}$

Point group: $\frac{2}{m}\frac{2}{m}\frac{2}{m}$

$(n, m, a \rightarrow m$ and $2_1 \rightarrow 2)$

"Representation" of the symmetry operations

Symmetry operations

(1) 1	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$	(3) $2(0,\frac{1}{2},0)$ $0,y,0$	(4) $2(\frac{1}{4},0,0)$ $x,\frac{1}{4},\frac{1}{4}$
(5) $\bar{1}$ 0,0,0	(6) a $x,y,\frac{1}{4}$	(7) m $x,\frac{1}{4},z$	(8) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$

2-fold rotation
followed by $\vec{t} = \frac{1}{2}\vec{c}$
i.e. axis $2_1 \parallel \vec{c}$

axis $\parallel \vec{c}$ at
$x = \frac{1}{4}$ et $y = 0$

Glide plane n
with $\vec{t} = \frac{1}{2}(\vec{b} + \vec{c})$

plane (x, y), i.e. $\perp \vec{a}$
with $x = \frac{1}{4}$

3. Space group symmetry: *space group Pnma – ITC*

CONTINUED **No. 62** ***P n m a***

Generators selected (1); *t*(1,0,0); *t*(0,1,0); *t*(0,0,1); (2); (3); (5)

Arbitrary choice of generators for the SG

Identity
Elementary translations
+ some of the symmetry
axes and planes

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	*d*	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$ (6) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}$ (7) $x,\bar{y}+\frac{1}{2},z$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$ (8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$
4	*c*	.*m*.	$x,\frac{1}{4},z$	$\bar{x}+\frac{1}{2},\frac{3}{4},z+\frac{1}{2}$	$\bar{x},\frac{3}{4},\bar{z}$	$x+\frac{1}{2},\frac{1}{4},\bar{z}+\frac{1}{2}$
4	*b*	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$
4	*a*	$\bar{1}$	$0,0,0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$

Symmetry of special projections

Along [001] $p\,2g\,m$
$\boldsymbol{a}'=\frac{1}{2}\boldsymbol{a}$ $\boldsymbol{b}'=\boldsymbol{b}$
Origin at $0,0,z$

Along [100] $c\,2m\,m$
$\boldsymbol{a}'=\boldsymbol{b}$ $\boldsymbol{b}'=\boldsymbol{c}$
Origin at $x,\frac{1}{4},\frac{1}{4}$

Along [010] $p\,2g\,g$
$\boldsymbol{a}'=\boldsymbol{c}$ $\boldsymbol{b}'=\boldsymbol{a}$
Origin at $0,y,0$

Reflection conditions

General:
$0kl$: $k+l=2n$
$hk0$: $h=2n$
$h00$: $h=2n$
$0k0$: $k=2n$
$00l$: $l=2n$

Special: as above, plus

no extra conditions

hkl : $h+l,k=2n$

hkl : $h+l,k=2n$

See Lecture III

Maximal non-isomorphic subgroups

I	[2]$P\,2_1\,2_1\,2_1$	1; 2; 3; 4
	[2]$P\,1\,1\,2_1/a$ ($P\,2_1/c$)	1; 2; 5; 6
	[2]$P\,1\,2_1/m\,1$ ($P\,2_1/m$)	1; 3; 5; 7
	[2]$P\,2_1/n\,1\,1$ ($P\,2_1/c$)	1; 4; 5; 8
	[2]$P\,n\,m\,2_1$ ($P\,m\,n\,2_1$)	1; 2; 7; 8
	[2]$P\,n\,2_1\,a$ ($P\,n\,a\,2_1$)	1; 3; 6; 8
	[2]$P\,2_1\,m\,a$ ($P\,m\,c\,2_1$)	1; 4; 6; 7
IIa	none	
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [3]$P\,n\,m\,a\,(\boldsymbol{a}'=3\boldsymbol{a})$; [3]$P\,n\,m\,a\,(\boldsymbol{b}'=3\boldsymbol{b})$; [3]$P\,n\,m\,a\,(\boldsymbol{c}'=3\boldsymbol{c})$

subgroups /supergroups, for crystallogr. transitions to a lower / higher symmetry phase
See Lecture II

See also www.cryst.ehu.es

Minimal non-isomorphic supergroups

I none

II [2]$A\,m\,m\,a\,(C\,m\,c\,m)$; [2]$B\,b\,m\,m\,(C\,m\,c\,m)$; [2]$C\,c\,m\,b\,(C\,m\,c\,a)$; [2]$I\,m\,m\,a$; [2]$P\,n\,m\,m\,(2\boldsymbol{a}'=\boldsymbol{a})\,(P\,m\,m\,n)$; [2]$P\,c\,m\,a\,(2\boldsymbol{b}'=\boldsymbol{b})\,(P\,b\,a\,m)$; [2]$P\,b\,m\,a\,(2\boldsymbol{c}'=\boldsymbol{c})\,(P\,b\,c\,m)$

page 2/2 of Pnma taken from the ITC, volume A

3. Space group symmetry: *space group Pnma – ITC*

Wyckoff sites: List of the different sites from the most general (*i.e.* less symmetrical) to the less general position (*i.e.* most symmetrical: special position)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	*d*	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(7) $x,\bar{y}+\frac{1}{2},z$	(8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$
4	*c*	$.m.$	$x,\frac{1}{4},z$	$\bar{x}+\frac{1}{2},\frac{3}{4},z+\frac{1}{2}$	$\bar{x},\frac{3}{4},\bar{z}$	$x+\frac{1}{2},\frac{1}{4},\bar{z}+\frac{1}{2}$
4	*b*	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$
4	*a*	$\bar{1}$	$0,0,0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$

Site name

Multiplicity of the site

Wyckoff letter

Symmetry of the site

Coordinates of all equivalent positions

3. Space group symmetry: *space group Pnma – ITC*

Wyckoff sites: List of the different sites from the most general (*i.e.* less symmetrical) to the less general position (*i.e.* most symmetrical: special position)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates			
8 *d*	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$
		(5) $\bar{x},\bar{y},\bar{z}$	(6) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(7) $x,\bar{y}+\frac{1}{2},z$	(8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$

Symmetry operations

(1) 1	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$	(3) $2(0,\frac{1}{2},0)$ $0,y,0$	(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},\frac{1}{4}$
(5) $\bar{1}$ $0,0,0$	(6) a $x,y,\frac{1}{4}$	(7) m $x,\frac{1}{4},z$	(8) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$

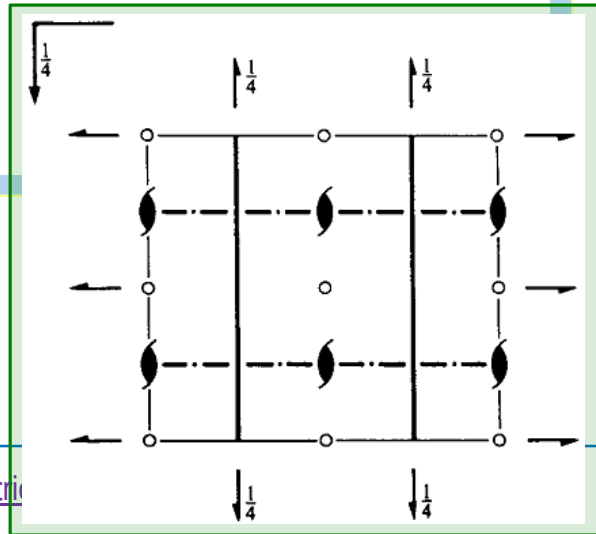
3. Space group symmetry: *space group Pnma – ITC*

Wyckoff sites: List of the different sites from the most general (*i.e.* less symmetrical) to the less general position (*i.e.* most symmetrical: special position)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	*d*	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(7) $x,\bar{y}+\frac{1}{2},z$	(8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$
4	*c*	.*m*.	$x,\frac{1}{4},z$	$\bar{x}+\frac{1}{2},\frac{3}{4},z+\frac{1}{2}$	$\bar{x},\frac{3}{4},\bar{z}$	$x+\frac{1}{2},\frac{1}{4},\bar{z}+\frac{1}{2}$
4	*b*	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$
4	*a*	$\bar{1}$	$0,0,0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$

Origin at $\bar{1}$ on $12_1 1$



3. Space group symmetry: *space group Pnma*

http://img.chem.ucl.ac.uk/sgp/

High-Resolution

Space Group Diagrams and Tables

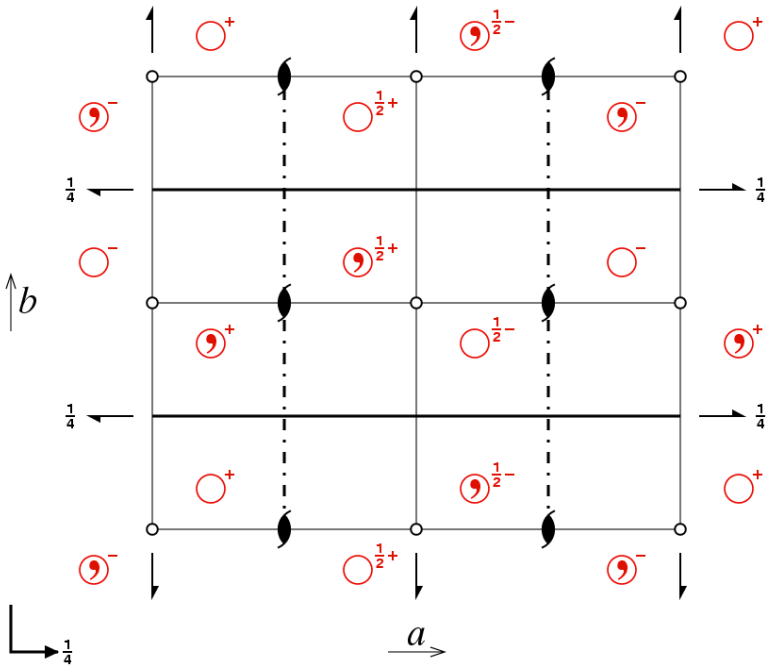
Return link to the main menu

Orthorhombic

(For a fuller list with alternative axes and origins click here)

61. *P b c a*	62. *P n m a*	63. *C m c m*	64. *C m c a*	65. *C m m m*
66. *C c c m*	67. *C m m a*	68. *C c c a*	69. *F m m m*	70. *F d d d*
71. *I m m m*	72. *I b a m*	73. *I b c a*	74. *I m m a*	

Pnma $P\,2_1/n\,2_1/m\,2_1/a$ *mmm* No. 62



Symmetry Operators

1	x, y, z	1	
2	$\frac{1}{2}-x, \frac{1}{2}+y, \frac{1}{2}+z$	n	$(\frac{1}{4}, y, z)\ [0, \frac{1}{2}, \frac{1}{2}]$
3	$x, \frac{1}{2}-y, z$	m	$(x, \frac{1}{4}, z)$
4	$\frac{1}{2}+x, y, \frac{1}{2}-z$	a	$(x, y, \frac{1}{4})\ [\frac{1}{2}, 0, 0]$
5	$\bar{x}, \bar{y}, \bar{z}$	$\bar{1}$	$(0, 0, 0)$
6	$\frac{1}{2}+x, \frac{1}{2}-y, \frac{1}{2}-z$	2_1	$(x, \frac{1}{4}, \frac{1}{4})\ [\frac{1}{2}, 0, 0]$
7	$\bar{x}, \frac{1}{2}+y, \bar{z}$	2_1	$(0, y, 0)\ [0, \frac{1}{2}, 0]$
8	$\frac{1}{2}-x, \bar{y}, \frac{1}{2}+z$	2_1	$(\frac{1}{4}, 0, z)\ [0, 0, \frac{1}{2}]$

Careful: different order as compared to the ITC!

3. Space group symmetry: *space group Pnma*

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Space-group symmetry

WYCKPOS

Wyckoff Positions of Group 62 (*Pnma*)

Multiplicity	Wyckoff letter	Site symmetry	Coordinates
8	d	1	(x,y,z) (-x+1/2,-y,z+1/2) (-x,y+1/2,-z) (x+1/2,-y+1/2,-z+1/2) (-x,-y,-z) (x+1/2,y,-z+1/2) (x,-y+1/2,z) (-x+1/2,y+1/2,z+1/2)
4	c	.m.	(x,1/4,z) (-x+1/2,3/4,z+1/2) (-x,3/4,-z) (x+1/2,1/4,-z+1/2)
4	b	-1	(0,0,1/2) (1/2,0,0) (0,1/2,1/2) (1/2,1/2,0)
4	a	-1	(0,0,0) (1/2,0,1/2) (0,1/2,0) (1/2,1/2,1/2)

Wyckoff position and site symmetry group of a specific point

Specify the point by its relative coordinates (in fractions or decimals)
Variable parameters (x,y,z) are also accepted

x = y = z =

Show

If you want to see the Wyckoff position in other setting, click here

http://www.cryst.ehu.es/

3. Space group symmetry: *space group Pnma*

ITC

8	*d*	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(7) $x,\bar{y}+\frac{1}{2},z$	(8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$

Symmetry operations

(1) 1	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$	(3) $2(0,\frac{1}{4},0)$ $0,y,0$	(4) $2(\frac{1}{4},0,0)$ $x,\frac{1}{4},\frac{1}{4}$
(5) $\bar{1}$ 0,0,0	(6) *a* $x,y,\frac{1}{4}$	(7) *m* $x,\frac{1}{4},z$	(8) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$

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Space-group symmetry

GENPOS

General Positions of the Group 62 (*Pnma*)

Click here to get the general positions in text format

No.	(x,y,z) form	Matrix form	Symmetry operation	
			ITA	Seitz
1	x,y,z	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	1	{ 1 | 0 }
2	-x+1/2,-y,z+1/2	$\begin{pmatrix} -1 & 0 & 0 & 1/2 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 1/2 \end{pmatrix}$	2 (0,0,1/2) 1/4,0,z	{ 2_{001} | 1/2 0 1/2 }

Same order

3. Space group symmetry: *space group $Pnma$ – $LaMnO_3$*

Example: $LaMnO_3$ (space group $Pnma$)

($\equiv Pbnm$ if $\vec{a} \to \vec{b} \to \vec{c} \to \vec{a}$)

	x	y	z	
La	0.518	0.25	0.007	$\to 4c$
Mn	0	0	0	$\to 4a$
O_1	-0.005	0.25	0.075	$\to 4c$
O_2	0.288	0.096	0.226	$\to 8d$

→ Motif = $La_4Mn_4O_{12}$

7 coordinates to determine out of (4+4+12)×3 = 60 !!!

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
O_2 8 d	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$
		(5) $\bar{x},\bar{y},\bar{z}$	(6) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(7) $x,\bar{y}+\frac{1}{2},z$	(8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$
La, O_1 4 c	$.m.$	$x,\frac{1}{4},z$	$\bar{x}+\frac{1}{2},\frac{3}{4},z+\frac{1}{2}$	$\bar{x},\frac{3}{4},\bar{z}$	$x+\frac{1}{2},\frac{1}{4},\bar{z}+\frac{1}{2}$
4 b	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$
Mn 4 a	$\bar{1}$	$0,0,0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$

3. Space group symmetry: *space group Pnma – $LaMnO_3$*

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Note: substructure search by SMILES is currently available in a subset of COD containing 157980 str

text (1 or 2 words)	
journal	
year	
volume	
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DOI	
Z (min, max)	
Z' (min, max)	
chemical formula (in Hill notation)	
1 to 8 elements	La Mn O
NOT these elements	
volume min and max	
number of distinct elements min and max	3
filters	has F_{obs} include duplicates include structures with errors include theoretical structures
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3. Space group symmetry: *space group Pnma – $LaMnO_3$*

.cif file for $LaMnO_3$

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#$Revision: 176429 $
#$URL: svn://www.crystallography.net/cod/cif/1/52/13/1521337.cif $
#------------------------------------------------------------------------
#
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-x+1/2,-y,z+1/2
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-x,y+1/2,-z
-x,-y,-z
x-1/2,y,-z-1/2
-x-1/2,y-1/2,z-1/2
x,-y-1/2,z
loop_
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_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_U_iso_or_equiv
Mn1 Mn+3 0 0 0.5 1 0.0
O2 O-2 0.194 0.537 0.223 1 0.0
La1 La+3 0.0495 0.25 -0.083 1 0.0
O1 O-2 0.474 0.25 0.07 1 0.0
```

3. Space group symmetry: *space group Pnma – $LaMnO_3$*

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				Search Effacer
Elements	**Element Count**	**Chem/Mineral Name**	**ANX/Pearson/S.Type**	**Cell Size/Mass**
La Mn O	3			
System	**Laue Class**	**Centering**	**Space Group**	**Wyckoff Sequence**
any	any	any		
Remarks	**Min. Distance**	**Distance Select**	**Distance Range**	**Co-ordin.**

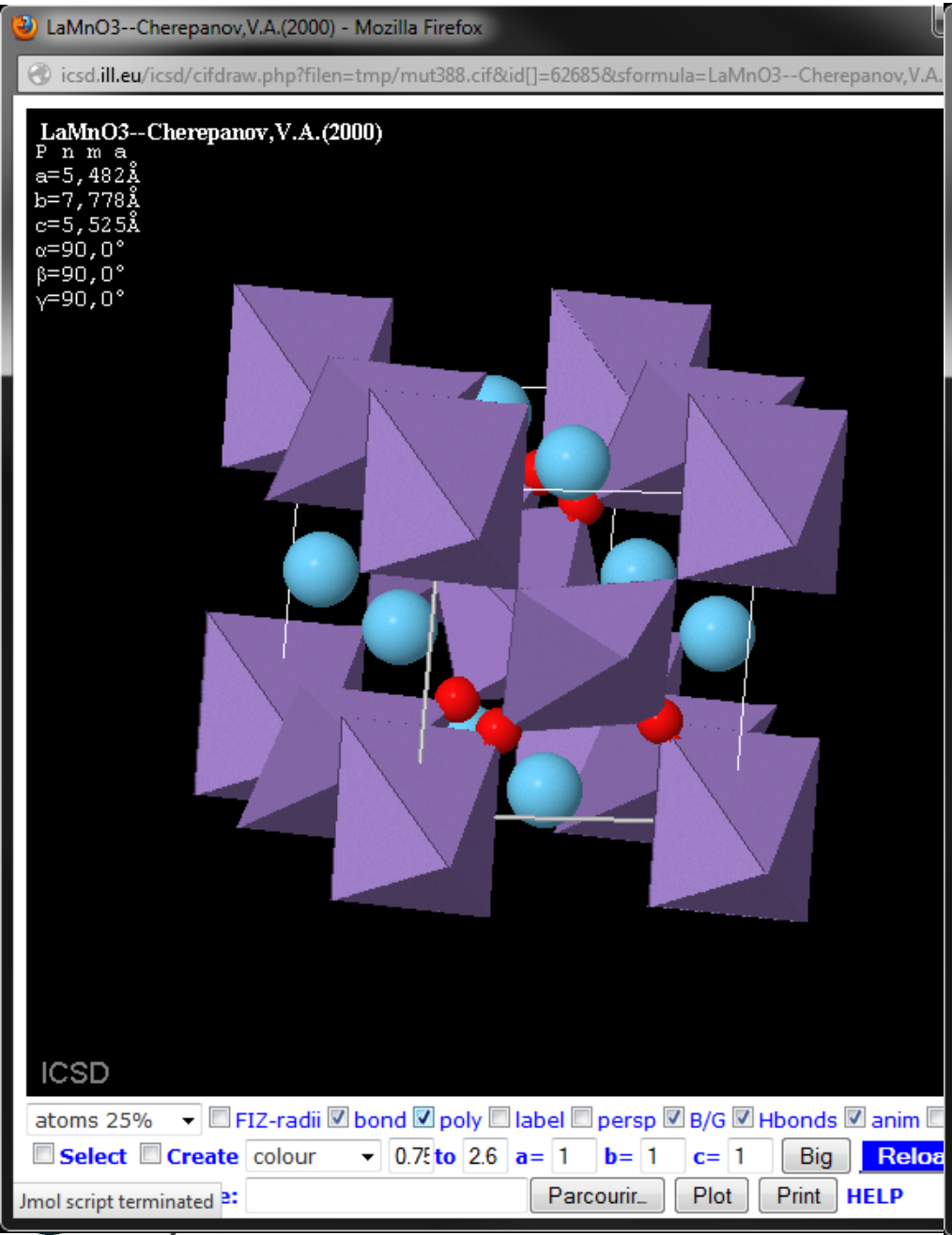
Query : (EL_COUNT = "3") AND icsd.sum_form RLIKE 'LA[0-9]' AND icsd.sum_form RLIKE 'MN[0-9]' AND icsd.sum_form RLIKE BINARY 'O[0-9]'

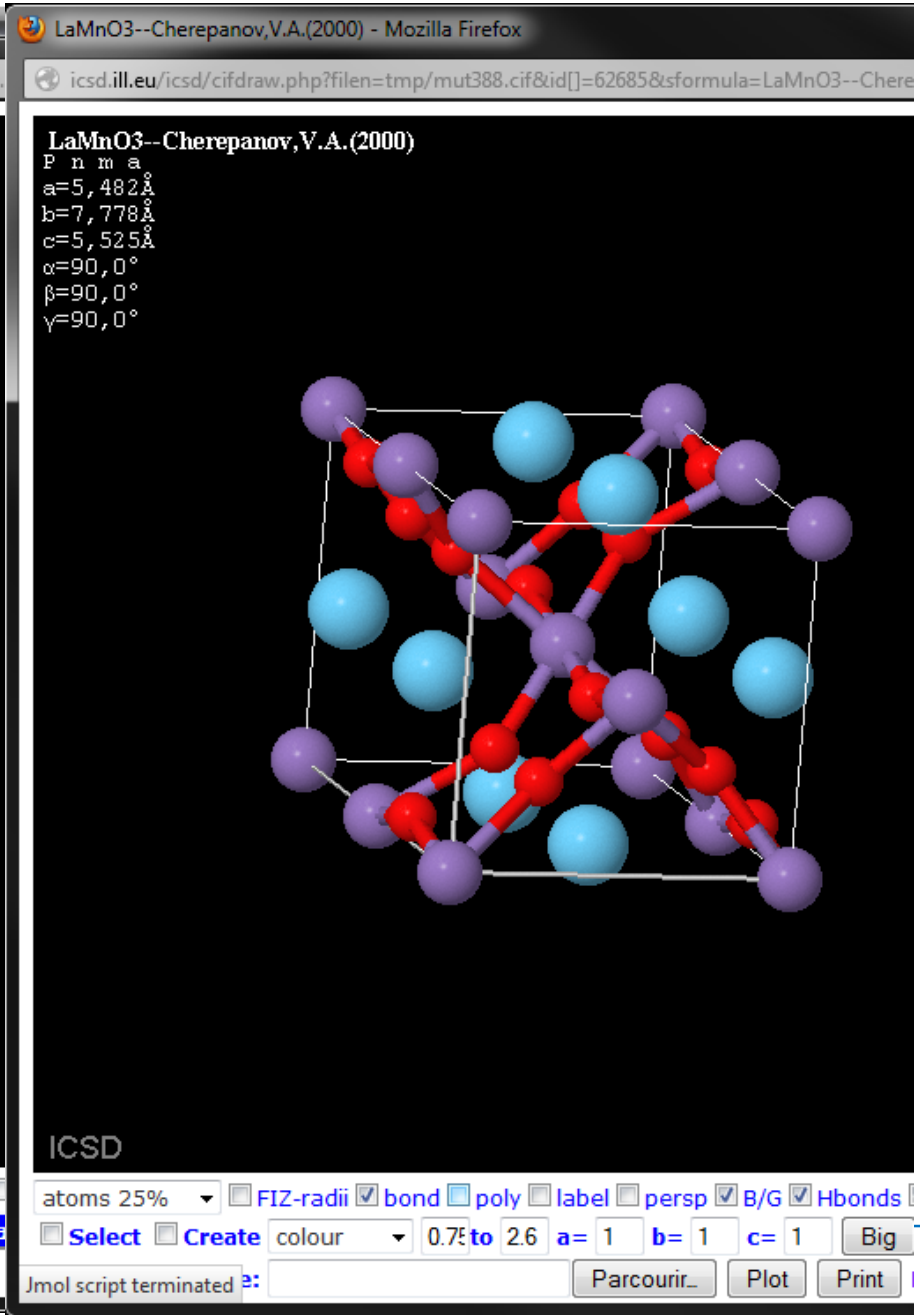
Select All / None *8 Results* References EndNote Details CIF Bonds Pattern Structure Jmol

Year	Authors	Title	Struct. Formula	sgr	Mineral
2004	Hansteen, O.H.; Breard, Y.; Fjellvag, H.; Hauback, B.C.;	Divalent manganese in reduced La Mn O3-d - effect of oxygen nonstoichiometry on structural and magnetic properties	La (Mn O2.78)	PNMA	
2000	Cherepanov, V.A.; Filonova, E.A.; Voronin, V.I.; Berger, I.F.;	Phase equilibria in the (La Co O3) - (La Mn O3) -(Ba Co Oz) (Ba Mn O3) system	La Mn O3	PNMA	
1999	Taguchi, H.; Matsu-ura, S.-I.; Nagao, M.; Kido, H.;	Electrical properties of perovskite-type La (Cr1-x Mnx) O3+d	La0.951 Mn0.951 O3	R3-CR	
1997	Ferris, V.; Goglio, G.; Brohan, L.; Joubert, O.; Molinie, P.; Ganne, M.; Dordor, P.;	Transport properties and magnetic behavior in the polycrystalline lanthanum-deficient manganate perovskite (La(1-x) Mn O3)	La0.91 (Mn0.99 O3)	R3CR	
1997	Alonso, J.A.; Martinez-Lopez, M.J.; Casais, M.T.; MacManus-Driscoll, J.L.; de Silva, P.S.I.P.N.; Cohen, L.F.; Fernandez-Diaz, M.T.;	Non-stoichiometry, structural defects and properties of La Mn O3+d with high d values (0.11	La0.969 Mn0.93 O3	R3-CH	
1996	Shimura, T.; Hayashi, T.; Inaguma, Y.; Itoh, M.;	Magnetic and electrical properties of Lay Ax Mnw O3 (A = Na, K, Rb and Sr) with perovskite-type structure	La0.953 Mn0.935 O3	R3-CH	
1996	Hauback, B.C.; Fjellvag, H.; Sakai, N.;	Effect of nonstoichiometry on properties of La1-t Mn O3+d. III. Magnetic order studied by neutron powder diffraction	La0.92 Mn O2.88	PNMA	
1996	Hauback, B.C.; Fjellvag, H.; Sakai, N.;	Effect of nonstoichiometry on properties of La1-x Mn O3+delta III. Magnetic order studied by powder neutron diffraction	La0.88 Mn O2.82	PNMA	

Page : [1](8 results) 10 results per page.

3. Space group symmetry: *space group $Pnma$ – $LaMnO_3$*





3. Space group symmetry: *space group Pnma – $LaMnO_3$*

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				Search Effacer
Elements	**Element Count**	**Chem/Mineral Name**	**ANX/Pearson/S.Type**	**Cell Size/Mass**
La Mn O	3			
System	**Laue Class**	**Centering**	**Space Group**	**Wyckoff Sequence**
any	any	any		
Remarks	**Min. Distance**	**Distance Select**	**Distance Range**	**Co-ordin.**

Query : (EL_COUNT = "3") AND icsd.sum_form RLIKE 'LA[0-9]' AND icsd.sum_form RLIKE 'MN[0-9]' AND icsd.sum_form RLIKE BINARY 'O[0-9]'

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1996	Hauback, B.C.; Fjellvag, H.; Sakai, N.;	Effect of nonstoichiometry on properties of La1-t Mn O3+d. III. Magnetic order studied by neutron powder diffraction	La0.92 Mn O2.88	PNMA	
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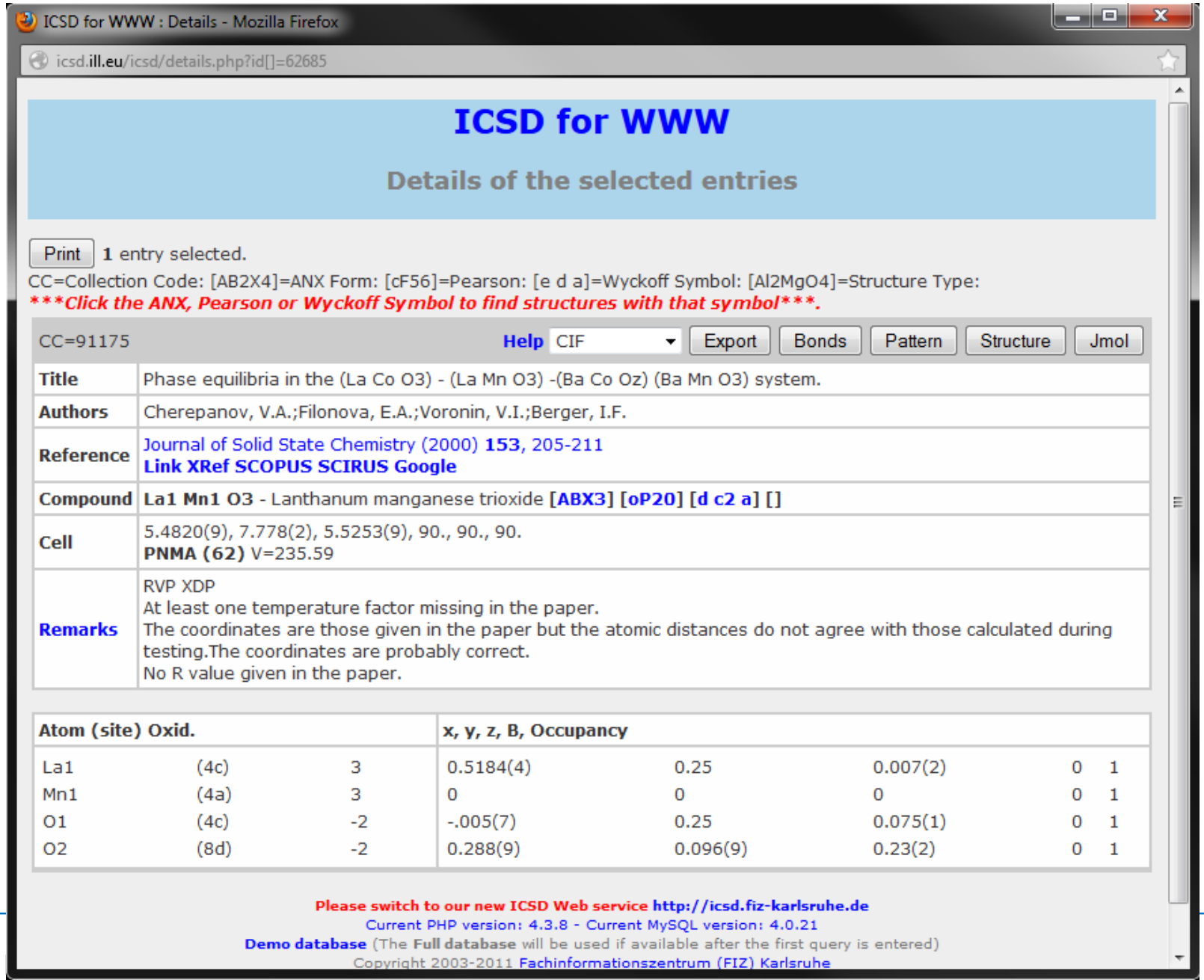
Page : [1](8 results) 10 results per page.

3. Space group symmetry: *space group Pnma – $LaMnO_3$*



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CC=Collection Code: [AB2X4]=ANX Form: [cF56]=Pearson: [e d a]=Wyckoff Symbol: [Al2MgO4]=Structure Type:

******Click the ANX, Pearson or Wyckoff Symbol to find structures with that symbol***.***

CC=91175 **Help** CIF Export Bonds Pattern Structure Jmol

Title	Phase equilibria in the (La Co O3) - (La Mn O3) -(Ba Co Oz) (Ba Mn O3) system.
Authors	Cherepanov, V.A.;Filonova, E.A.;Voronin, V.I.;Berger, I.F.
Reference	Journal of Solid State Chemistry (2000) **153**, 205-211 **Link XRef SCOPUS SCIRUS Google**
Compound	**La1 Mn1 O3** - Lanthanum manganese trioxide **[ABX3] [oP20] [d c2 a] []**
Cell	5.4820(9), 7.778(2), 5.5253(9), 90., 90., 90. **PNMA (62)** V=235.59
Remarks	RVP XDP At least one temperature factor missing in the paper. The coordinates are those given in the paper but the atomic distances do not agree with those calculated during testing.The coordinates are probably correct. No R value given in the paper.

Atom (site) Oxid.			**x, y, z, B, Occupancy**				
La1	(4c)	3	0.5184(4)	0.25	0.007(2)	0	1
Mn1	(4a)	3	0	0	0	0	1
O1	(4c)	-2	-.005(7)	0.25	0.075(1)	0	1
O2	(8d)	-2	0.288(9)	0.096(9)	0.23(2)	0	1

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Current PHP version: 4.3.8 - Current MySQL version: 4.0.21

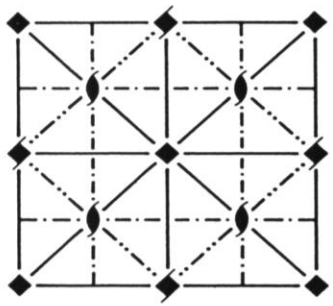
Demo database (The **Full database** will be used if available after the first query is entered)

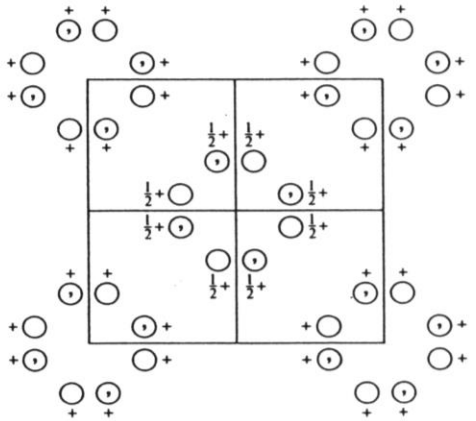
3. Space group symmetry: *space group I4mm*

Symmorphic SG

$I\,4\,m\,m$ $\quad C_{4v}^{9}$ $\quad 4\,m\,m$ $\quad$ Tetragonal

No. 107 $\quad I\,4\,m\,m$ $\quad$ Patterson symmetry $I\,4/m\,m\,m$





Origin on $4m\,m$

Asymmetric unit $0\le x\le\frac{1}{2};\ 0\le y\le\frac{1}{2};\ 0\le z\le\frac{1}{2};\ x\le y$

Symmetry operations

For (0,0,0)+ set

(1) 1	(2) 2 0,0,z	(3) 4^+ 0,0,z	(4) 4^- 0,0,z
(5) m x,0,z	(6) m 0,y,z	(7) m $x,\bar{x},z$	(8) m x,x,z

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$+ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{2},\frac{1}{2},z$	(3) $4^+(0,0,\frac{1}{2})$ $0,\frac{1}{2},z$	(4) $4^-(0,0,\frac{1}{2})$ $\frac{1}{2},0,z$
(5) $n(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{2},z$	(6) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{2},y,z$	(7) c $x+\frac{1}{2},\bar{x},z$	(8) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,z

Bravais lattice: body centered (I) tetragonal

Axis $4 \parallel \vec{c}$; mirrors $m \perp$ <100> ; mirrors $m \perp$ <110>

3. Space group symmetry: *space group I4mm*

Symmetry operations

4-fold rotation applied 2, 1, and 3 times, resp.

For (0,0,0)+ set

(1) 1	(2) 2 0,0,z	(3) 4⁺ 0,0,z	(4) 4⁻ 0,0,z
(5) m x,0,z	(6) m 0,y,z	(7) m x,x̄,z	(8) m x,x,z

For (½,½,½)+ set

(1) t(½,½,½)	(2) 2(0,0,½) ¼,¼,z	(3) 4⁺(0,0,½) 0,½,z	(4) 4⁻(0,0,½) ½,0,z
(5) n(½,0,½) x,¼,z	(6) n(0,½,½) ¼,y,z	(7) c x+½,x̄,z	(8) n(½,½,½) x,x,z

I lattice

Generators selected (1); t(1,0,0); t(0,1,0); t(0,0,1); t(½,½,½); (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates (0,0,0)+	(½,½,½)+		
16	e	1	(1) x,y,z	(2) x̄,ȳ,z	(3) ȳ,x,z	(4) y,x̄,z
			(5) x,ȳ,z	(6) x̄,y,z	(7) ȳ,x̄,z	(8) y,x,z
8	d	.m.	x,0,z	x̄,0,z	0,x,z	0,x̄,z
8	c	..m	x,x,z	x̄,x̄,z	x̄,x,z	x,x̄,z
4	b	2mm.	0,½,z	½,0,z		
2	a	4mm	0,0,z			

I lattice

Add (0,0,0) and (½ ½ ½) to these coordinates → 8 × 2 atomic coordinates

Summary

Point group symmetry:
Allows to predict the existence or not of some macroscopic physical properties
And in the case they do exist, the direction of the vectorial quantity or form of the tensor, …

Translation symmetry:
Responsible for diffraction → see lecture III

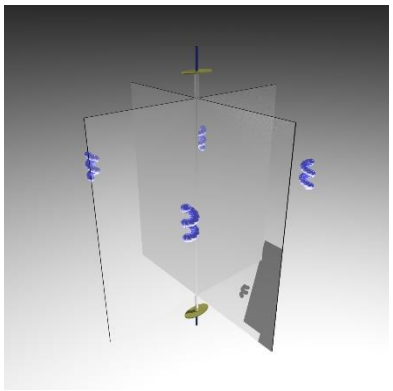
Structure completely described by:
Space group + lattice parameters + asymetric unit
Then use Wyckoff positions to calculate the coordinates of the other atoms of the motif, and last the lattice translations

The same approach can be done for magnetic structures → see lecture II

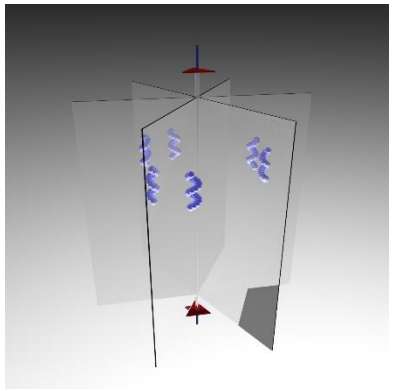
Point group: to go further …

From crystallographic point groups …

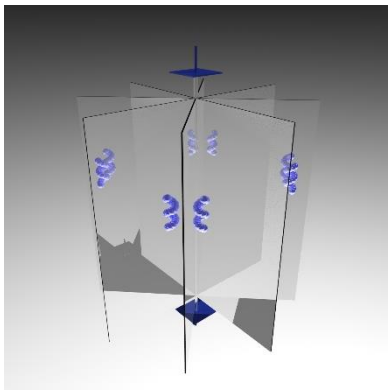
http://materials.cmu.edu/degraef/pg/



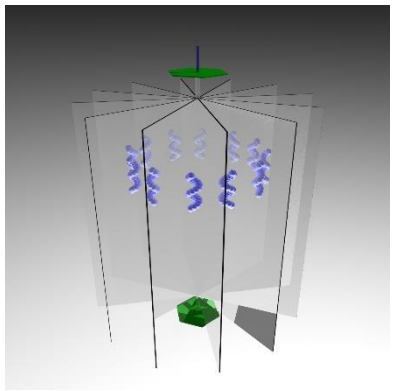
$2mm$



$3m$



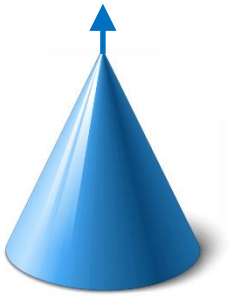
$4mm$



$6mm$

… to Curie point groups

∞m



Thank you …

et bonne dégustation