



1- Estructura de la Materia



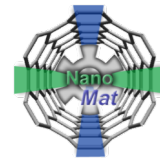
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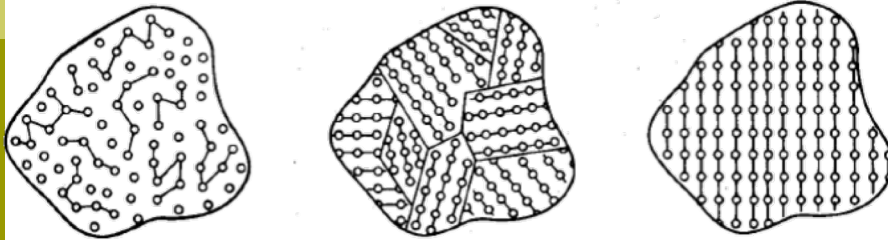


Punteo

- ❑ Cristales y Retículos
- ❑ Elementos de Simetría
- ❑ Grupos Puntuales
- ❑ Grupos Espaciales
- ❑ Cristales y Polimorfismo

1. Materiales Cristalinos

Son aquellos que se componen de átomos dispuestos en un modelo que se repite periódicamente en tres dimensiones. Lo que permite establecer orden de largo alcance.



1. Definición de Cristal

reference.iucr.org/dictionary/Crystal

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Crystal

Definition

A material is a crystal if it has **essentially** a sharp diffraction pattern. The word **essentially** means that most of the intensity of the diffraction is concentrated in relatively sharp **Bragg peaks**, besides the always present diffuse scattering. In all cases, the positions of the diffraction peaks can be expressed by

$$\mathbf{H} = \sum_{i=1}^n h_i \mathbf{a}_i^* \quad (n \geq 3)$$

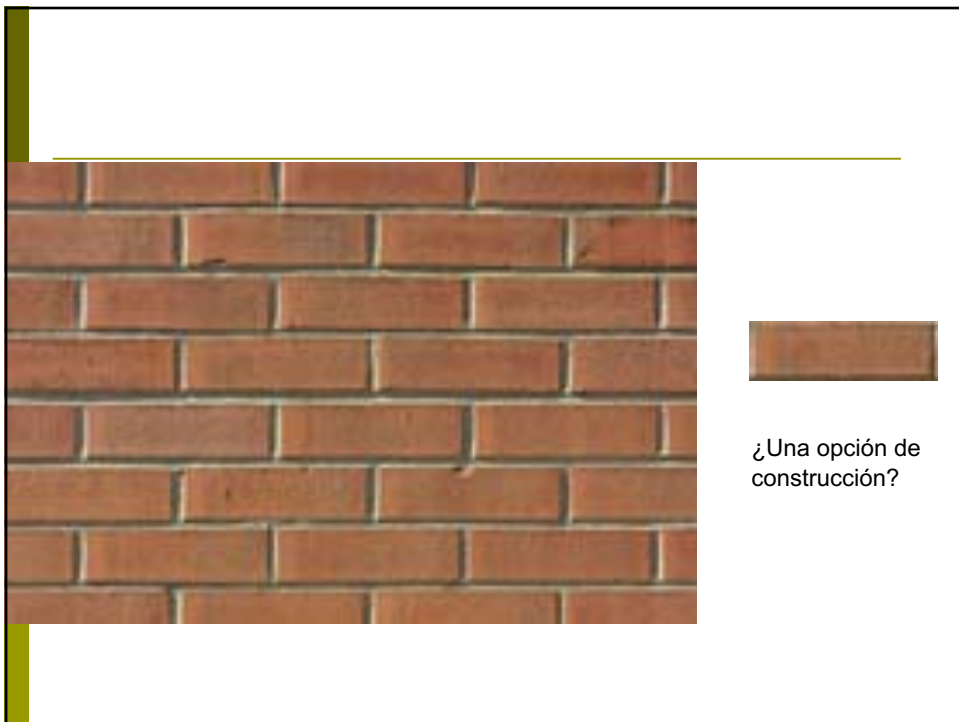
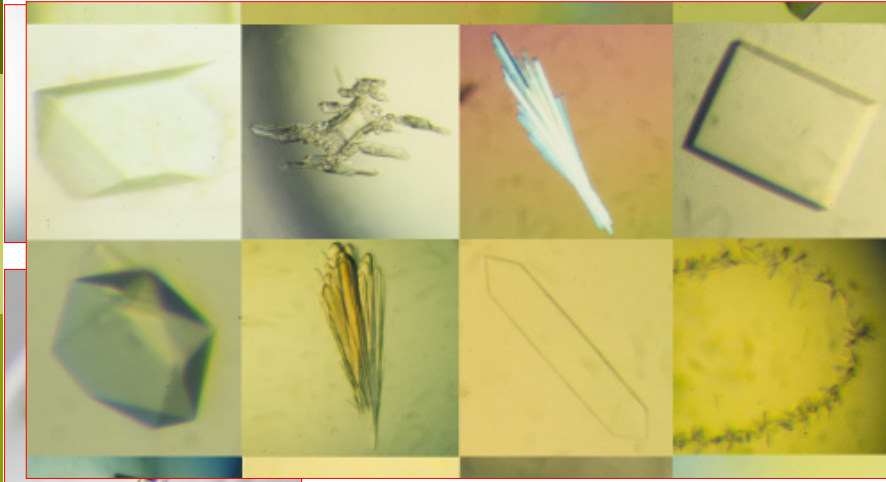
Here \mathbf{a}_i^* and h_i are the basis vectors of the reciprocal lattice and integer coefficients respectively and the number n is the minimum for which the positions of the peaks can be described with integer coefficient h_i .

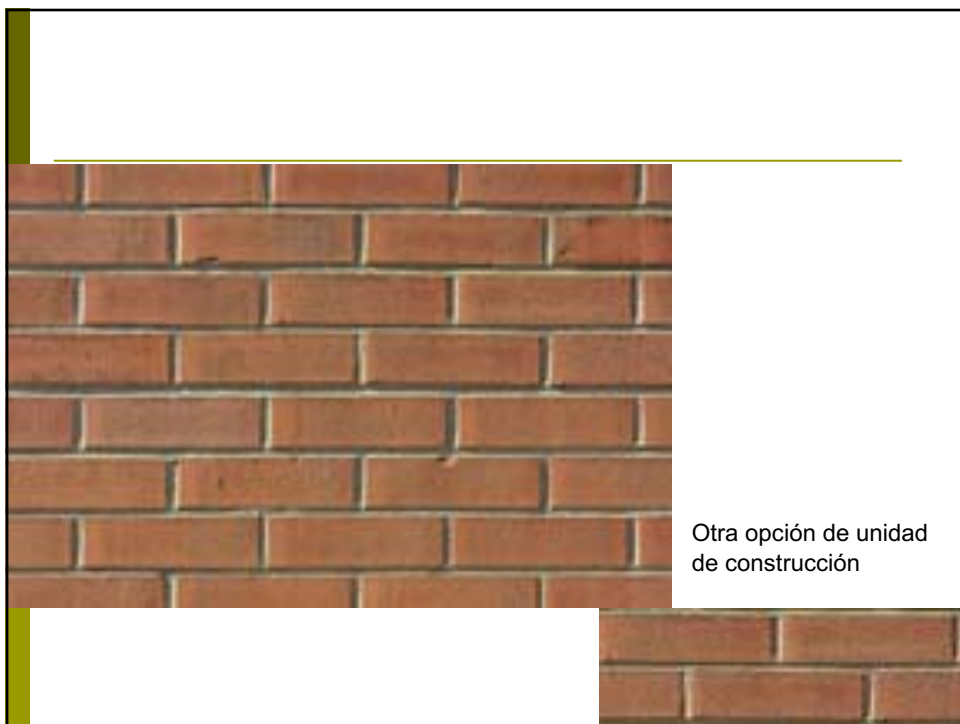
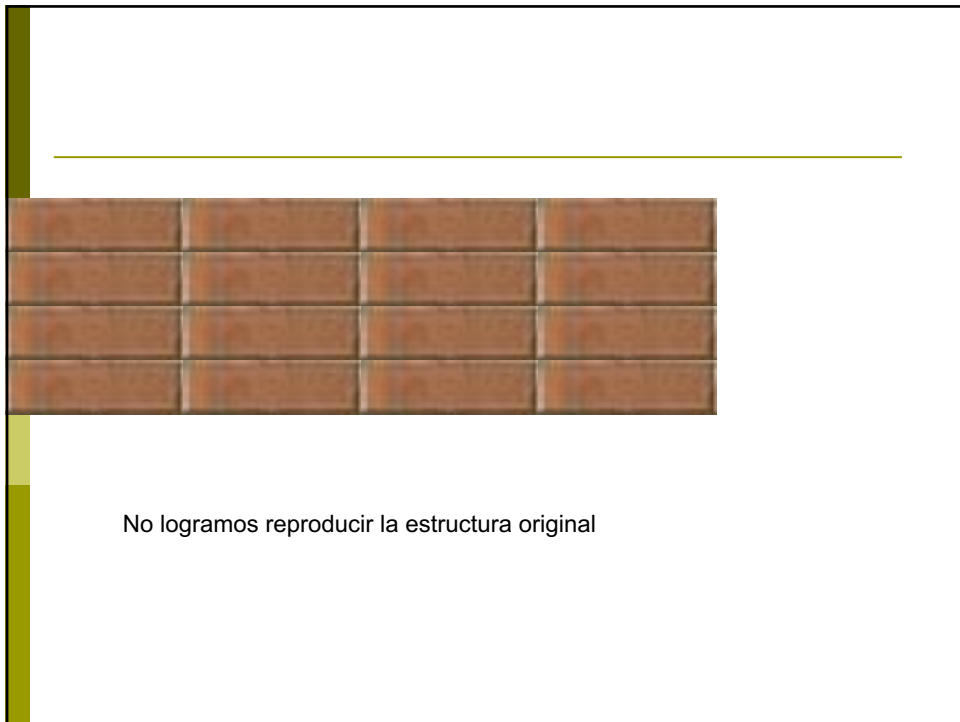
The conventional crystals are a special class, though very large, for which $n = 3$.

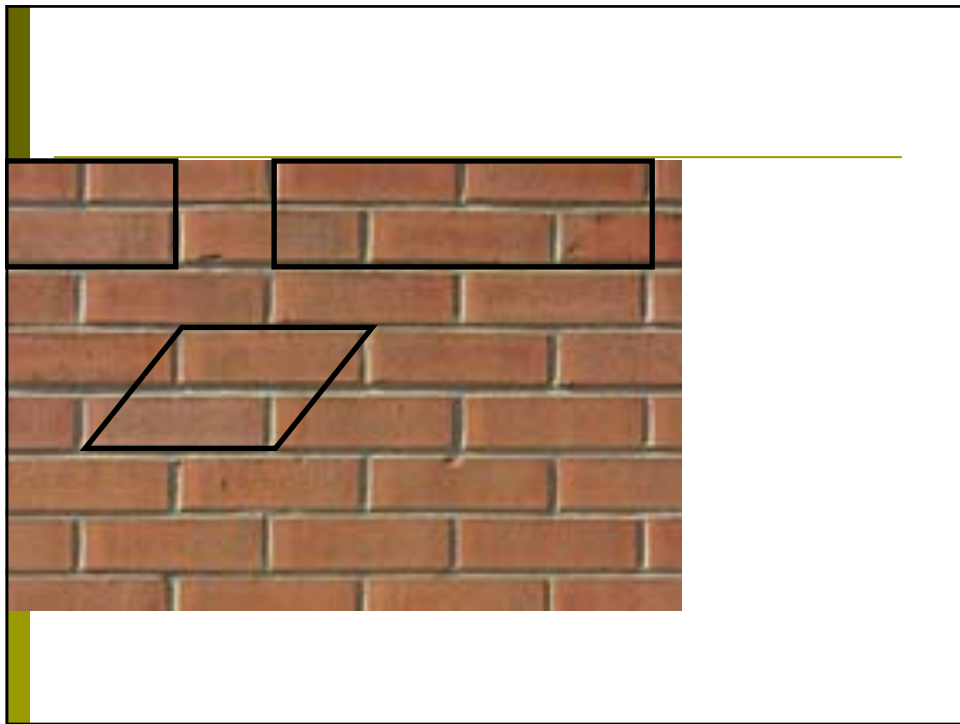
See also

Acta Cryst. (1992), **A48**, 928 where the definition of a crystal [Ⓔ] appears in the **Terms of reference** of the IUCr commission on aperiodic crystals

Category: Fundamental crystallography

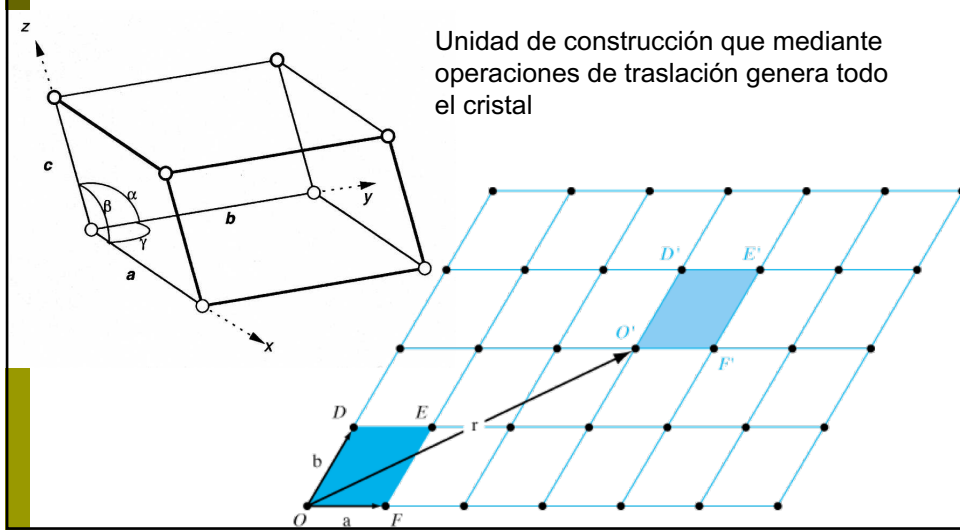






1. Celda Unitaria

Unidad de construcción que mediante operaciones de traslación genera todo el cristal



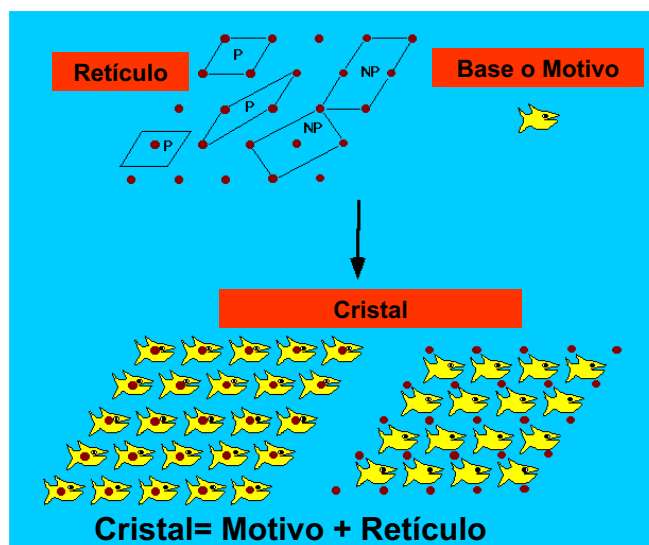
1. Convenciones para la CU

- El origen de la celda debe coincidir con el elemento de mayor simetría
- En lo posible los ejes deben estar vinculados por la simetría de la red
- En lo posible la C-U debería tener el menor volumen posible.

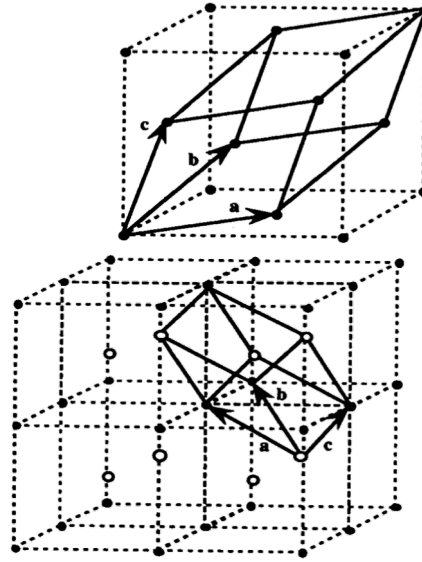
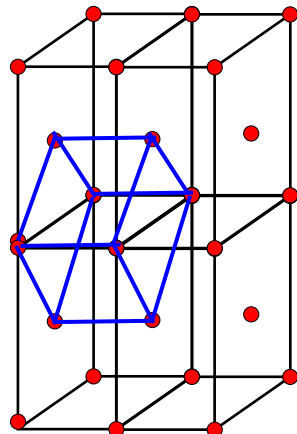
1. Definición de Retículo

Arreglo de nodos.
Los nodos son todos equivalentes entre sí y poseen el mismo entorno

Permite definir todos los vectores de traslación entre elementos equivalentes para todo el cristal



1. Celdas Primitivas y Convencionales



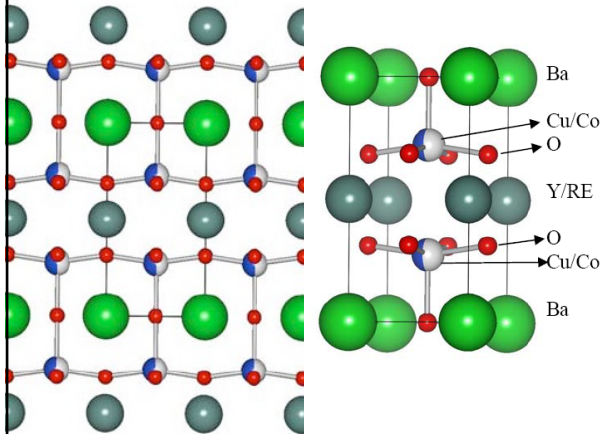
1. Sistemas Cristalinos y Retículos de Bravais

CUBIC $a = b = c$ $\alpha = \beta = \gamma = 90^\circ$			
TETRAGONAL $a = b \neq c$ $\alpha = \beta = \gamma = 90^\circ$			
ORTHORHOMBIC $a \neq b \neq c$ $\alpha = \beta = \gamma = 90^\circ$			
HEXAGONAL $a = b \neq c$ $\alpha = \beta = 90^\circ$ $\gamma = 120^\circ$		TRIGONAL $a = b = c$ $\alpha = \beta = \gamma \neq 90^\circ$	
MONOCLINIC $a \neq b \neq c$ $\alpha = \gamma = 90^\circ$ $\beta \neq 90^\circ$			
TRICLINIC $a \neq b \neq c$ $\alpha \neq \beta \neq \gamma \neq 90^\circ$			

4 Types of Unit Cell
 P = Primitive
 I = Body-Centred
 F = Face-Centred
 C = Side-Centred
 +
 7 Crystal Classes
 → 14 Bravais Lattices

1. Coordenadas Atómicas

□ Coordenadas Fraccionales



Atomo	Wyckoff	x	y	z
Ba	1a	0	0	0
RE/Y	1b	0	0	½
Cu	2h	½	½	z_{Cu}
Co	2h	½	½	z_{Co}
O1	1c	½	½	0
O2	4i	½	0	½
O3	1d	½	½	½

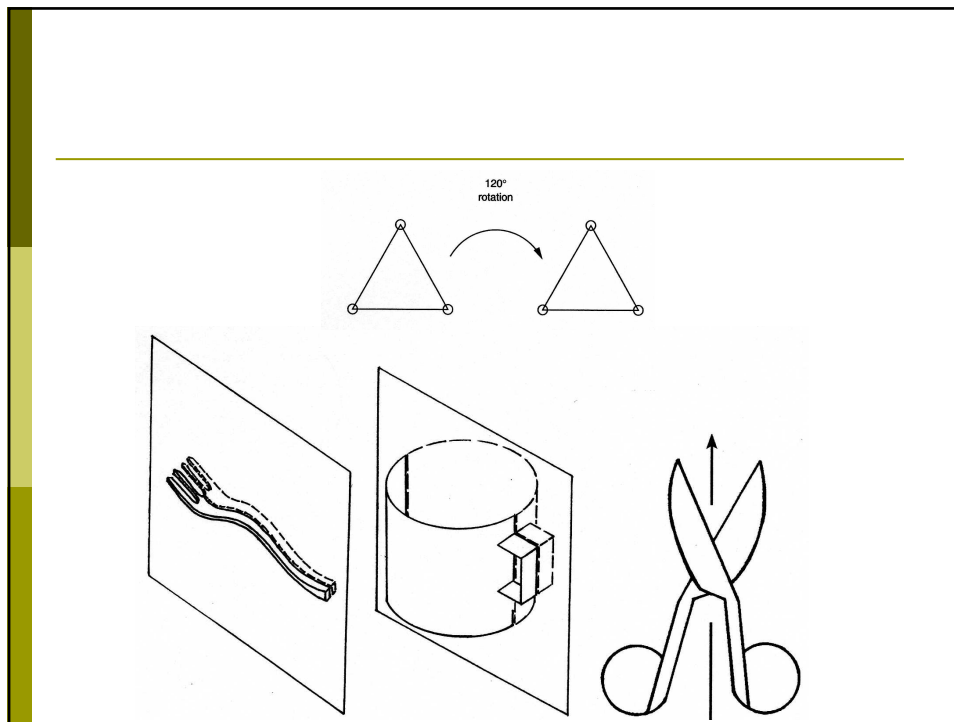
2. Simetría

□ Simetría externa del cristal

□ Simetría interna del cristal

□ Definición:

- Un objeto tiene simetría si algún movimiento u operación sobre esta lo deja en una posición indistinguible de su posición original



2. Simetría: Definiciones

- Elemento de simetría:
 - Punto, línea o plano a partir del cual se puede aplicar una operación de simetría
- Operación de simetría
 - Movimiento real o imaginario aplicado a un cuerpo respecto de un elemento de simetría, que al final genera una imagen coincidente con el cuerpo original.

2. Simetría: Operaciones

- Identidad
 - Simetría que tiene cualquier objeto, rotación 360°
- Centro de Inversión
 - Simetría central o simetría de punto. Hay cambio de quiralidad
- Rotación Propia
 - Rotación entorno a una línea que no cambia la quiralidad de un objeto
- Rotación Impropia
 - Rotación entorno a una línea seguida de una inversión, que cambia la quiralidad de un objeto
- Reflexión
 - Simetría especular respecto a un plano, hay cambio de quiralidad
- Combinaciones de rotación-traslación y reflexión-traslación

2. Simbología de Grupos Espaciales

- Hermann-Mauguin
- Schoenflies

2. Elementos de Simetría: Rotaciones

Rotación Propia: Rotación en $360^\circ/n$.

Roto-traslación: Rotación en $360^\circ/n$ + traslación $d(m/n)$

d =parámetro de celda

Rotación Propia

	Símbolo	(n)
Orden-dos		2
Orden-tres		3
Orden-cuatro		4
Orden-seis		6

Roto-traslación

Símbolo	(nm)
	2 ₁
	3 ₁ , 3 ₂
	4 ₁ , 4 ₂ , 4 ₃
	6 ₁ , 6 ₂ , 6 ₃ , 6 ₄ , 6 ₅

2. Elementos de Simetría: Rotaciones Compuestas

Rotaciones

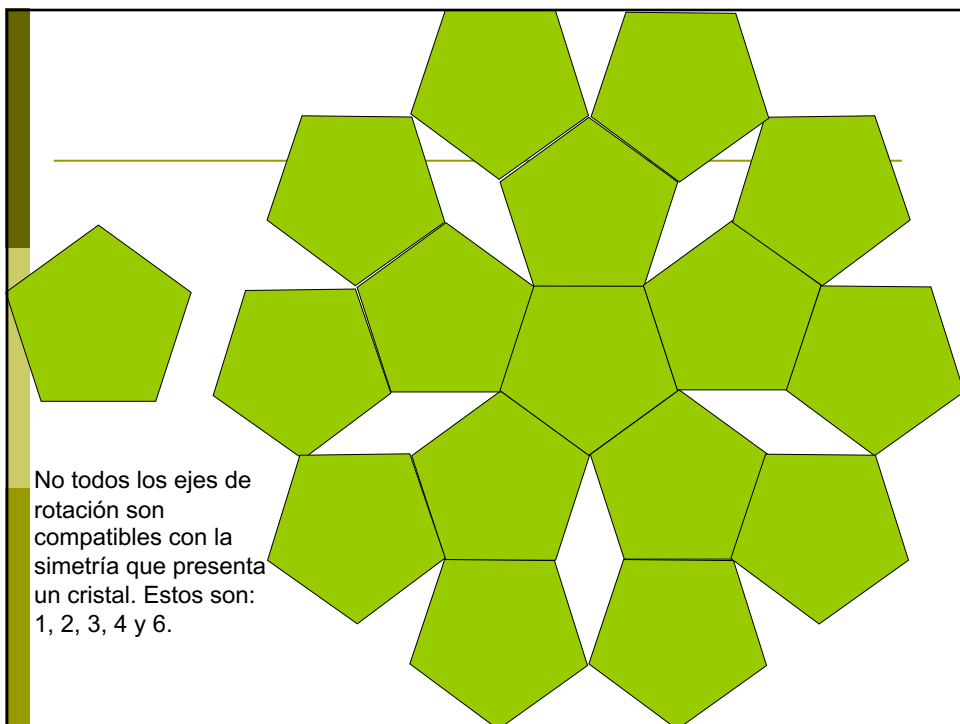
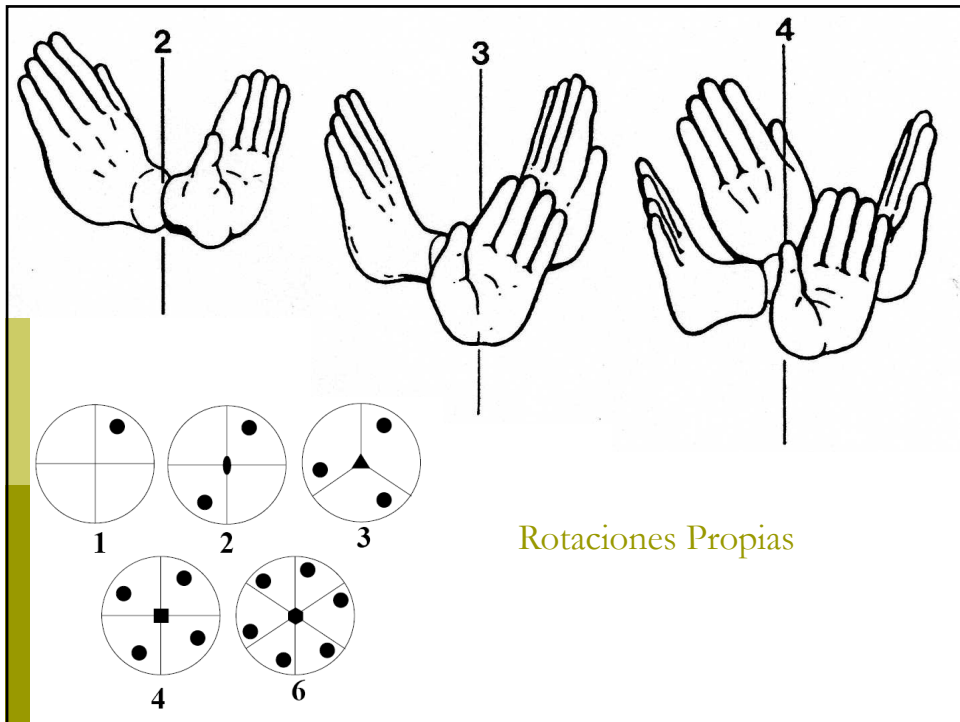
	2	
	2 ₁	
	4	
	4 ₂	

Planos espejo Planos con deslizamiento

	$\bar{1}$	
	m	
	a, b	
	c	
	n	

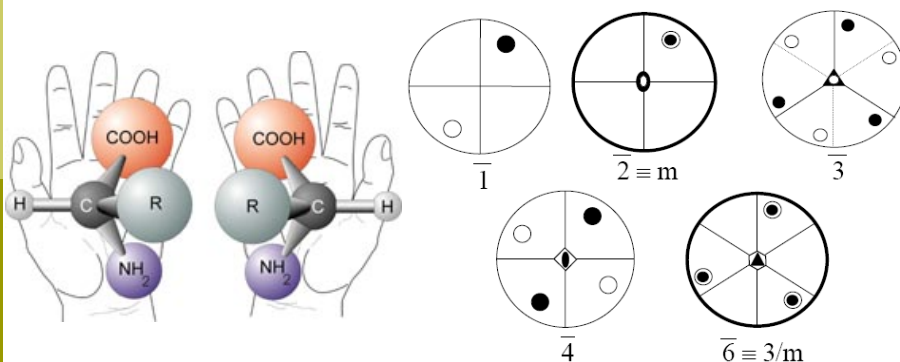
Rotaciones Impropias

	2 + $\bar{1}$
	2 ₁ + $\bar{1}$
	4 ₂ + $\bar{1}$

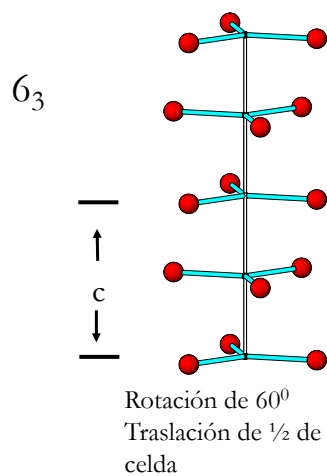
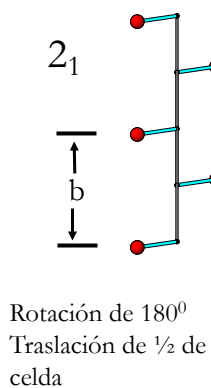
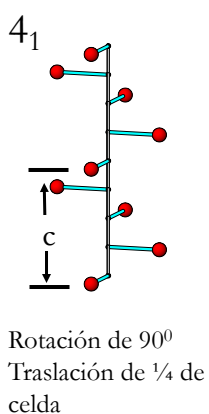


2. Operaciones Propias e Impropias

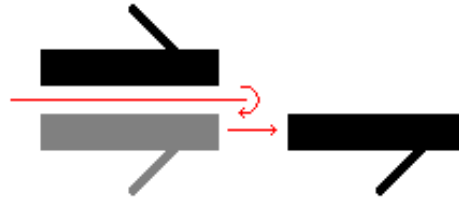
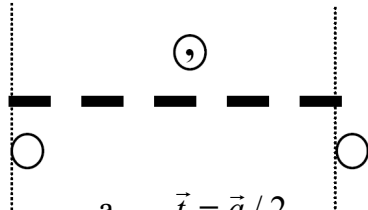
Las operaciones de simetría impropia establecen el cambio de quiralidad de los objetos presentes.



2. Elementos de Simetría: Ejes tornillo



2. Elementos de Simetría: Planos con Deslizamiento



a $\vec{t} = \vec{a} / 2$

b $\vec{t} = \vec{b} / 2$

c $\vec{t} = \vec{c} / 2$

n $\vec{t} = (\vec{a} + \vec{b}) / 2$ $\vec{t} = (\vec{b} + \vec{c}) / 2$ $\vec{t} = (\vec{a} + \vec{c}) / 2$

d $\vec{t} = (\vec{a} + \vec{b}) / 4$ $\vec{t} = (\vec{b} + \vec{c}) / 4$ $\vec{t} = (\vec{a} + \vec{c}) / 4$

2. Elementos de Simetría: Ejes Tornillo

Rotación Propia: Rotación en $360^\circ/n$.

Roto-traslación: Rotación en $360^\circ/n$ + traslación $d(m/n)$

d =parámetro de celda

Rotación Propia

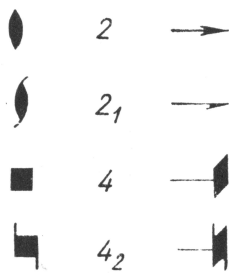
	Símbolo	(n)
Orden-dos		2
Orden-tres		3
Orden-cuatro		4
Orden-seis		6

Roto-traslación

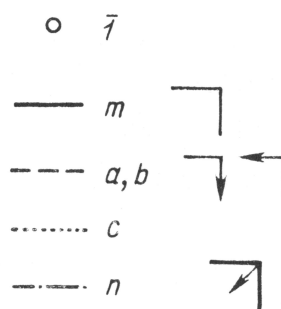
Símbolo	(nm)
	21
	31, 32
	41, 42, 43
	61, 62, 63, 64, 65

Elementos de Simetría: Otros Elementos

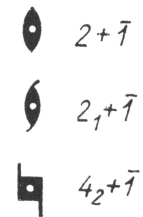
Rotaciones



Planos espejo Planos con deslizamiento

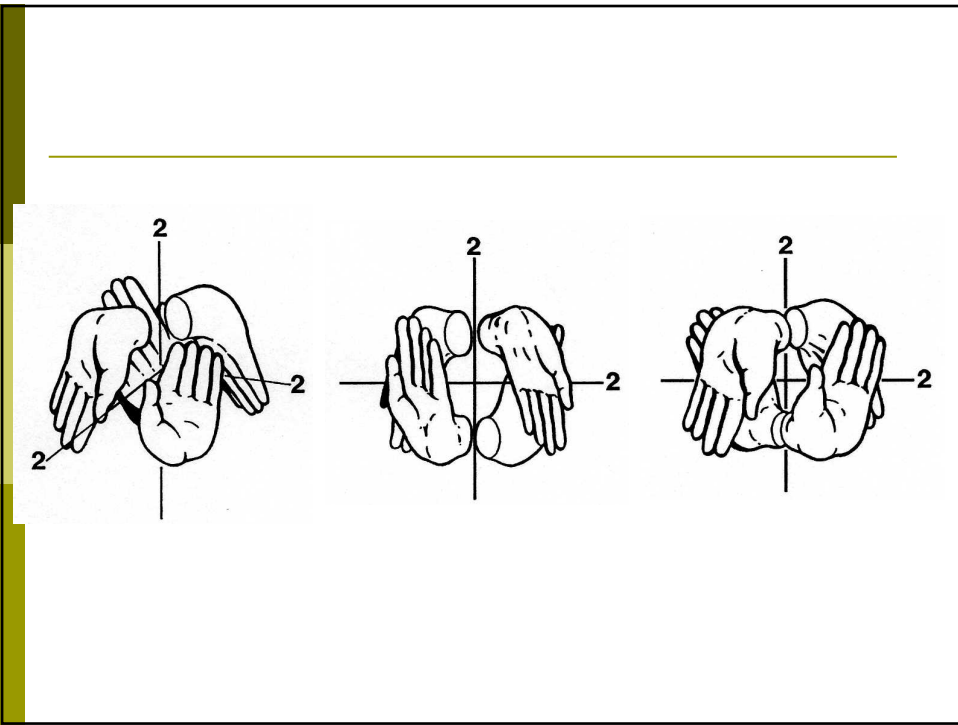
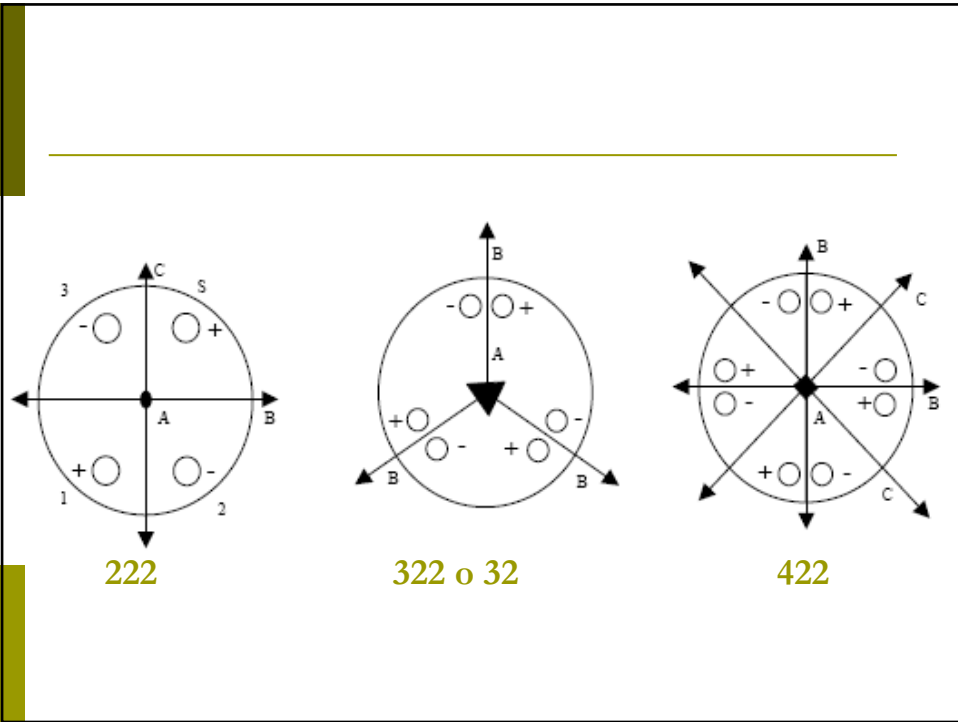


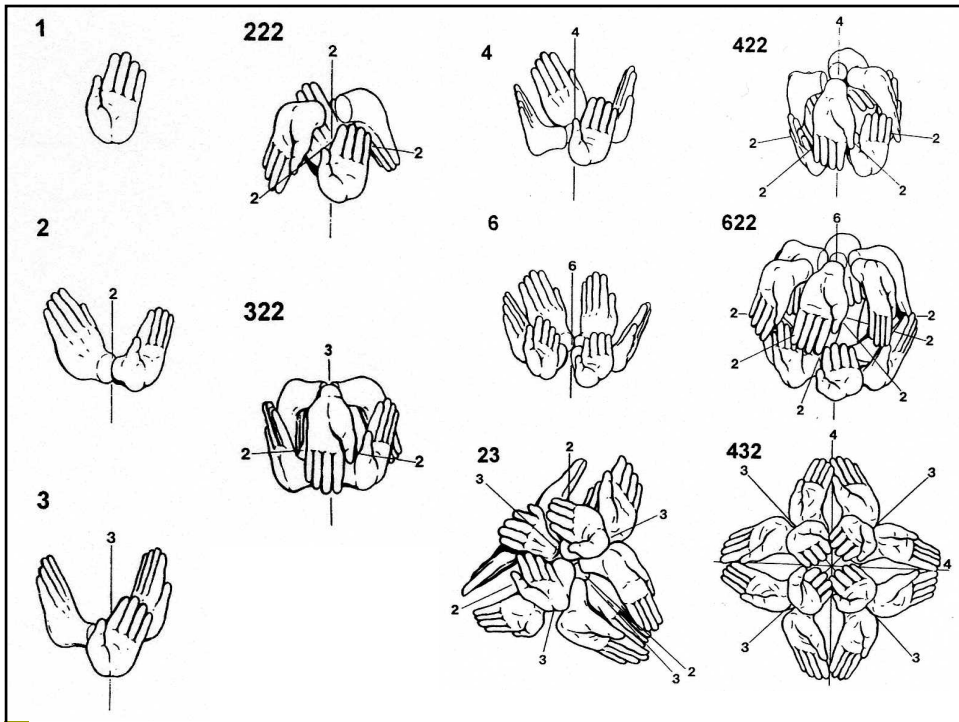
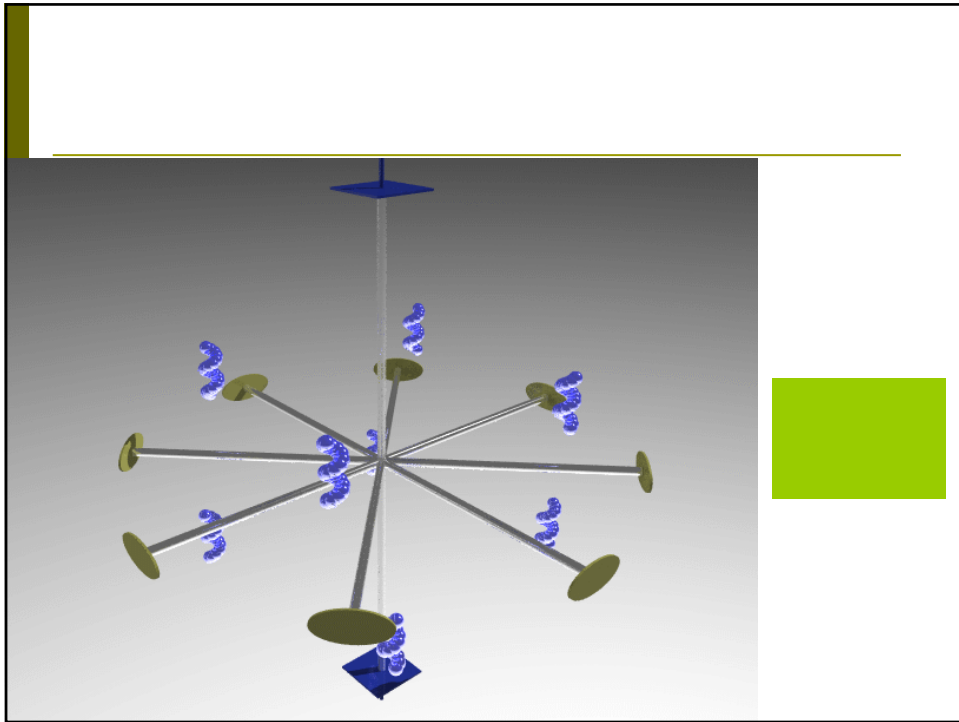
Rotaciones Impropias


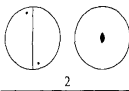
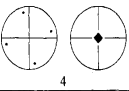
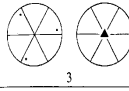
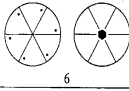
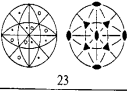
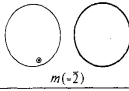
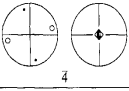
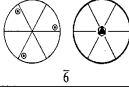

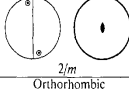
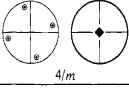
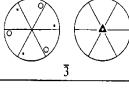
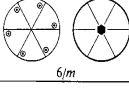
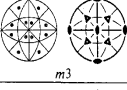

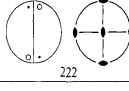

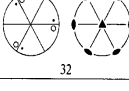
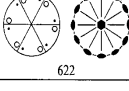
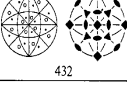

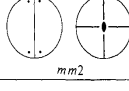
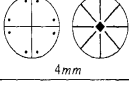
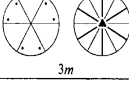
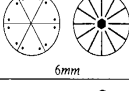
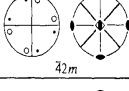
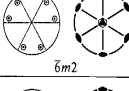
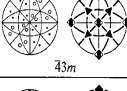

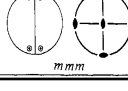
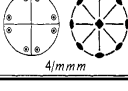
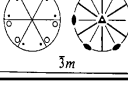

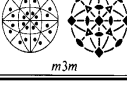


3. Grupos Puntuales de Simetría

- Combinación de elementos de simetría que deja uno de sus puntos in cambiados y dónde se encuentran todos los elementos.
- Reflejan la simetría no traslacional del cristal





	Triclinic	Monoclinic (1st setting)	Tetragonal	Trigonal	Hexagonal	Cubic	
X	 1	 $m(-2)$	 4	 3	 6	 23	X
\bar{X} (even)	—	 $m(-2)$	 4	—	 $\bar{6}$	—	\bar{X} (even)
\bar{X} (even) plus centre and \bar{X} (odd)	 1	 $2/m$	 $4/m$	 3	 $6/m$	 $m3$	\bar{X} (even) plus centre and \bar{X} (odd)
$X2$	 2	 222	 422	 32	 622	 432	$X2$
Xm	 m	 $mm2$	 $4mm$	 $3m$	 $6mm$	—	Xm
$\bar{X}2$ (even) or $\bar{X}m$ (even)	—	—	 $42m$	—	 $6m2$	 $43m$	$\bar{X}2$ (even) or $\bar{X}m$ (even)
$X2$ or Xm plus centre and $\bar{X}m$ (odd)	 $2/m$	 mmm	 $4/mmm$	 $3m$	 $6/mmm$	 $m3m$	$X2$ or Xm plus centre and $\bar{X}m$ (odd)

3. Grupos Puntuales

□ 32 Grupos Puntuales

- 11 son centrosimétricos (clases de Laue)
- 21 son no-centrosimétricos

Esta simetría es la que se refleja en la morfología del cristal

4. Grupos Espaciales

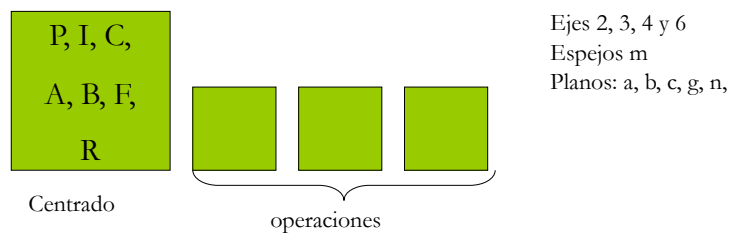
Al combinar los 14 Retículos de Bravais con los 32 Grupos Puntuales se obtiene 230 combinaciones independientes

73 carecen de traslación: simórficos

230 Grupos Espaciales

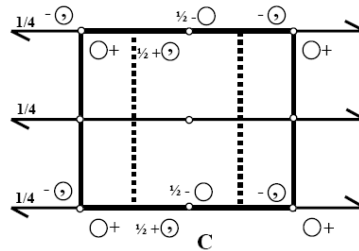
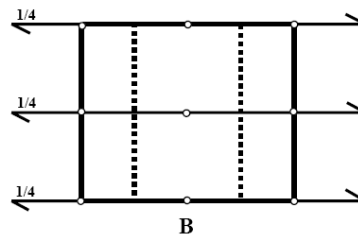
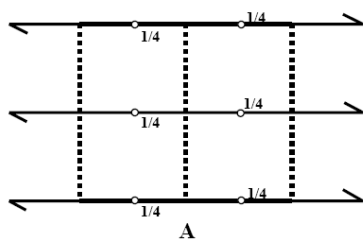
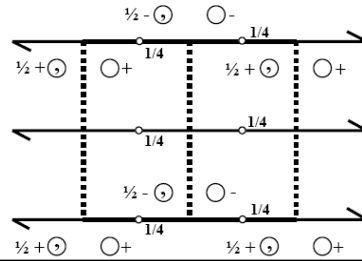
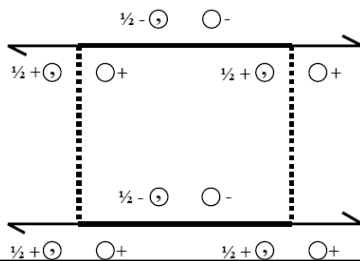
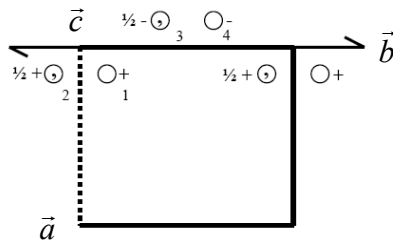
4. Tablas Internacionales de Cristalografía

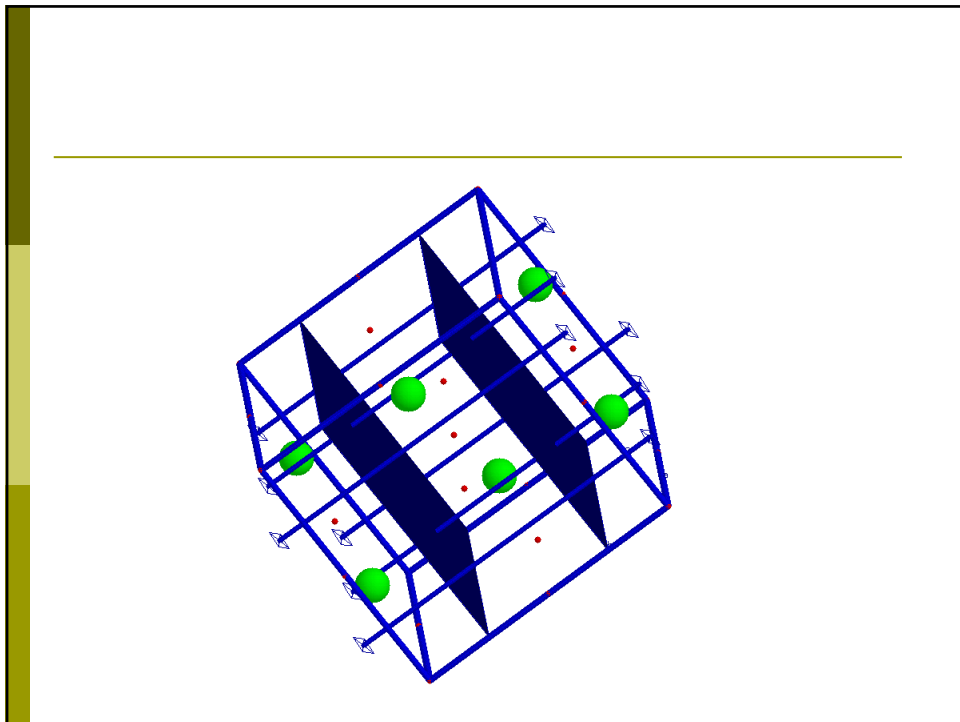
Se desarrollaron en 1890 por Federov y Schoenflies 1891.
Simbología de Hermann-Mauguin



4. Derivación del GE $P2_1/c$

Eje 2_1 paralelo al eje \vec{b}
 Plano-c perpendicular a \vec{b}
 con traslación $c/2$





4. Ejemplos de Grupos Espaciales

Triclínico

- $P1$ o $P \bar{1}$

Monoclínico

- $P121 = P2$
- $C121 = C2$

Ortorrómbico

- $Pca2_1$

Tetragonal

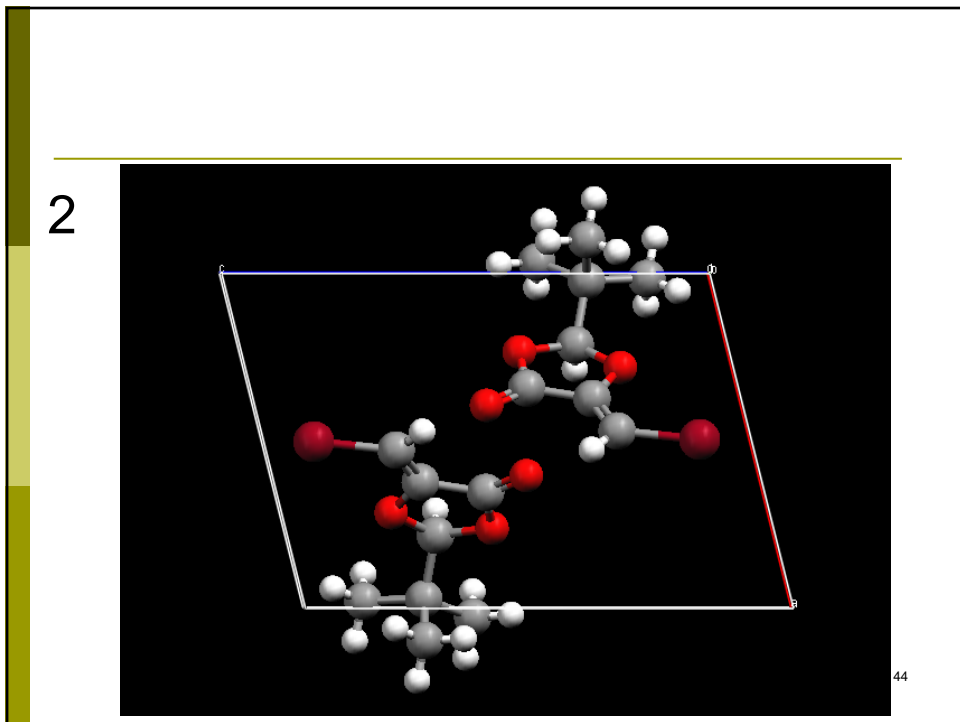
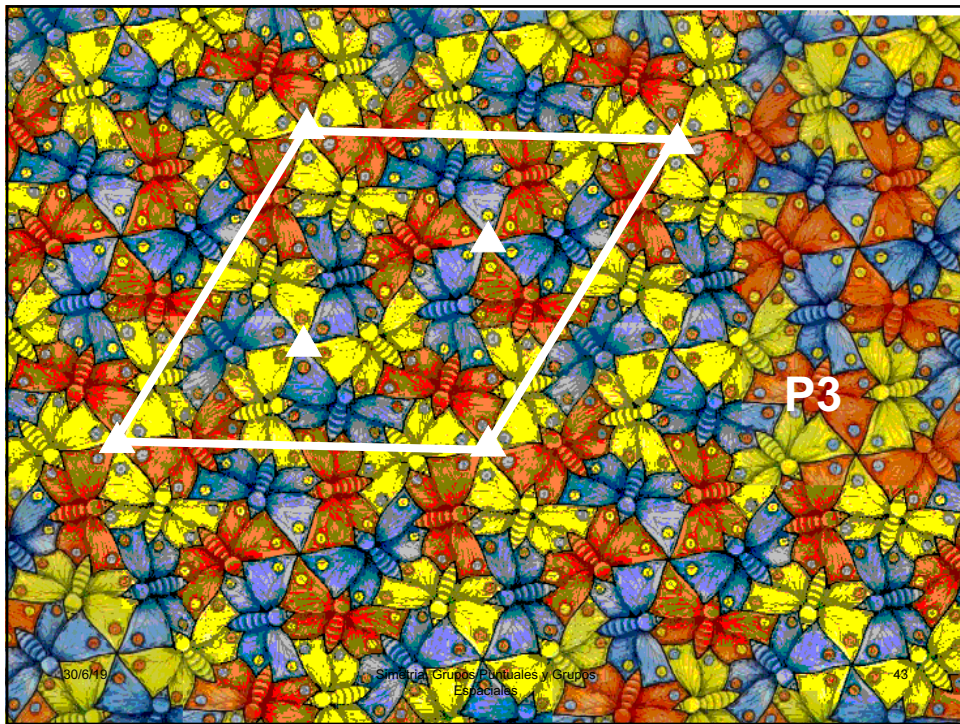
- $P4_2/nbc$ ($c, a, (a+b)$)

Trigonal y Hexagonal

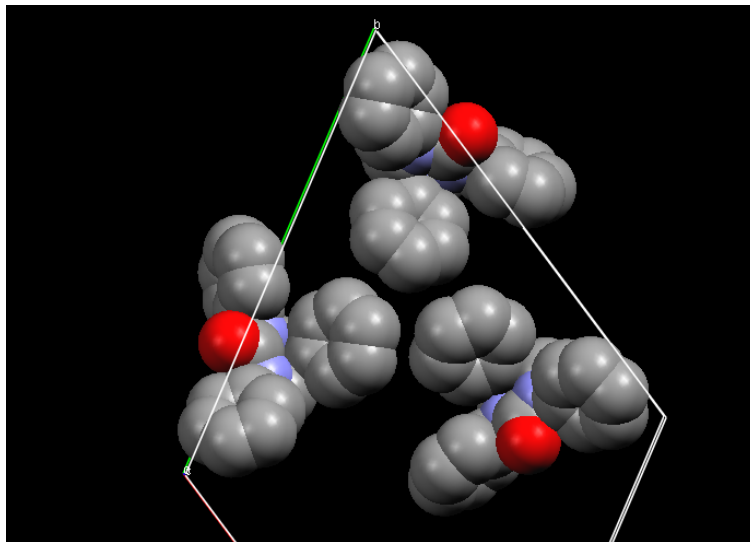
- $P6_3/mmc$ ($c, a, [1-10]$)
- $P312$

Cúbico

- $Im\bar{3}m$ ($a, [111], [110]$)

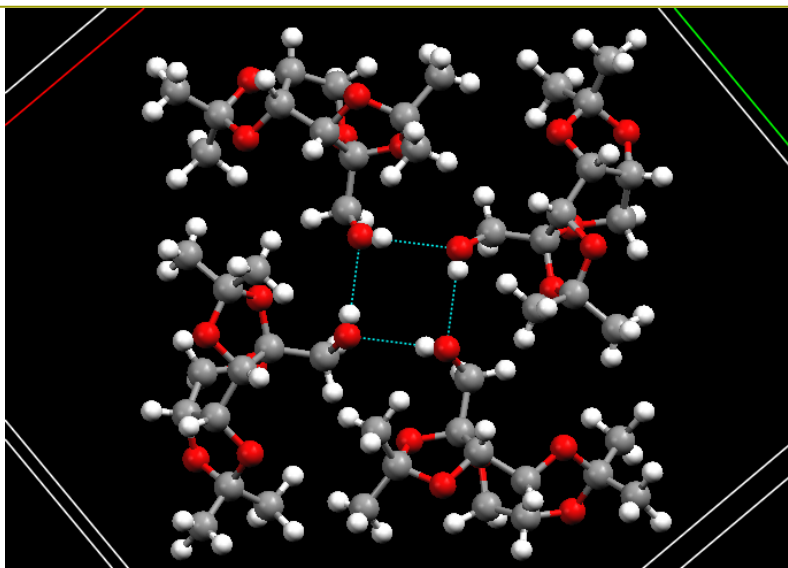


3



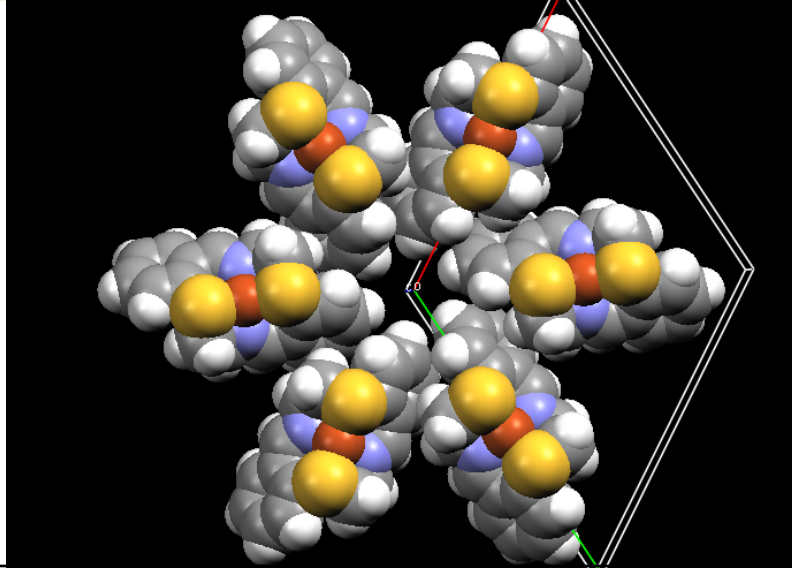
45

4

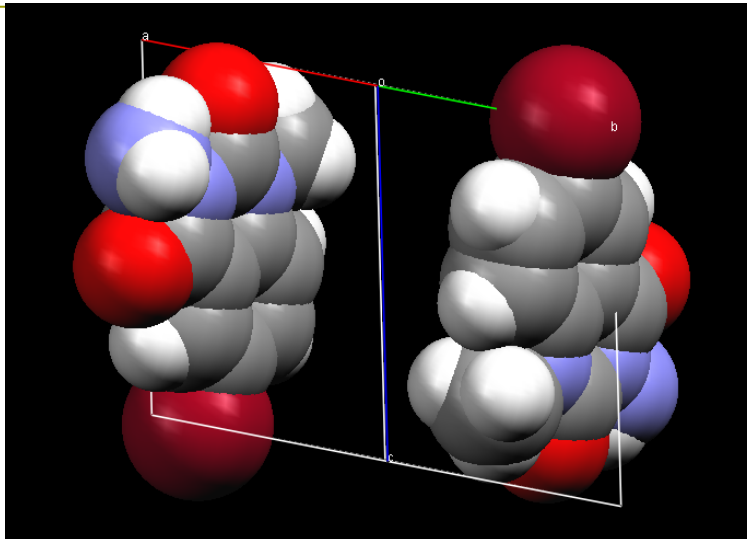


46

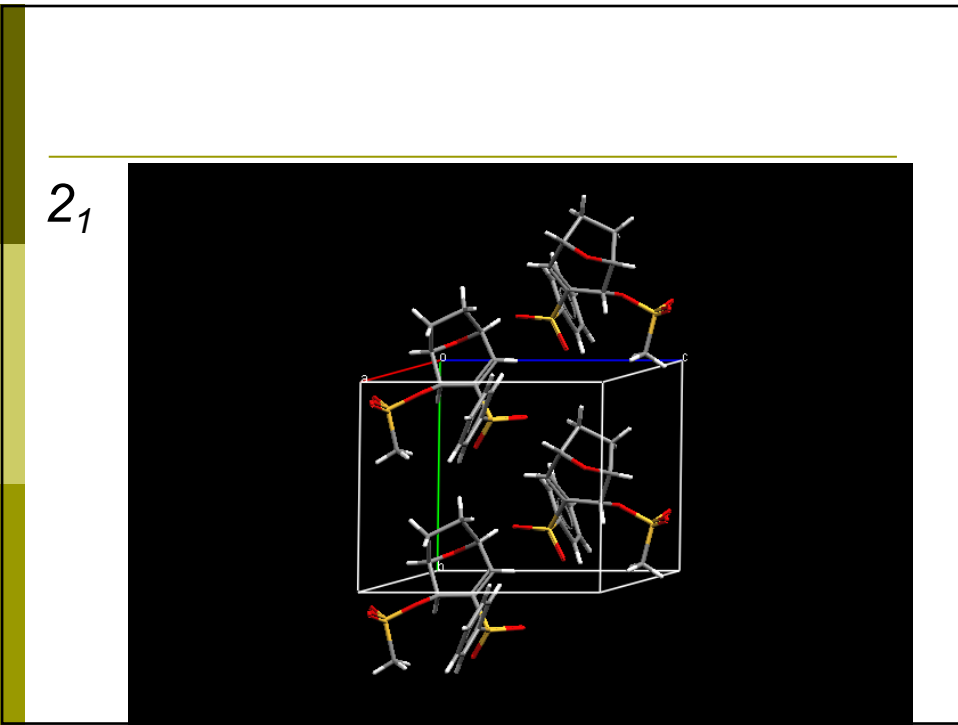
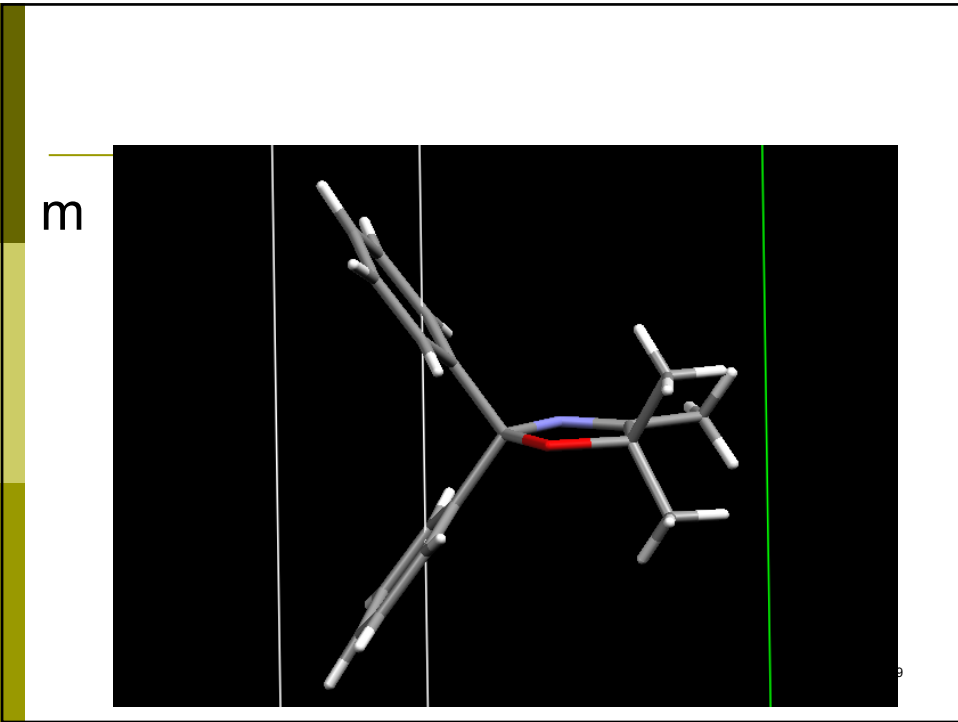
6



-1 Inversion



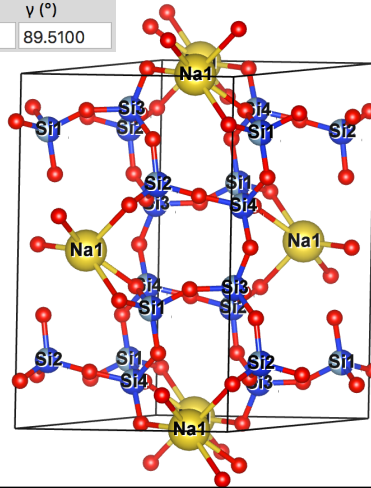
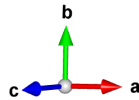
48



Albite

GE: C -1

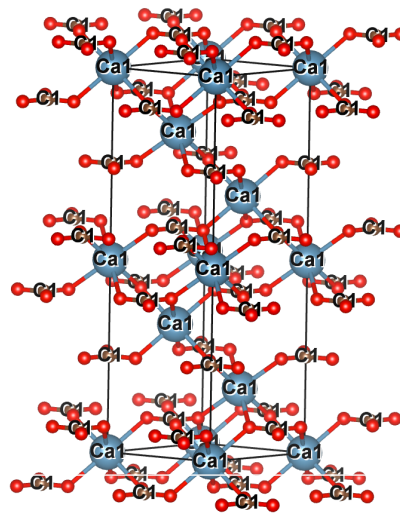
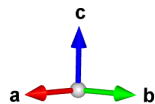
a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)
8.14900	12.84000	7.12000	93.8300	116.4700	89.5100



Calcita

GE: R -3 c

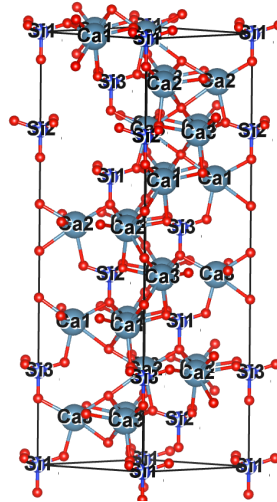
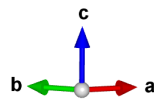
a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)
4.98900	4.98900	17.06200	90.0000	90.0000	120.0000



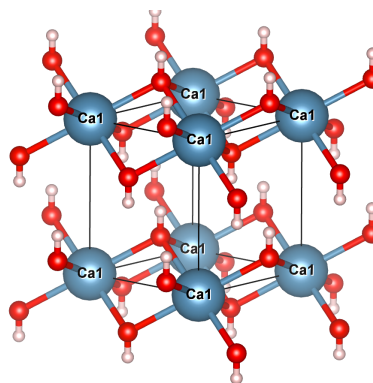
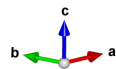
Ca₃SiO₅

GE: R-3 m

a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)
7.00000	7.00000	25.00000	90.0000	90.0000	120.0000



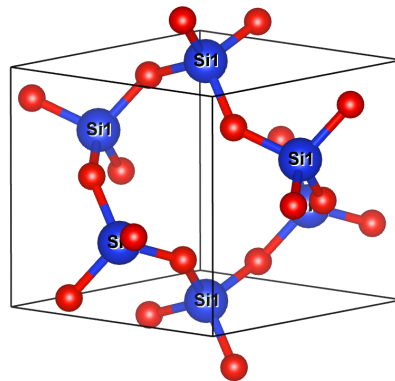
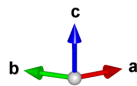
Portlandite



Cuarzo

a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)
4.83200	4.83200	5.34700	90.0000	90.0000	120.0000

GE: $P3_2 2 1$



Struvite

Struvite: $\text{NH}_4\text{MgPO}_4 \cdot 6\text{H}_2\text{O}$

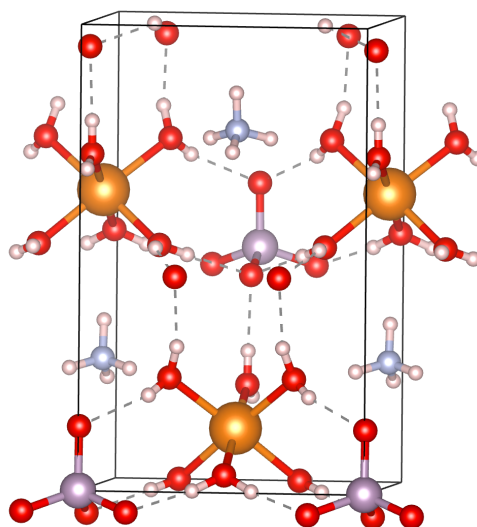
Grupo Espacial: $P m n 2_1$

$a=6.966 \text{ \AA}$

$b=6.142 \text{ \AA}$

$c=11.217 \text{ \AA}$

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



Uric Acid

Ucidite: $C_5H_4N_4O_3$

Grupo Espacial: $P 2_1/a$

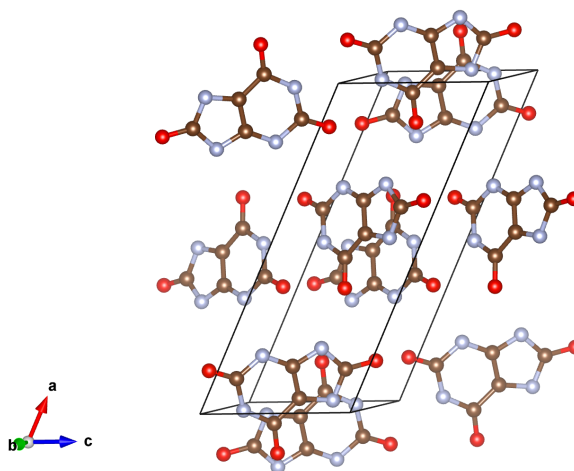
$a=14.464 \text{ \AA}$

$b= 7.404 \text{ \AA}$

$c= 6.208 \text{ \AA}$

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

$\beta= 65.1^\circ$



Apatite

Apatite:

$Ca_5(PO_4)_3(OH)$

Grupo Espacial: $P 6_3/m$

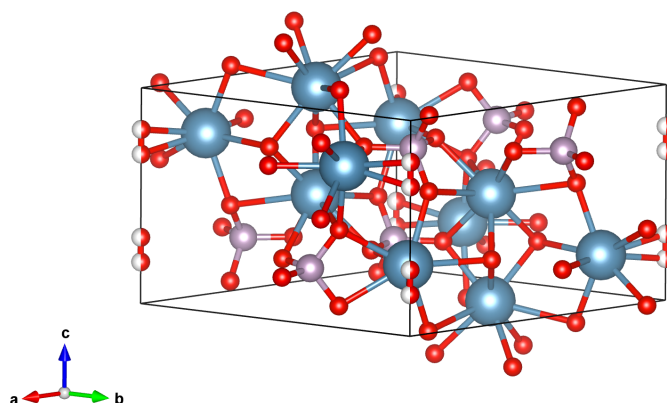
$P 6_3/m$

$a=b=9.342 \text{ \AA}$

$c= 6.881 \text{ \AA}$

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

$\gamma= 120^\circ$



Carbo-apatite

Carbo-Apatite

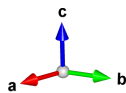
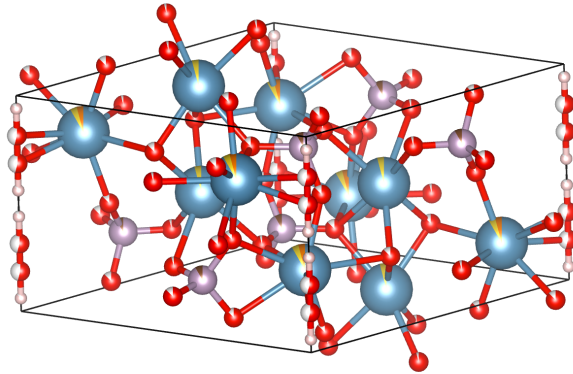
Grupo Espacial: $P 6_3/m$

$a=b= 9.4564 \text{ \AA}$

$c= 6.88210 \text{ \AA}$

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

$\beta= 120^\circ$



Brushite

Brushite:

$\text{CaHPO}_4 \cdot 2\text{H}_2\text{O}$

Grupo Espacial: $I 2/a$

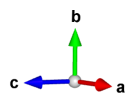
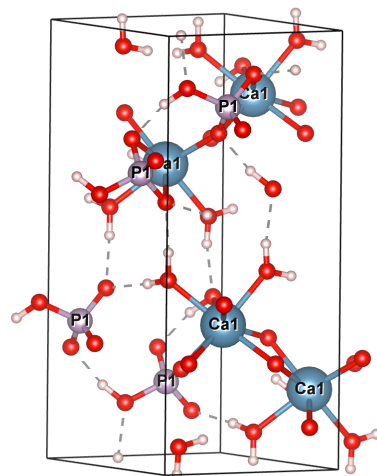
$a=5.81200 \text{ \AA}$

$b = 15.18000 \text{ \AA}$

$c = 6.23900 \text{ \AA}$

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

$\beta= 116.4300^\circ$

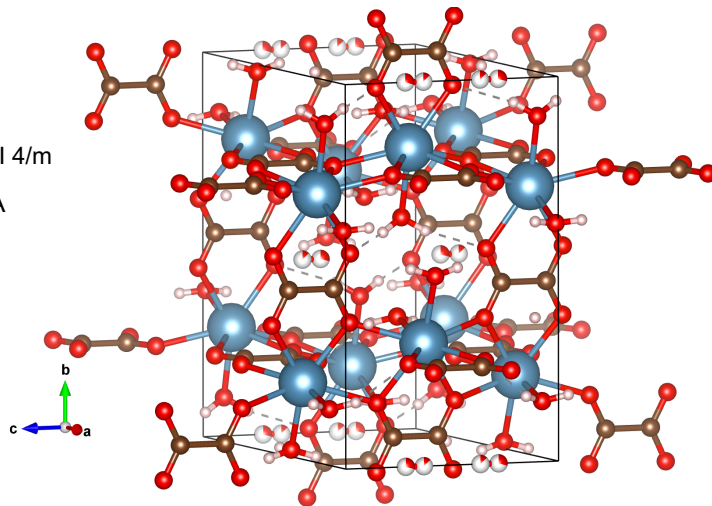


Weddellite

Weddellite:
CaC2O4·2H2O

Grupo Espacial: $I 4/m$

$a = b = 12.35430 \text{ \AA}$
 $c = 7.35470 \text{ \AA}$
 $\alpha = \beta = \gamma = 90^\circ$

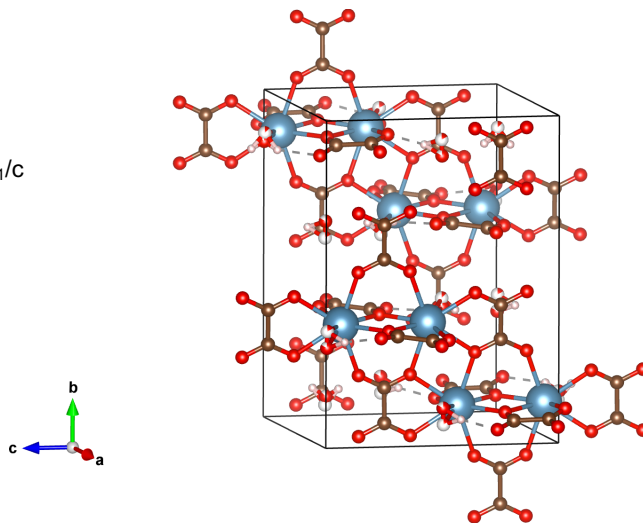


Whewellite

Whewellite:
CaC2O4·H2O

Grupo Espacial: $P 2_1/c$

$a = 6.29000 \text{ \AA}$
 $b = 14.58300 \text{ \AA}$
 $c = 10.11600 \text{ \AA}$
 $\alpha = \gamma = 90^\circ$
 $\beta = 109.4600^\circ$



Cystine

Cystine:
C6H12N2O4S2

Grupo Espacial: P 6₁ 2 2

a=b= 5.41200 Å
c = 55.95600 Å
 $\alpha = \beta = 90^\circ$
 $\gamma = 120^\circ$

