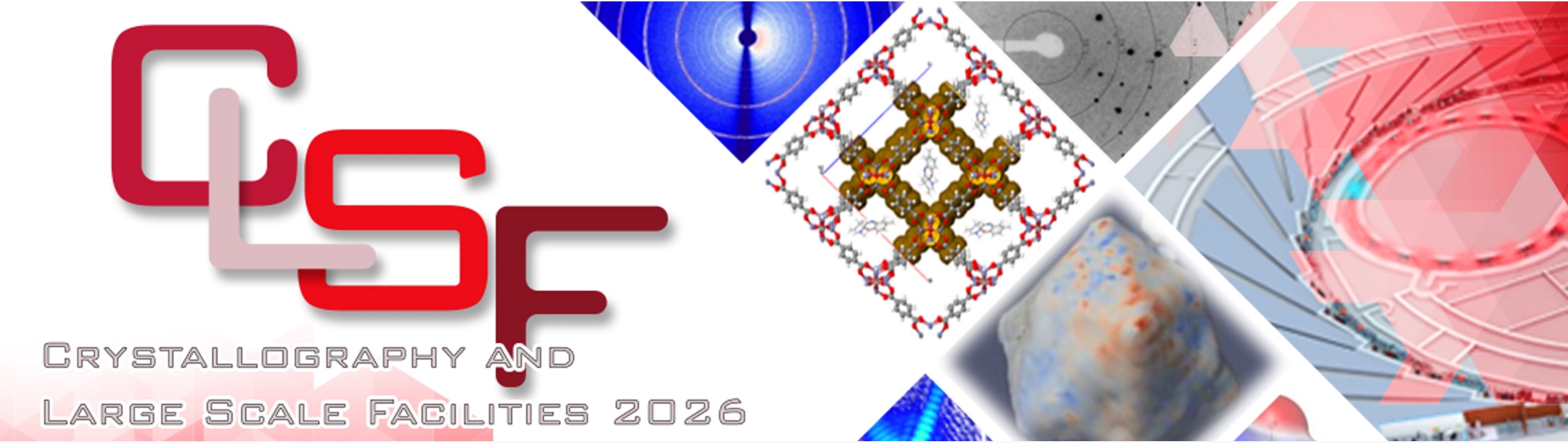


How to describe the crystal state?

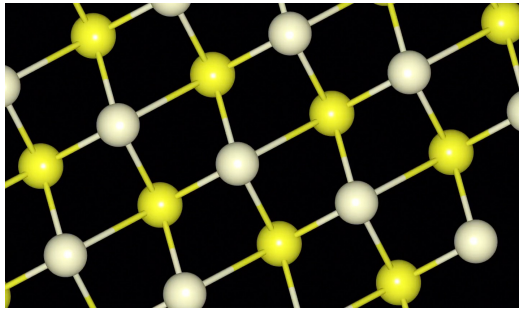
Geometric Crystallography, symmetries

Delphine Cabaret, IMPMC

delphine.cabaret@sorbonne-universite.fr

Introduction: what is a crystal?

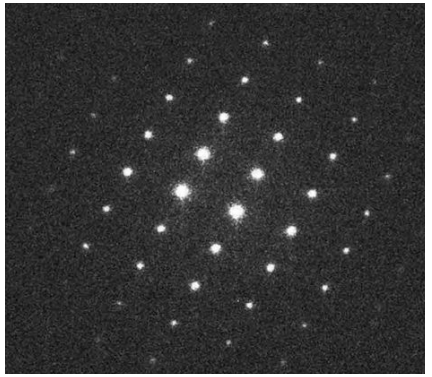
A crystal is a solid composed of atoms arranged in a motif (or a *pattern*) that is periodic in 3 dimensions.



Since 1992 (IUCR) :

« A material is a crystal if it has ***essentially*** ***a sharp diffraction pattern*** *»*

➔ All solids with long range order
(translation symmetry in spaces of **dimension ≥ 3**)



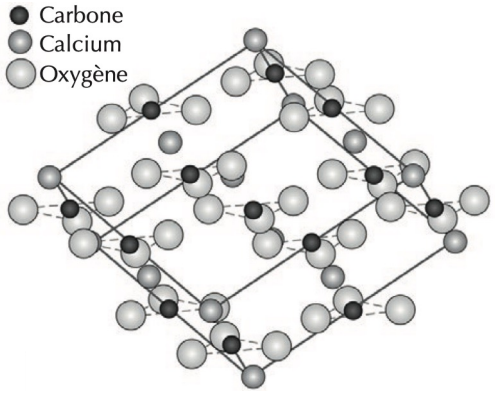
Nature Materials 10, 890–896 (2011)

cf. article de B. Toudic, Reflets de la Physique 2015, vol 44-45

Introduction: the periodic crystals

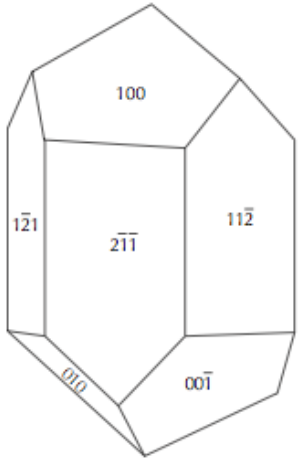
translation symmetry

ex: $CaCO_3$ (calcite)

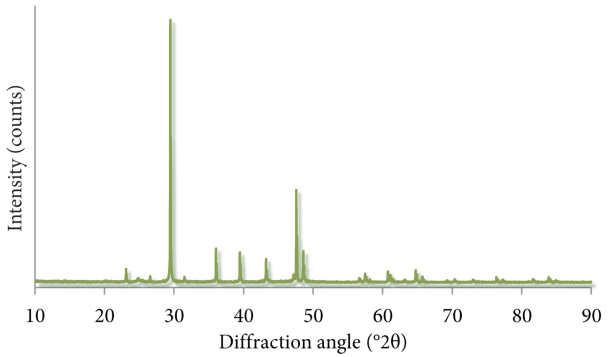


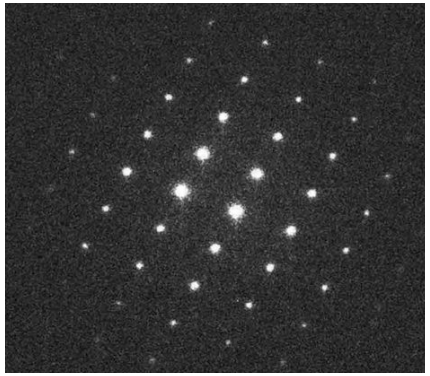


B. Toudic, Reflets de la Physique 2015, vol 44-45



law of rational indices





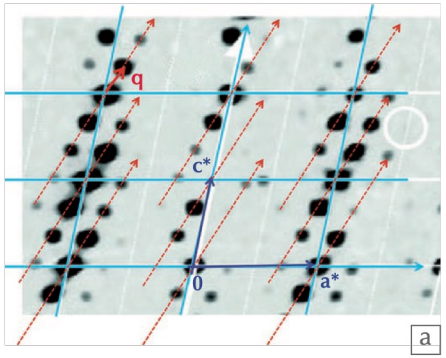
Nature Materials 10, 890–896 (2011)

Introduction: aperiodic crystals

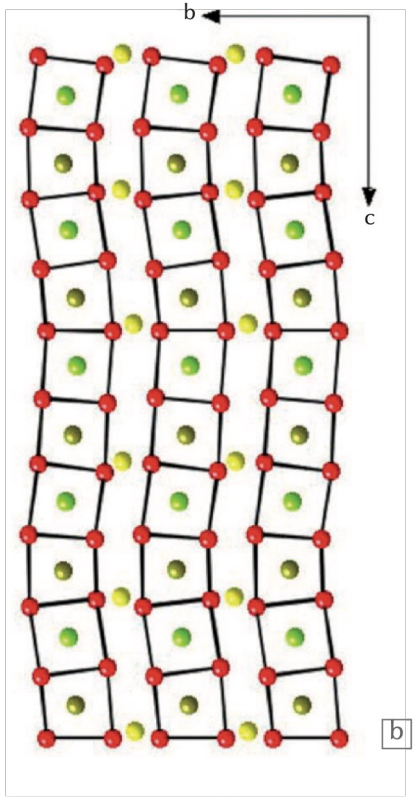
No translation symmetry in the **3D space**

incommensurate crystals, modulated phases

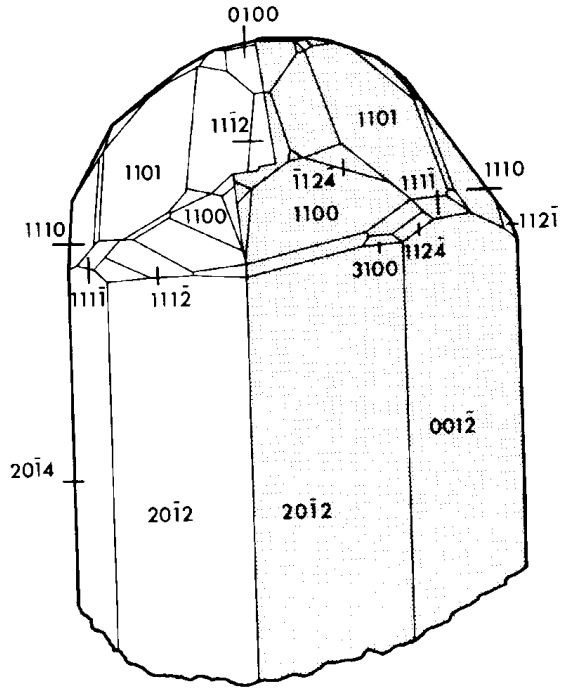
Periodicity (order at infinite) cannot be described in a 3D space



3. Structure incommensurable modulée du carbonate de sodium γ-Na_2CO_3.
(a) Plan de diffraction (a^*, c^*) du réseau réciproque de γ-Na_2CO_3. Il est constitué de pics de Bragg, preuve d'un ordre à grande distance, mais requiert pour son indexation complète un vecteur de base complémentaire, $\mathbf{q} = \alpha\,\mathbf{a}^* + \gamma\,\mathbf{c}^*$. On observe les pics de Bragg du réseau périodique moyen (aux sommets des parallélogrammes bleus), et les pics satellites alignés le long des flèches rouges (parallèles à **q**).
(b) La solution structurale modulée, projetée selon **a** (atomes d'oxygène en rouge, atomes de sodium en jaune et vert, les atomes de carbone sont omis). Une onde statique de déplacements transversaux (parallèles à **b**) apparaît dans la direction **c**. La longueur d'onde de la modulation est $2\pi/q$.



B. Toudic, Reflets de la Physique 2015, vol 44-45



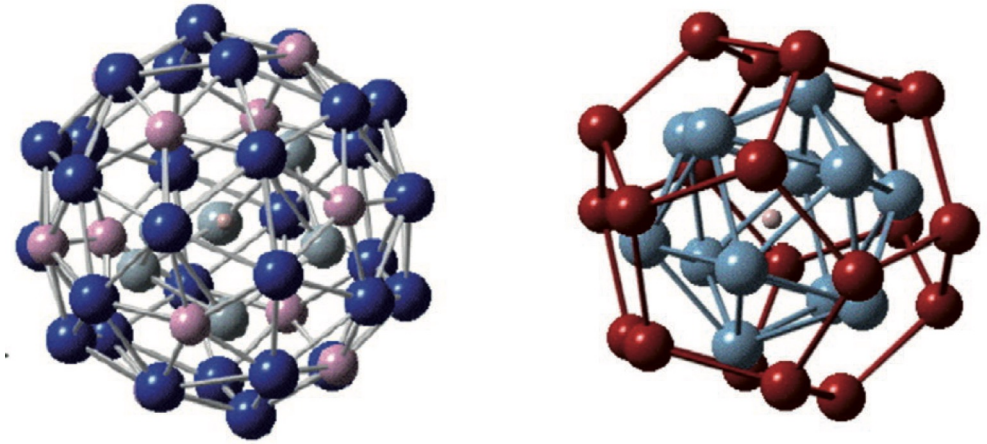
calaverite $Au_{1-x}Ag_xTe$

Introduction: aperiodic crystals

No translation symmetry in the **3D space**

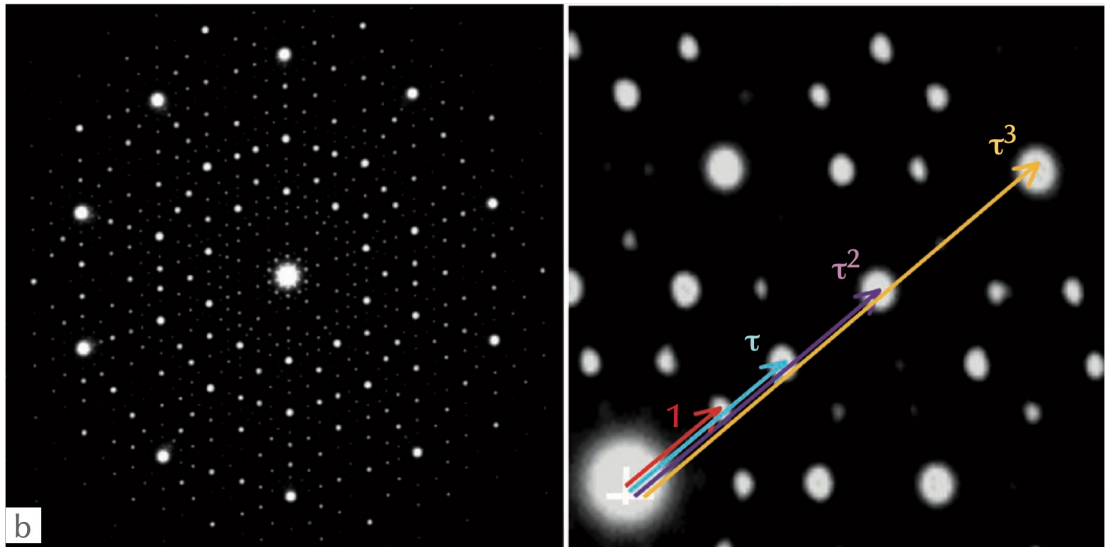
quasicrystals (1982, Nobel prize in chemistry in 2011)

ex : alloy AlPdMn



9. Amas atomiques dont est constitué principalement un alliage quasicristallin de type AlMnPd. À gauche, amas de type Mackay (51 atomes) ; à droite, amas de type Bergman (33 atomes).

$$\tau = 2\cos(2\pi/10)$$

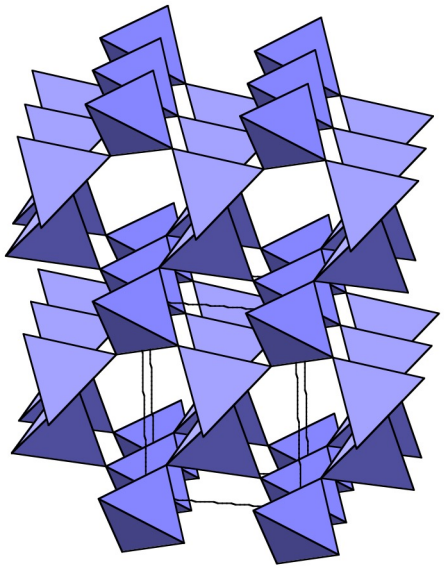


B. Toudic, Reflets de la Physique 2015, vol 44-45

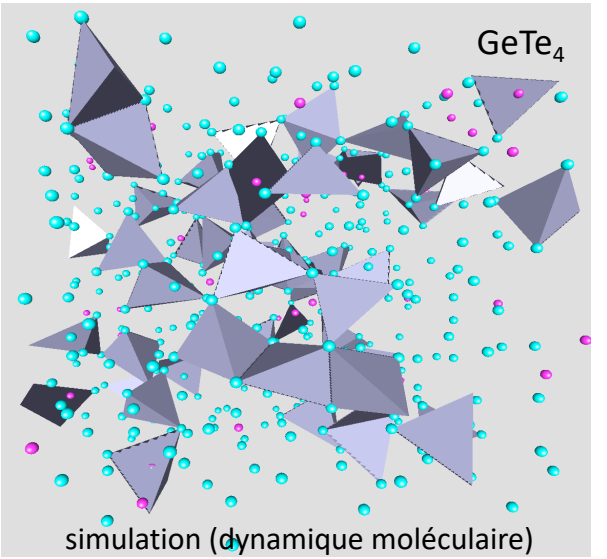
Introduction: what is a crystal?



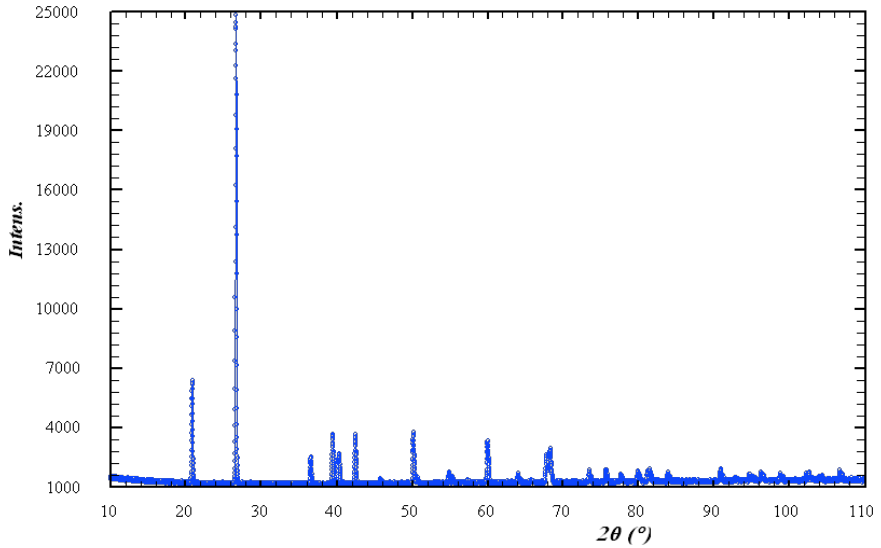
quartz

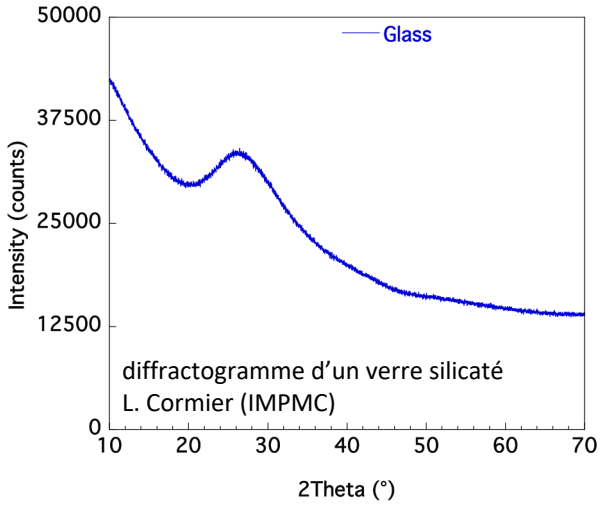


crystal ≠ glass



simulation (dynamique moléculaire)





diffractogramme d'un verre silicaté
L. Cormier (IMPMC)

What you should have learnt at the end of the day

example 1

Inorganic Chemistry

Article

pubs.acs.org/IC

Crystal Structures of $Li_6B_4O_9$ and $Li_3B_{11}O_{18}$ and Application of the Dimensional Reduction Formalism to Lithium Borates

Gwenaëlle Rousse,*[,†,‡] Benoît Baptiste,[†] and Gérald Lelong*[,†]

[†]Institut de Minéralogie, de Physique des Matériaux, et de Cosmochimie (IMPMC), Sorbonne Universités-UPMC Univ Paris 06, UMR CNRS 7590, Muséum National d'Histoire Naturelle, IRD UMR 206, 4 Place Jussieu, F-75005 Paris, France

[‡]FRE 3677, Chimie du Solide et Energie, Collège de France, 11 Place Marcelin Berthelot, and Réseau sur le Stockage Electrochimique de l'Energie (RS2E), FR CNRS 3459, 75231 Paris Cedex 05, France

$Li_3B_{11}O_{18}$ crystallizes in the $P2_1/c$ space group with lattice parameters a = 17.7607(8) Å, b = 7.7737(4) Å, c = 9.6731(4) Å, and β = 100.906(4)°. The lithium, boron, and oxygen atoms are distributed in the general 4*e* Wyckoff site (see Table 4 for the complete list of atomic positions). The

?

?

What you should have learnt at the end of the day

example 2

PHYSICAL REVIEW B **89**, 064305 (2014)

Accuracy of generalized gradient approximation functionals for density-functional perturbation theory calculations

Lianhua He,[1] Fang Liu,[2] Geoffroy Hautier,[3,4] Micael J. T. Oliveira,[3,5] Miguel A. L. Marques,[3,6] Fernando D. Vila,[7] J. J. Rehr,[7] G.-M. Rignanese,[3,4] and Aihui Zhou[1]

? ? ? ?

The unit cell of α-quartz is trigonal (space group $P3_221$). It contains nine atoms: the Si atoms are located at $(u,0,0)$ on the $3a$ Wyckoff sites, while the O atoms are located at (x,y,z) on the $6c$ Wyckoff sites. Hence, four internal coordinates u, x, y, z are required, besides the two lattice constants a and c, in order to completely determine the structure. The theoretical value

α-quartz = α-SiO_2

? ?

Periclase = MgO

The space group of periclase is $Fm3m$. The O atom occupies the $4a$ Wyckoff site (0,0,0) and the Mg atom is located at $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ occupying the $4b$ Wyckoff sites. In Table II,

What you should have learnt at the end of the day

example 3

PHYSICAL REVIEW B **78**, 195103 (2008)

X-ray linear dichroism in cubic compounds: The case of Cr^{3+} in $MgAl_2O_4$

Amélie Juhin,[1,*] Christian Brouder,[1] Marie-Anne Arrio,[1] Delphine Cabaret,[1] Philippe Sainctavit,[1] Etienne Balan,[1,2]
Amélie Bordage,[1] Ari P. Seitsonen,[1] Georges Calas,[1] Sigrid G. Eeckhout,[3] and Pieter Glatzel[3]

?

?

?

mechanical properties.[13] In $MgAl_2O_4$ spinel ($Fd\bar{3}m$ space-group symmetry), Al^{3+} cations occur at octahedral sites, which exhibit D_{3d} (or $\bar{3}m$) symmetry and build chains aligned along the six twofold axis of the cubic structure.[14] The number of equivalent octahedral sites in the unit cell is four, denoted hereafter as sites A, B, C, and D, depending on their direction of distortion, either $[\bar{1}11]$, $[11\bar{1}]$, $[111]$, or $[1\bar{1}1]$, respectively (Fig. 1 and Table. I). During the Al to Cr

What you should have learnt at the end of the day

example 3

Extract of the space-group table of spinel

$F\,d\,\bar{3}\,m$	O_h^7	$m\bar{3}m$	Cubic
No. 227	$F\ 4_1/d\ \bar{3}\ 2/m$	Patterson symmetry $F\,m\bar{3}\,m$	

ORIGIN CHOICE 2

Positions

Multiplicity, Wyckoff letter, Site symmetry

Coordinates

$(0,0,0)+$ $(0,\frac{1}{2},\frac{1}{2})+$ $(\frac{1}{2},0,\frac{1}{2})+$ $(\frac{1}{2},\frac{1}{2},0)+$

Reflection conditions

h,k,l permutable

General:

192	i	1	(1) x,y,z	(2) $\bar{x}+\frac{3}{4},\bar{y}+\frac{1}{4},z+\frac{1}{2}$	(3) $\bar{x}+\frac{1}{4},y+\frac{1}{2},\bar{z}+\frac{3}{4}$	(4) $x+\frac{1}{2},\bar{y}+\frac{3}{4},\bar{z}+\frac{1}{4}$	hkl :	$h+k=2n$ and $h+l,k+l=2n$
			(5) z,x,y	(6) $z+\frac{1}{2},\bar{x}+\frac{3}{4},\bar{y}+\frac{1}{4}$	(7) $\bar{z}+\frac{3}{4},\bar{x}+\frac{1}{4},y+\frac{1}{2}$	(8) $\bar{z}+\frac{1}{4},x+\frac{1}{2},\bar{y}+\frac{3}{4}$	$0kl$:	$k+l=4n$ and $k,l=2n$
			(9) y,z,x	(10) $\bar{y}+\frac{1}{4},z+\frac{1}{2},\bar{x}+\frac{3}{4}$	(11) $y+\frac{1}{2},\bar{z}+\frac{3}{4},\bar{x}+\frac{1}{4}$	(12) $\bar{y}+\frac{3}{4},\bar{z}+\frac{1}{4},x+\frac{1}{2}$	hhl :	$h+l=2n$
			(13) $y+\frac{3}{4},x+\frac{1}{4},\bar{z}+\frac{1}{2}$	(14) $\bar{y},\bar{x},\bar{z}$	(15) $y+\frac{1}{4},\bar{x}+\frac{1}{2},z+\frac{3}{4}$	(16) $\bar{y}+\frac{1}{2},x+\frac{3}{4},z+\frac{1}{4}$	$h00$:	$h=4n$
			(17) $x+\frac{3}{4},z+\frac{1}{4},\bar{y}+\frac{1}{2}$	(18) $\bar{x}+\frac{1}{2},z+\frac{3}{4},y+\frac{1}{4}$	(19) $\bar{x},\bar{z},\bar{y}$	(20) $x+\frac{1}{4},\bar{z}+\frac{1}{2},y+\frac{3}{4}$		
			(21) $z+\frac{3}{4},y+\frac{1}{4},\bar{x}+\frac{1}{2}$	(22) $z+\frac{1}{4},\bar{y}+\frac{1}{2},x+\frac{3}{4}$	(23) $\bar{z}+\frac{1}{2},y+\frac{3}{4},x+\frac{1}{4}$	(24) $\bar{z},\bar{y},\bar{x}$		
			(25) $\bar{x},\bar{y},\bar{z}$	(26) $x+\frac{1}{4},y+\frac{3}{4},\bar{z}+\frac{1}{2}$	(27) $x+\frac{3}{4},\bar{y}+\frac{1}{2},z+\frac{1}{4}$	(28) $\bar{x}+\frac{1}{2},y+\frac{1}{4},z+\frac{3}{4}$		
			(29) $\bar{z},\bar{x},\bar{y}$	(30) $\bar{z}+\frac{1}{2},x+\frac{1}{4},y+\frac{3}{4}$	(31) $z+\frac{1}{4},x+\frac{3}{4},\bar{y}+\frac{1}{2}$	(32) $z+\frac{3}{4},\bar{x}+\frac{1}{2},y+\frac{1}{4}$		
			(33) $\bar{y},\bar{z},\bar{x}$	(34) $y+\frac{3}{4},\bar{z}+\frac{1}{2},x+\frac{1}{4}$	(35) $\bar{y}+\frac{1}{2},z+\frac{1}{4},x+\frac{3}{4}$	(36) $y+\frac{1}{4},z+\frac{3}{4},\bar{x}+\frac{1}{2}$		
			(37) $\bar{y}+\frac{1}{4},\bar{x}+\frac{3}{4},z+\frac{1}{2}$	(38) y,x,z	(39) $\bar{y}+\frac{3}{4},x+\frac{1}{2},\bar{z}+\frac{1}{4}$	(40) $y+\frac{1}{2},\bar{x}+\frac{1}{4},\bar{z}+\frac{3}{4}$		
			(41) $\bar{x}+\frac{1}{4},\bar{z}+\frac{3}{4},y+\frac{1}{2}$	(42) $x+\frac{1}{2},\bar{z}+\frac{1}{4},\bar{y}+\frac{3}{4}$	(43) x,z,y	(44) $\bar{x}+\frac{3}{4},z+\frac{1}{2},\bar{y}+\frac{1}{4}$		
			(45) $\bar{z}+\frac{1}{4},\bar{y}+\frac{3}{4},x+\frac{1}{2}$	(46) $\bar{z}+\frac{3}{4},y+\frac{1}{2},\bar{x}+\frac{1}{4}$	(47) $z+\frac{1}{2},\bar{y}+\frac{1}{4},\bar{x}+\frac{3}{4}$	(48) z,y,x		
							Special: as above, plus	
96	h	. . 2	$0,y,\bar{y}$	$\frac{3}{4},\bar{y}+\frac{1}{4},\bar{y}+\frac{1}{2}$	$\frac{1}{4},y+\frac{1}{2},y+\frac{3}{4}$	$\frac{1}{2},\bar{y}+\frac{3}{4},y+\frac{1}{4}$		no extra conditions
			$\bar{y},0,y$	$\bar{y}+\frac{1}{2},\frac{3}{4},\bar{y}+\frac{1}{4}$	$y+\frac{3}{4},\frac{1}{4},y+\frac{1}{2}$	$y+\frac{1}{4},\frac{1}{2},\bar{y}+\frac{3}{4}$		
			$y,\bar{y},0$	$\bar{y}+\frac{1}{4},\bar{y}+\frac{1}{2},\frac{3}{4}$	$y+\frac{1}{2},y+\frac{3}{4},\frac{1}{4}$	$\bar{y}+\frac{3}{4},y+\frac{1}{4},\frac{1}{2}$		
			$0,\bar{y},y$	$\frac{1}{4},y+\frac{3}{4},y+\frac{1}{2}$	$\frac{3}{4},\bar{y}+\frac{1}{2},\bar{y}+\frac{1}{4}$	$\frac{1}{2},y+\frac{1}{4},\bar{y}+\frac{3}{4}$		
			$y,0,\bar{y}$	$y+\frac{1}{2},\frac{1}{4},y+\frac{3}{4}$	$\bar{y}+\frac{1}{4},\frac{3}{4},\bar{y}+\frac{1}{2}$	$\bar{y}+\frac{3}{4},\frac{1}{2},y+\frac{1}{4}$		
			$\bar{y},y,0$	$y+\frac{3}{4},y+\frac{1}{2},\frac{1}{4}$	$\bar{y}+\frac{1}{2},\bar{y}+\frac{1}{4},\frac{3}{4}$	$y+\frac{1}{4},\bar{y}+\frac{3}{4},\frac{1}{2}$		
96	g	. . m	x,x,z	$\bar{x}+\frac{3}{4},\bar{x}+\frac{1}{4},z+\frac{1}{2}$	$\bar{x}+\frac{1}{4},x+\frac{1}{2},\bar{z}+\frac{3}{4}$	$x+\frac{1}{2},\bar{x}+\frac{3}{4},\bar{z}+\frac{1}{4}$		no extra conditions
			z,x,x	$z+\frac{1}{2},\bar{x}+\frac{3}{4},\bar{x}+\frac{1}{4}$	$\bar{z}+\frac{3}{4},\bar{x}+\frac{1}{4},x+\frac{1}{2}$	$\bar{z}+\frac{1}{4},x+\frac{1}{2},\bar{x}+\frac{3}{4}$		
			x,z,x	$\bar{x}+\frac{1}{4},z+\frac{1}{2},\bar{x}+\frac{3}{4}$	$x+\frac{1}{2},\bar{z}+\frac{3}{4},\bar{x}+\frac{1}{4}$	$\bar{x}+\frac{3}{4},\bar{z}+\frac{1}{4},x+\frac{1}{2}$		
			$x+\frac{3}{4},x+\frac{1}{4},\bar{z}+\frac{1}{2}$	$\bar{x},\bar{x},\bar{z}$	$x+\frac{1}{4},\bar{x}+\frac{1}{2},z+\frac{3}{4}$	$\bar{x}+\frac{1}{2},x+\frac{3}{4},z+\frac{1}{4}$		
			$x+\frac{3}{4},z+\frac{1}{4},\bar{x}+\frac{1}{2}$	$\bar{x}+\frac{1}{2},z+\frac{3}{4},x+\frac{1}{4}$	$\bar{x},\bar{z},\bar{x}$	$x+\frac{1}{4},\bar{z}+\frac{1}{2},x+\frac{3}{4}$		
			$z+\frac{3}{4},x+\frac{1}{4},\bar{x}+\frac{1}{2}$	$z+\frac{1}{4},\bar{x}+\frac{1}{2},x+\frac{3}{4}$	$\bar{z}+\frac{1}{2},x+\frac{3}{4},x+\frac{1}{4}$	$\bar{z},\bar{x},\bar{x}$		
48	f	2 . mm	$x,\frac{1}{8},\frac{1}{8}$	$\bar{x}+\frac{3}{4},\frac{1}{8},\frac{5}{8}$	$\frac{1}{8},x,\frac{1}{8}$	$\frac{5}{8},\bar{x}+\frac{3}{4},\frac{1}{8}$	$\frac{1}{8},\frac{1}{8},x$	$\frac{1}{8},\frac{5}{8},\bar{x}+\frac{3}{4}$	hkl :	$h=2n+1$
			$\frac{7}{8},x+\frac{1}{4},\frac{3}{8}$	$\frac{7}{8},\bar{x},\frac{7}{8}$	$x+\frac{3}{4},\frac{3}{8},\frac{3}{8}$	$\bar{x}+\frac{1}{2},\frac{7}{8},\frac{3}{8}$	$\frac{7}{8},\frac{3}{8},\bar{x}+\frac{1}{2}$	$\frac{3}{8},\frac{3}{8},x+\frac{3}{4}$	or	$h+k+l=4n$
32	e	. 3 m	x,x,x	$\bar{x}+\frac{3}{4},\bar{x}+\frac{1}{4},x+\frac{1}{2}$						no extra conditions
			$\bar{x}+\frac{1}{4},x+\frac{1}{2},\bar{x}+\frac{3}{4}$	$x+\frac{1}{2},\bar{x}+\frac{3}{4},\bar{x}+\frac{1}{4}$						
			$x+\frac{3}{4},x+\frac{1}{4},\bar{x}+\frac{1}{2}$	$\bar{x},\bar{x},\bar{x}$						
			$x+\frac{1}{4},\bar{x}+\frac{1}{2},x+\frac{3}{4}$	$\bar{x}+\frac{1}{2},x+\frac{3}{4},x+\frac{1}{4}$						
16	d	. $\bar{3}$ m	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},0$	$\frac{3}{4},0,\frac{1}{4}$	$0,\frac{1}{4},\frac{3}{4}$			hkl :	$h=2n+1$
16	c	. $\bar{3}$ m	$0,0,0$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$	$\frac{1}{4},\frac{1}{2},\frac{3}{4}$	$\frac{1}{2},\frac{3}{4},\frac{1}{4}$			or	$h,k,l=4n+2$
									or	$h,k,l=4n$
8	b	$\bar{4}$ 3 m	$\frac{3}{8},\frac{3}{8},\frac{3}{8}$	$\frac{1}{8},\frac{5}{8},\frac{1}{8}$					hkl :	$h=2n+1$
8	a	$\bar{4}$ 3 m	$\frac{1}{8},\frac{1}{8},\frac{1}{8}$	$\frac{7}{8},\frac{3}{8},\frac{3}{8}$					or	$h+k+l=4n$

What you should have learnt at the end of the day

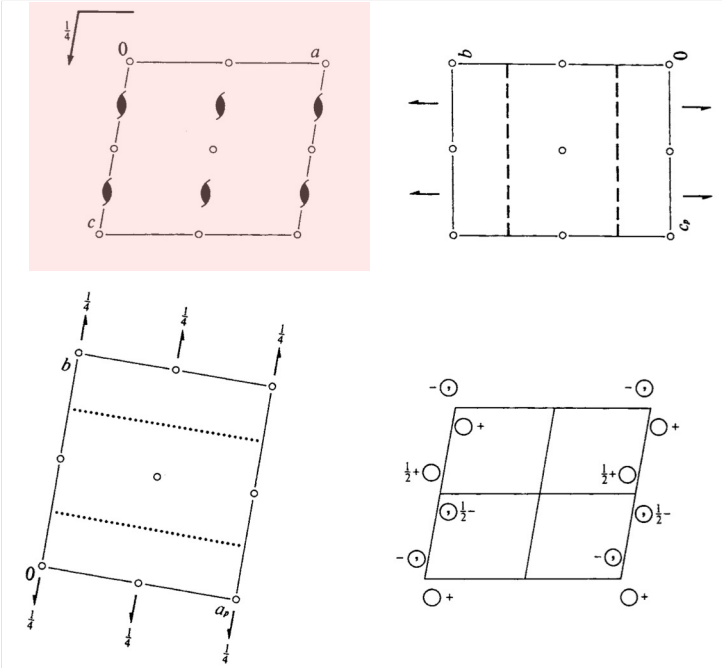
example 1

Space-group table of the Li-borate

$P2_1/c$	C_{2h}^5	$2/m$	Monoclinic

No. 14 $P12_1/c1$ Patterson symmetry $P12/m1$

UNIQUE AXIS b, CELL CHOICE 1



Origin at $\bar{1}$

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le \frac{1}{4};\quad 0 \le z \le 1$

Symmetry operations

(1) 1 (2) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{4}$ (3) $\bar{1}$ $0,0,0$ (4) c $x,\frac{1}{4},z$

CONTINUED No. 14 $P2_1/c$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	e	1	(1) x,y,z	(2) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	$h0l$: $l=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
2	d	$\bar{1}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			hkl : $k+l=2n$
2	c	$\bar{1}$	$0,0,\frac{1}{2}$	$0,\frac{1}{2},0$			hkl : $k+l=2n$
2	b	$\bar{1}$	$\frac{1}{2},0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $k+l=2n$
2	a	$\bar{1}$	$0,0,0$	$0,\frac{1}{2},\frac{1}{2}$			hkl : $k+l=2n$

Symmetry of special projections

Along [001] $p2gm$
$\mathbf{a}' = \mathbf{a}_p$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p2gg$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}_p$
Origin at $x,0,0$

Along [010] $p2$
$\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $P1c1$ (Pc, 7) 1; 4
[2] $P12_11$ ($P2_1$, 4) 1; 2
[2] $P\bar{1}$ (2) 1; 3

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [2] $P12_1/c1$ ($\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{a}' = 2\mathbf{a}, \mathbf{c}' = 2\mathbf{a}+\mathbf{c}$) ($P2_1/c$, 14); [3] $P12_1/c1$ ($\mathbf{b}' = 3\mathbf{b}$) ($P2_1/c$, 14)

Minimal non-isomorphic supergroups

I [2] $Pnna$ (52); [2] $Pmna$ (53); [2] $Pcca$ (54); [2] $Pbam$ (55); [2] $Pccn$ (56); [2] $Pbcm$ (57); [2] $Pnnm$ (58); [2] $Pbcn$ (60); [2] $Pbca$ (61); [2] $Pnma$ (62); [2] $Cmce$ (64)

II [2] $A12/m1$ ($C2/m$, 12); [2] $C12/c1$ ($C2/c$, 15); [2] $I12/c1$ ($C2/c$, 15); [2] $P12_1/m1$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) ($P2_1/m$, 11); [2] $P12/c1$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) ($P2/c$, 13)

Course outline

1- Symmetry observation in natural crystals

2- Internal cause of the natural crystal shape

3 – Crystal lattice, cell, motif

4 – Lattice direction and planes

5 – Reciprocal lattice

6 – Crystal lattice & symmetries

7 – Conventional cell (unit cell)

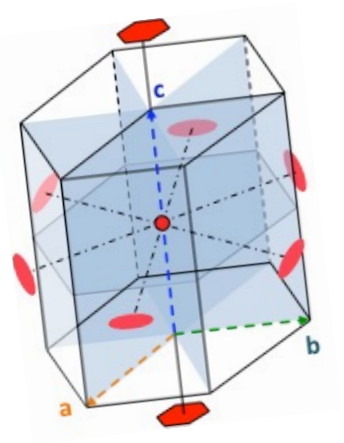
8 – The 32 crystallographic point groups

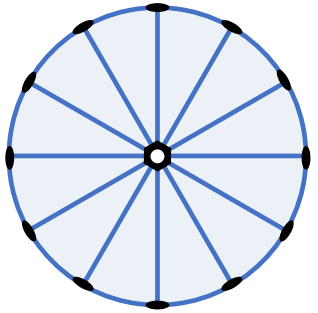
9 – The 7 crystal systems

10 – The 14 Bravais lattices

11 – The 230 space-groups



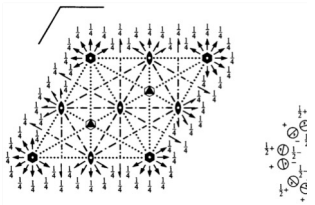




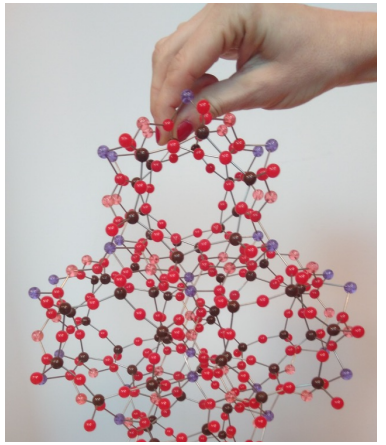
$$\frac{6}{m}mm$$

$P6/mcc$ D^2_{6h}

No. 192 $P\ 6/m\ 2/c\ 2/c$



Origin at centre $(6/m)$ at $6/mcc$



Course outline

1- Symmetry observation in natural crystals

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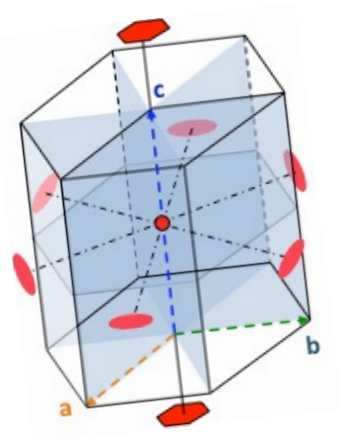
8 – The 32 crystallographic point groups

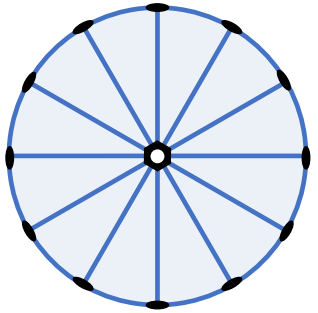
9 – The 7 crystal systems

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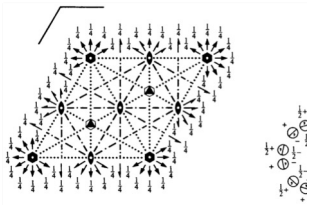




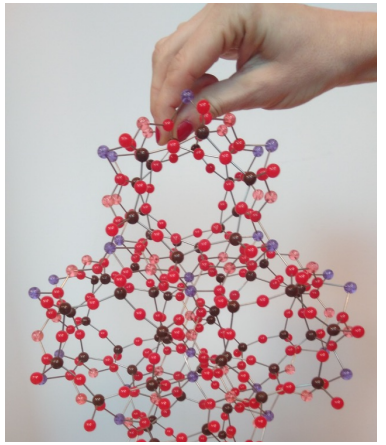
$\frac{6}{m}mm$

$P6/mcc$ D^2_{6h}

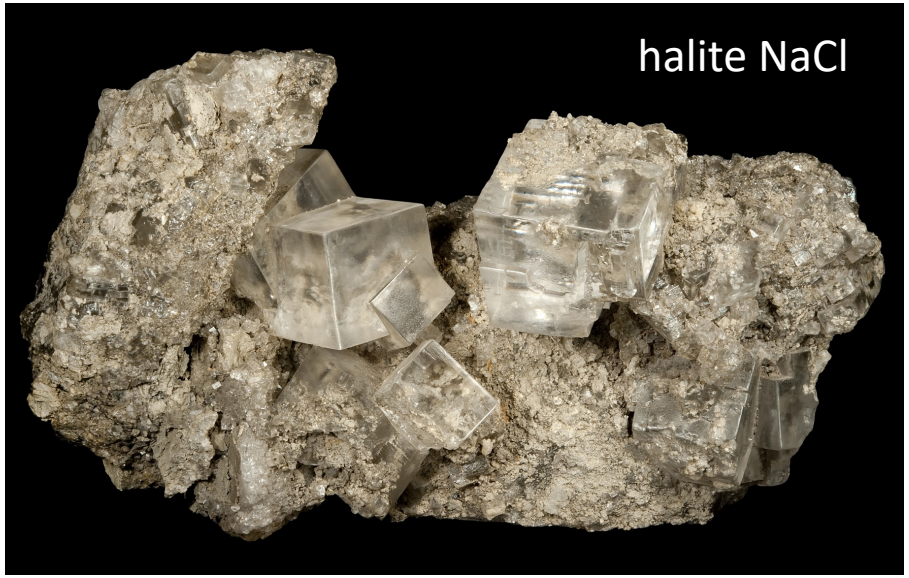
No. 192 $P\ 6/m\ 2/c\ 2/c$

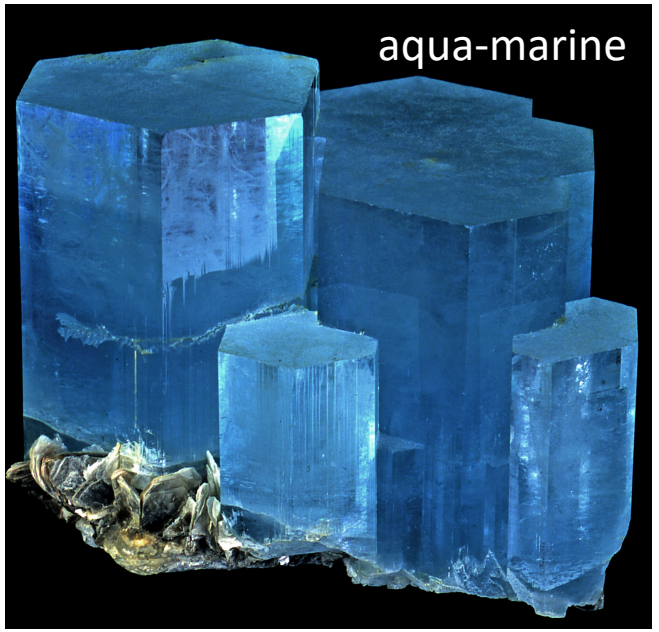


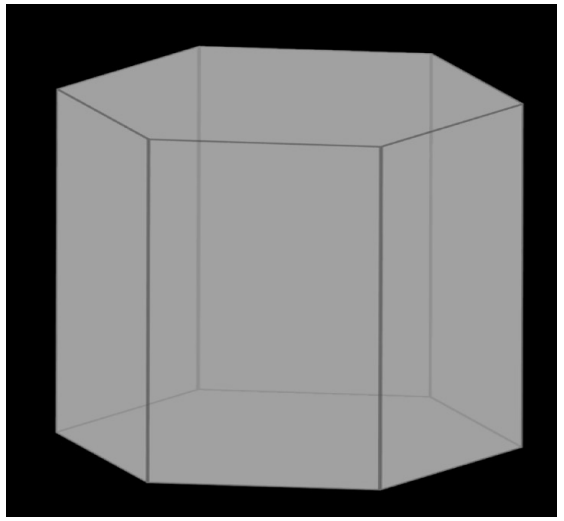
Origin at centre $(6/m)$ at $6/mcc$

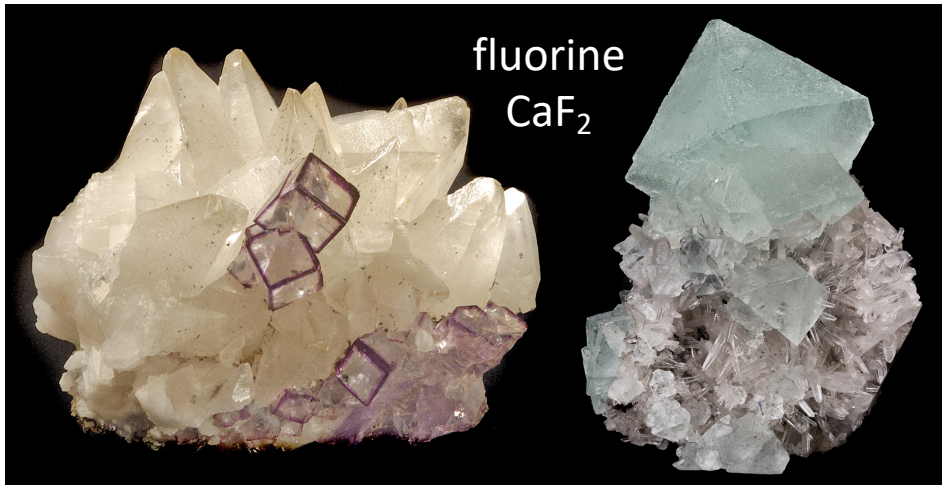


1- Symmetry observation in natural crystals

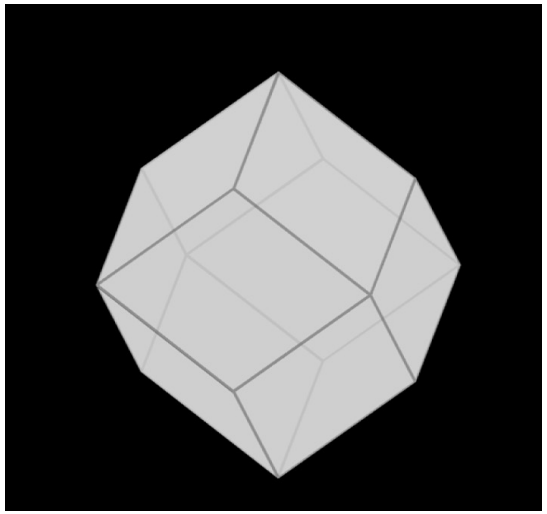








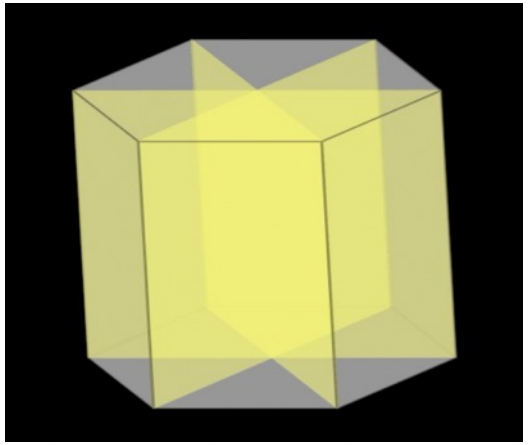


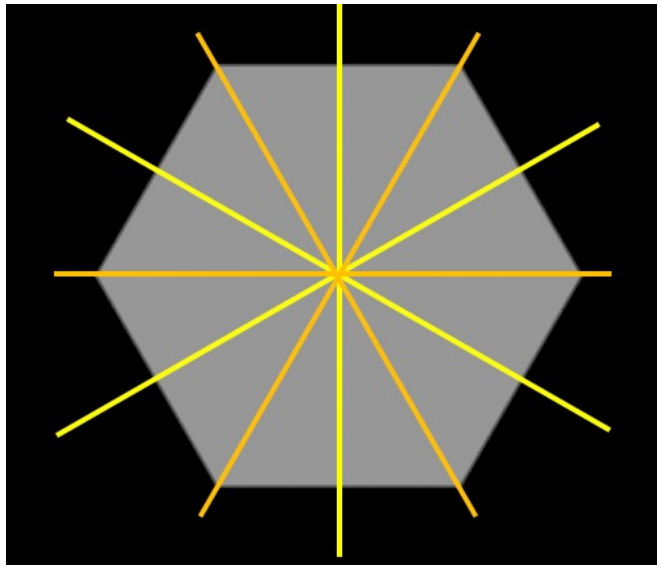


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Highlighting mirror planes

aquamarine model: hexagonal-based straight prism

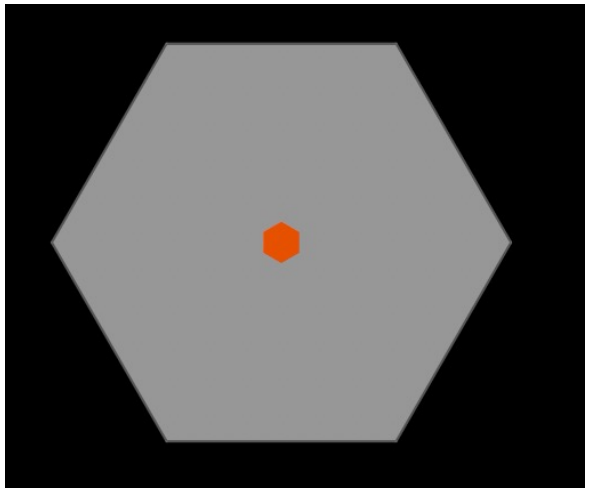


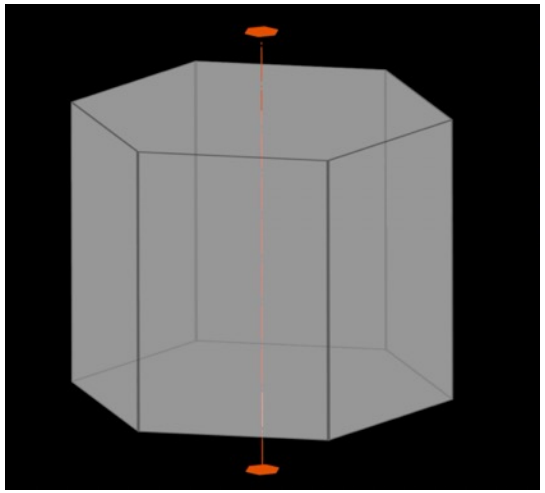


- **3 mirror planes**
  parallel to vertical edges
  and cutting the hexagonal face
  edges in the middle

- **3 mirror planes**
  parallel to the vertical edges and
  joining two corners opposite
  in the hexagonal face

Highlighting 6-fold rotation axis





axis A_6 or 6

$$\varphi = 60\,^{\circ} = \frac{2\pi}{6}$$

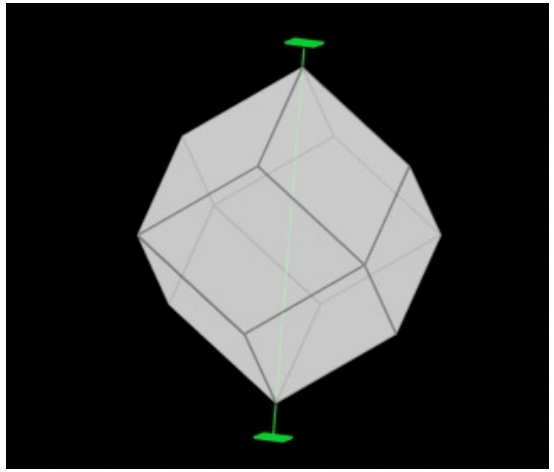
Highlighting 4-fold, 3-fold and 2-fold rotation axes



rhombododecahedron

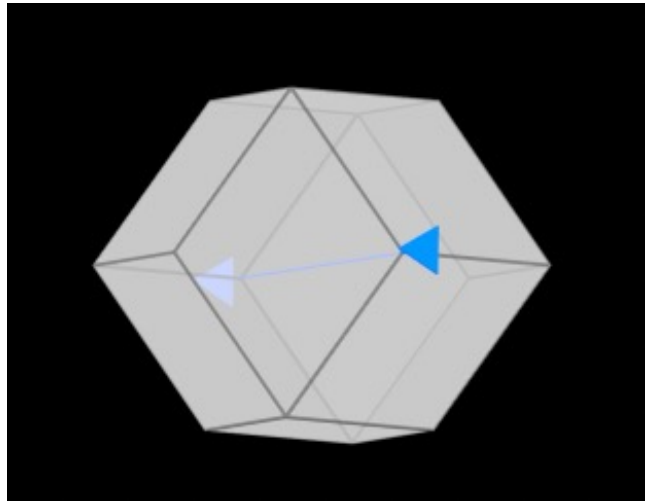
(12-face polyhedron)

Highlighting 4-fold, 3-fold and 2-fold rotation axes



axis A_4 or 4

$$\varphi = 90\,° = \frac{2\pi}{4}$$

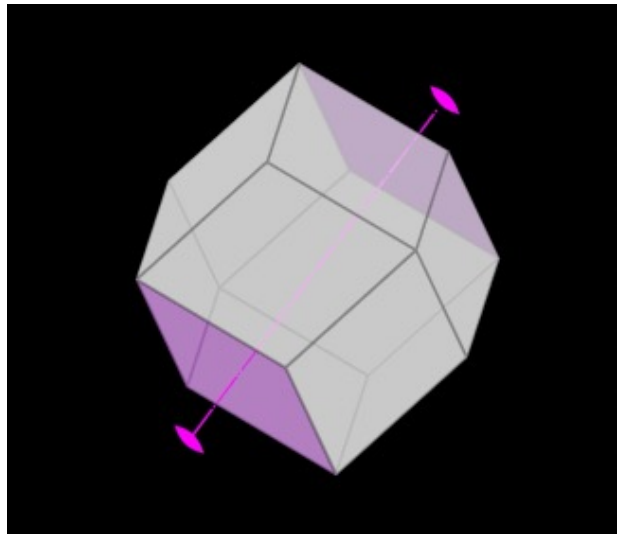


axis A_3 or 3

$$\varphi = 120\,° = \frac{2\pi}{3}$$

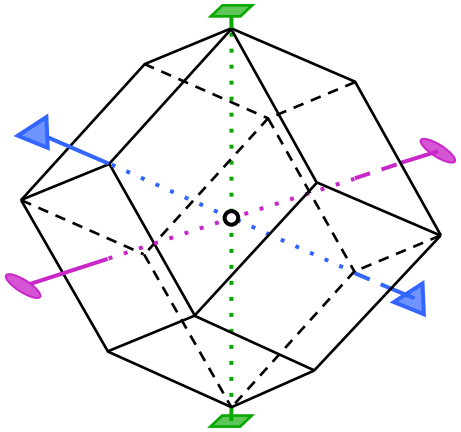
axis A_2 or 2

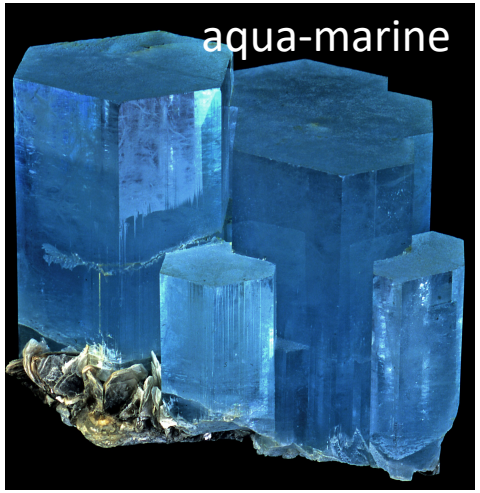
$$\varphi = 180\,° = \frac{2\pi}{2}$$

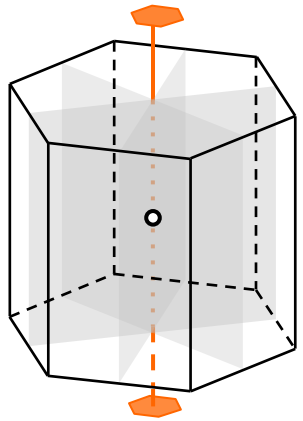


1- Symmetry observation in natural crystals









rotations

A_2 A_3 A_4 A_6

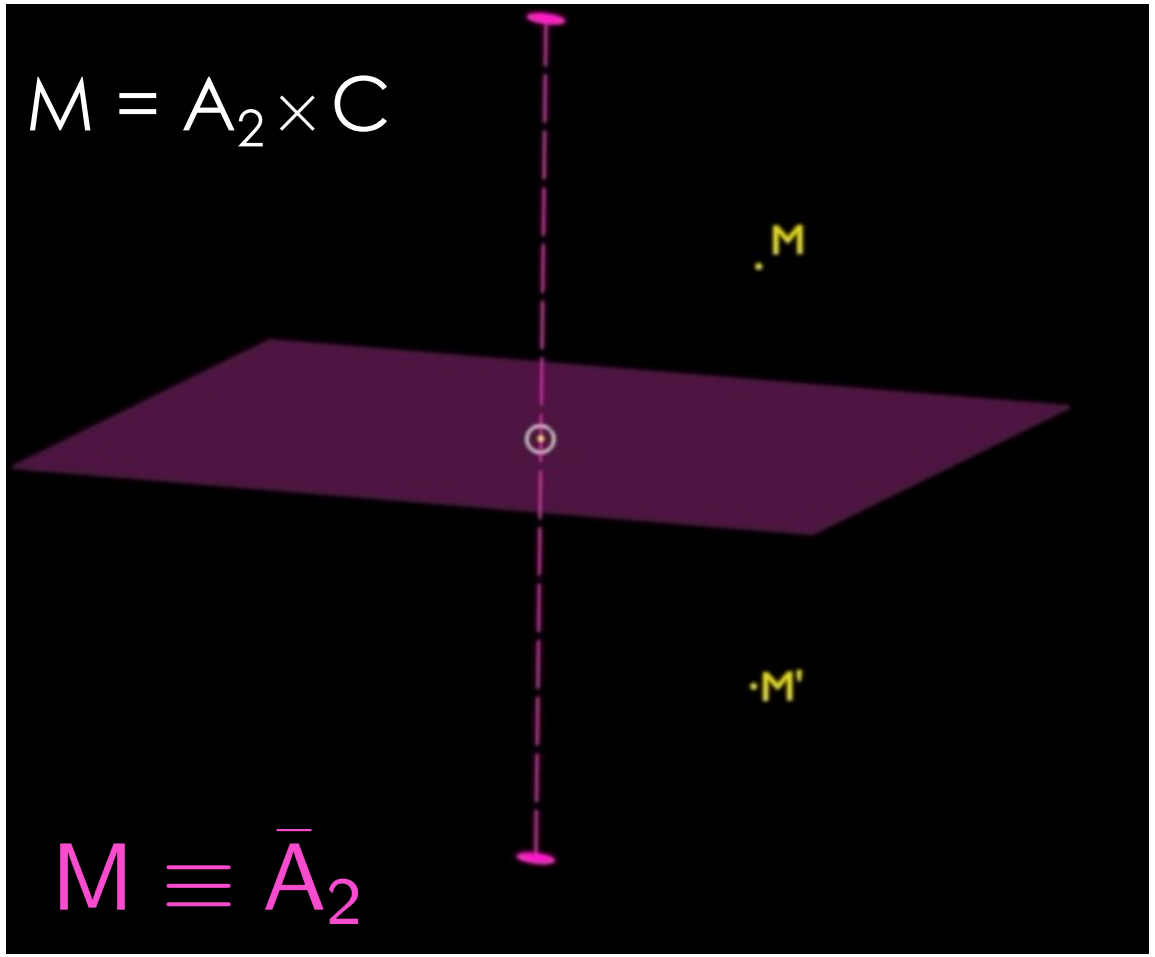
mirror plane

M

symmetry centre

C

What is a mirror plane?



The mirror plane is a roto-inversion of order 2

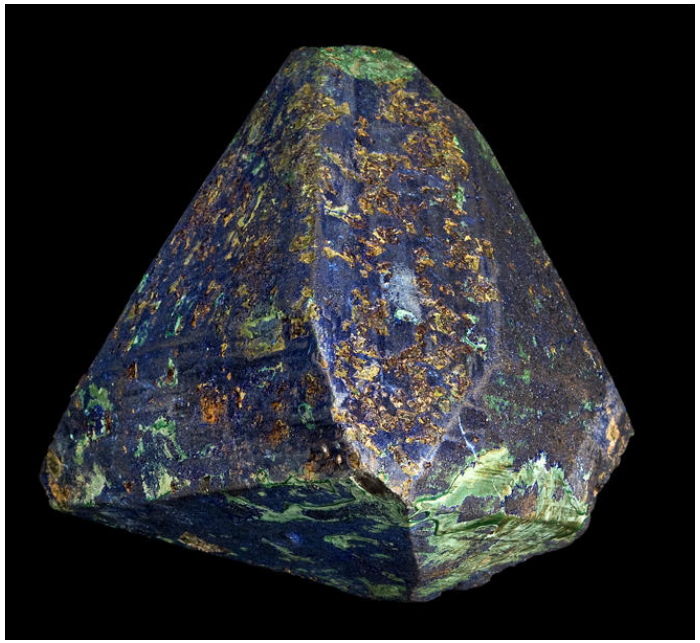
rotations and roto-inversions

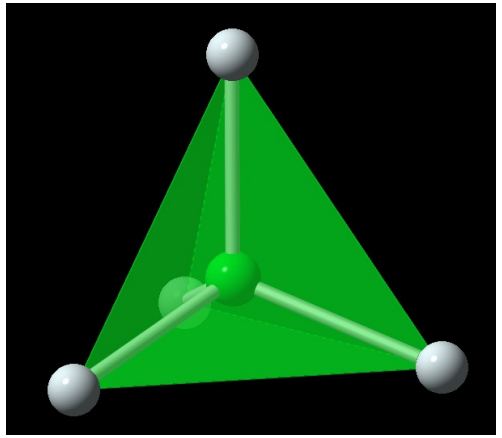
rotations	A_1	A_2	A_3	A_4	A_6	← this course symbols
	identity					
	1	2	3	4	6	← Hermann-Mauguin symbols
roto-inversions	$C \equiv \bar{A}_1$	$M \equiv \bar{A}_2$	$\bar{A}_3$	$\bar{A}_4$	$\bar{A}_6$	← this course symbols
	centre					
	$\bar{1}$	m	$\bar{3}$	$\bar{4}$	$\bar{6}$	← Hermann-Mauguin symbols

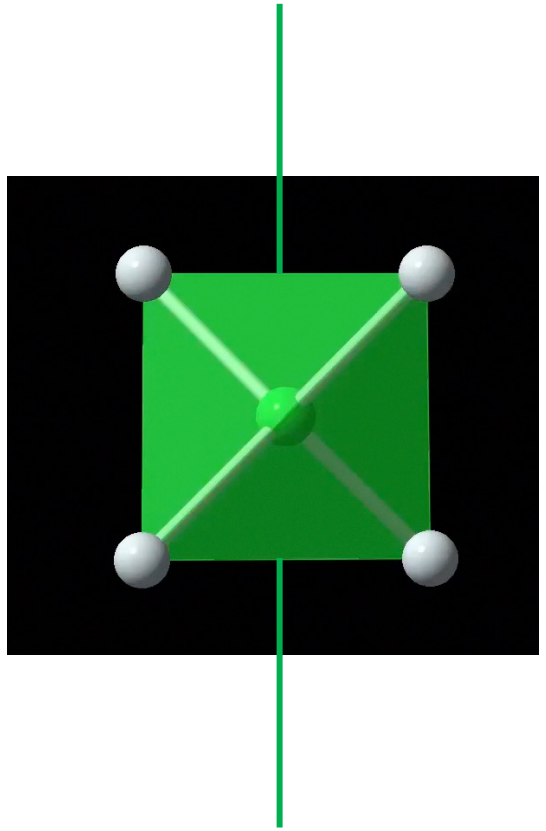
$$\bar{n} = \text{rotation } \frac{2\pi}{n} \times \text{inversion}$$

1- Symmetry observation in natural crystals

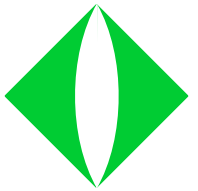
roto-inversions







axis $\bar{4}$



tetrahedrite ©mineral collection Sorbonne University

Course outline

1- Symmetry observation in natural crystals

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5 – Reciprocal lattice

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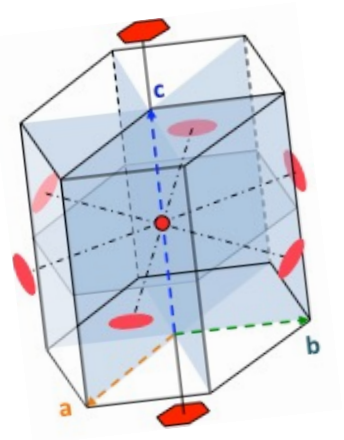
8 – The 32 crystallographic point groups

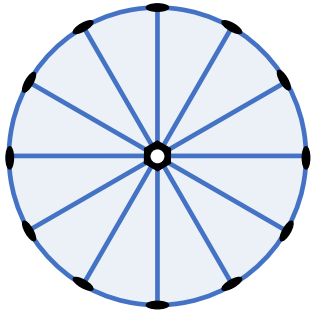
9 – The 7 crystal systems

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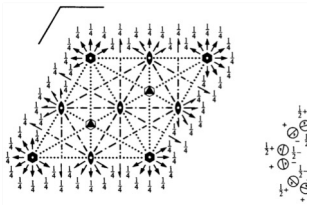




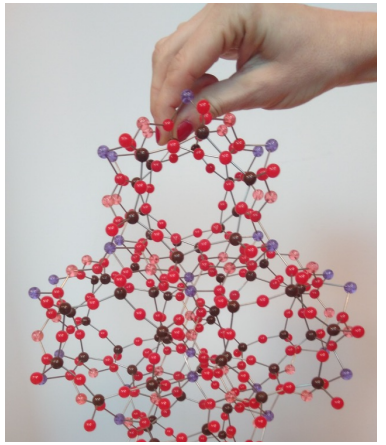
$\frac{6}{m}mm$

$P6/mcc$ D^2_{6h}

No. 192 $P\ 6/m\ 2/c\ 2/c$



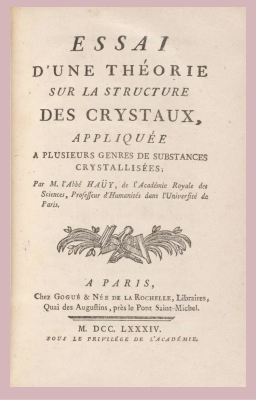
Origin at centre $(6/m)$ at $6/mcc$



2- Internal cause of the natural crystal shape

René-Just Haüy (1784)

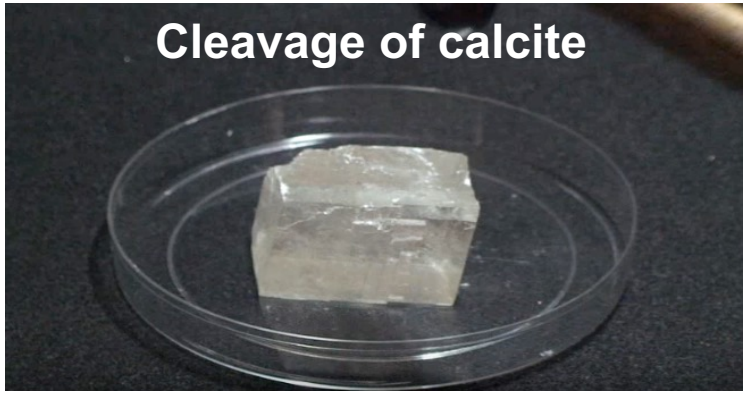




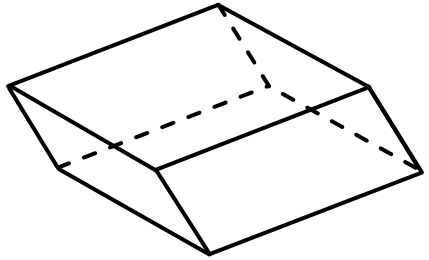
ESSAI
D'UNE THÉORIE
SUR LA STRUCTURE
DES CRYSTAUX,
APPLIQUÉE
A PLUSIEURS GENRES DE SUBSTANCES
CRYSTALLISÉES;
Par M. l'Abbé HAÜY, de l'Académie Royale des Sciences, Professeur d'Humanités dans l'Université de Paris.
A PARIS,
Chez Gogué & Née de la Rochelle, Libraires, Quai des Augustins, près le Pont Saint-Michel.
M. DCC. LXXXIV.
AVEC LE PRIVILÈGE DE L'ACADÉMIE.

Torbern Bergman





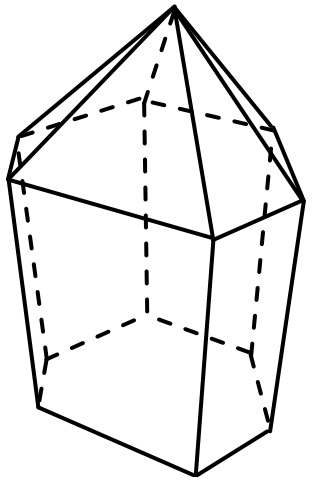
Rhombohedron



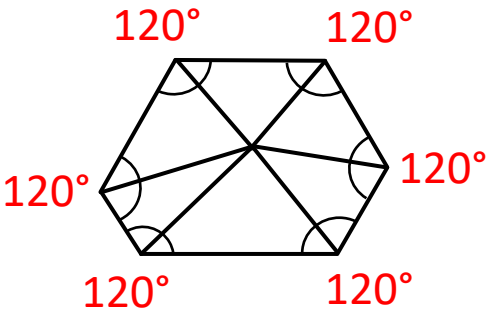
Jean-Baptiste Romé de l'Isle



Law of constancy of interfacial angles



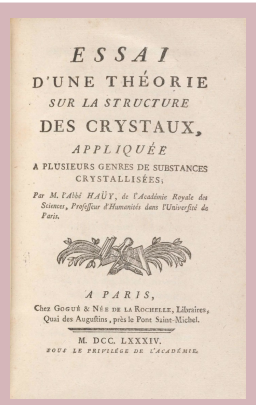
crystal of quartz



2- Internal cause of the natural crystal shape

René-Just Haüy (1784)



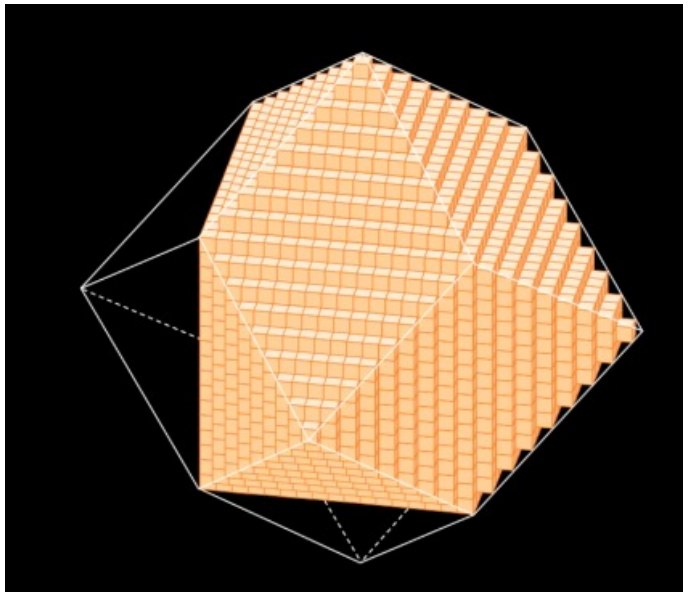


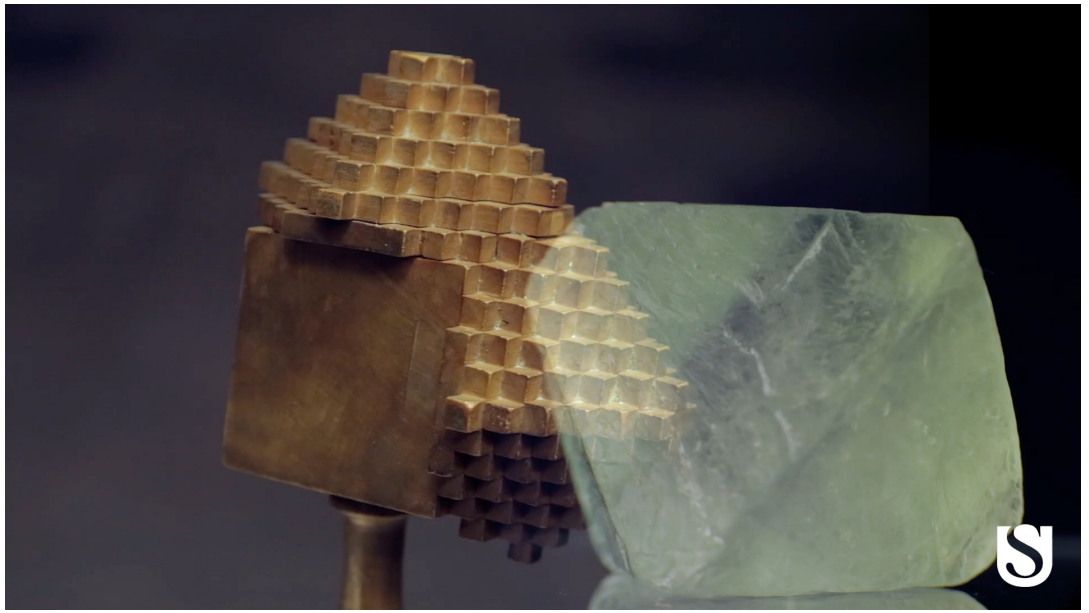
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primitive solid

''molécule intégrante''

law of rational decrements

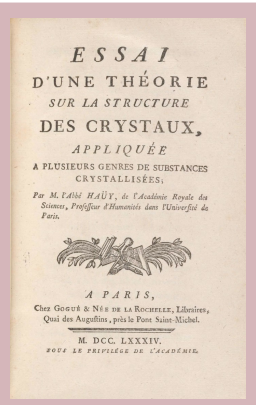




2- Internal cause of the natural crystal shape

René-Just Haüy (1784)





ESSAI
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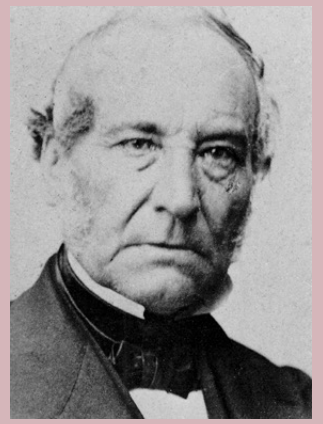
↓

''molécule intégrante''

↓

law of rational decrements

Gabriel Delafosse



cell

lattice

motif



Auguste Bravais (1848)

Course outline

1- Symmetry observation in natural crystals

2- Internal cause of the natural crystal shape

3 – Crystal lattice, cell, motif

4 – Lattice direction and planes

5 – Reciprocal lattice

6 – Crystal lattice & symmetries

7 – Conventional cell (unit cell)

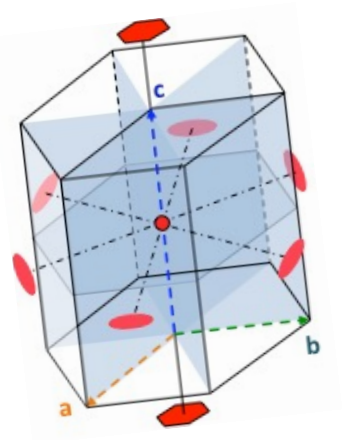
8 – The 32 crystallographic point groups

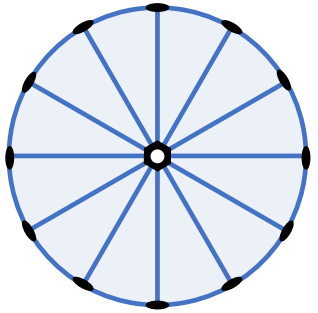
9 – The 7 crystal systems

10 – The 14 Bravais lattices

11 – The 230 space-groups



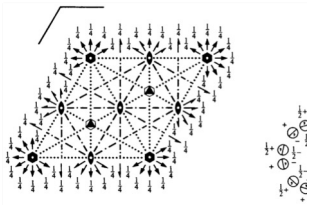




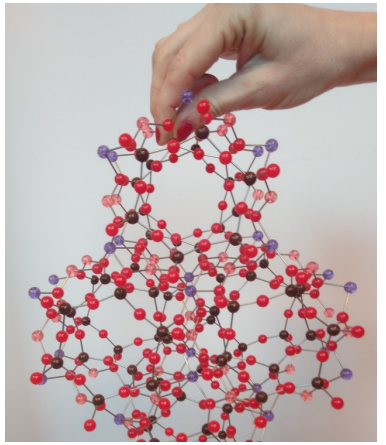
$\frac{6}{m}mm$

$P6/mcc$ D^2_{6h}

No. 192 $P\ 6/m\ 2/c\ 2/c$



Origin at centre $(6/m)$ at $6/mcc$

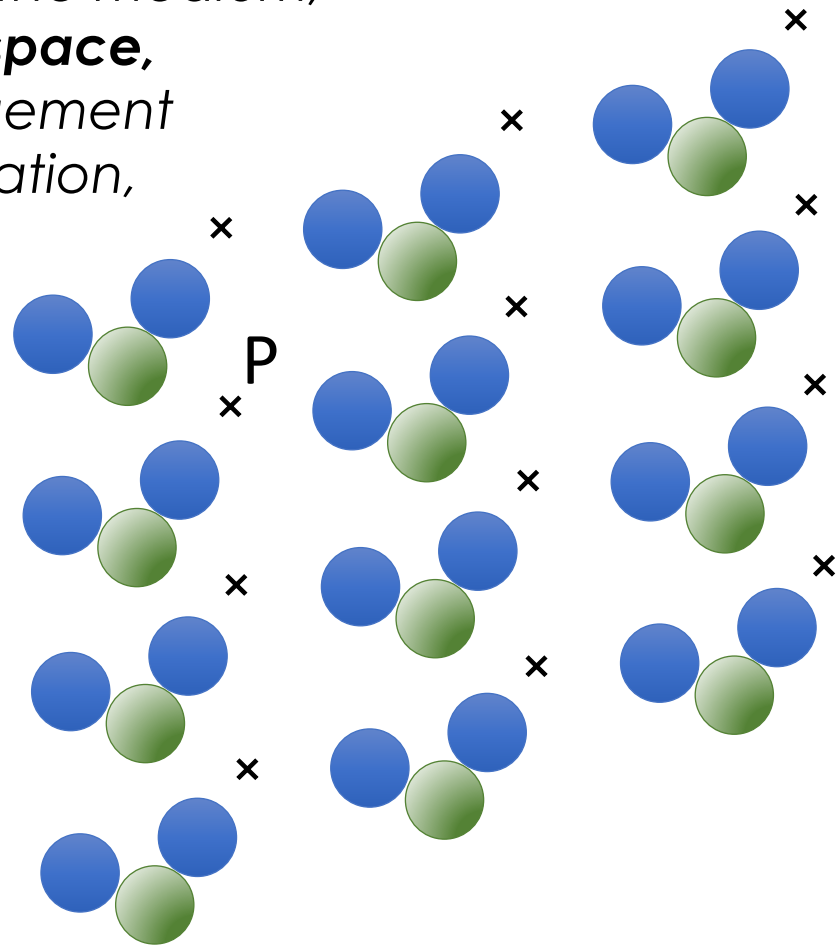


3 – Crystal lattice, cell, motif



The Bravais postulate

''Given any P point in a crystal, there is in the medium, ***a discrete, unlimited in the 3 directions of space, number of points*** *around which the arrangement of atoms is the same, with the same orientation, as around point P.''*



- All the points define the **lattice**.
- The points are called **lattice points** (or nodes).

The **lattice points** do not correspond to any physical entity.

Do not make the confusion between lattice points and atoms!

lattice ➔ basis vectors

The lattice is defined, in 3D, by **3 basis vecteurs** $\vec{a}$, $\vec{b}$ and $\vec{c}$ that are non colinear.

All the lattice points are obtained by linear combination:

$$\vec{t} = u\,\vec{a} + v\,\vec{b} + w\,\vec{c}$$

u, v , w: relative integers

lattice translation

3 – Crystal lattice, cell, motif

lattice ➔ how to identify a lattice point

$\vec{t} = \vec{a} + \vec{b} + \vec{c}$

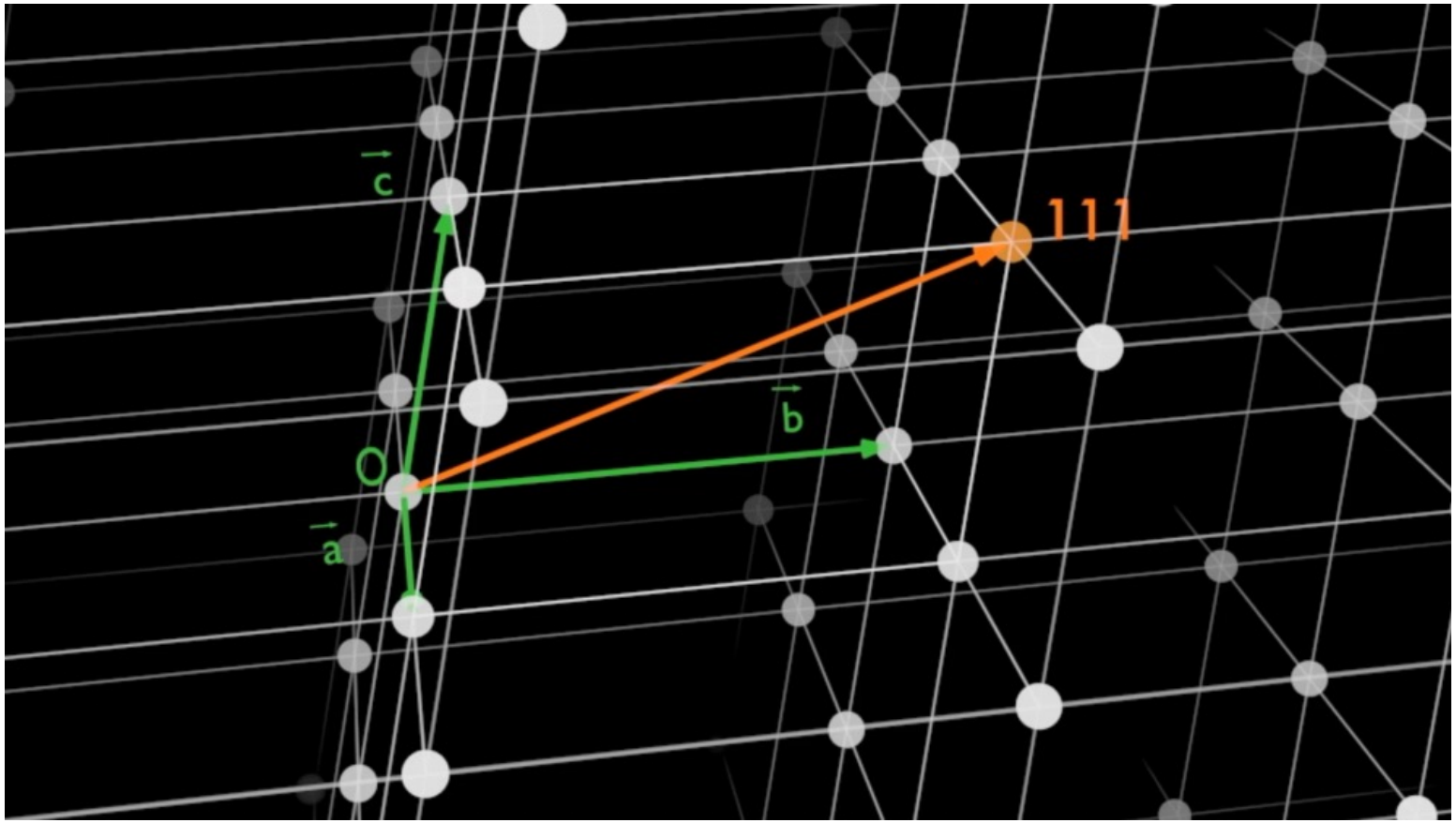
➔ lattice point 111

$\vec{t} = -\vec{a} + 2\vec{b}$

➔ lattice point $\bar{1}20$

$\vec{t} = \vec{a} - \vec{b} + 2\vec{c}$

➔ lattice point $1\bar{1}2$



3 – Crystal lattice, cell, motif

basis vectors ➔ cell

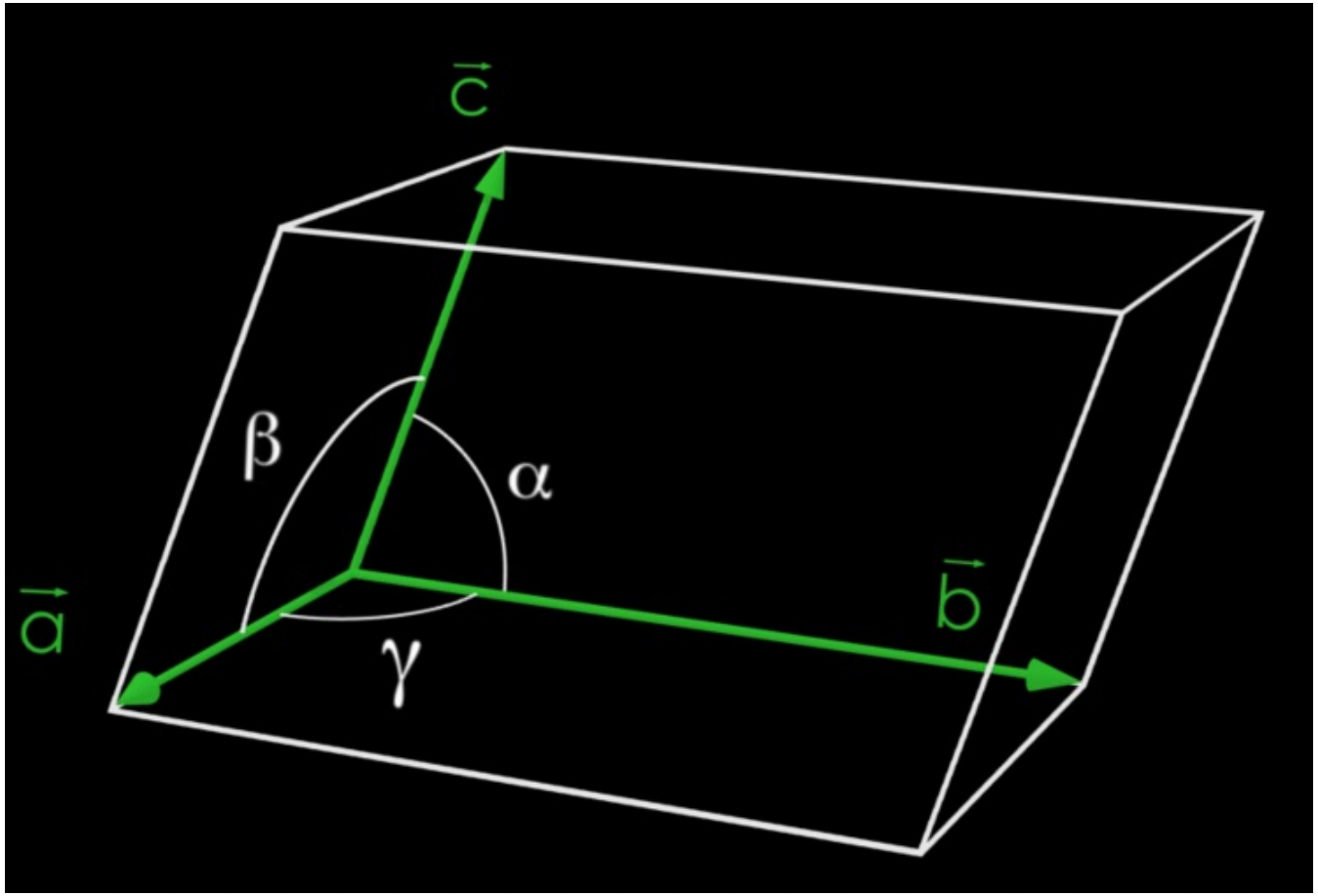
3 basis vectors: $\vec{a}$, $\vec{b}$ and $\vec{c}$

6 parameters:

- 3 lengths a, b, c
- 3 angles α, β et γ

volume:

$$V = (\vec{a}, \vec{b}, \vec{c}) = \vec{a} \cdot (\vec{b} \times \vec{c})$$



3 – Crystal lattice, cell, motif

2D cell

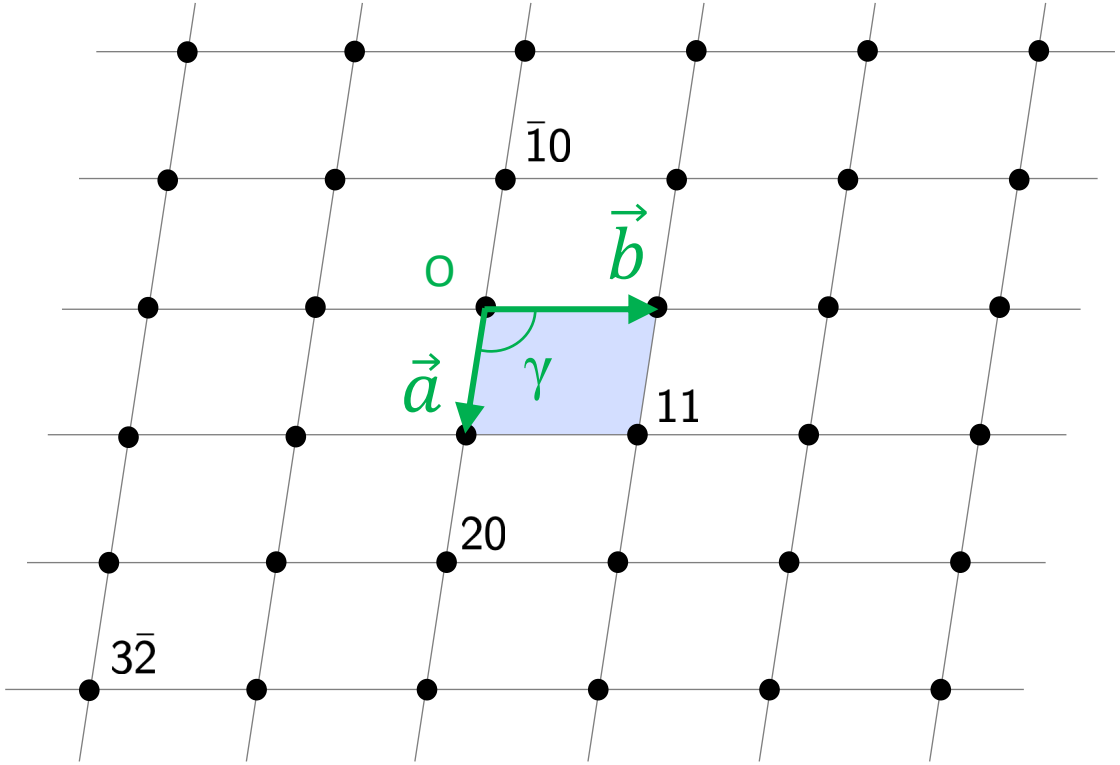
2 basis vectors: $\vec{a}$ and $\vec{b}$

3 parameters:

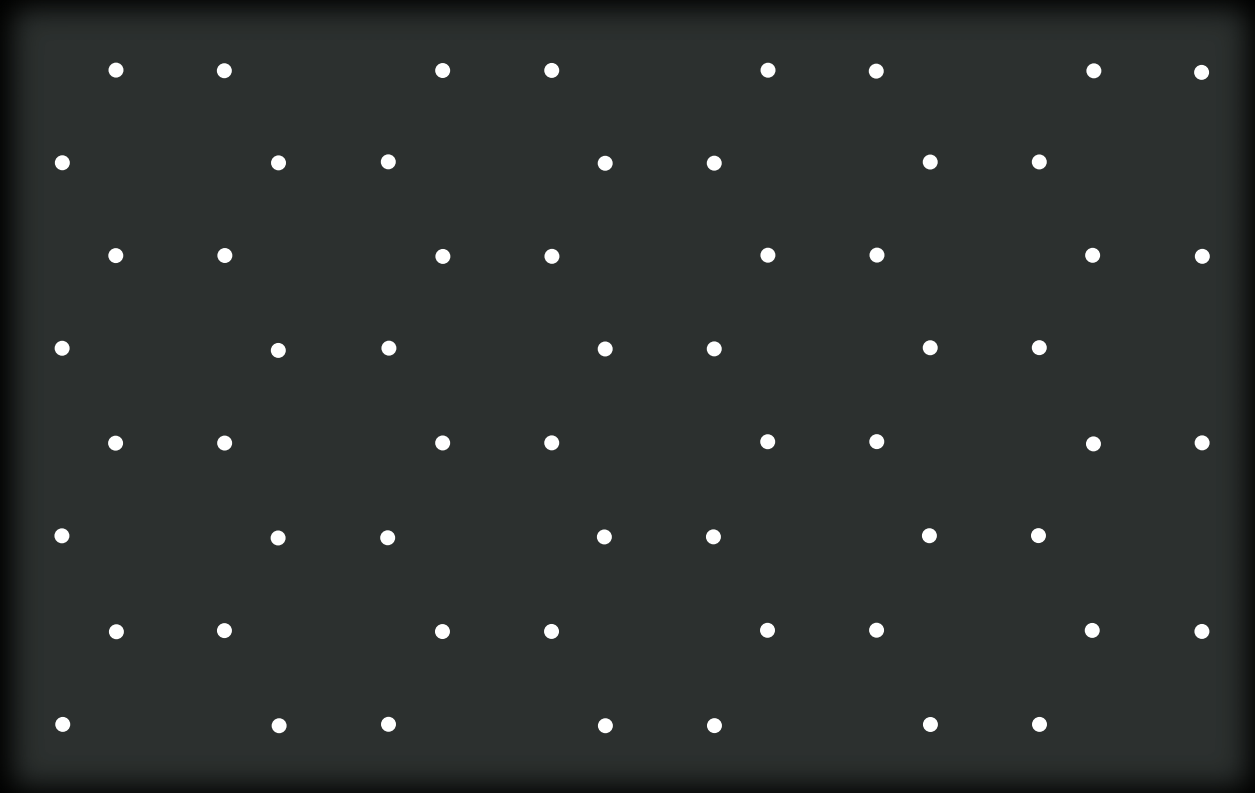
- 2 lengths a, b
- 1 angle $\gamma \geq 90°$

surface:

$$S = |\vec{a} \times \vec{b}|$$

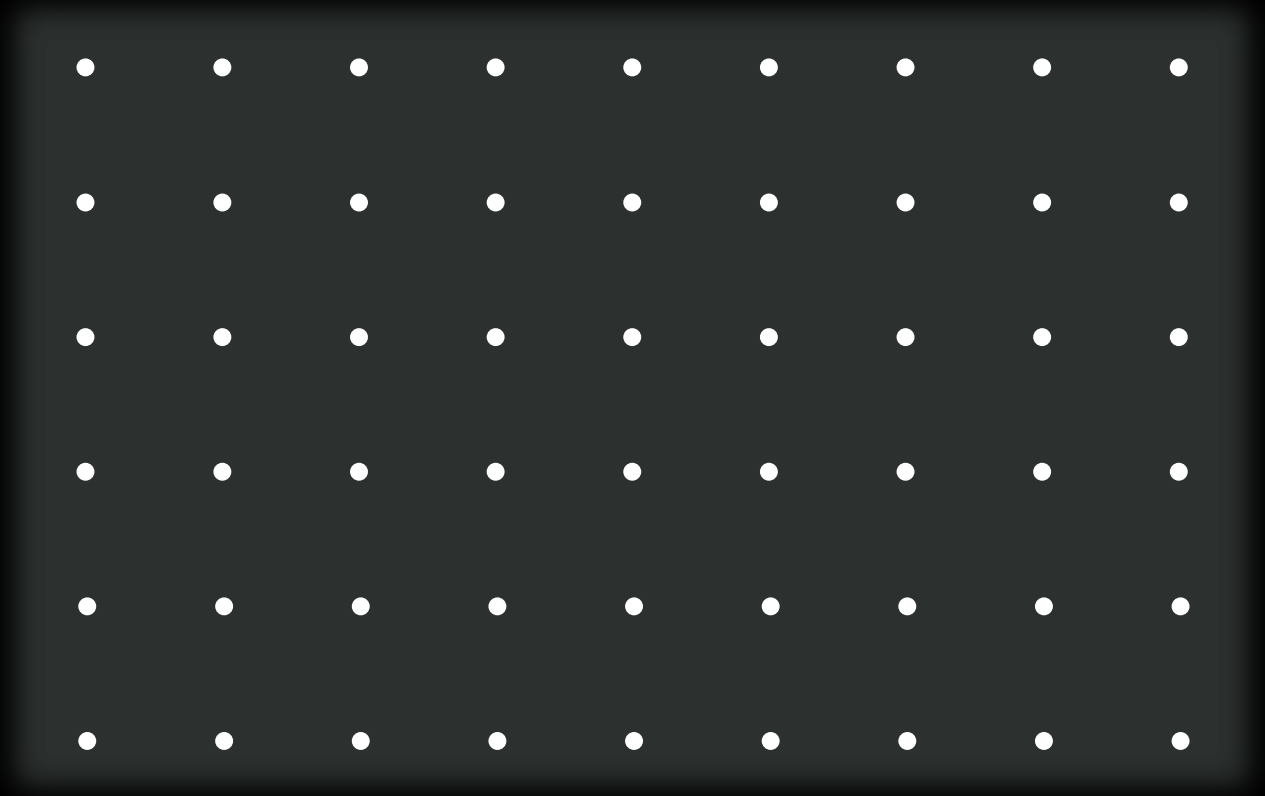


Exercize



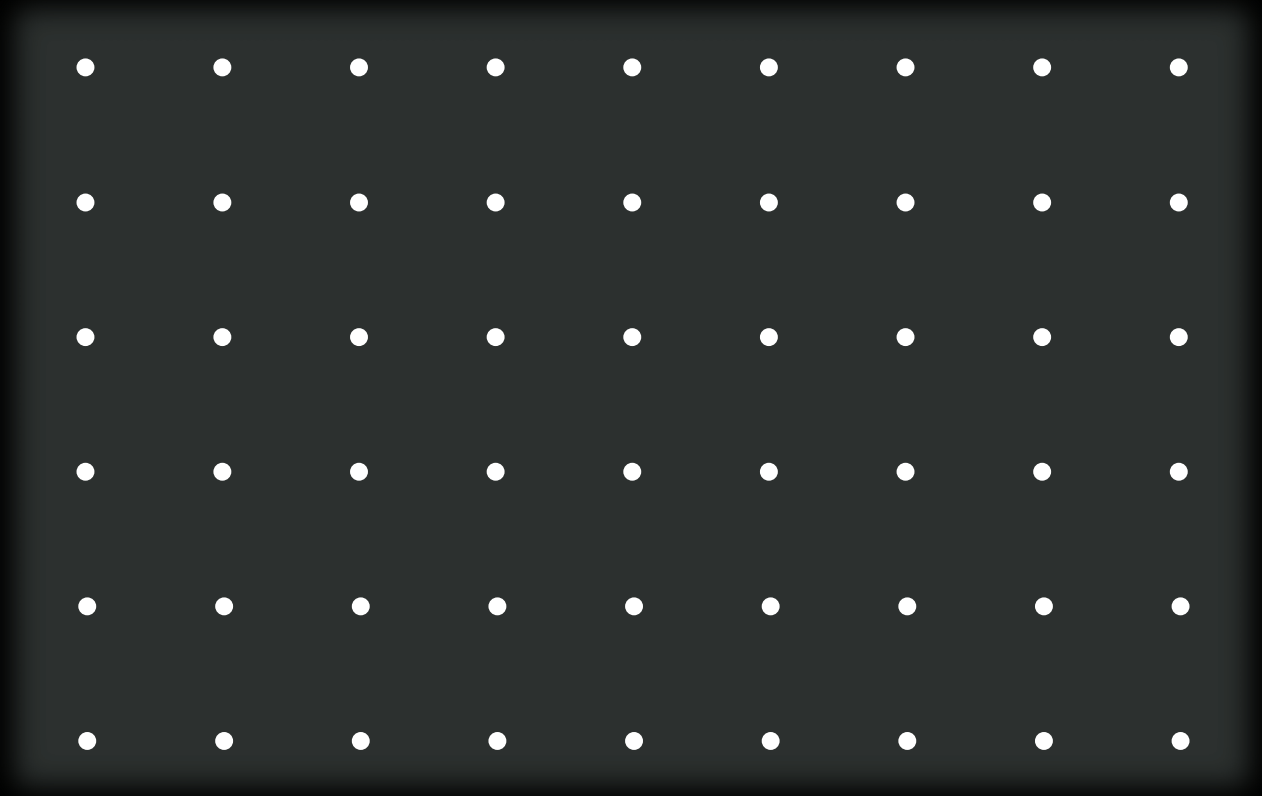
Does this **set of points** define a **lattice**?

Exercize



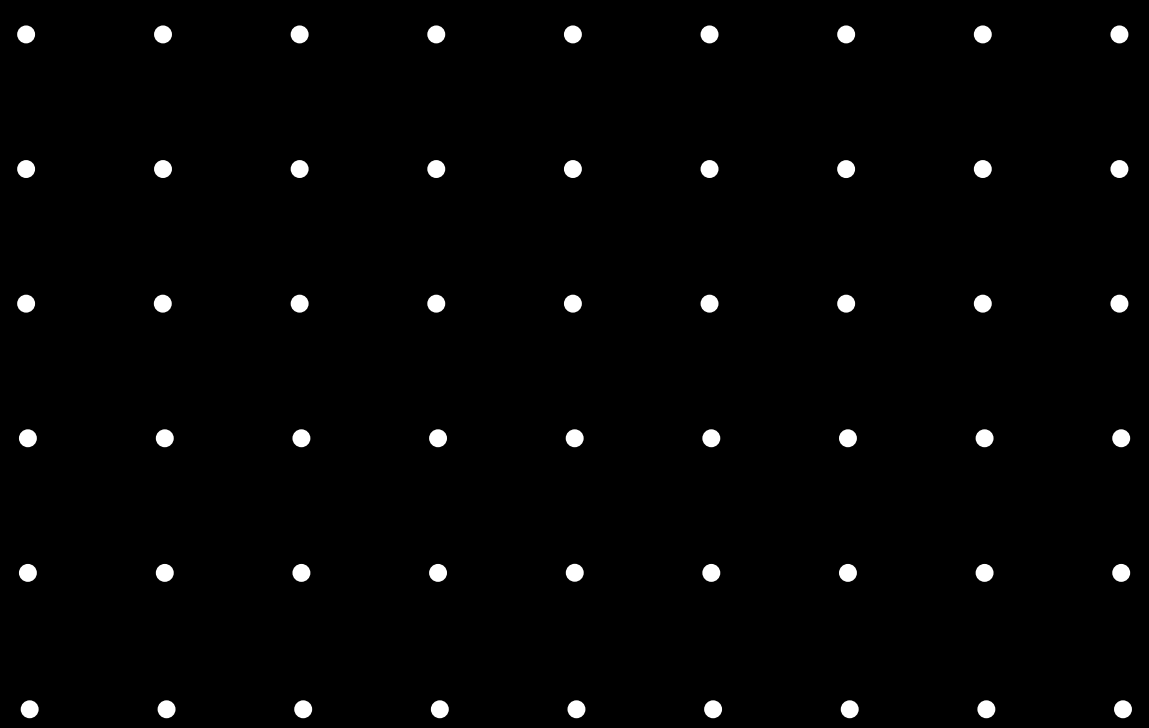
Does this **set of points** define a **lattice**?

Exercize



View a primitive square cell

Exercize



View a **square** cell that contains **2 lattice points**

3 – Crystal lattice, cell, motif

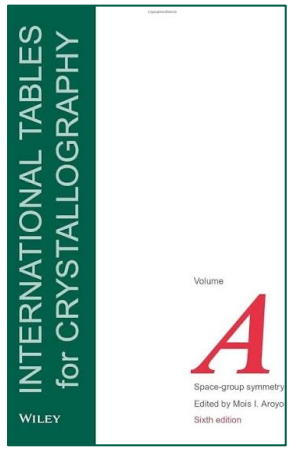
primitive cell and supercells

Conventional centring types of one-, two- and three-dimensional cells

2D cells

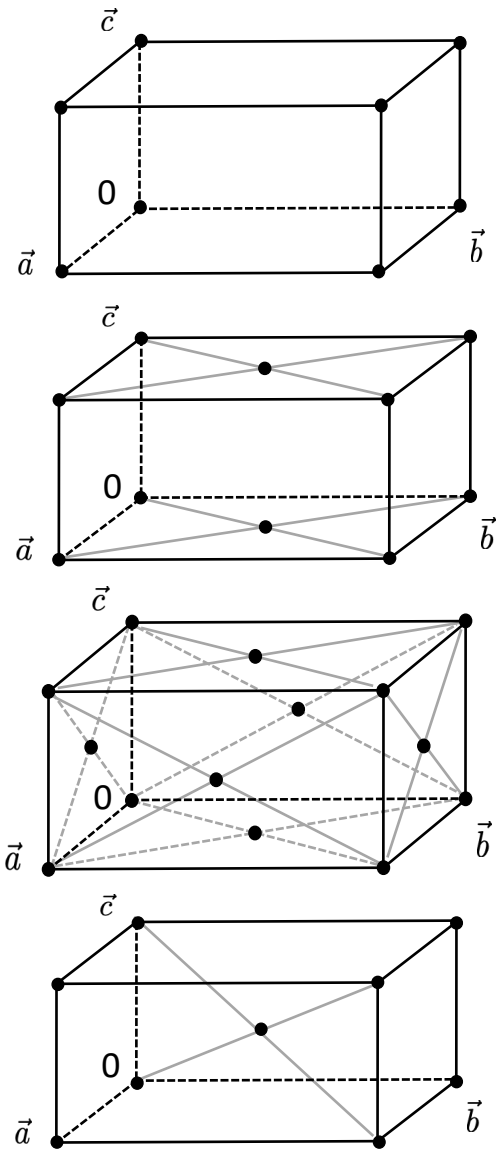
3D cells

Printed symbol	Centring type of cell	Number of lattice points per cell	Coordinates of lattice points within cell
Two dimensions			
p	Primitive	1	0, 0
c	Centred	2	0, 0; $\frac{1}{2}, \frac{1}{2}$
Three dimensions			
P	Primitive	1	0, 0, 0
C	*C*-face centred	2	0, 0, 0; $\frac{1}{2}, \frac{1}{2}$, 0
A	*A*-face centred	2	0, 0, 0; 0, $\frac{1}{2}, \frac{1}{2}$
B	*B*-face centred	2	0, 0, 0; $\frac{1}{2}$, 0, $\frac{1}{2}$
I	Body centred	2	0, 0, 0; $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$
F	All-face centred	4	0, 0, 0; $\frac{1}{2}, \frac{1}{2}$, 0; 0, $\frac{1}{2}, \frac{1}{2}; \frac{1}{2}$, 0, $\frac{1}{2}$



tab.1.2.1

3 – Crystal lattice, cell, motif



3D primitive cell and supercells

Translations	Cell	Lattice type	Cell Multiplicity
$\vec{a},\ \vec{b},\ \vec{c}$	primitive (*or simple*)	P	1
$\vec{a},\ \vec{b},\ \vec{c},\ \frac{\vec{b}+\vec{c}}{2}$	centred on face $(\vec{b},\ \vec{c})$	A	2
$\vec{a},\ \vec{b},\ \vec{c},\ \frac{\vec{a}+\vec{c}}{2}$	centred on face $(\vec{a},\ \vec{c})$	B	2
$\vec{a},\ \vec{b},\ \vec{c},\ \frac{\vec{a}+\vec{b}}{2}$	centred on face $(\vec{a},\ \vec{b})$	C	2
$\vec{a},\ \vec{b},\ \vec{c},\ \frac{\vec{a}+\vec{b}}{2},\ \frac{\vec{b}+\vec{c}}{2},\ \frac{\vec{a}+\vec{c}}{2}$	all-faces centred	F	4
$\vec{a},\ \vec{b},\ \vec{c},\ \frac{\vec{a}+\vec{b}+\vec{c}}{2}$	body centred	I	2

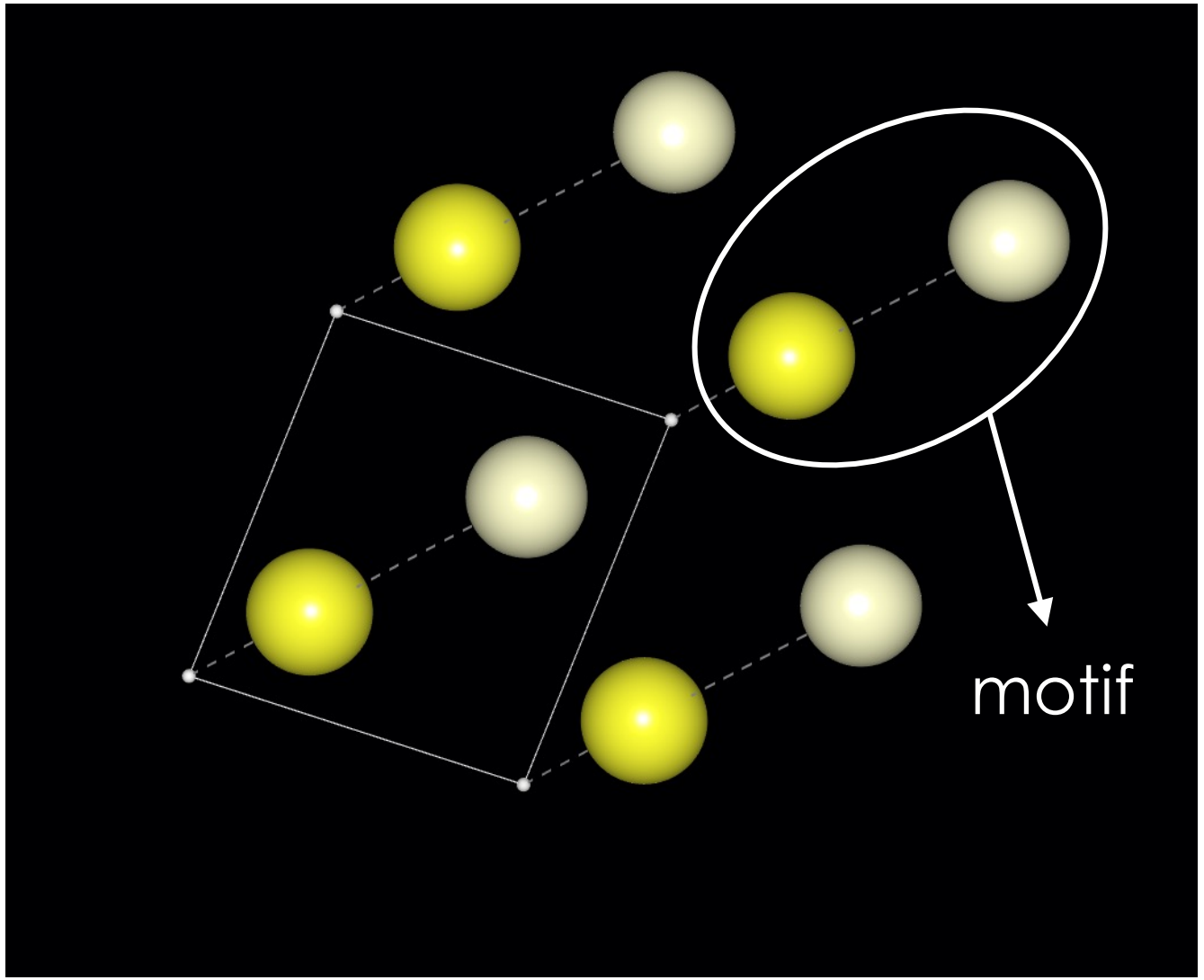
➔ **4 lattice types** (i.e. 4 translation groups)

3 – Crystal lattice, cell, motif

motif

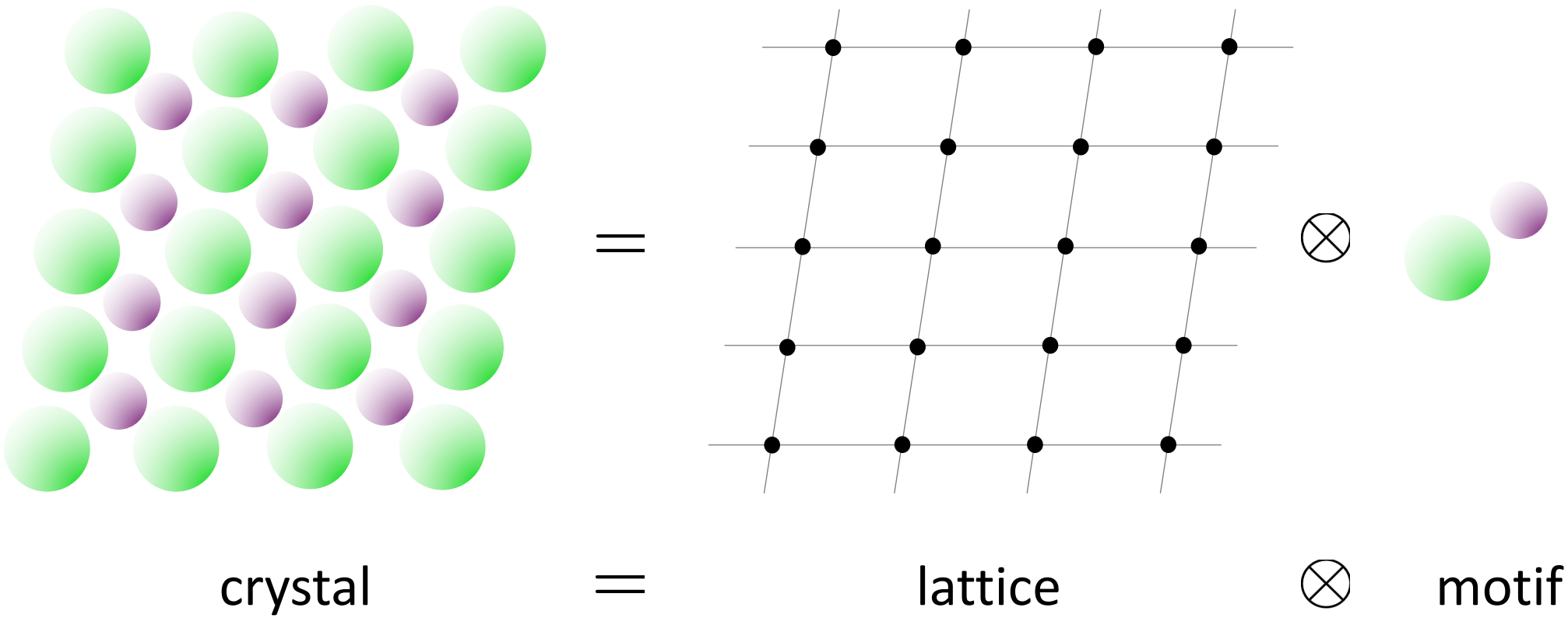
primitive-cell content

one atom or a set of atoms attached to each lattice point



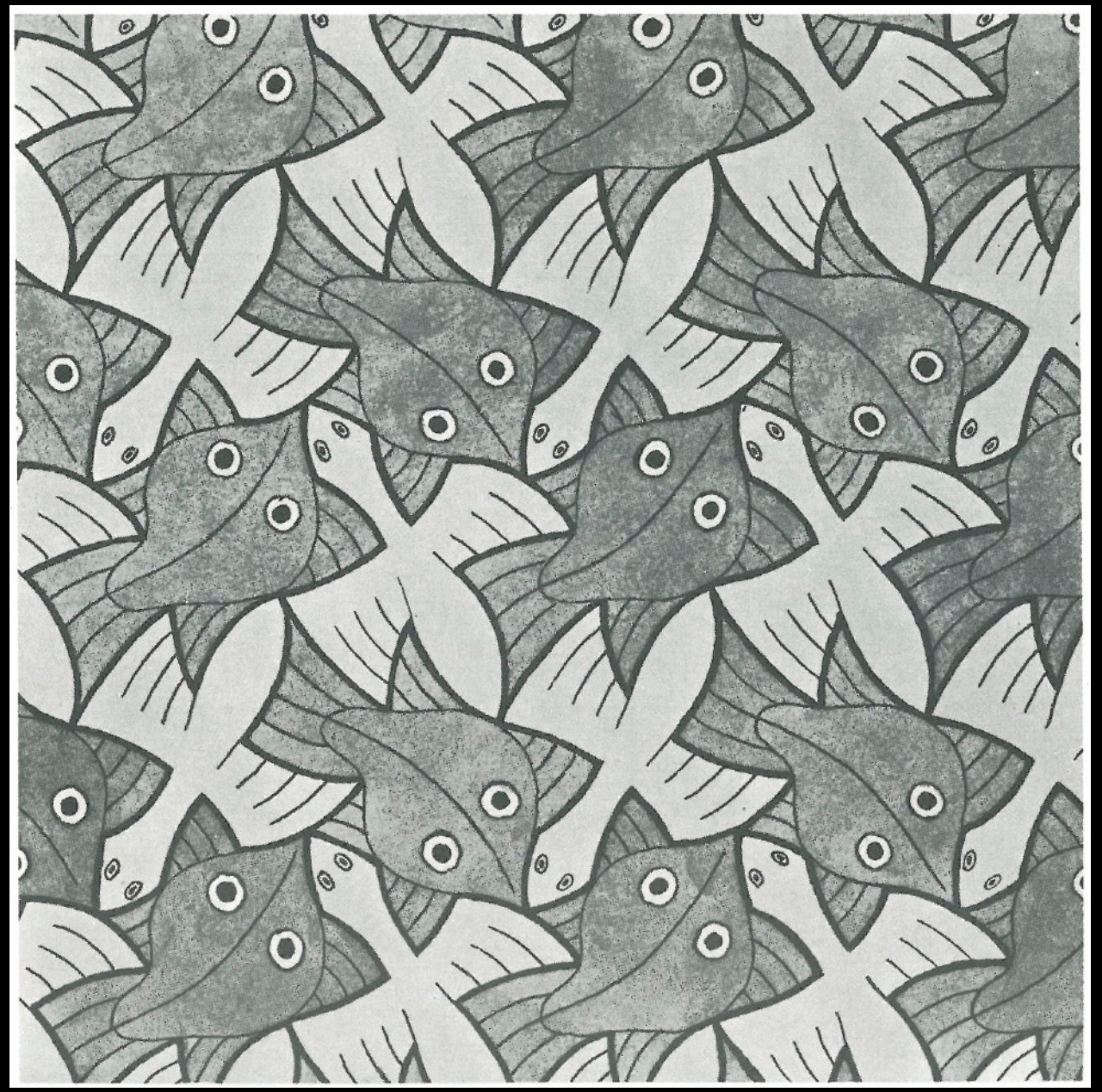
3 – Crystal lattice, cell, motif

crystal



crystal = lattice ⊗ motif

Exercize



Determine the motif

reproduction of periodic drawing n°110
by Escher
(ink and watercolor, 1961)

Course outline

1- Symmetry observation in natural crystals

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7 – Conventional cell (unit cell)

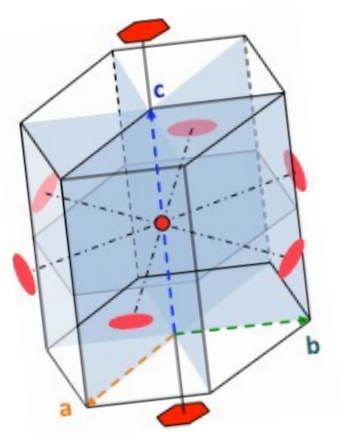
8 – The 32 crystallographic point groups

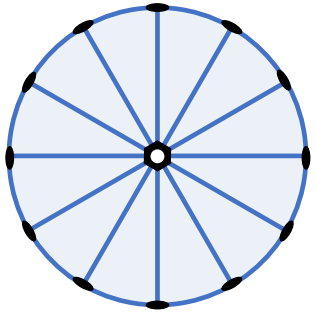
9 – The 7 crystal systems

10 – The 14 Bravais lattices

11 – The 230 space-groups



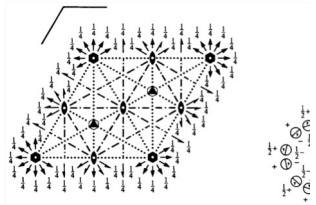




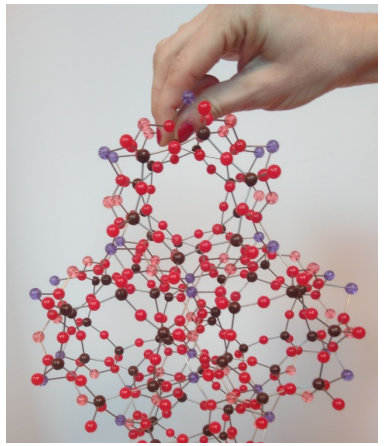
$\frac{6}{m}mm$

$P6/mcc$ D^2_{6h}

No. 192 $P\ 6/m\ 2/c\ 2/c$



Origin at centre $(6/m)$ at $6/mcc$



lattice direction

A line passing through two lattice points corresponds to a lattice direction

→ It contains an infinity of lattice points

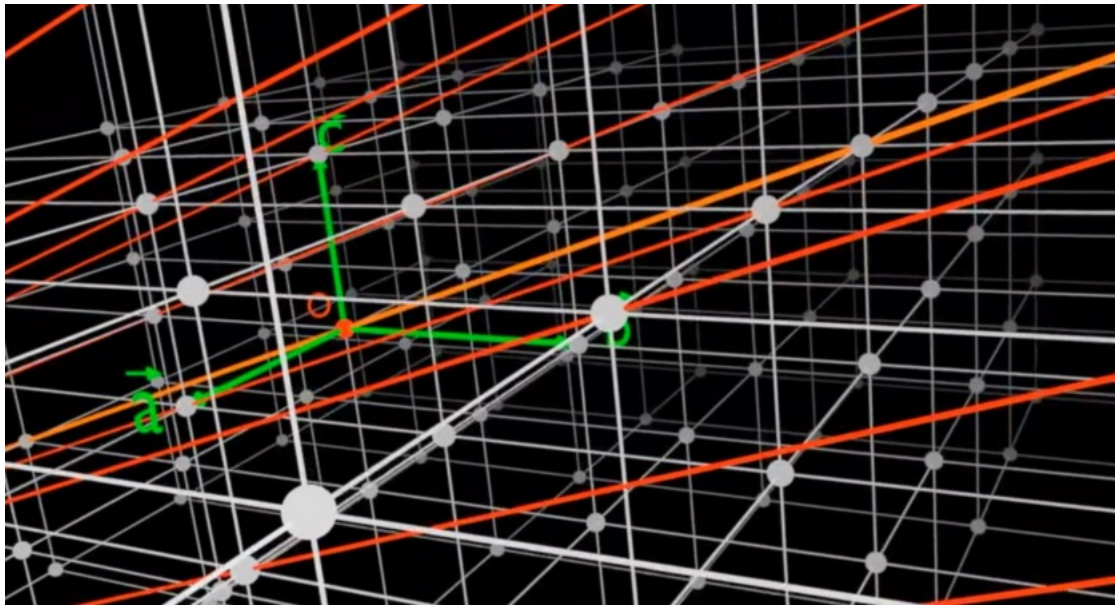
Indexing directions:

Any line is parallel to a particular line passing
through the **origin lattice point** and
through **another lattice point** of coordinates (u, v, w).

→ lattice direction [uvw]

4 – Lattice direction and planes

lattice direction

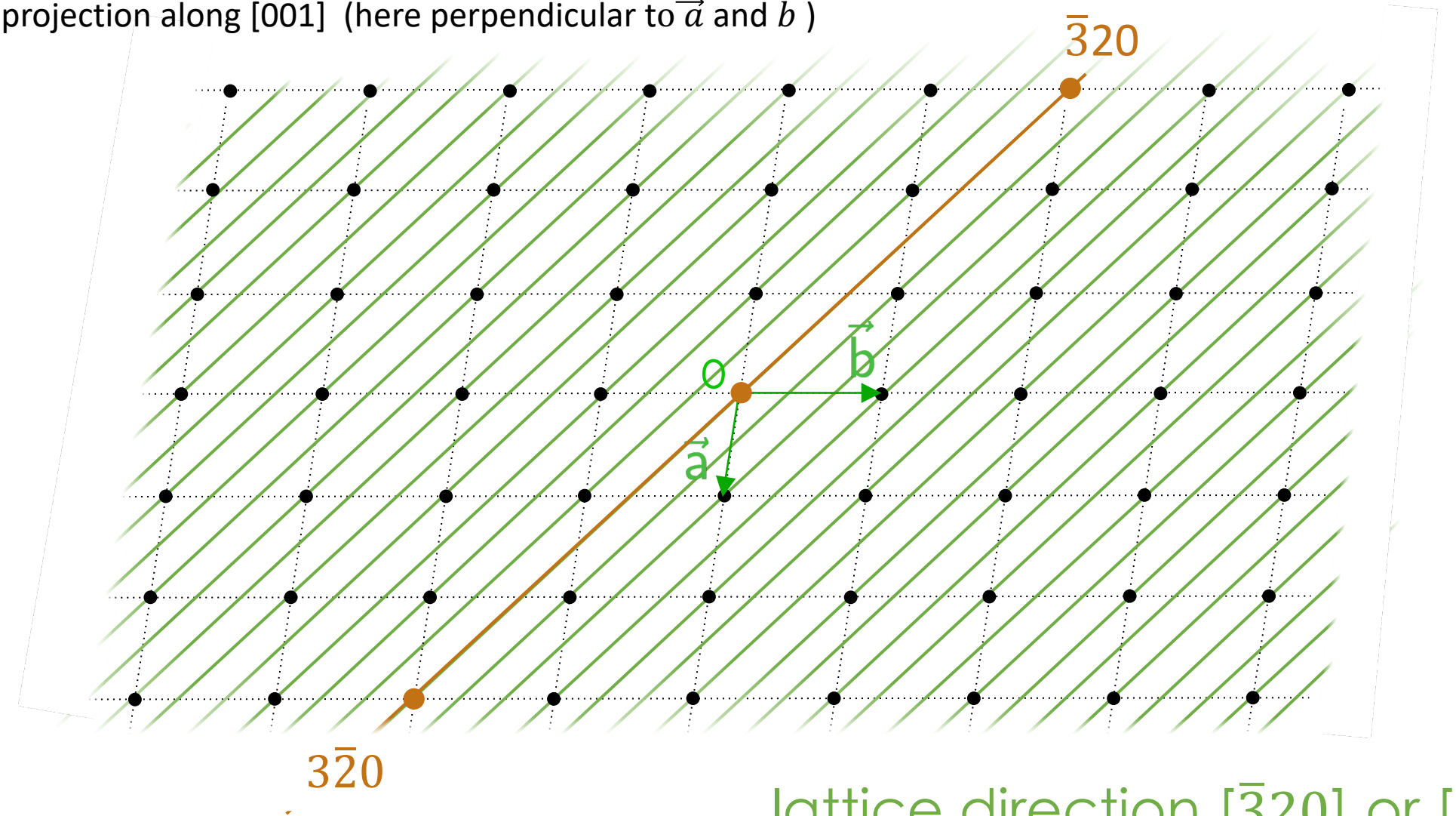


lattice direction [021]

4 – Lattice direction and planes

lattice direction

in projection along [001] (here perpendicular to $\vec{a}$ and $\vec{b}$)

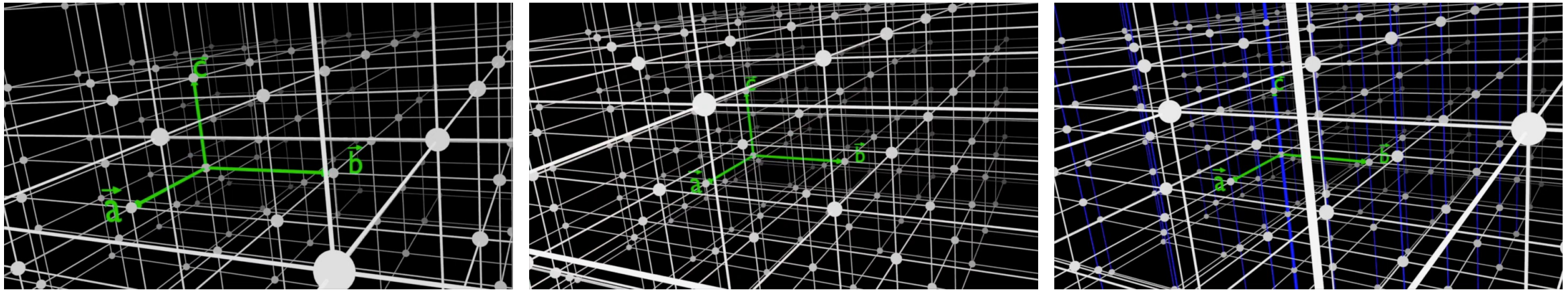


lattice direction $[\bar{3}20]$ or $[3\bar{2}0]$

4 – Lattice direction and planes

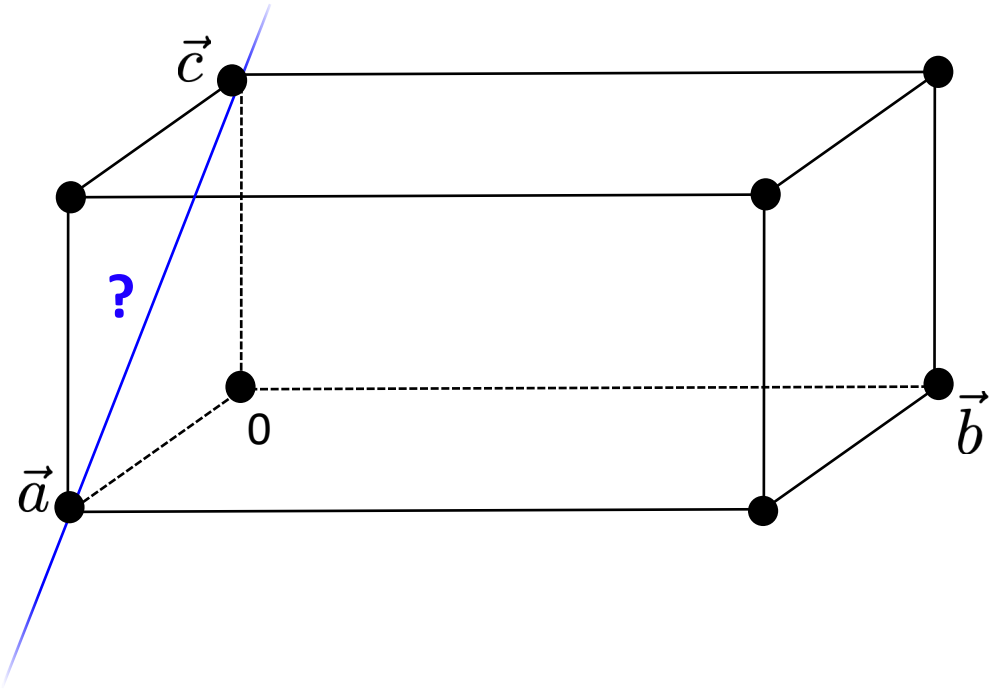
lattice direction

[100] [010] [001]



Exercize

Give the [uvw] indices of the lattice direction corresponding to the line passing through lattice points 100 and 001 .

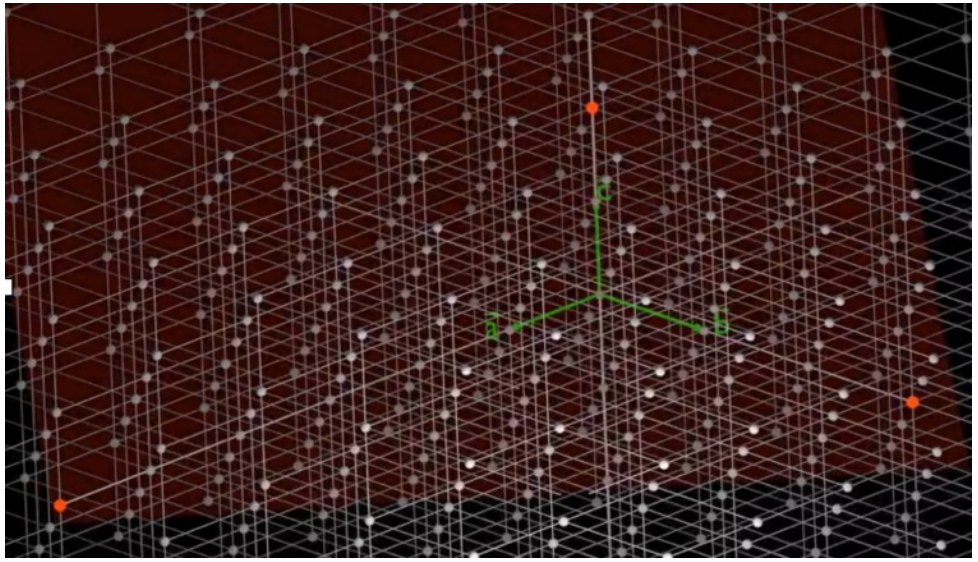


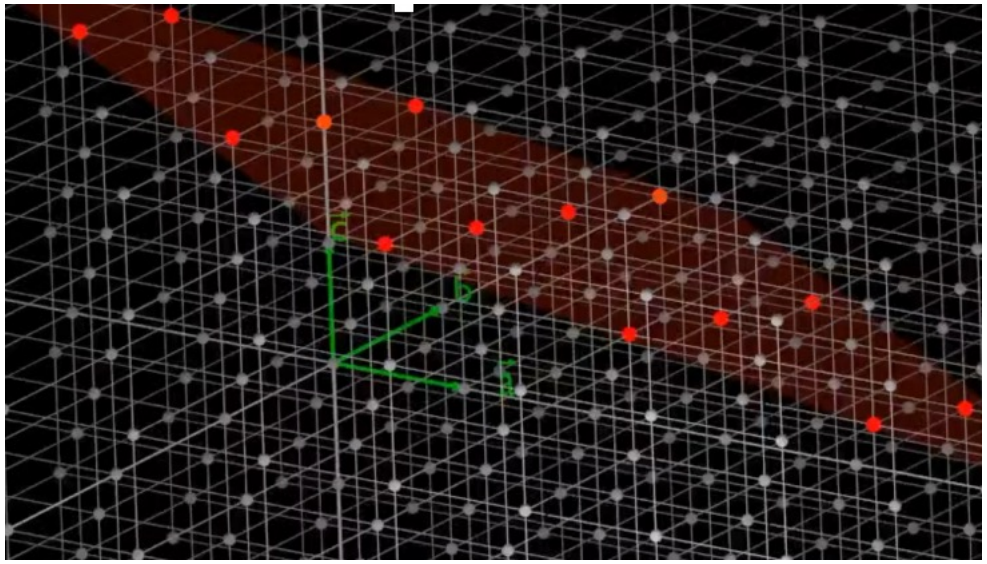
4 – Lattice direction and planes

lattice planes

Lattice plane: any plane passing through 3 non colinear lattice points

→ A lattice plane contains an infinity of lattice points and forms a 2D lattice.

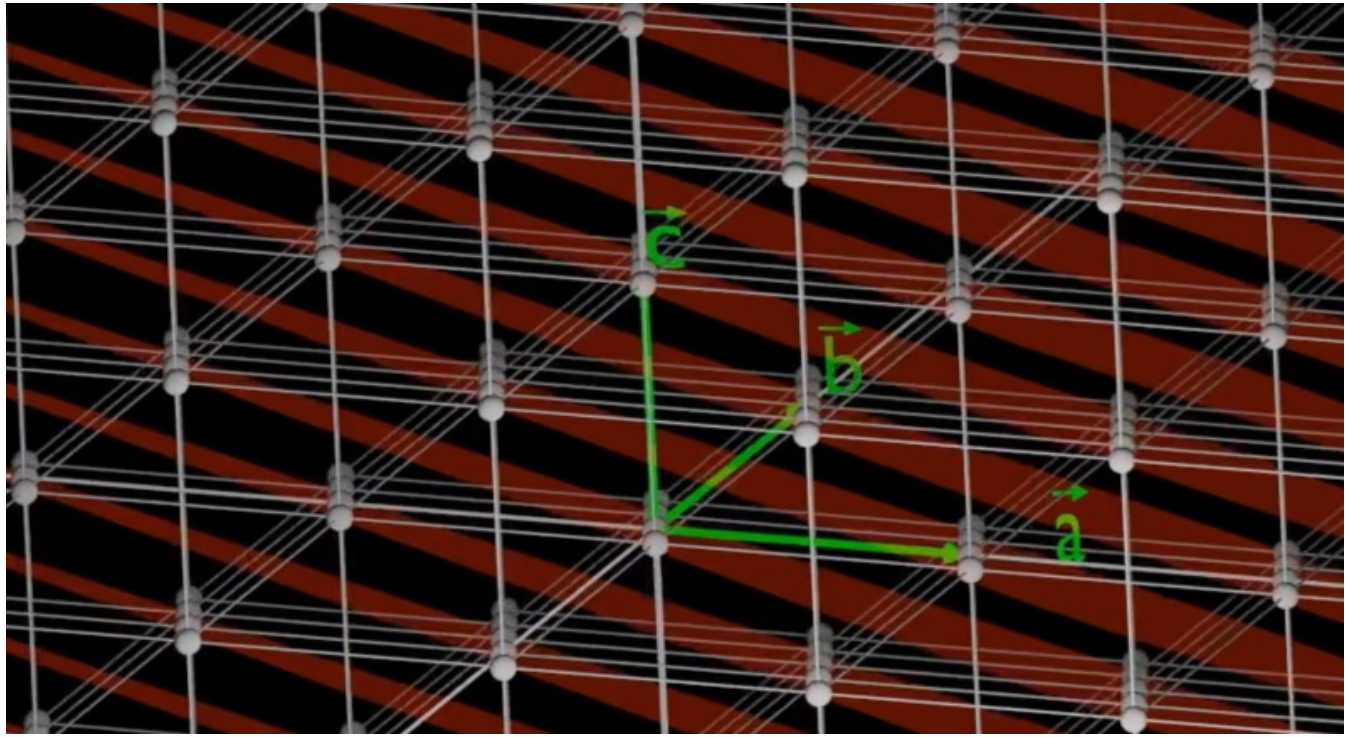




lattice planes

Lattice-plane family: infinity of equidistant and parallel lattice planes.

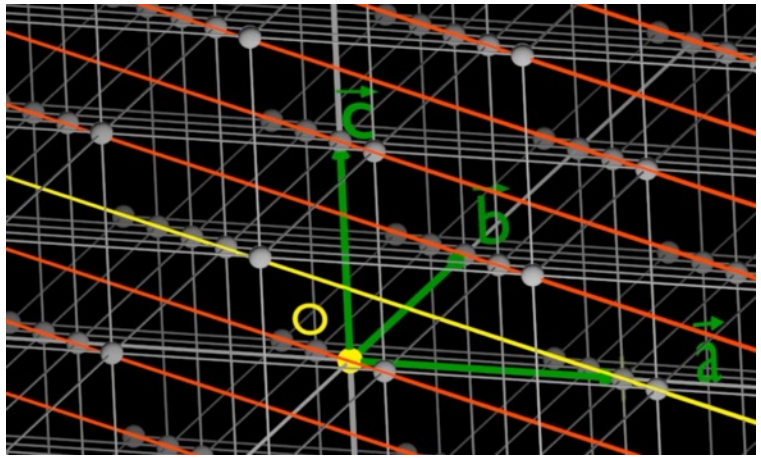
→ A lattice-plane family contains all the lattice points of the 3D lattice.

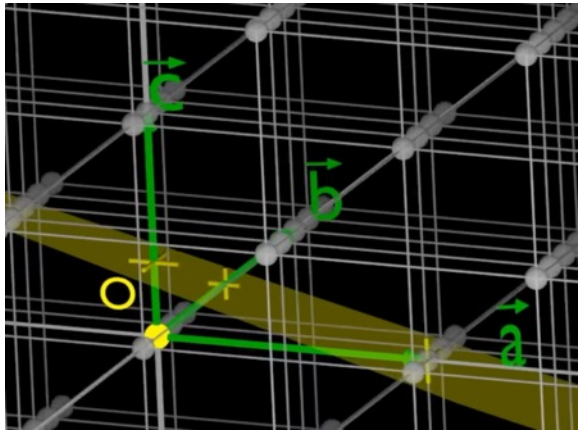


lattice planes

A **lattice-plane family** is labeled (hkl)

h, k and l are Miller indices, which are **relative prime integer numbers**.





axis [100] cut in a/1
axis [010] cut in b/2
axis [001] cut in c/3

➔ lattice-plane family (123)

lattice planes

A **lattice-plane family** is labeled (hkl)

(hkl) refers to as the lattice-plane family

such as the plane of the family that is

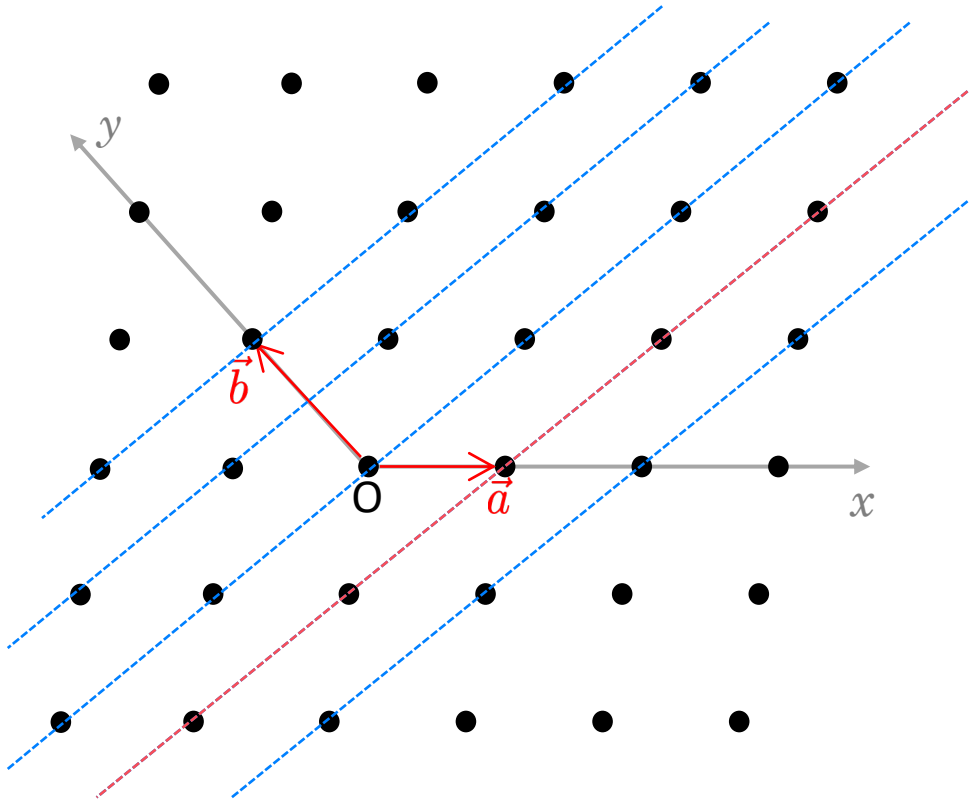
the closest to the lattice-origin point,

cuts (O*x*) axis in a/h,

(O*y*) axis in b/k and

(O*z*) axis in c/l.

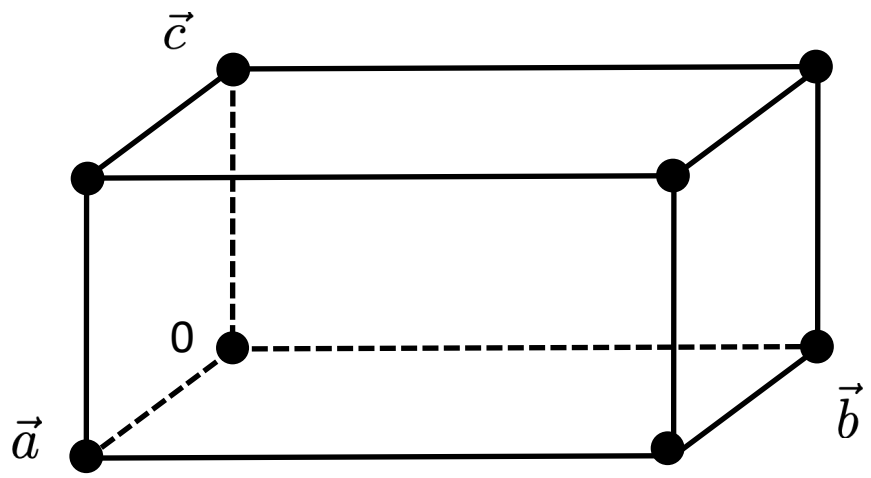
here $h = 1$, $k = -2$ and $l = 0$
→ lattice-plane family $(1\bar{2}0)$



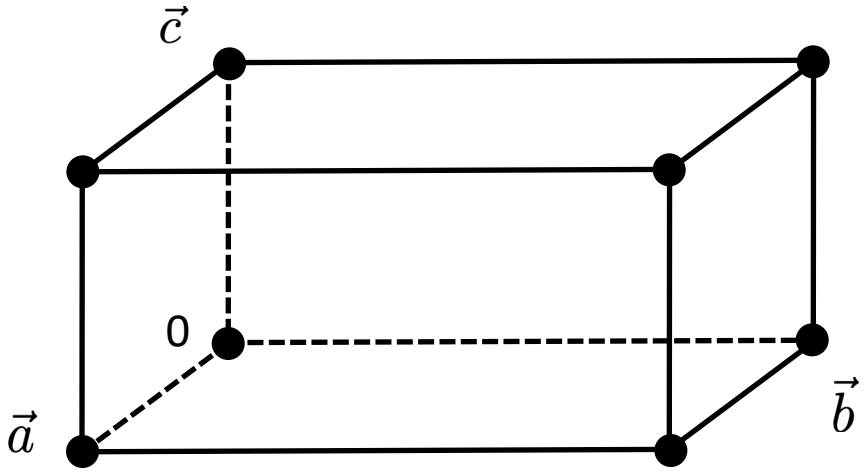
projection in plane (0, ***a***, ***b***)

Exercize

1. Trace a plane of the (001) family



2. Trace a plane of the (221) family



lattice planes

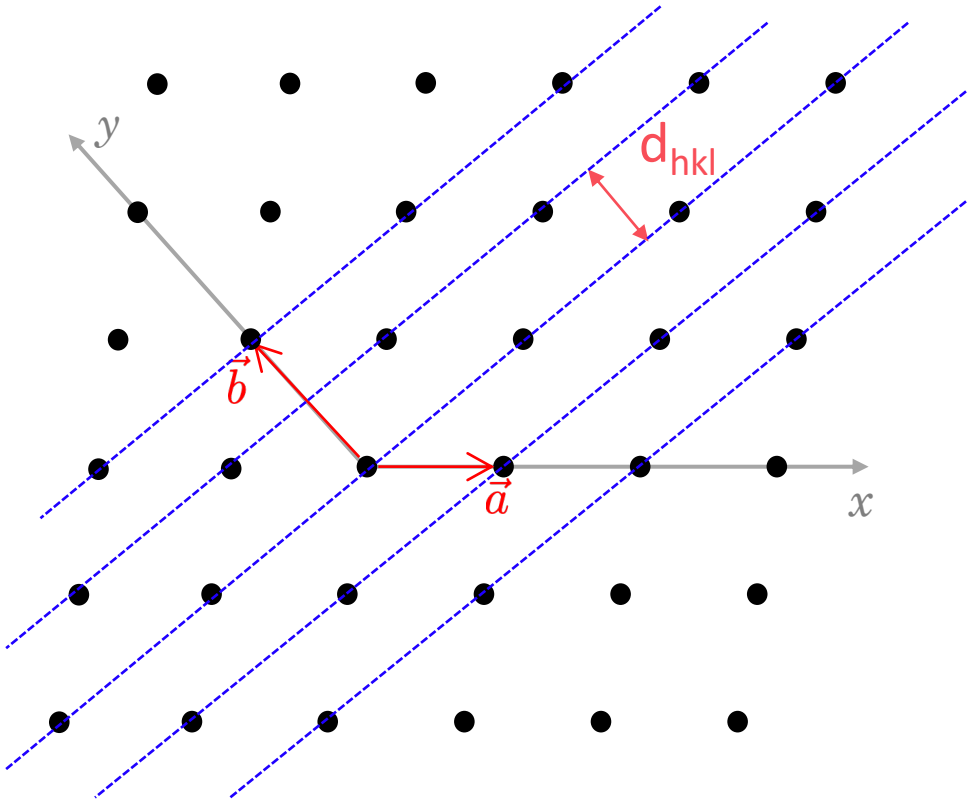
d-spacing:

distance between

two consecutive planes belonging to

the same (hkl) family,

noted d_{hkl}.



projection in plane (001)

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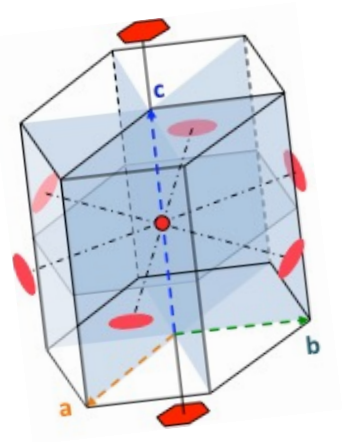
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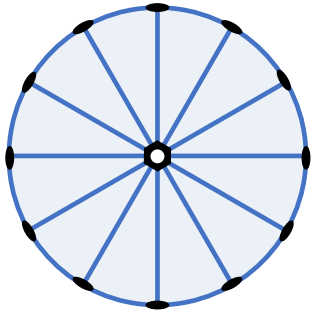
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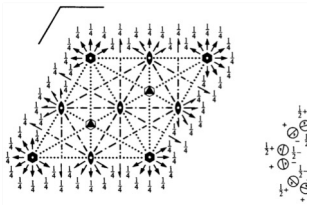




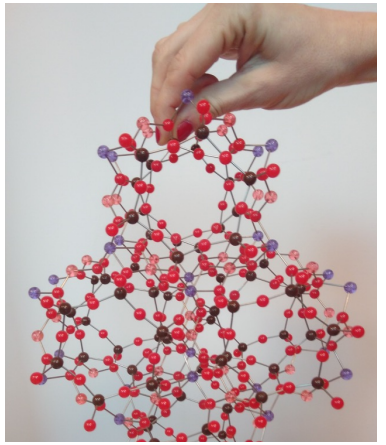
$\frac{6}{m}mm$

$P6/mcc$ D_{6h}^2

No. 192 $P\ 6/m\ 2/c\ 2/c$



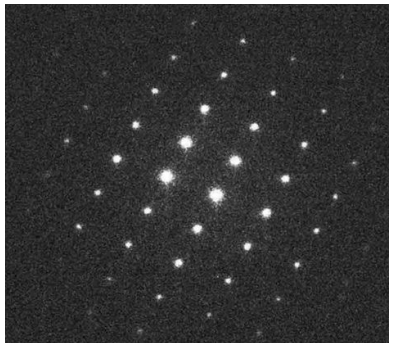
Origin at centre $(6/m)$ at $6/mcc$



5 – Reciprocal lattice

- makes easier some crystallographic calculations
- naturally derived from the diffraction theory

for any radiation (X, neutrons, electrons)



Nature Materials 10, 890–896 (2011)

Définition

Given a direct lattice with basis vectors $\vec{a}, \vec{b}$ and $\vec{c}$.
The corresponding reciprocal lattice is defined by $\vec{a}^\star$, $\vec{b}^\star$ and $\vec{c}^\star$ such that:

$$\begin{array}{lll} \vec{a}\cdot\vec{a}^\star = \sigma & \vec{a}\cdot\vec{b}^\star = 0 & \vec{a}\cdot\vec{c}^\star = 0 \\ \vec{b}\cdot\vec{a}^\star = 0 & \vec{b}\cdot\vec{b}^\star = \sigma & \vec{b}\cdot\vec{c}^\star = 0 \\ \vec{c}\cdot\vec{a}^\star = 0 & \vec{c}\cdot\vec{b}^\star = 0 & \vec{c}\cdot\vec{c}^\star = \sigma \end{array}$$

In crystallography: $\boxed{\sigma = 1}$

In solid-state physics: $\sigma = 2\pi$

5 – Reciprocal lattice

$$\vec{b} \cdot \vec{a}^{\star} = 0 \quad \Longrightarrow \vec{a}^{\star} \perp \vec{b}$$

$$\vec{c} \cdot \vec{a}^{\star} = 0 \quad \Longrightarrow \vec{a}^{\star} \perp \vec{c}$$

so $\vec{a}^{\star} = \alpha' \, \vec{b} \times \vec{c}$ where α' is a constant

then $\vec{a} \cdot \vec{a}^{\star} = \alpha' \, \underbrace{\vec{a} \cdot \left(\vec{b} \times \vec{c} \right)}_{V}$

we know that $\vec{a} \cdot \vec{a}^{\star} = 1$

hence $\alpha' = \dfrac{1}{V}$

Hence $\boxed{\vec{a}^{\star} = \dfrac{\vec{b} \times \vec{c}}{V}}$

And in the same way:

$\boxed{\vec{b}^{\star} = \dfrac{\vec{c} \times \vec{a}}{V}}$ $\boxed{\vec{c}^{\star} = \dfrac{\vec{a} \times \vec{b}}{V}}$

length unit: $Å^{-1}$ or nm^{-1}

relationship with the direct lattice

- We can show[1]: $V V^{\star} = 1$

[1] *To do so, we express V as a function of a, b and c.*
Then, we use the following formula of the 3-vector product: $\mathbf{A}\times(\mathbf{B}\times\mathbf{C})=(\mathbf{A}.\mathbf{C})\mathbf{B}-(\mathbf{A}.\mathbf{B})\mathbf{C}$

- We can show:

Any plane of the direct lattice belonging to the family (hkl) corresponds to a direction of the reciprocal lattice of the same indices, [hkl]*, which is perpendicular to (hkl).

$$[hkl]^{\star} \perp (hkl)$$

relationship with the direct lattice

$[hkl]^\star \perp (hkl)$

examples

Reciprocal space			Direct space	
$\vec{a}^\star$	// [100]*	$\perp$	$(\vec{b}, \vec{c})$	= (100)
$\vec{b}^\star$	// [010]*	$\perp$	$(\vec{c}, \vec{a})$	= (010)
$\vec{c}^\star$	// [001]*	$\perp$	$(\vec{a}, \vec{b})$	= (001)

relationship with the direct lattice

- d-spacing calculation:

$$d_{hkl} \quad \| \vec{t}^{\star}_{hkl} \| = 1$$

where $\vec{t}^{\star}_{hkl} \parallel [hkl]^{\star}$ and $\vec{t}^{\star}_{hkl} = h\vec{a}^{\star} + k\vec{b}^{\star} + l\vec{c}^{\star}$

In a cubic lattice:

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

In a hexagonal lattice:

$$d_{hkl} = \frac{1}{\sqrt{\frac{4}{3}\left(\frac{h^2+k^2+hk}{a^2}\right) + \frac{l^2}{c^2}}}$$

relationship with the direct lattice

- Condition to have (hkl) **parallel** to [uvw]:

$\vec{t}^{\star}_{hkl} \perp \vec{t}_{uvw}$ ➔ scalar product equal to zero

with $\vec{t}^{\star}_{hkl} = h\vec{a}^{\star} + k\vec{b}^{\star} + l\vec{c}^{\star}$

and $\vec{t}_{uvw} = u\,\vec{a} + v\,\vec{b} + w\,\vec{c}$

thus $\boxed{h\,u + k\,v + l\,w = 0}$

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7 – Conventional cell (unit cell)

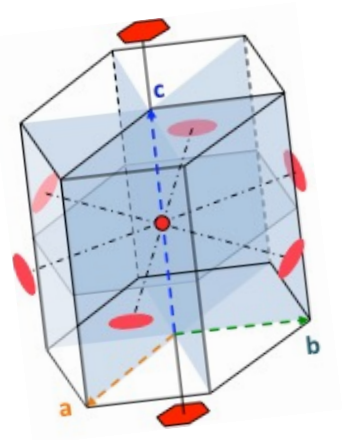
8 – The 32 crystallographic point groups

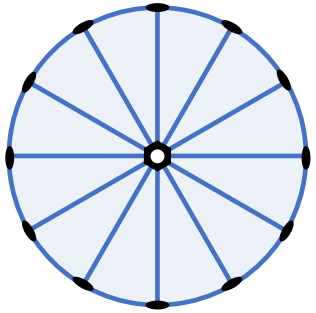
9 – The 7 crystal systems

10 – The 14 Bravais lattices

11 – The 230 space-groups



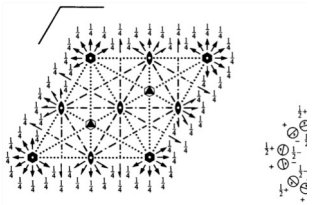




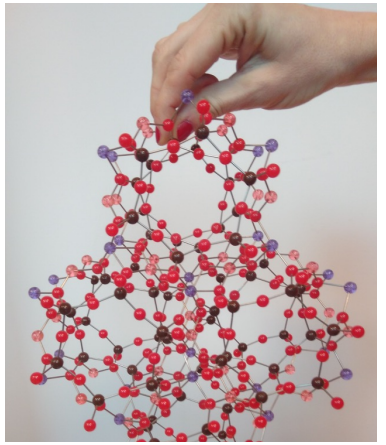
$\frac{6}{m}mm$

$P6/mcc$ D^2_{6h}

No. 192 $P\ 6/m\ 2/c\ 2/c$



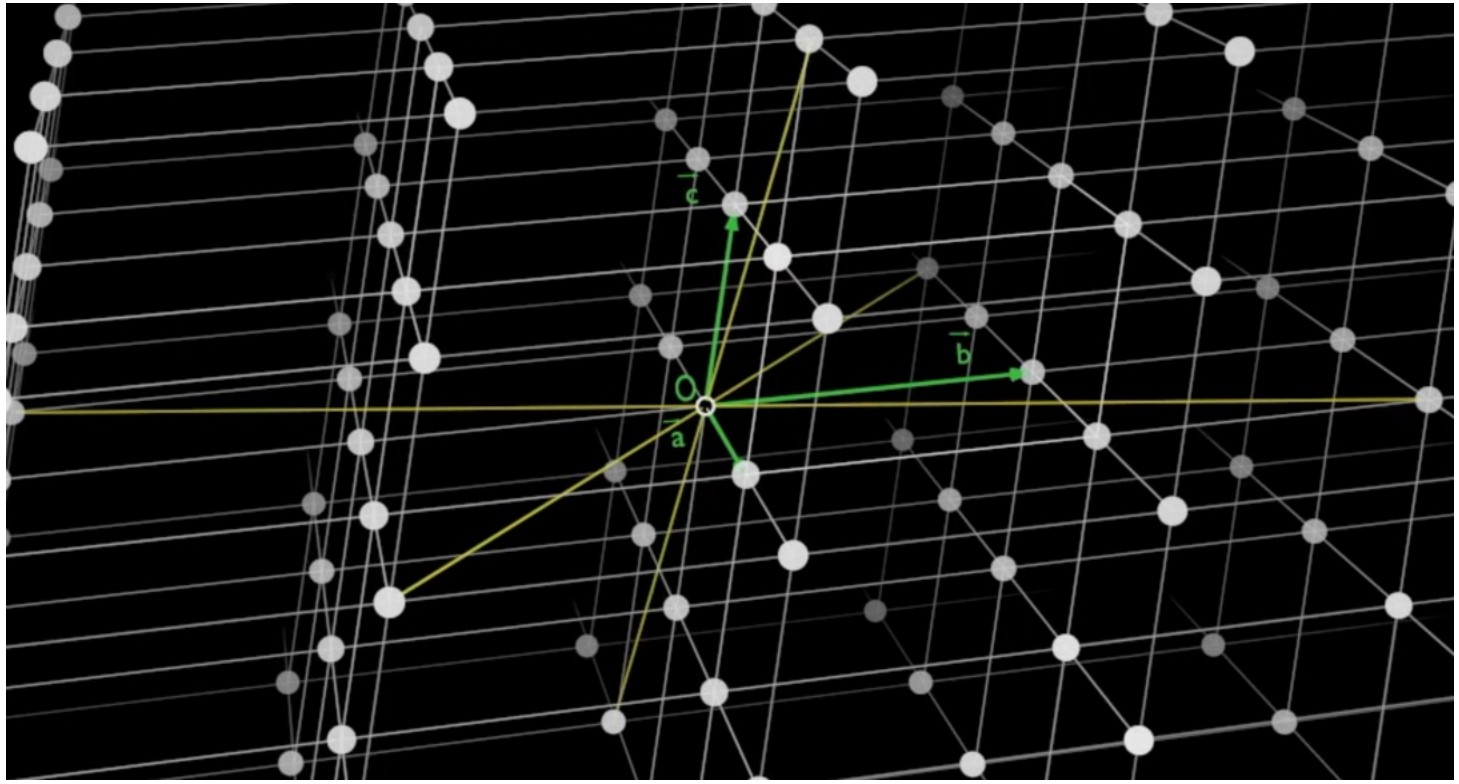
Origin at centre $(6/m)$ at $6/mcc$



centrosymmetry

Any lattice is **centrosymmetric** with centres:

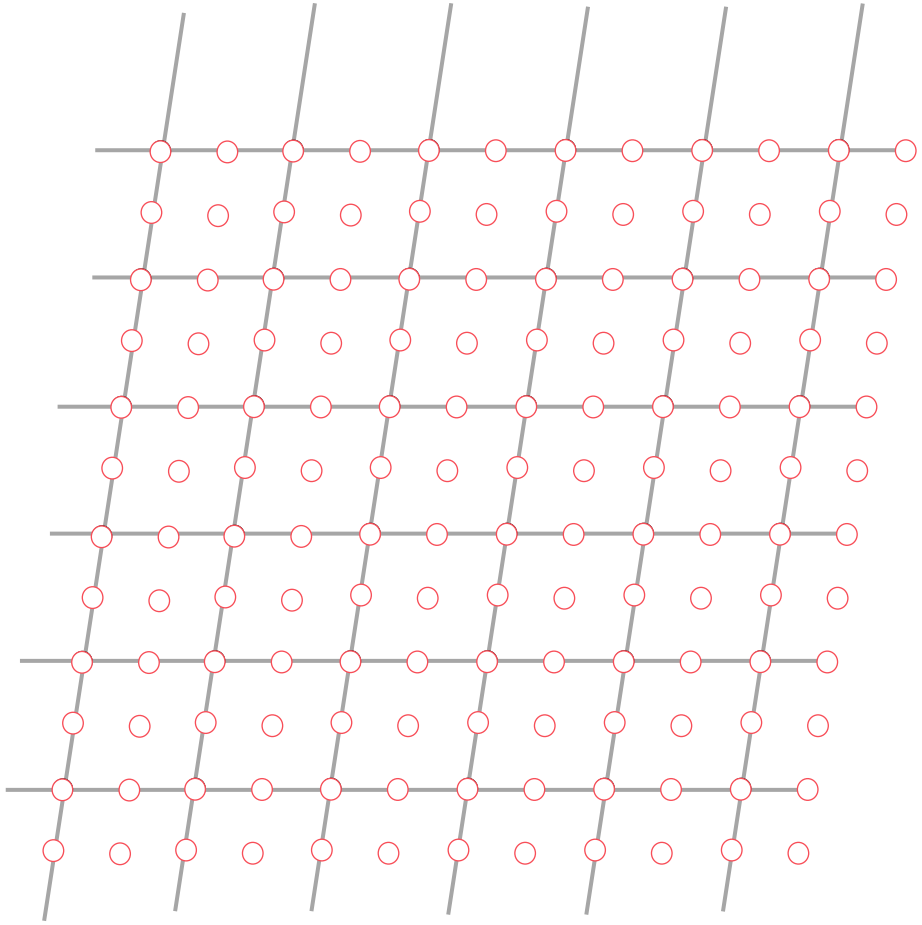
- on each lattice point
- in the middle of each cell edge
- in the middle of each cell face
- in the center of each cell



centrosymmetry

Any lattice is
centrosymmetric
with centres:

- on each lattice point
- in the middle of each cell edge
- in the middle of each cell face
- in the middle of each cell



The rotation axes compatible with the crystal lattice

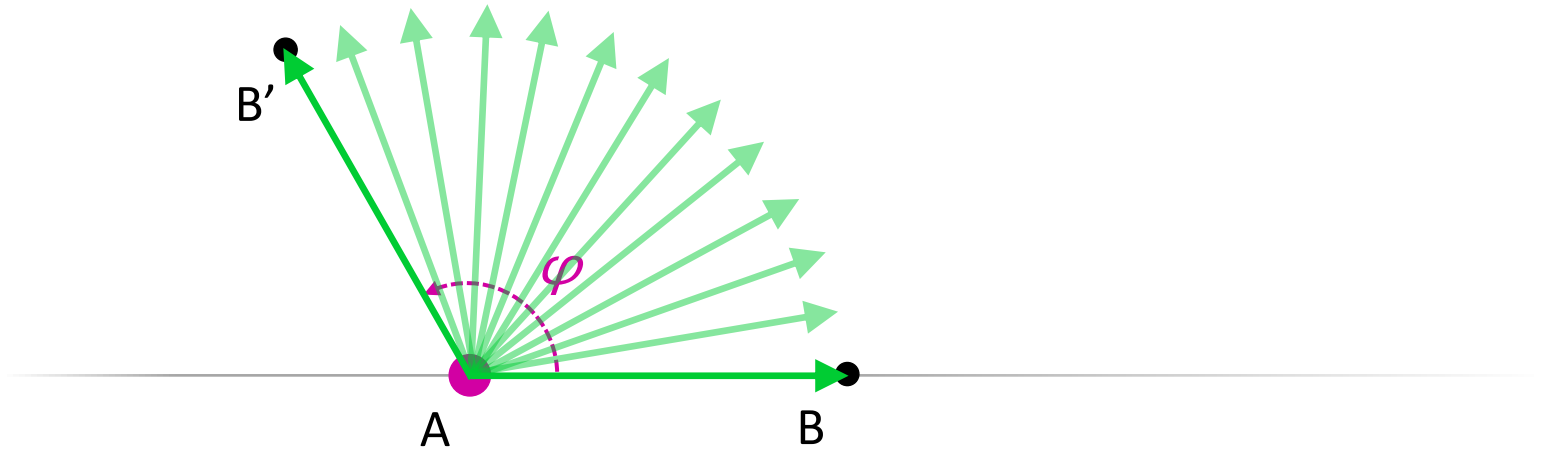
rotation axes $\mathbf{A_n}$ of angle $\varphi = \frac{2\pi}{n}$



Are other values of n possible?

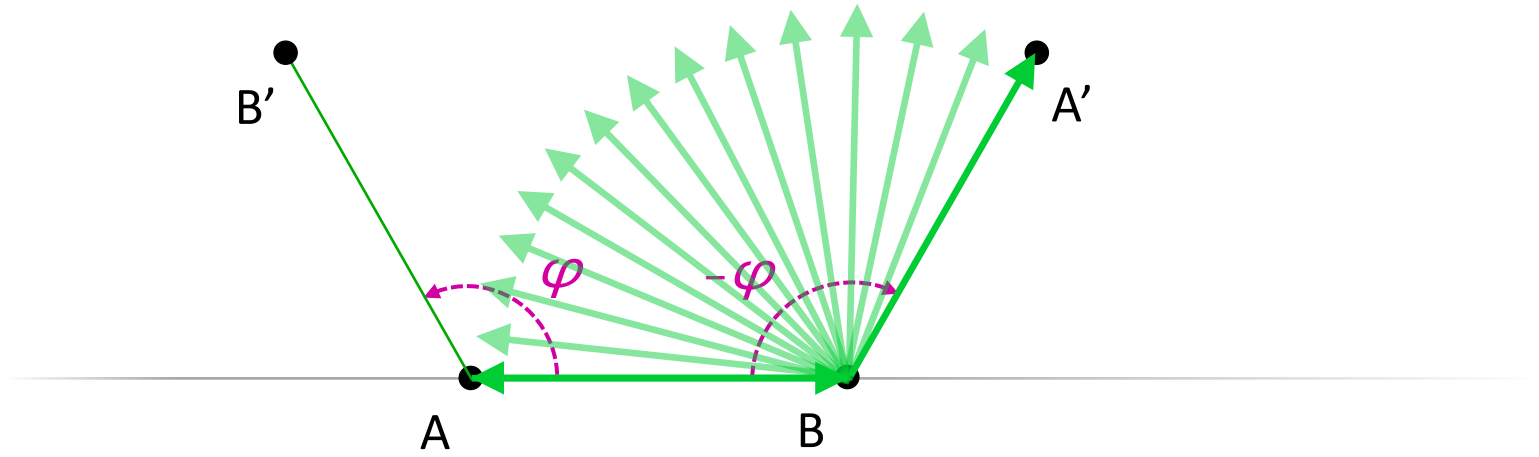
The rotation axes compatible with the crystal lattice

axis A_n of angle φ **in A**



The rotation axes compatible with the crystal lattice

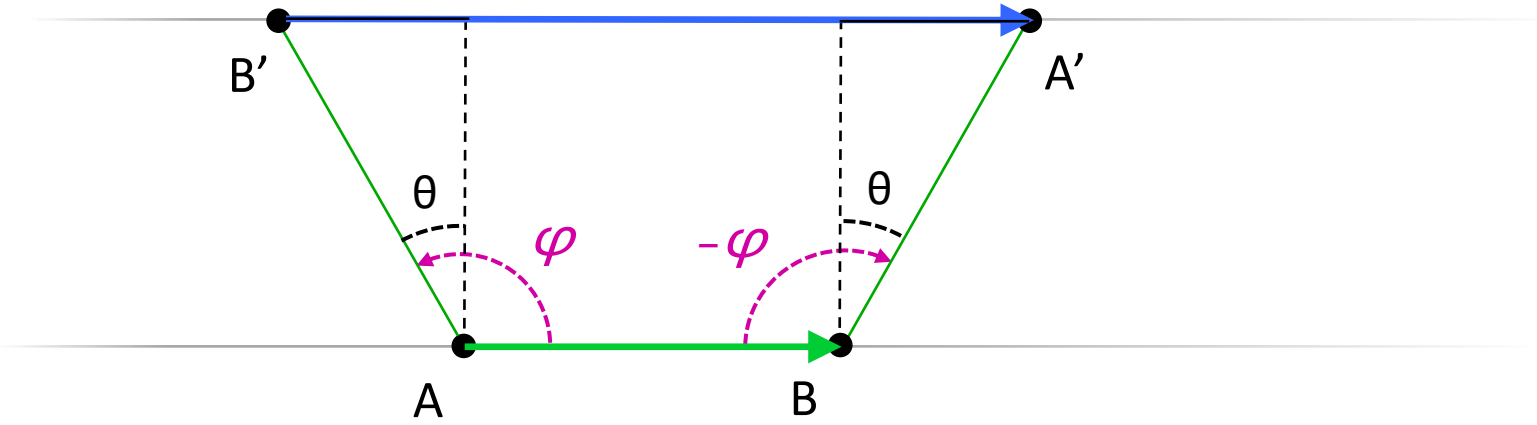
axis A_n of angle φ | in A | in B



The rotation axes compatible with the crystal lattice

What are the possible values of φ?

$$\varphi = \frac{2\pi}{n} \quad ?$$



B'A' = k AB with k an integer

B'A' = AB² + 2 AB' sinθ where θ= φ − π/2

= AB (1 – 2 cos φ)

The rotation axes compatible with the crystal lattice

What are the possible values of φ?

$$\varphi = \frac{2\pi}{n} \quad ?$$

$B'A' = k\,AB$ $\qquad$ $B'A' = (1 - 2\cos\varphi)\,AB$

identification

$$\cos\varphi = \frac{1 - k}{2}$$

with $-1 \leq \cos\varphi \leq +1$

The rotation axes compatible with the crystal lattice

k	0	1	2	3	4	-1
$\cos\varphi = \frac{1-k}{2}$	$\frac{1}{2}$	0	$-\frac{1}{2}$	-1	impossible!	1
$\varphi = \frac{2\pi}{n}$	$\frac{\pi}{3}$	$\frac{\pi}{2}$	$\frac{2\pi}{3}$	π		0
n	6	4	3	2		1
						identity

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6 – Crystal lattice & symmetries

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8 – Stereographic projection

9 – Roto-inversions

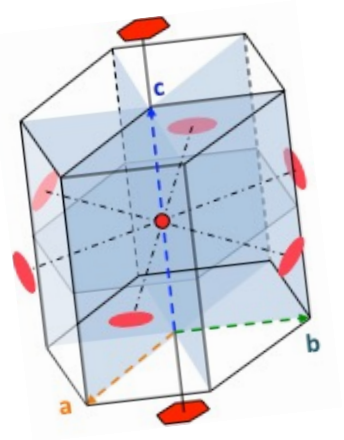
10 – The 32 crystallographic point groups

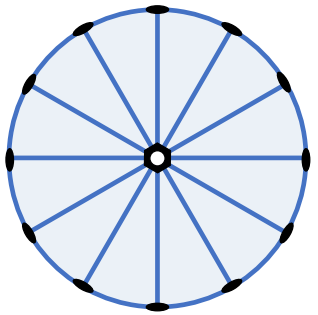
11 – The 7 crystal systems

12 – The 14 Bravais lattices

13 – The 230 space-groups



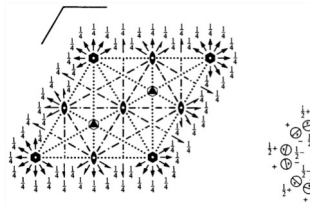




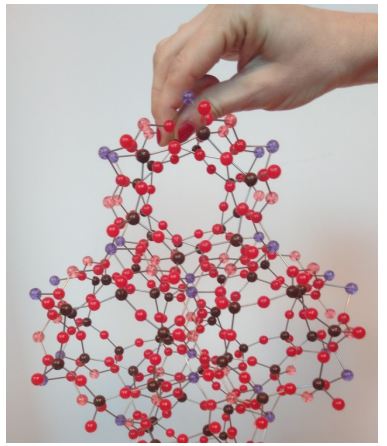
$$\frac{6}{m}mm$$

$P6/mcc$ D^2_{6h}

No. 192 $P\ 6/m\ 2/c\ 2/c$



Origin at centre $(6/m)$ at $6/mcc$



7 – Conventional cell (=unit cell)

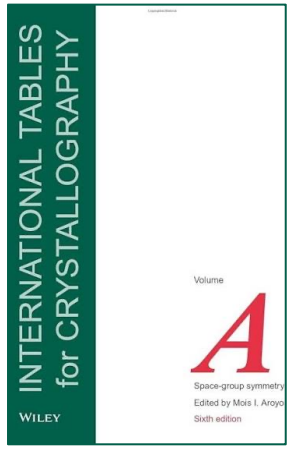
primitive cell and supercells

Conventional centring types of one-, two- and three-dimensional cells

2D cells

3D cells

Printed symbol	Centring type of cell	Number of lattice points per cell	Coordinates of lattice points within cell
Two dimensions			
p	Primitive	1	0, 0
c	Centred	2	0, 0; $\frac{1}{2}$, $\frac{1}{2}$
Three dimensions			
P	Primitive	1	0, 0, 0
C	*C*-face centred	2	0, 0, 0; $\frac{1}{2}$, $\frac{1}{2}$, 0
A	*A*-face centred	2	0, 0, 0; 0, $\frac{1}{2}$, $\frac{1}{2}$
B	*B*-face centred	2	0, 0, 0; $\frac{1}{2}$, 0, $\frac{1}{2}$
I	Body centred	2	0, 0, 0; $\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$
F	All-face centred	4	0, 0, 0; $\frac{1}{2}$, $\frac{1}{2}$, 0; 0, $\frac{1}{2}$, $\frac{1}{2}$; $\frac{1}{2}$, 0, $\frac{1}{2}$

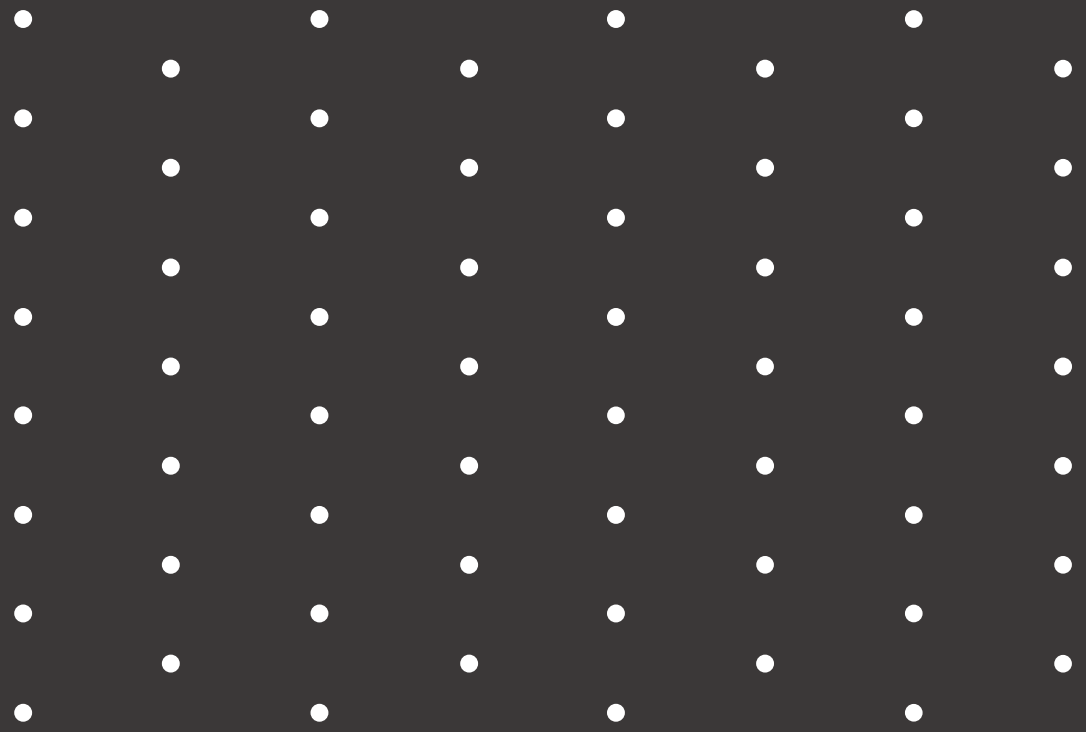


The unit cell can be a larger cell than the primitive cell…

7 – Conventional cell (=unit cell)

Exercize

View 2 primitive cells of different shapes

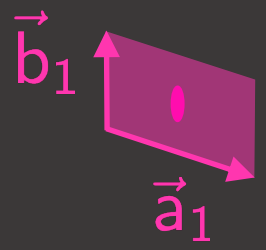


View a **centred cell**

7 – Conventional cell (=unit cell)

cell 1: primitive

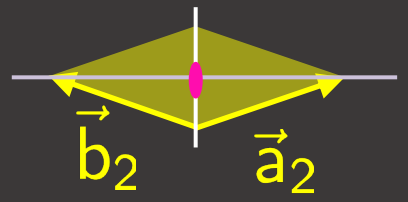
$a_1 \neq b_1$, $\gamma_1 \neq 90°$



A_2

cell 2: primitive

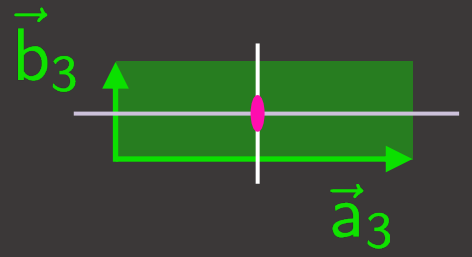
$a_2 = b_2$, $\gamma_2 \neq 90°$



A_2 M M'

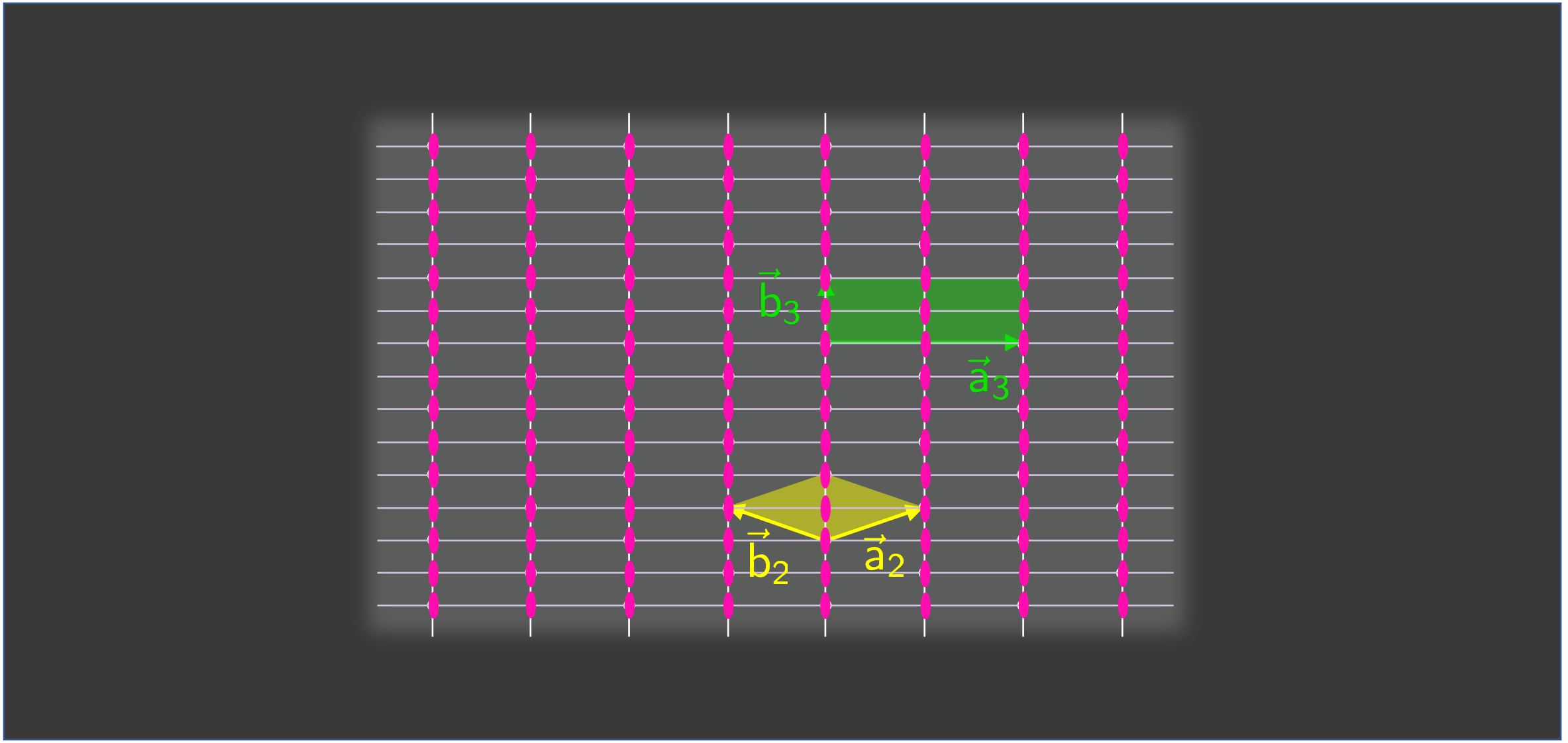
cell 3: double

$a_3 \neq b_3$, $\gamma_3 = 90°$



A_2 M M'

7 – Conventional cell (=unit cell)



7 – Conventional cell (=unit cell)

conventional cell or unit cell

- it has the symmetry as the lattice
- its axes are parallel
  to symmetry directions of the lattice
- it can be a supercell (it is not always primitive)

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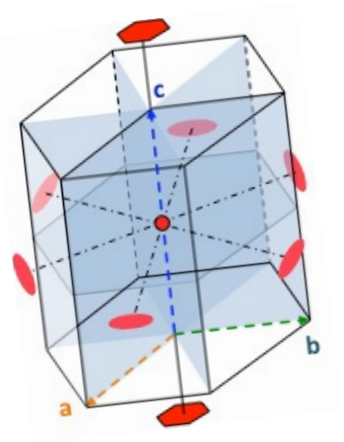
8 – The 32 crystallographic point groups

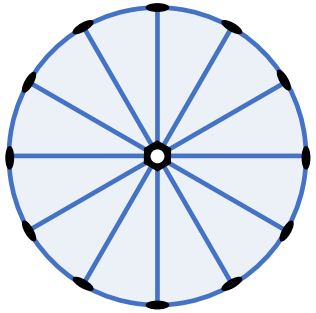
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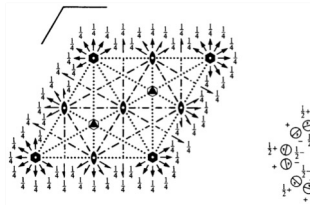




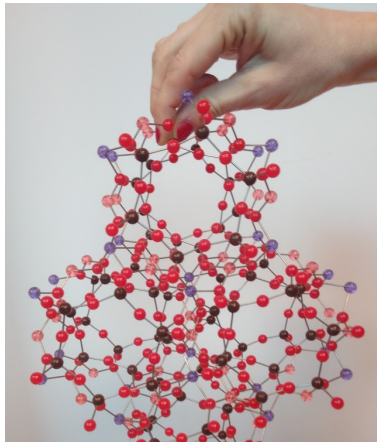
$\frac{6}{m}mm$

$P6/mcc$ D_{6h}^2

No. 192 $P\ 6/m\ 2/c\ 2/c$



Origin at centre $(6/m)$ at $6/mcc$



8 – The 32 crystallographic point groups

The possible ‘’combinations’’ of the 10 rotations and roto-inversions form the **32 crystallographic point groups**, also called the **32 classes of orientation symmetry**.

crystallographic point group: set of symmetry elements that leave a central point fixed

The symmetry of the macroscopic **physical properties** of a crystal is governed by its crystallographic point group.

↳ physical properties sensitive to direction symmetries (invariant under translations)

➔ *it is important to know, for a given point group, the equivalent directions by the symmetry operations that define the group.*

8 – The 32 crystallographic point groups

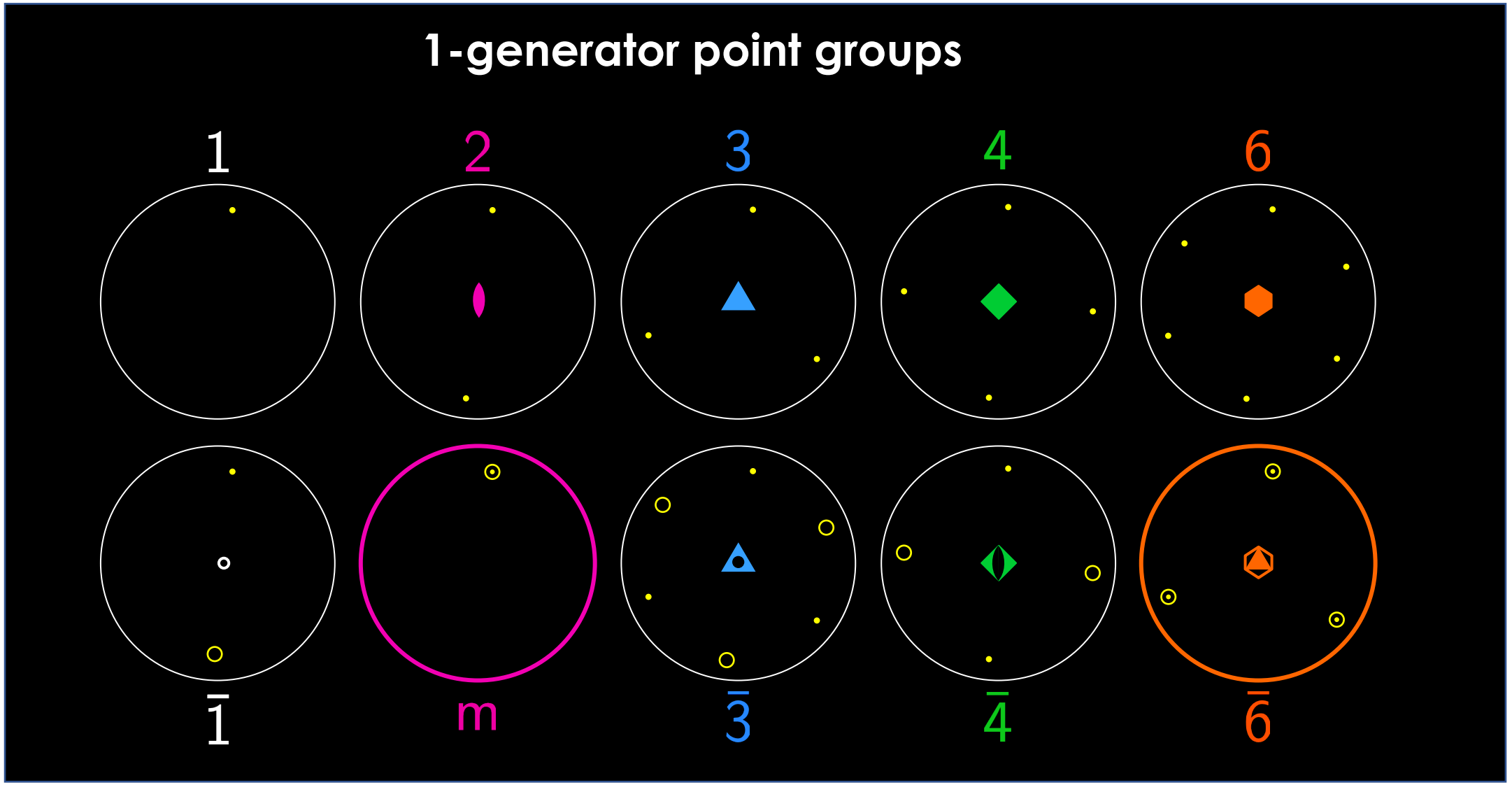
2 CATEGORIES:

- The groups containing MORE than one A_n axis with n>2
  ➔ **the 5 cubic groups**

- The other groups
  ➔ **the 27 non-cubic groups**

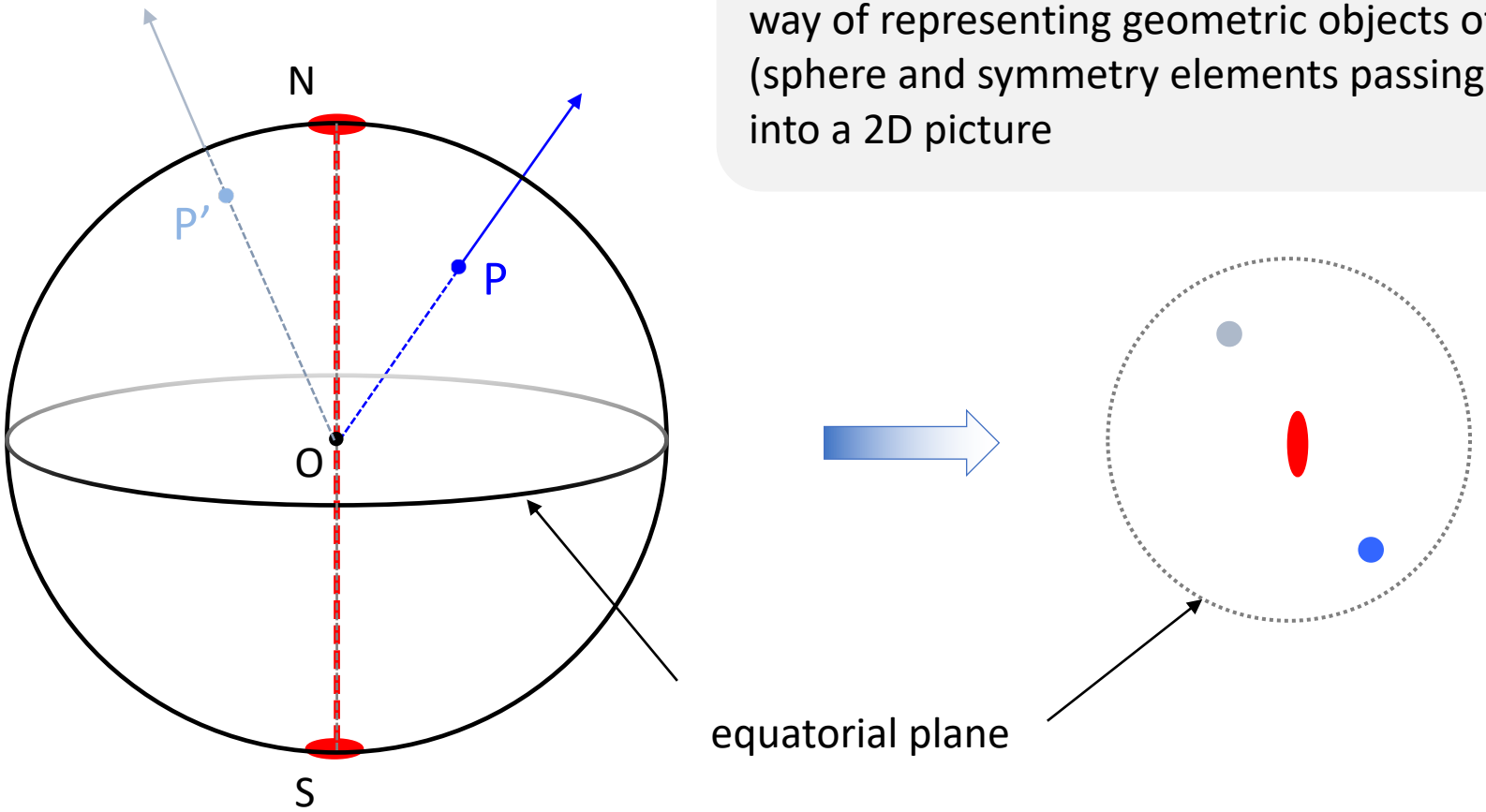
- We already know 10! ➔ 1-generator group
- 2- or 3-generator groups

8 – The 32 crystallographic point groups



stereographic projection

A useful tool: the stereographic projection
way of representing geometric objects of the 3D space (sphere and symmetry elements passing through its centre) into a 2D picture



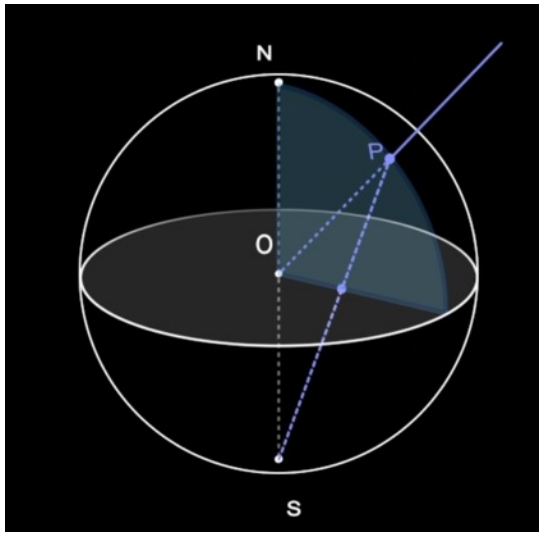
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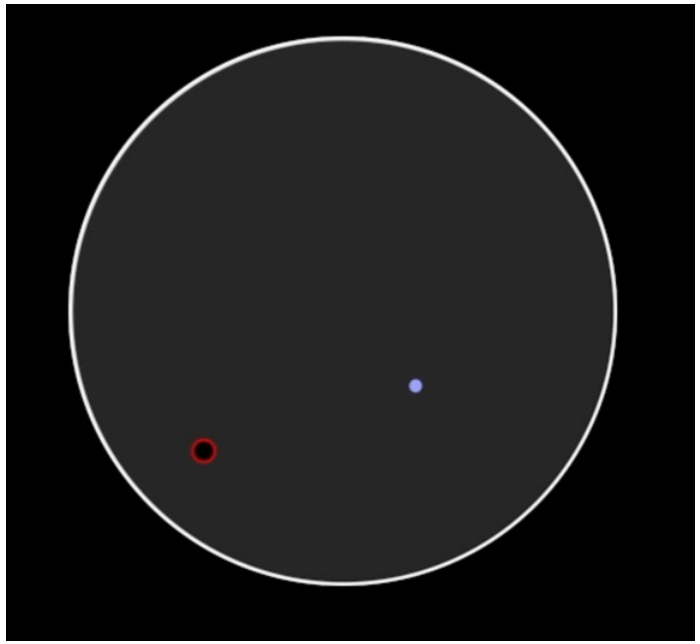
stereographic projection

• Given a half-line OP in the North hemisphere starting from O and crossing the sphere in point P.

• The stereographic projection of OP is the intersection point of [PS] with the equatorial plane.

• It is represented (here) by a dot: ●.

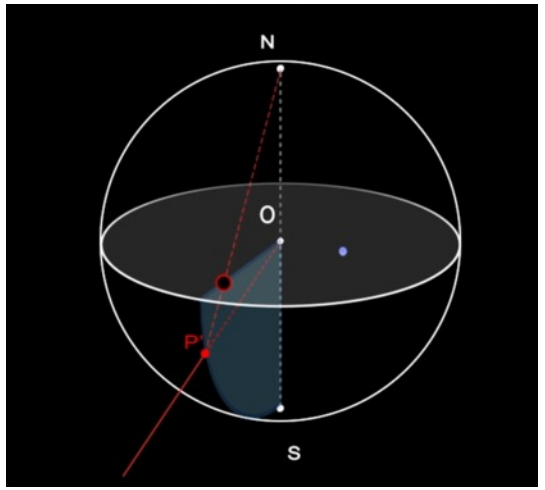




• Given a half-line OP' in the South hemisphere starting from O and crossing the sphere in point P'.

•The stereographic projection of OP' is the intersection point of [P'N] with the equatorial plane.

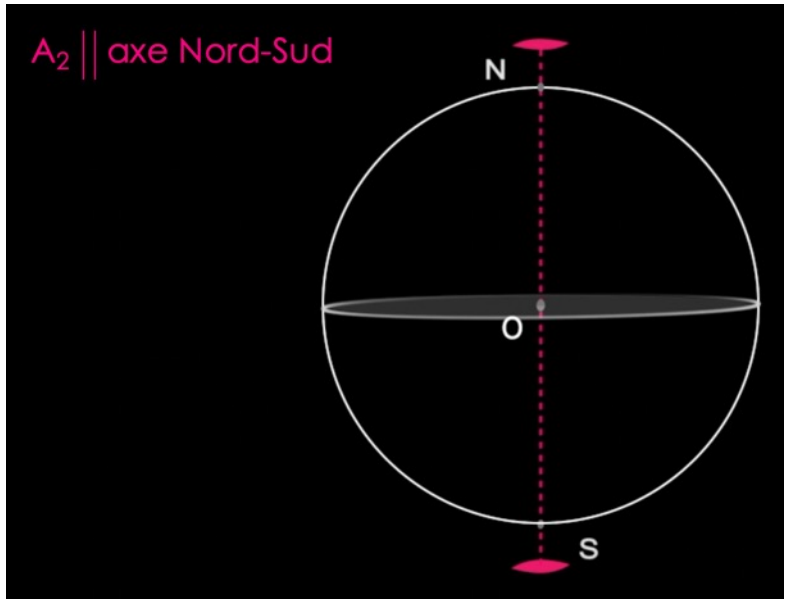
• It is represented by a small circle: ○.

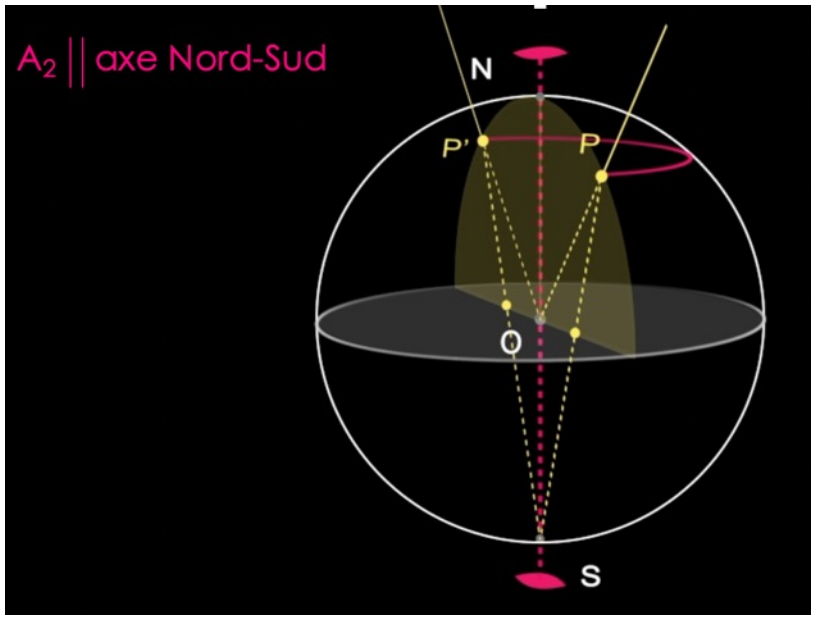


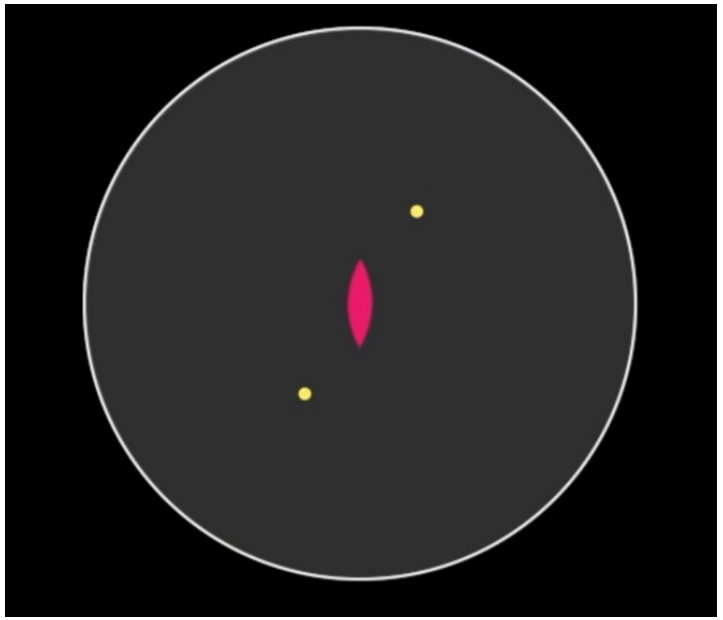
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stereographic projection

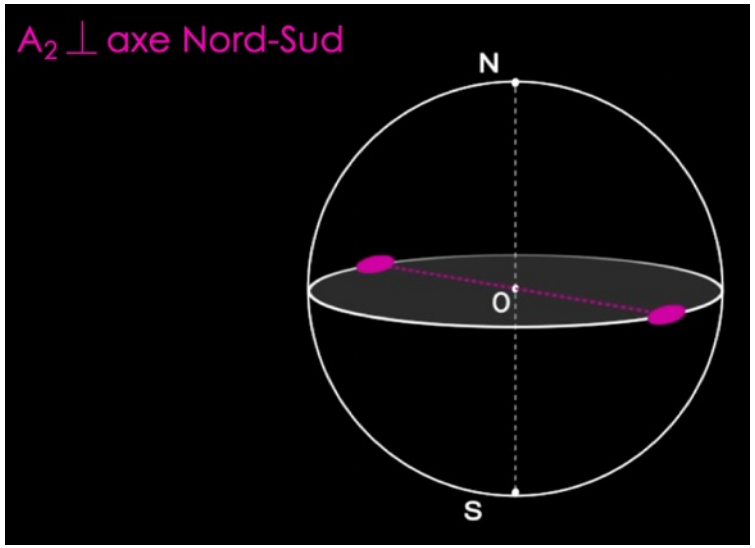
A_2 || North-South axis



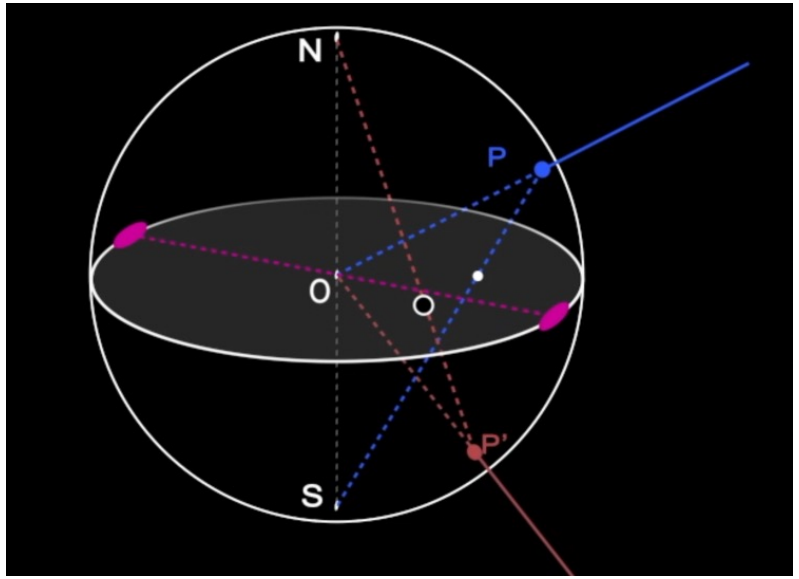


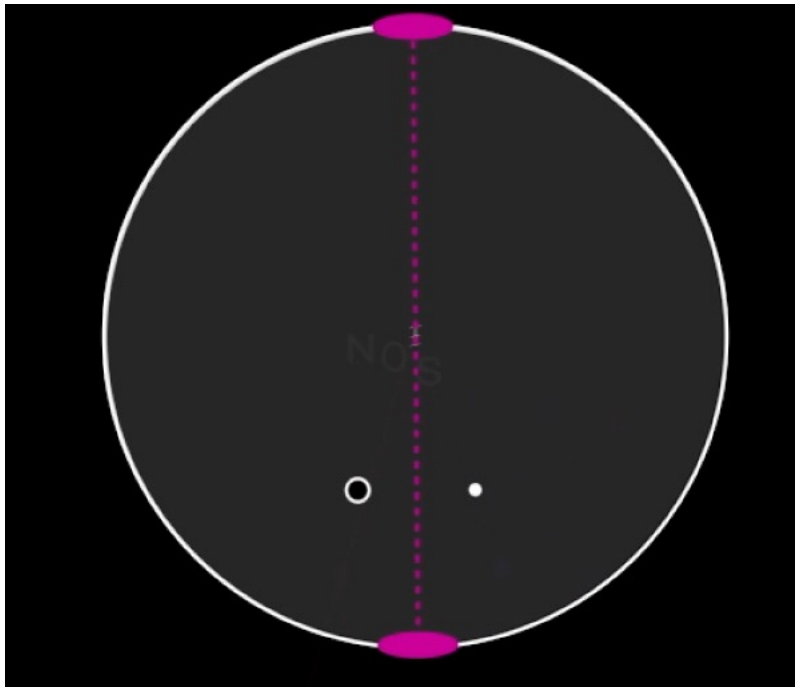


stereographic projection

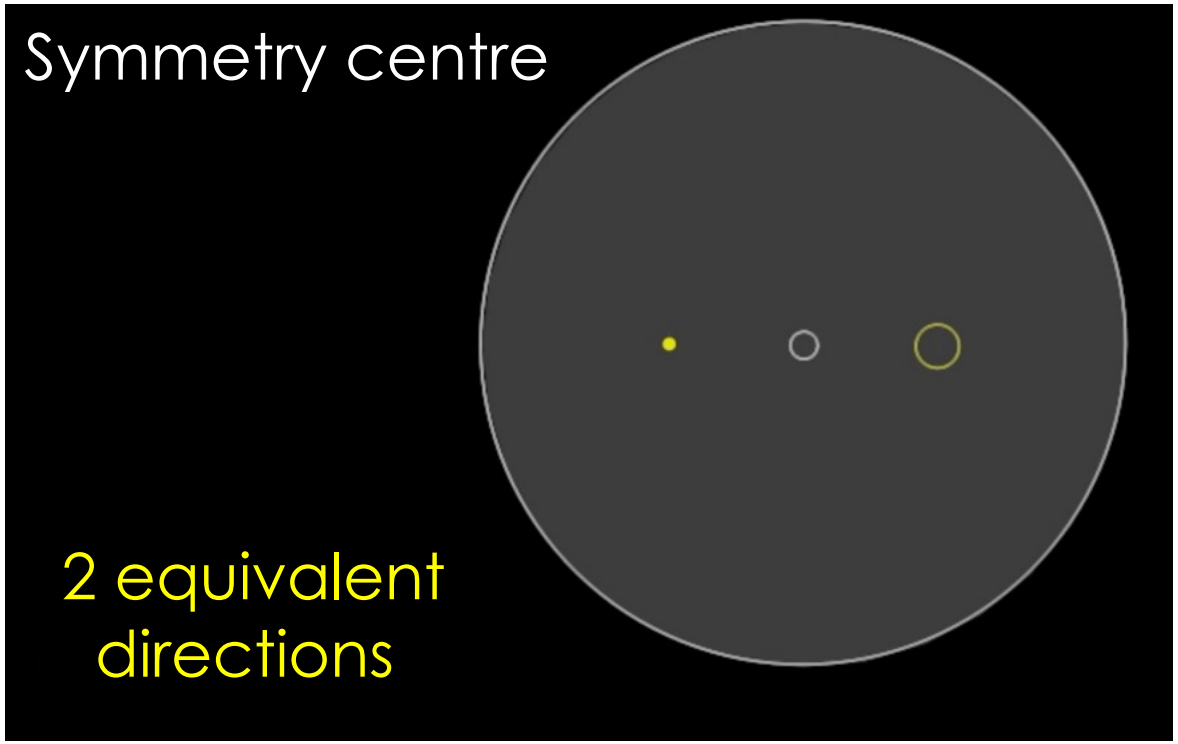


$A_2 \perp$ North-South axis

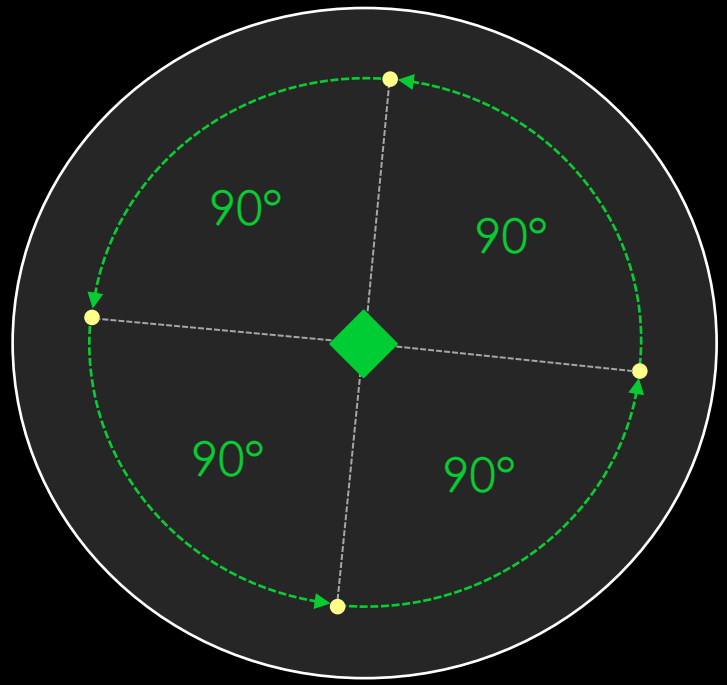




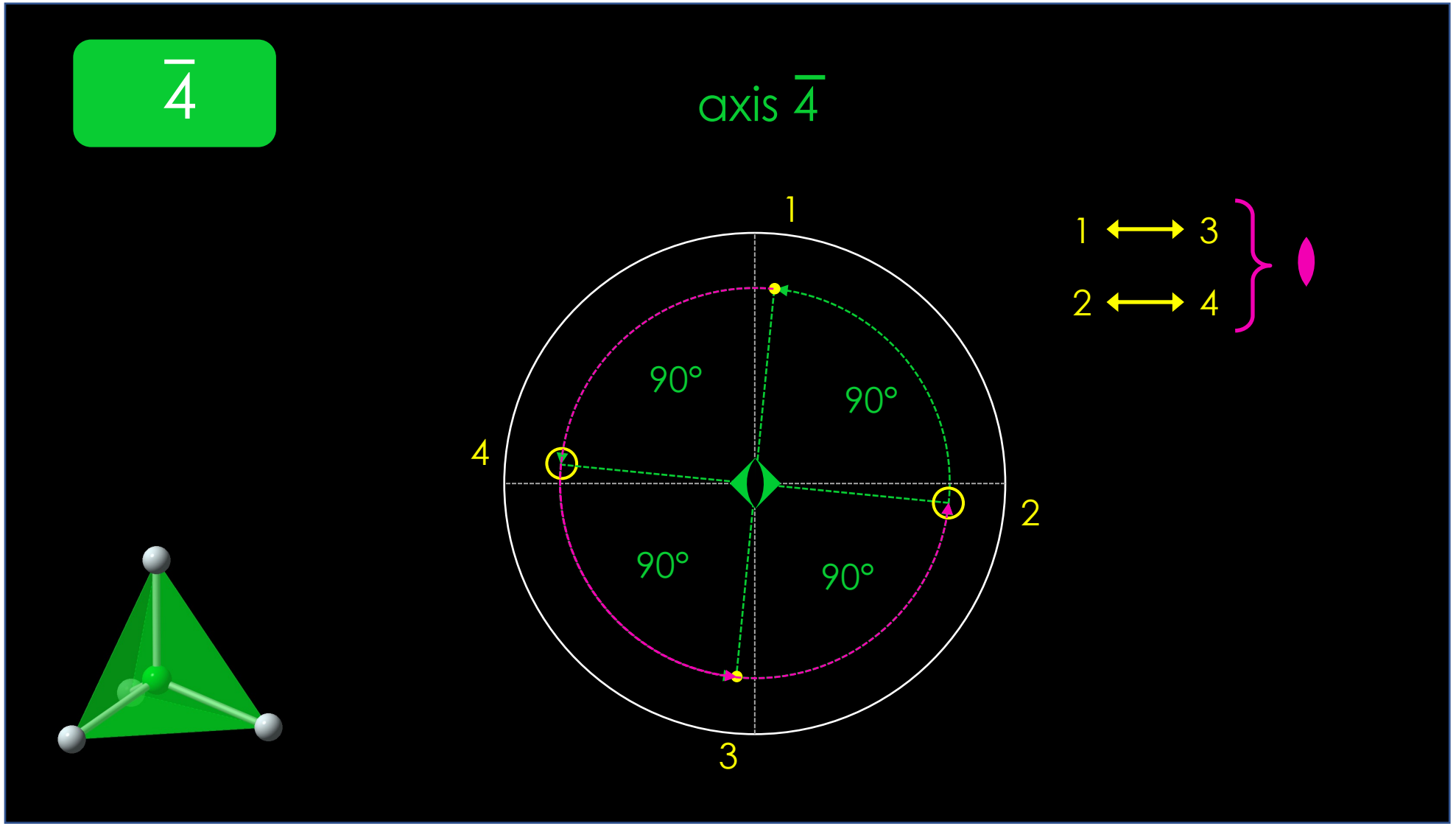
stereographic projection



A_4 || North-South axis

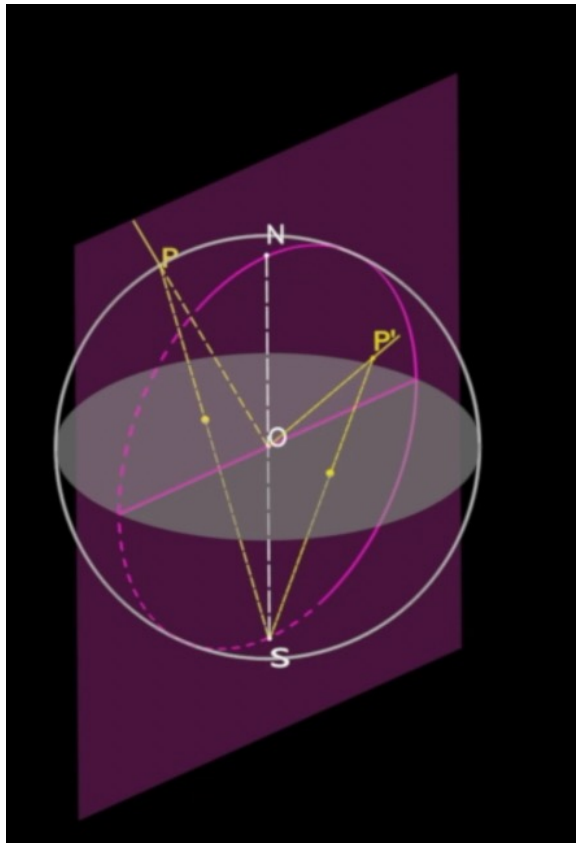


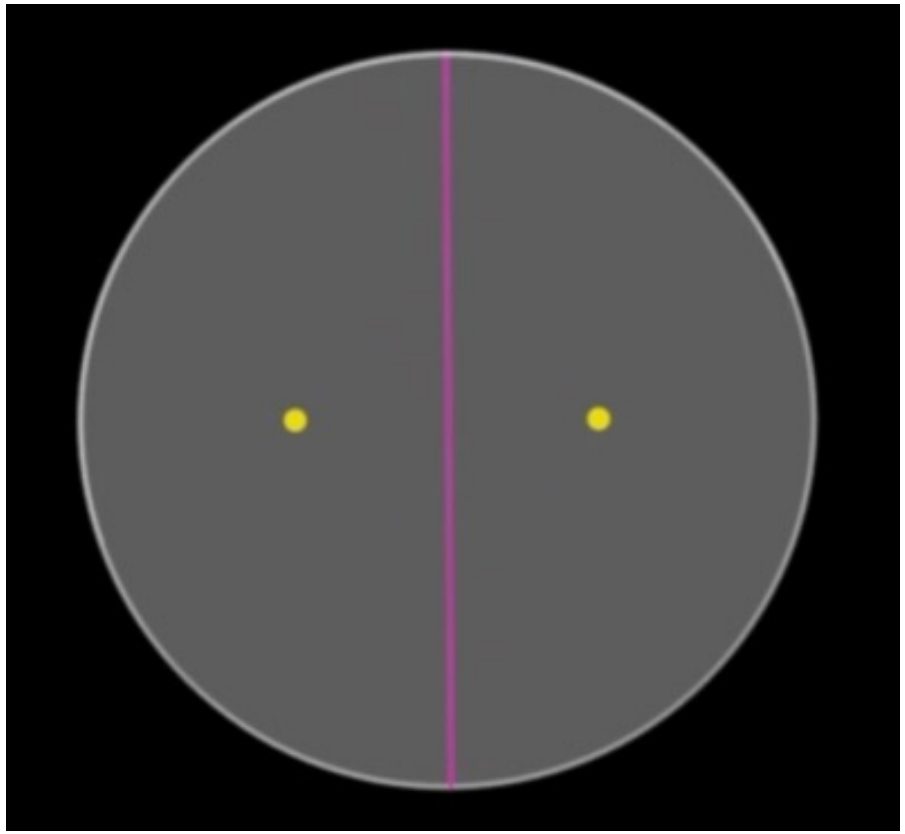
stereographic projection



stereographic projection

M || North-South axis

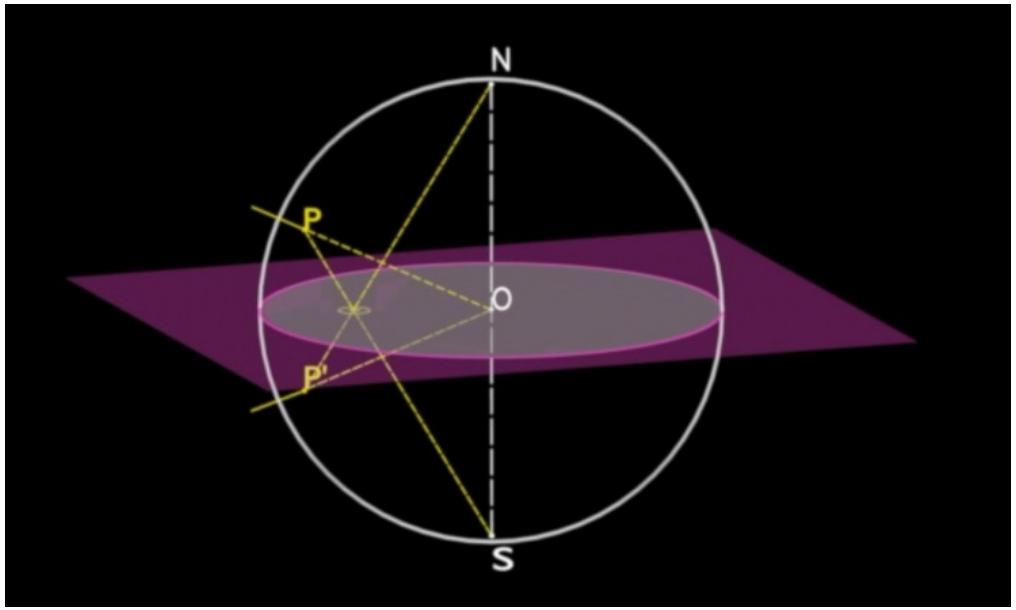


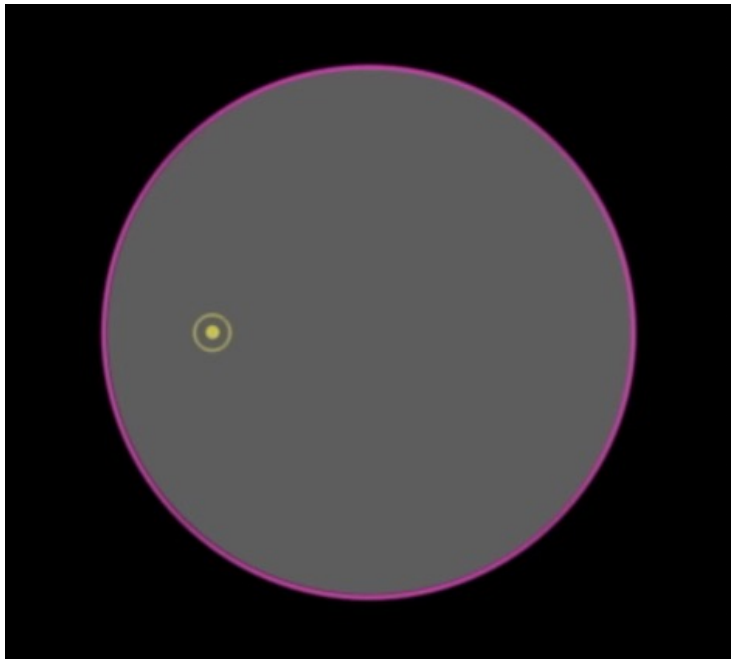


8 – The 32 crystallographic point groups

stereographic projection

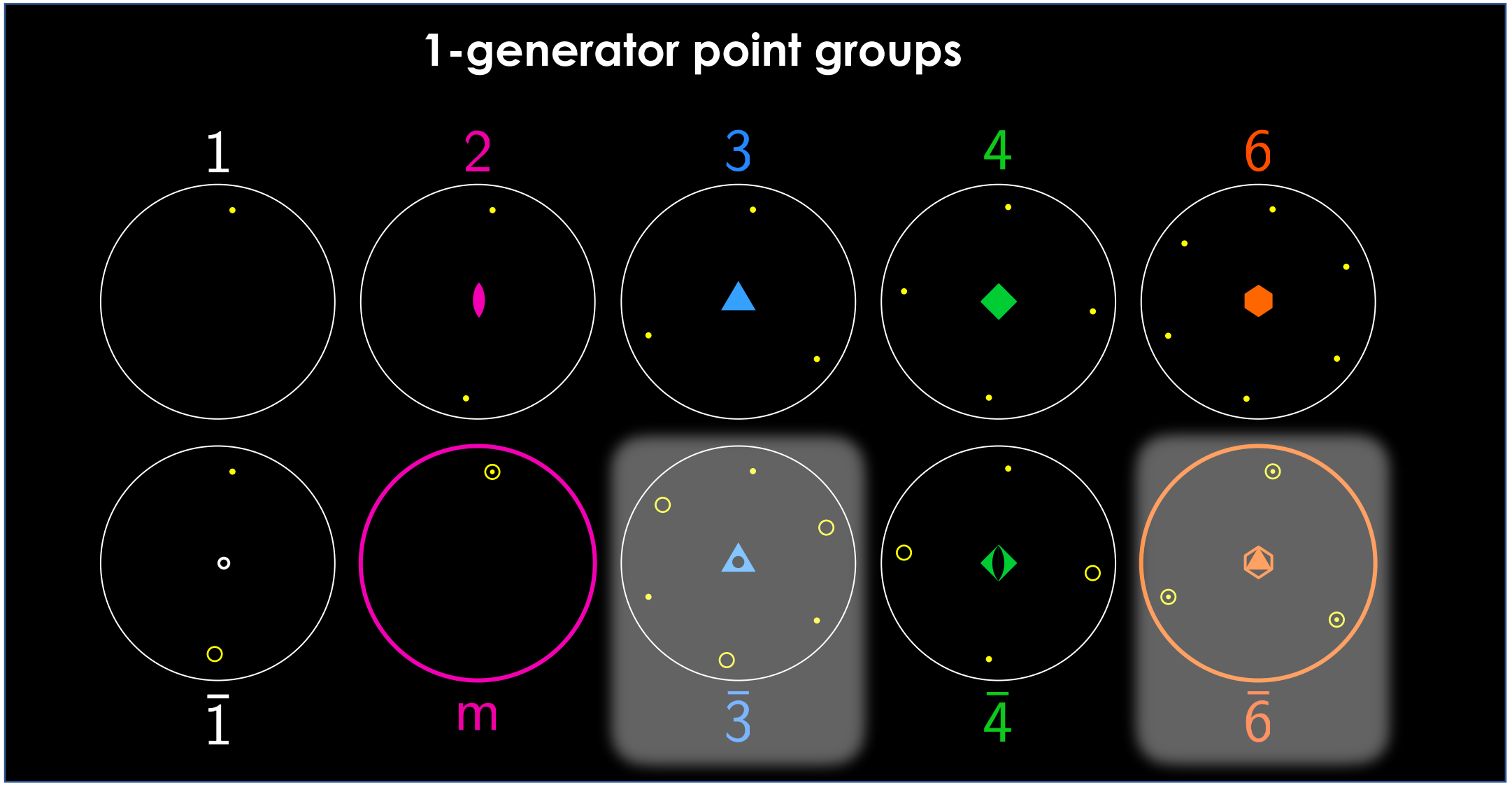
M ⊥ North-South axis



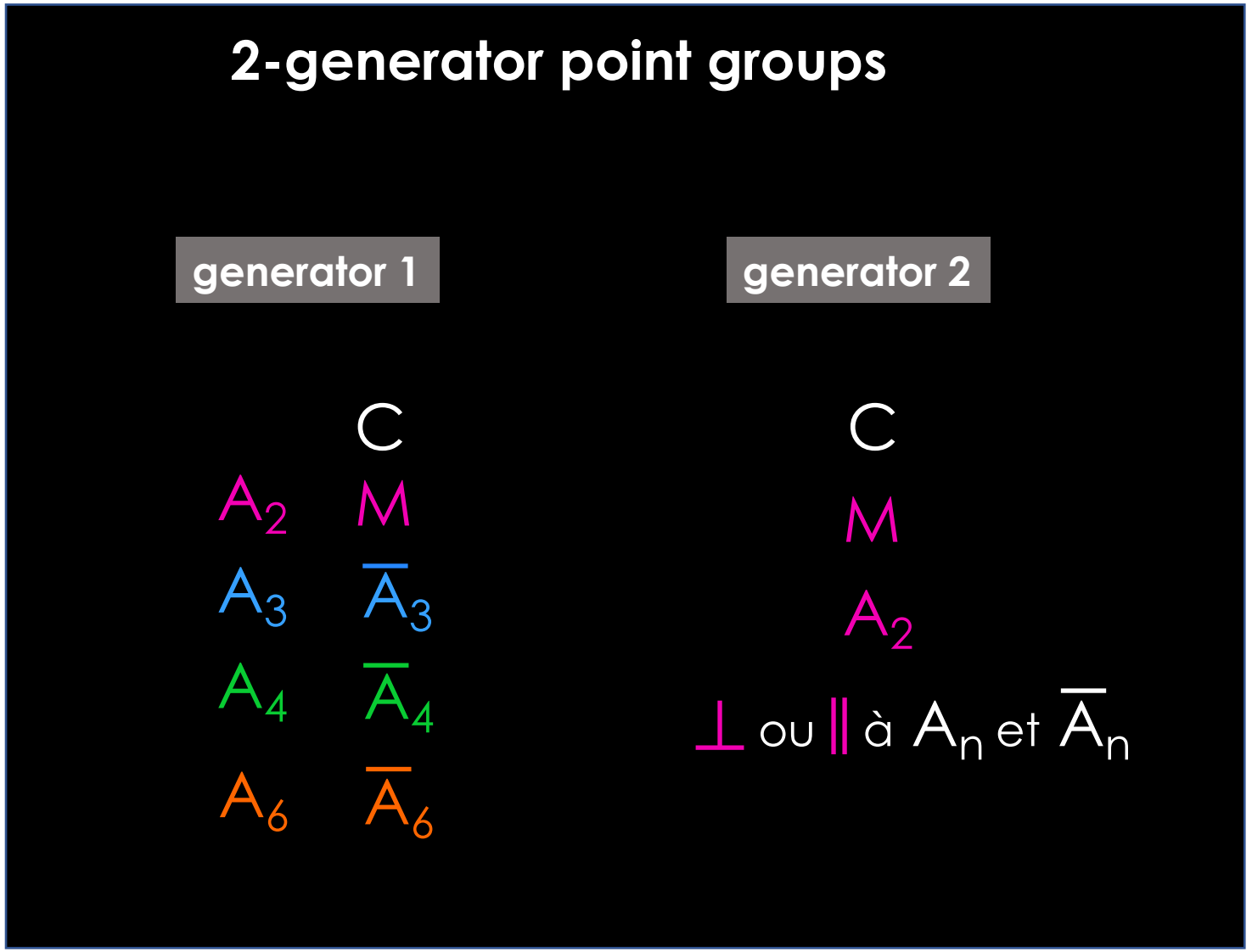


8 – The 32 crystallographic point groups

stereographic projection



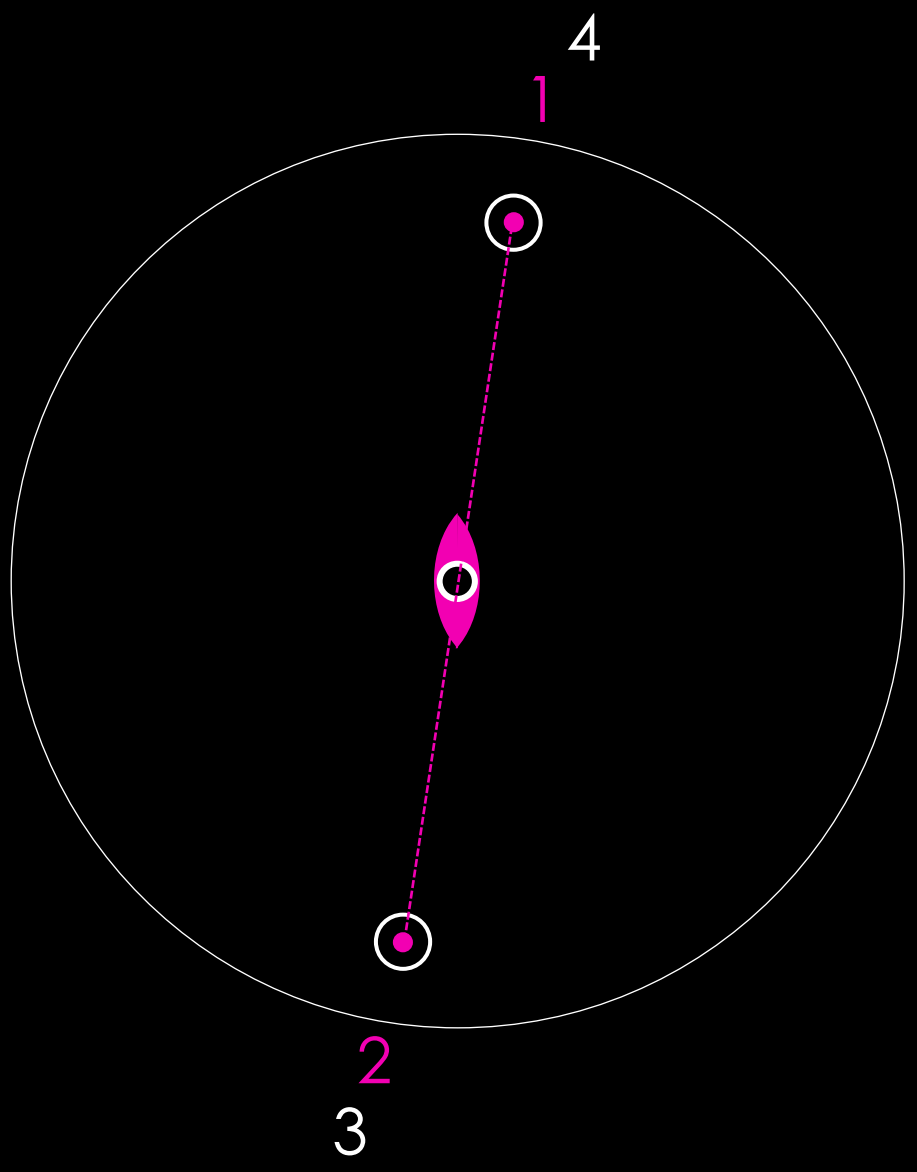
8 – The 32 crystallographic point groups



14 non-cubic point groups with 2 generators

Exercize

A_2 & C



1 ⟶ 2 : ?

1 ⟶ 3 : ?

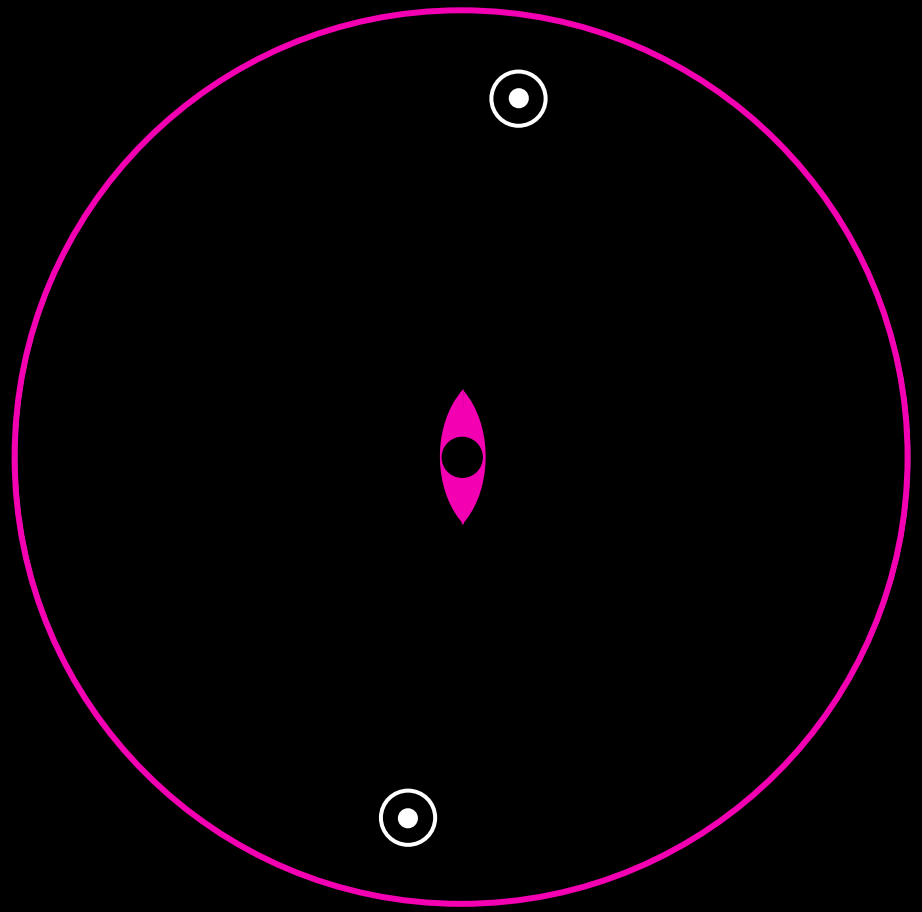
1 ⟶ 4 : ?

Exercize

A_2 & C

$\frac{A_2}{M}C$

$\frac{2}{m}$



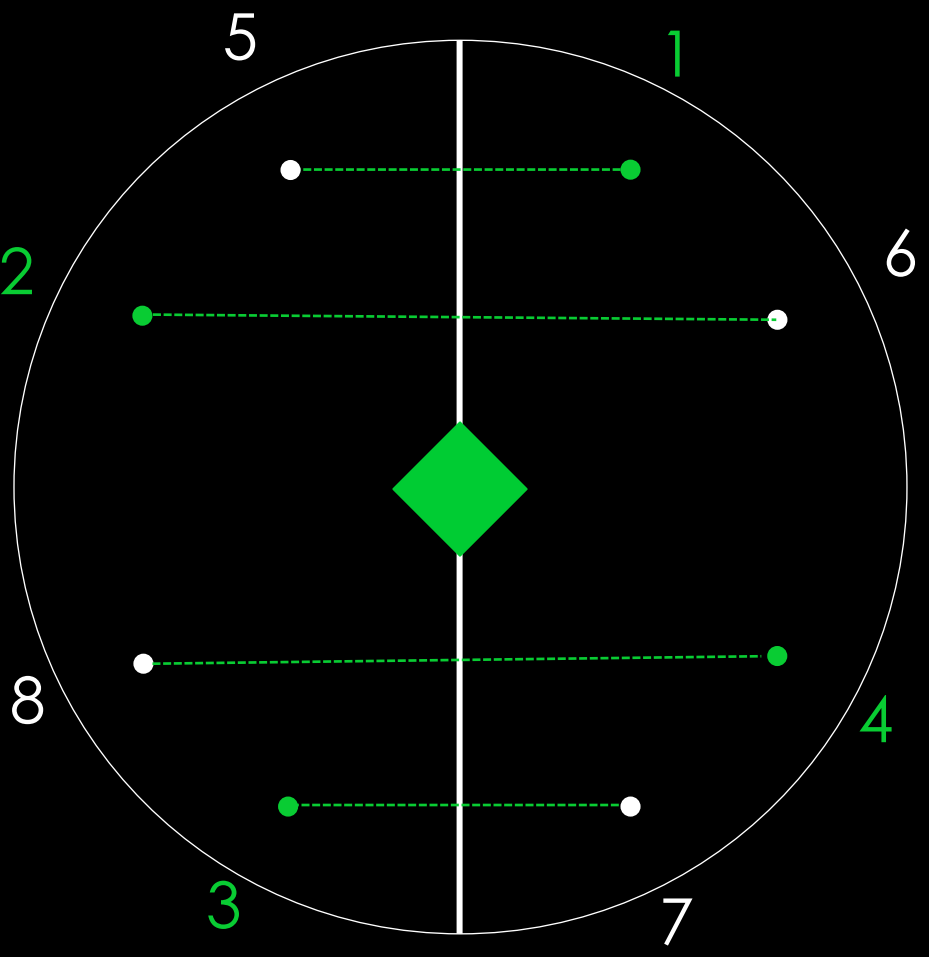
1 ⟶ 2 :

1 ⟶ 3 :

1 ⟶ 4 : M

Exercize

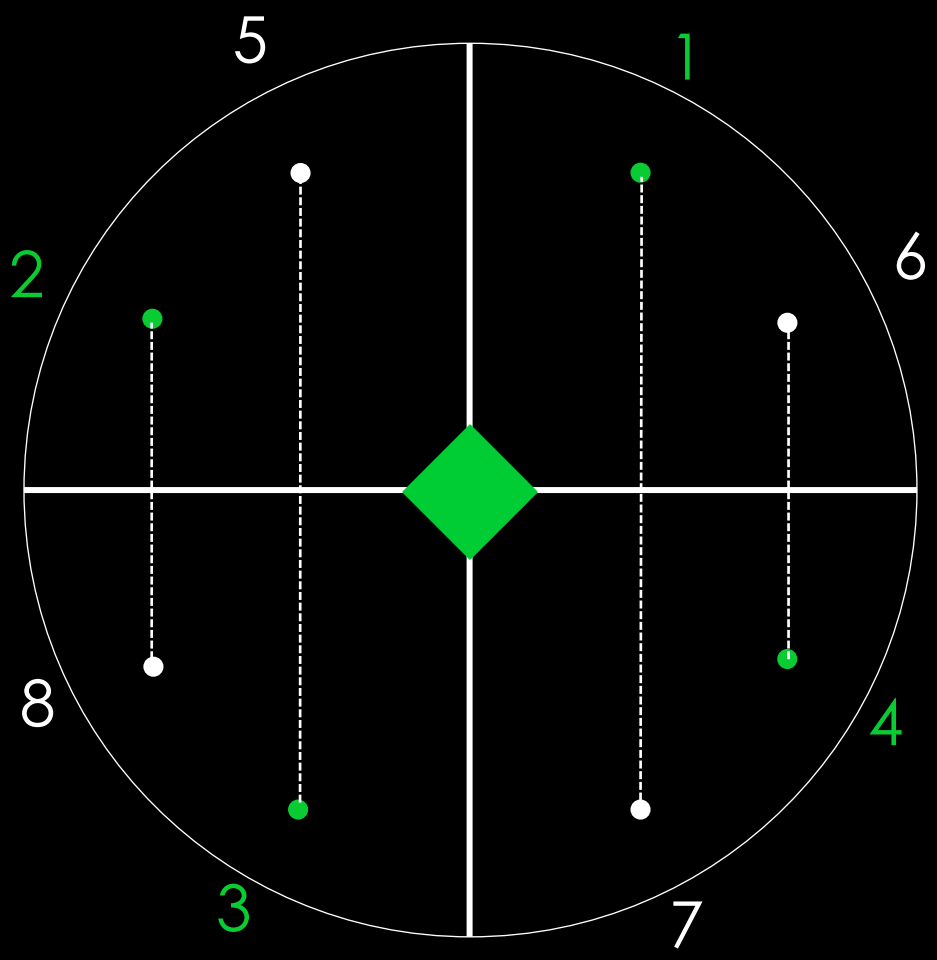
A_4 & M ||



8 equivalent directions

Exercize

A_4 & M ||



$1 \longrightarrow 7$

$2 \longrightarrow 8$

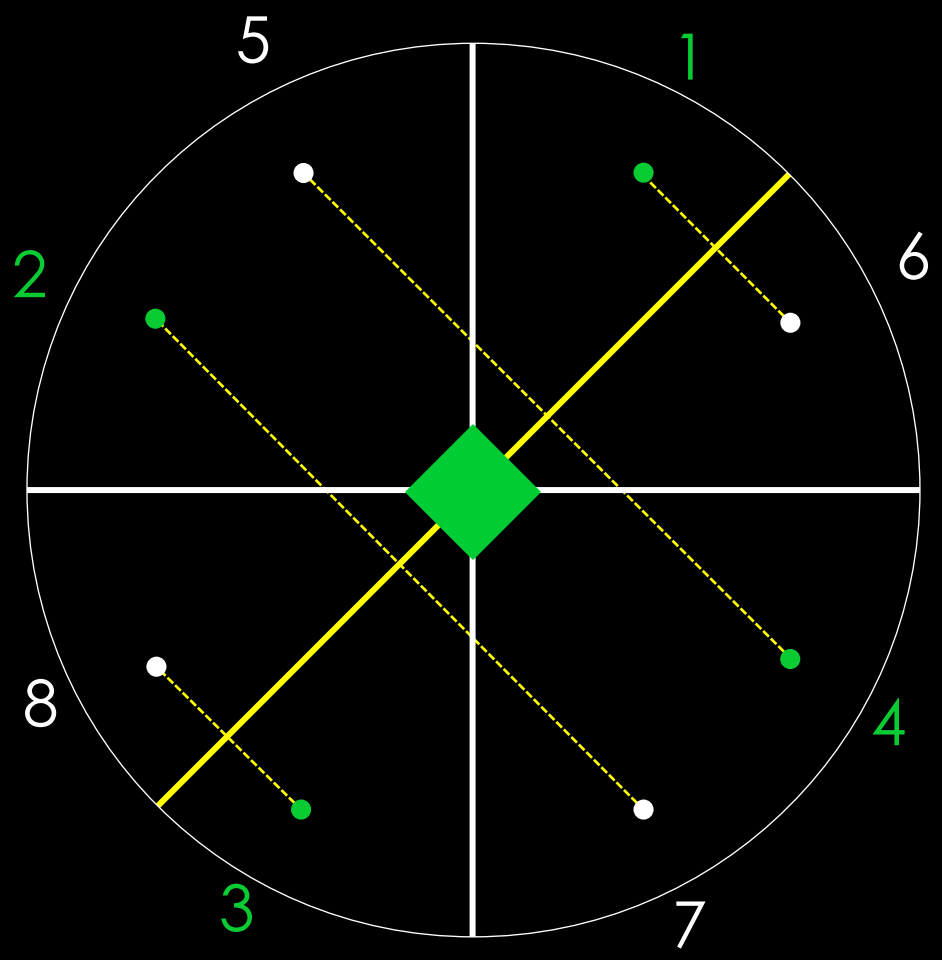
$3 \longrightarrow 5$

$4 \longrightarrow 6$

$\Big\} M -$

Exercize

A_4 & M ||

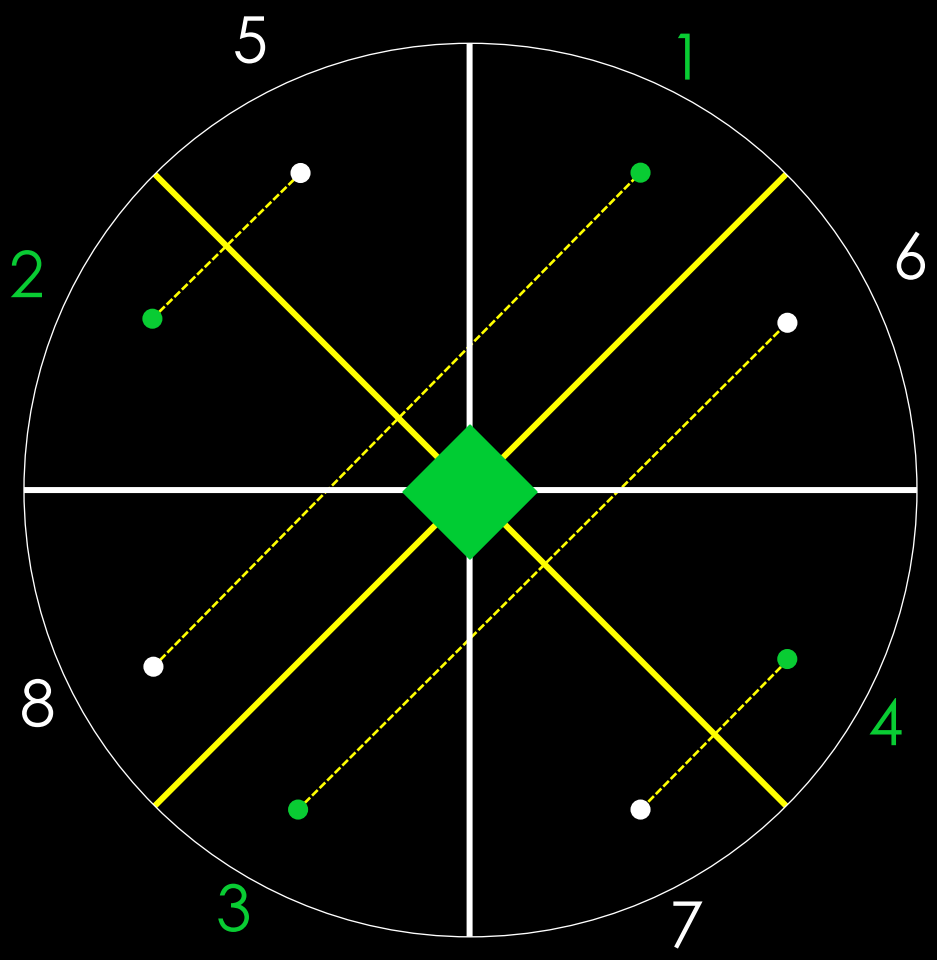


1 → 6
2 → 7
3 → 8
4 → 5

M' //

Exercize

A_4 & M ||

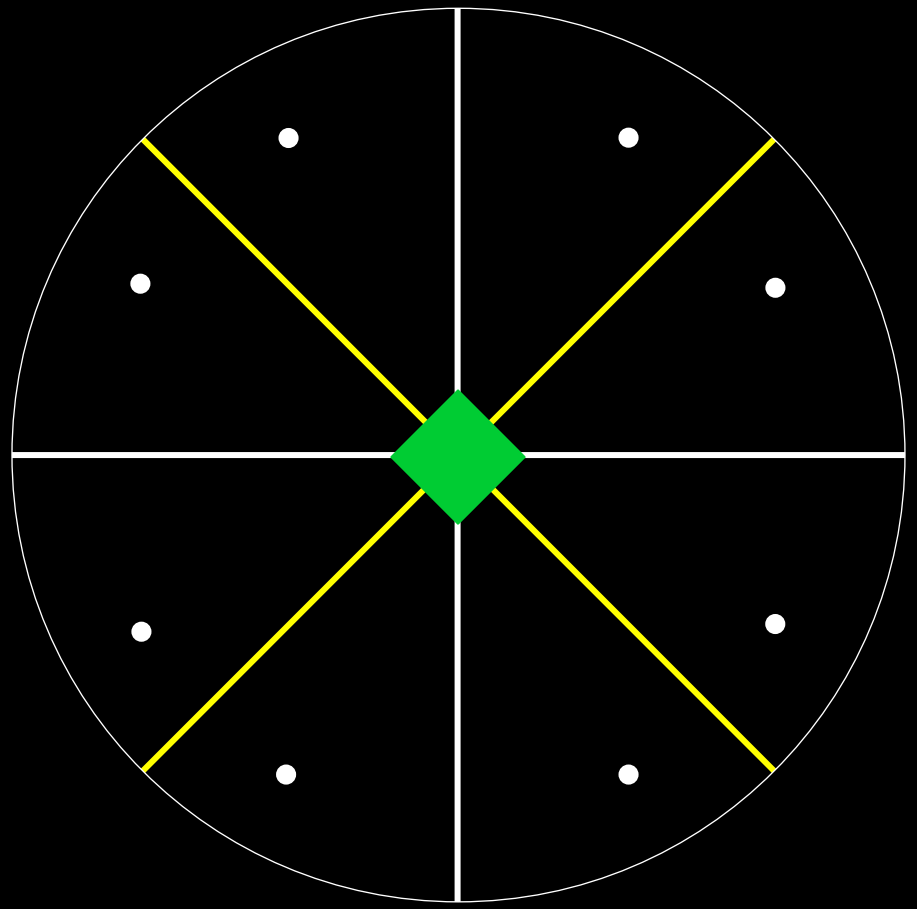


1 → 8
2 → 5
3 → 6
4 → 7

M' \

Exercize

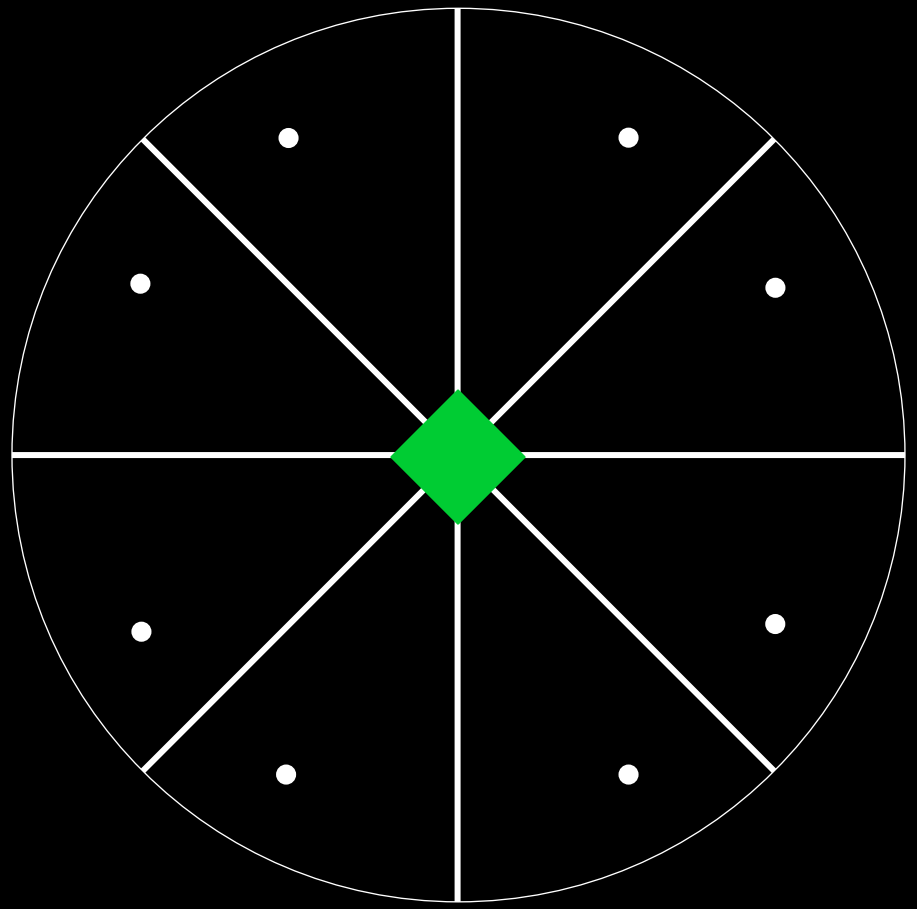
A_4 & M ||



A_4 2 M 2 M'

Exercize

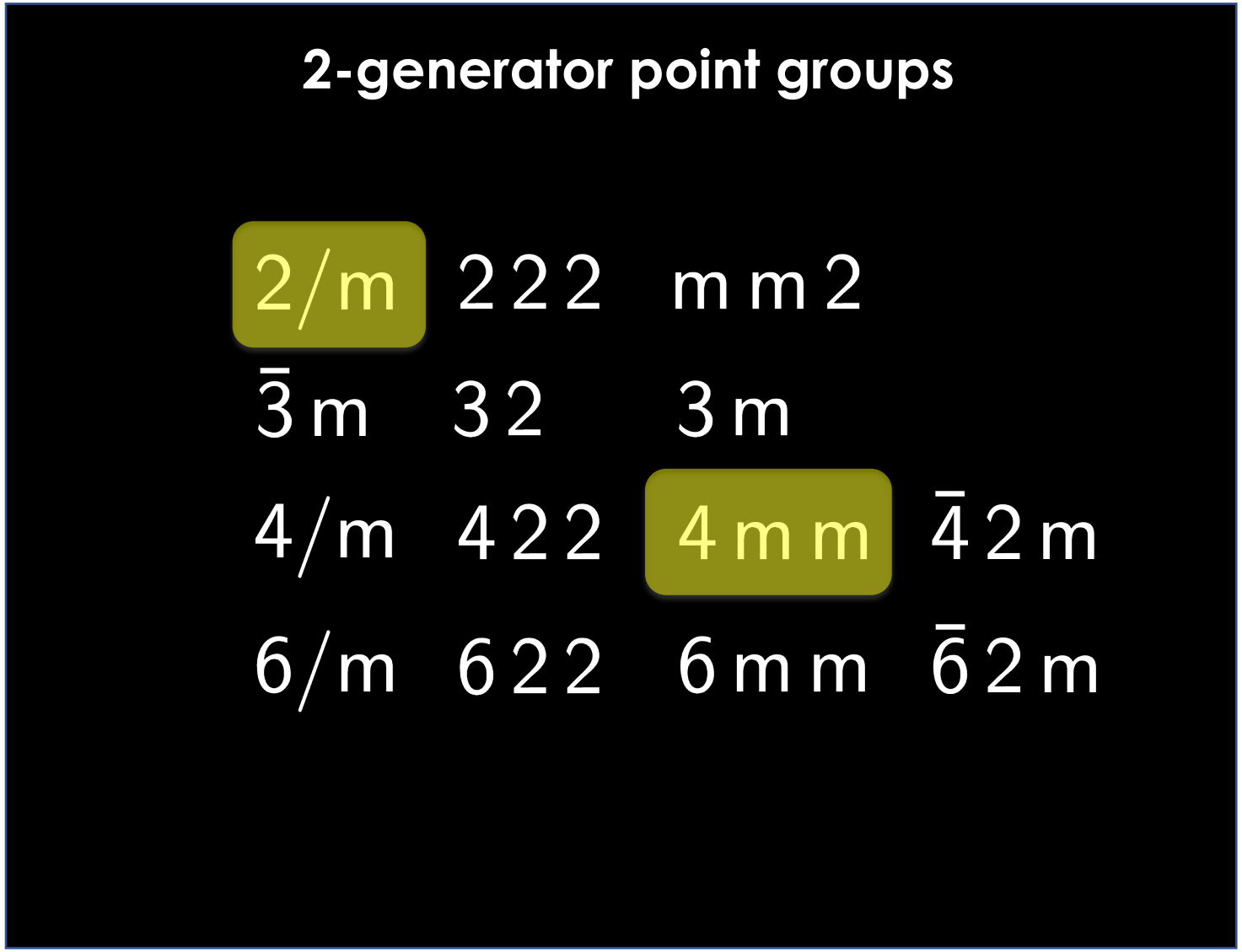
A_4 & M ||



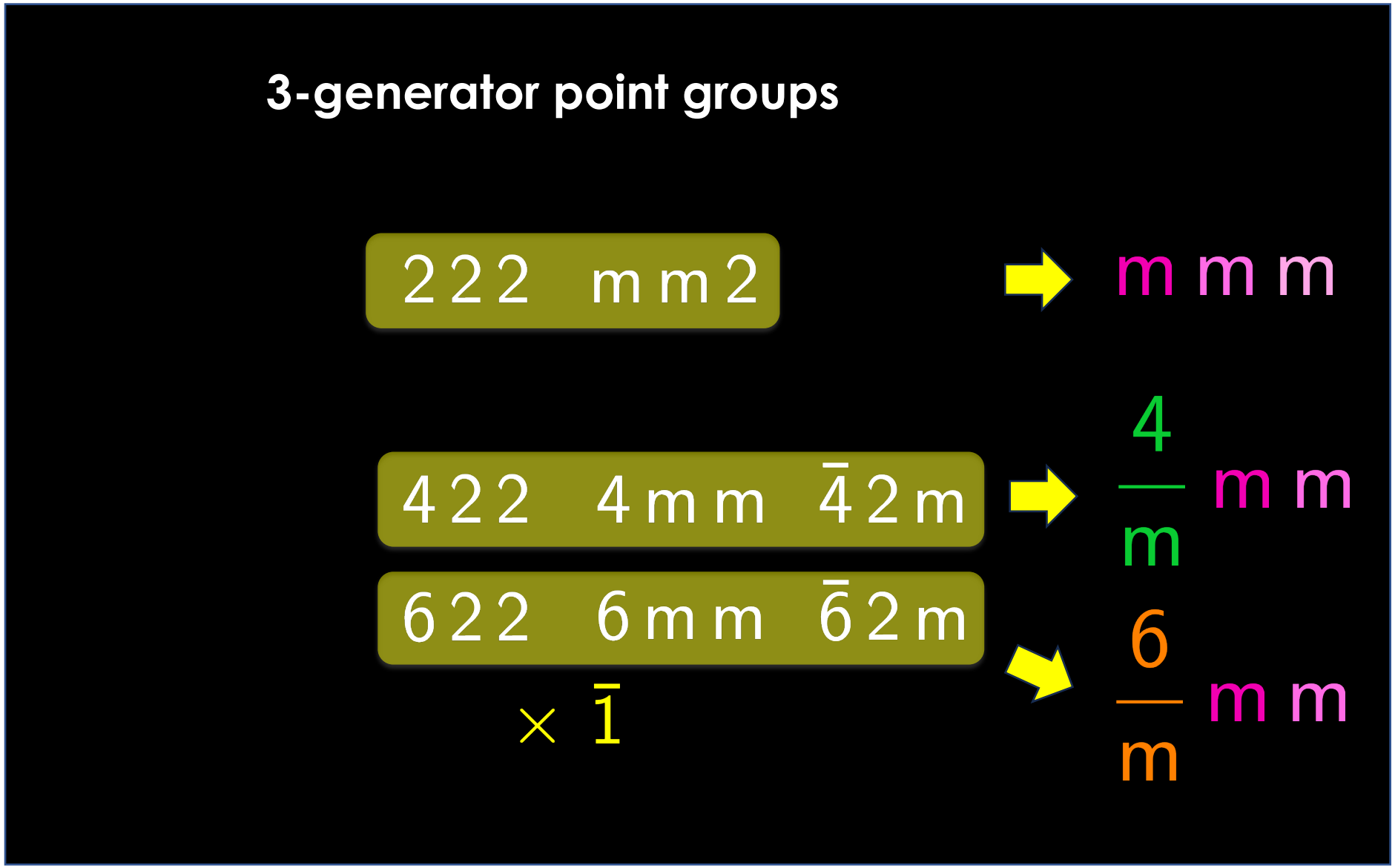
A_4 2 M 2 M'

4 m m

8 – The 32 crystallographic point groups

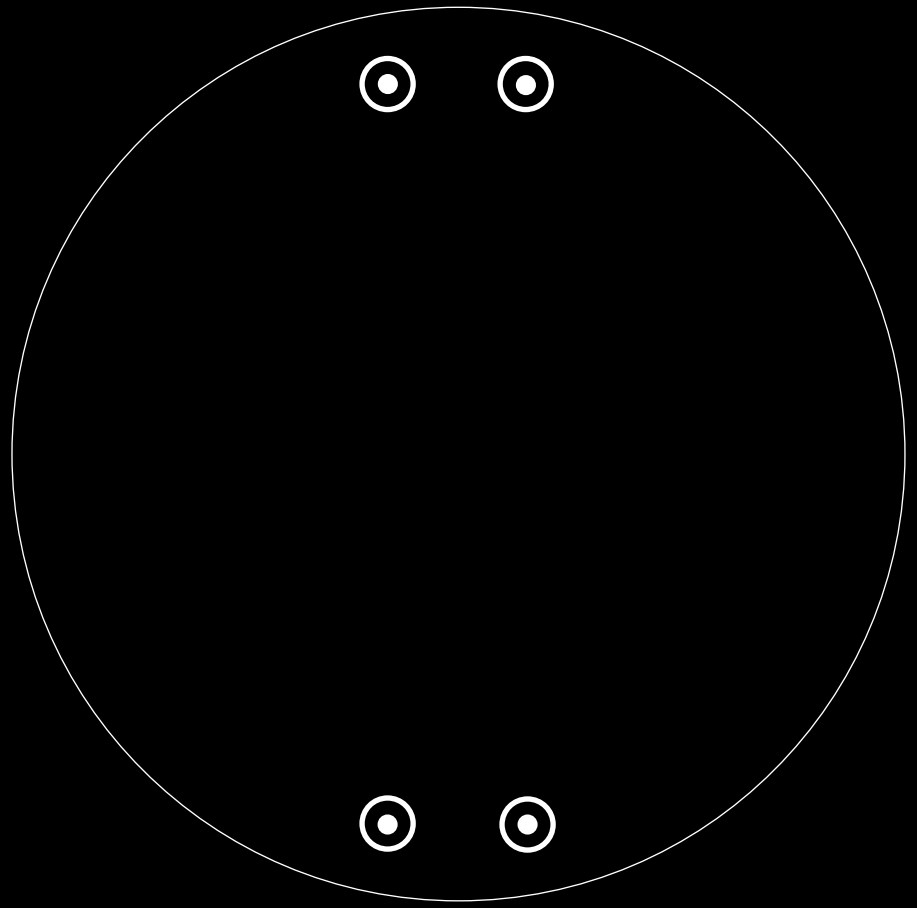


8 – The 32 crystallographic point groups



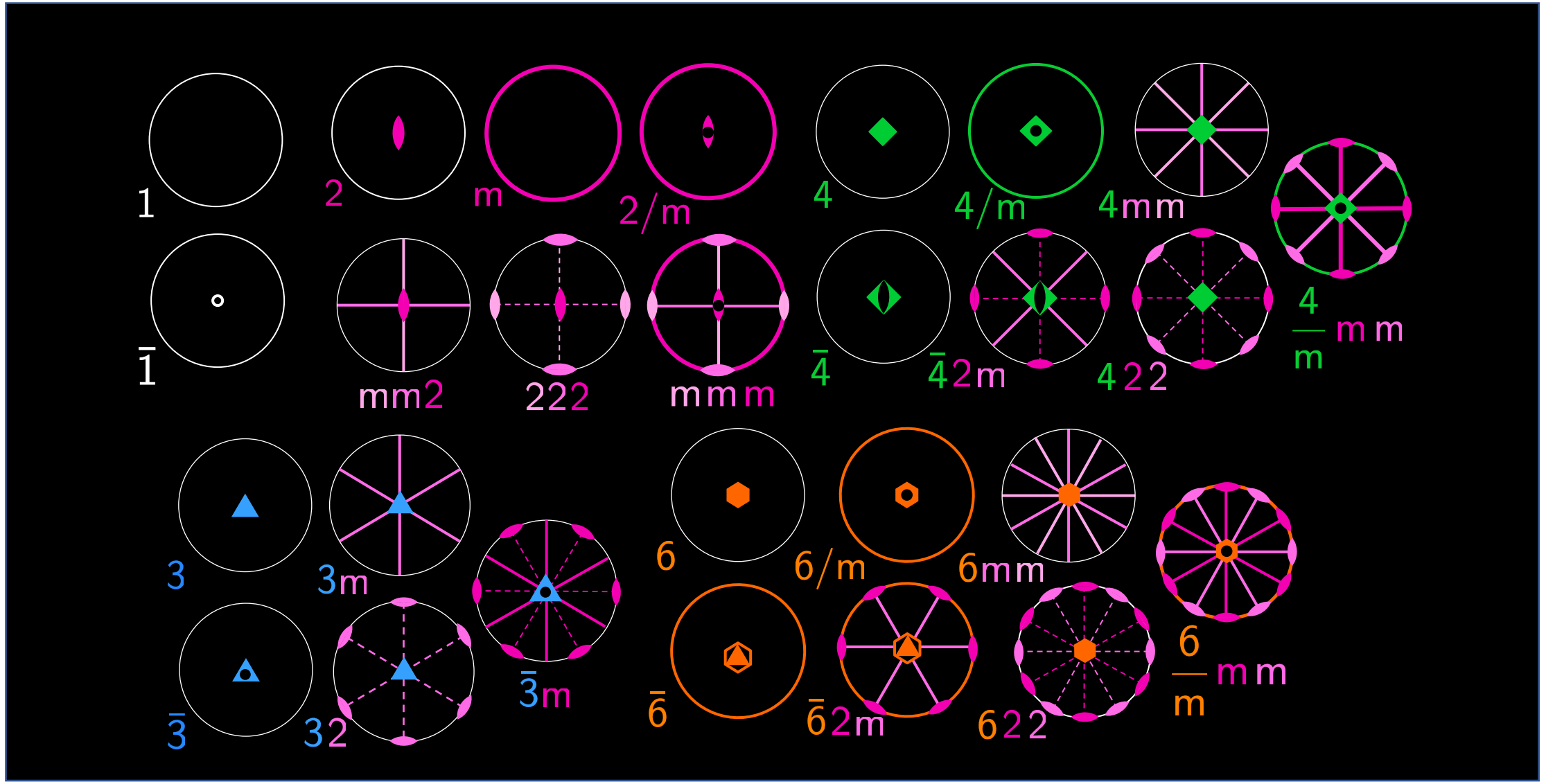
Exercize

Determine the symmetry operations that lead to the 8 equivalent directions



8 – The 32 crystallographic point groups

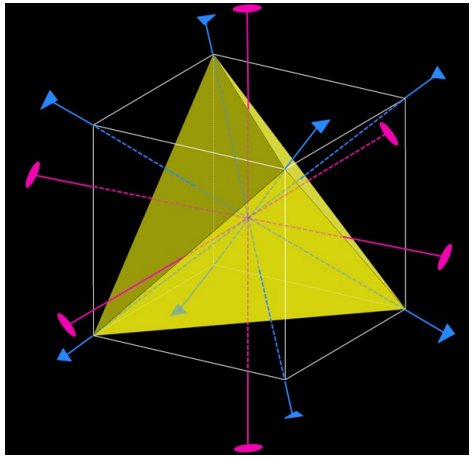
27 non-cubic point groups



8 – The 32 crystallographic point groups

5 cubic point groups

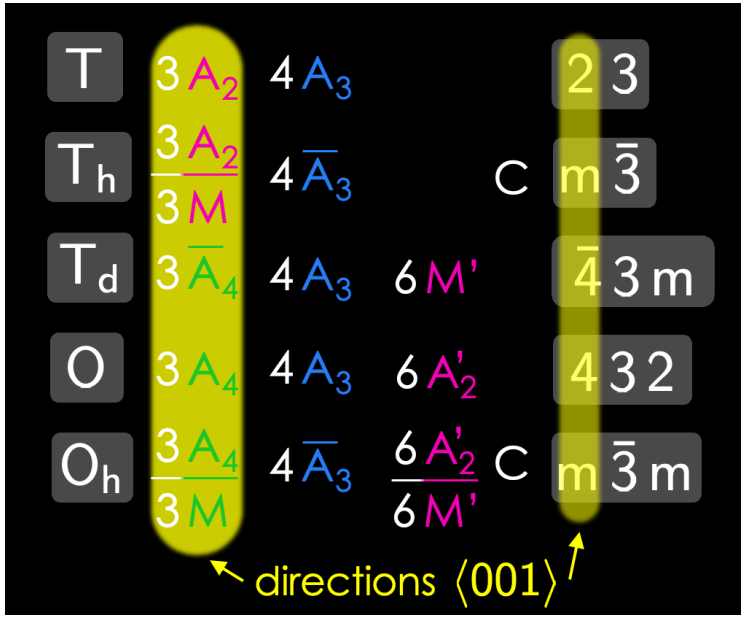
They contain **at least 4 A_3** (oriented along the <111> directions) and **3 A_2** (oriented along the <100> directions)

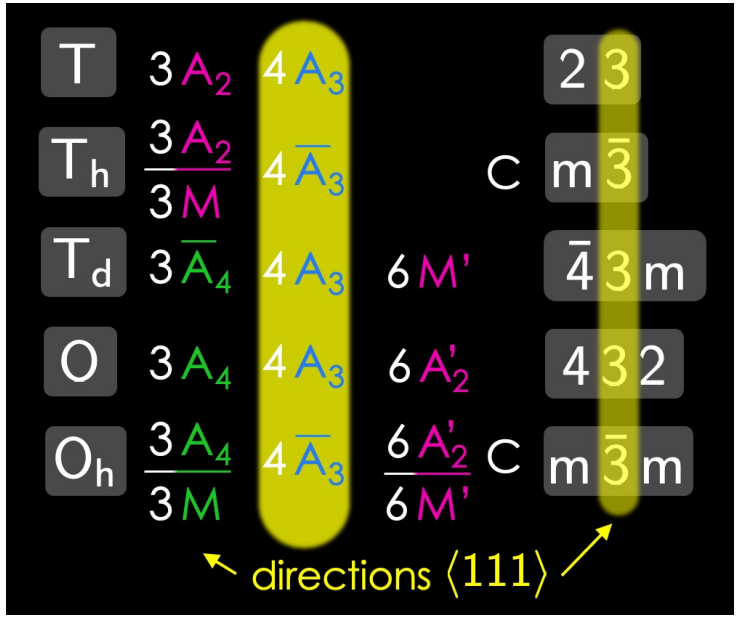


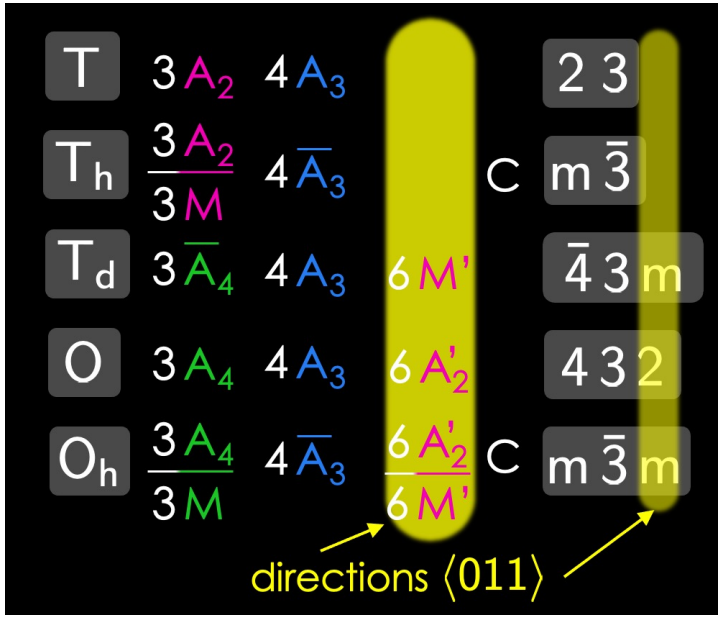
$3\,A_2\ 4\,A_3$	2 3	T	**rotation group of the regular tetrahedron**
$\frac{3\,A_2}{3\,M}\ 4\,\bar{A}_3\ C$	m $\bar{3}$	T_h	obtained by adding a centre to 2 3
$3\,\bar{A}_4\ 4\,A_3\ 6\,M'$	$\bar{4}$ 3 m	T_d	obtained from 2 3 by replacing A_2 par $\overline{A_4}$ **symmetry group of the regular tetrahedron**
$3\,A_4\ 4\,A_3\ 6\,A'_2$	4 3 2	O	obtained from 2 3 by replacing A_2 by A_4 **rotation group of the regular octahedron**
$\frac{3\,A_4}{3\,M}\ 4\,\bar{A}_3\ \frac{6\,A'_2}{6\,M'}\ C$	m $\bar{3}$ m	O_h	obtained by adding a centre to 4 3 2 **symmetry group of the regular octahedron**

8 – The 32 crystallographic point groups

5 cubic point groups









Course outline

1- Symmetry observation in natural crystals

2- Internal cause of the natural crystal shape

3 – Crystal lattice, cell, motif

4 – Lattice direction and planes

5 – Reciprocal lattice

6 – Crystal lattice & symmetries

7 – Conventional cell (unit cell)

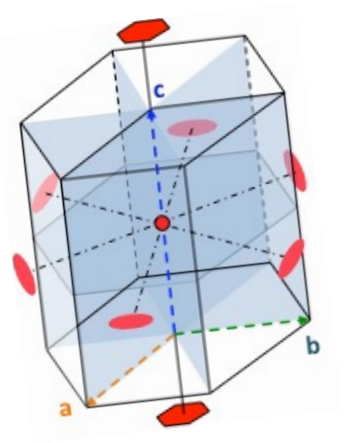
8 – The 32 crystallographic point groups

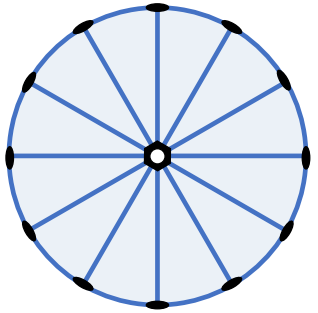
9 – The 7 crystal systems

10 – The 14 Bravais lattices

11 – The 230 space-groups



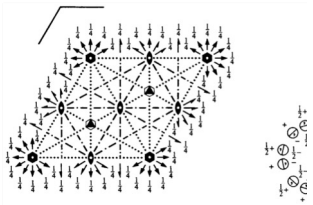




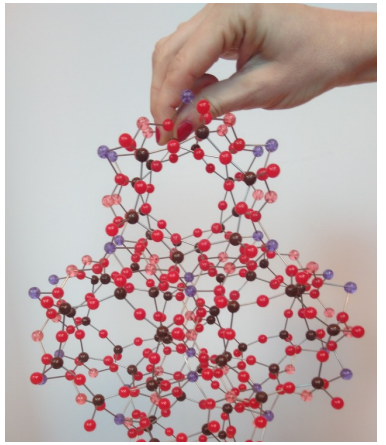
$$\frac{6}{m}mm$$

$P6/mcc$ D^2_{6h}

No. 192 $P\ 6/m\ 2/c\ 2/c$



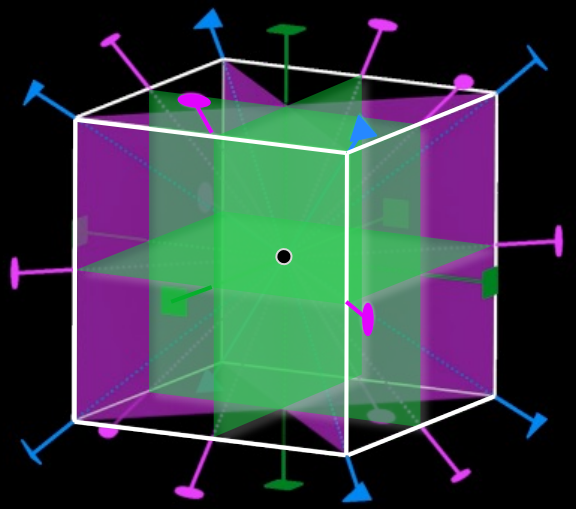
Origin at centre $(6/m)$ at $6/mcc$



9 – The 7 crystal systems

We can classify the **32 crystallographic point groups** in **7 crystal systems**.

cubic system



2 3

m $\bar{3}$

$\bar{4}$ 3 m

4 3 2

m $\bar{3}$ m ← holohedry

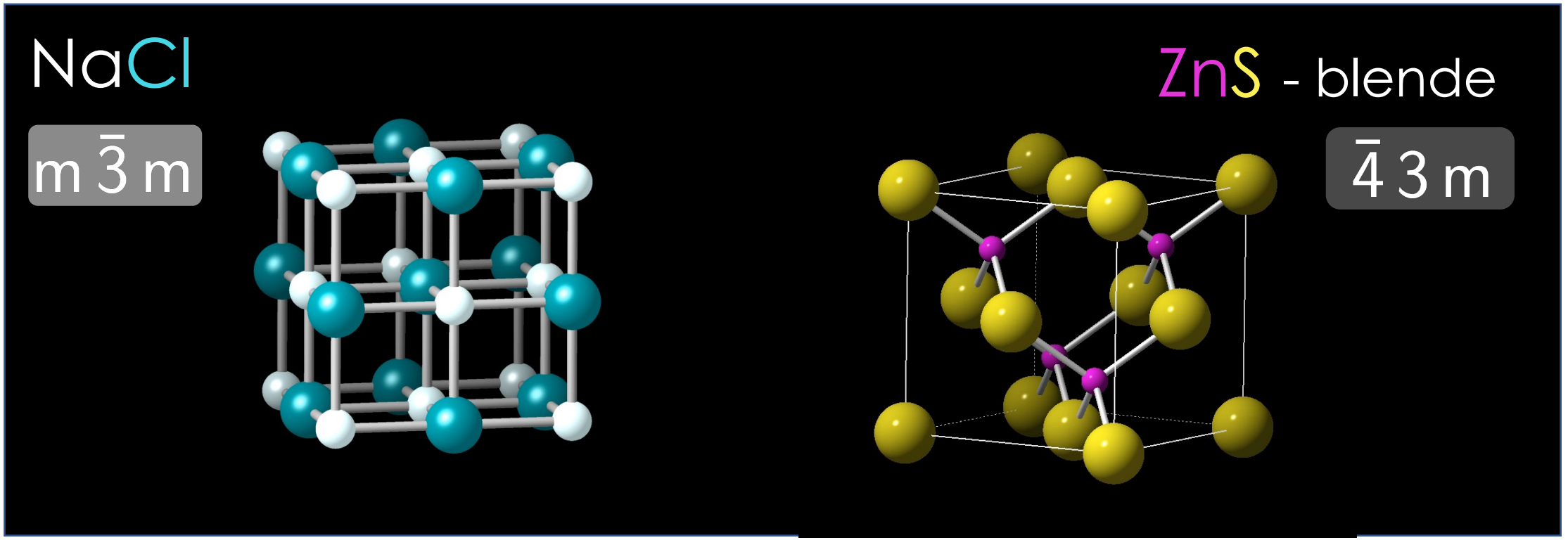
$a = b = c$

$\alpha = \beta = \gamma = 90°$

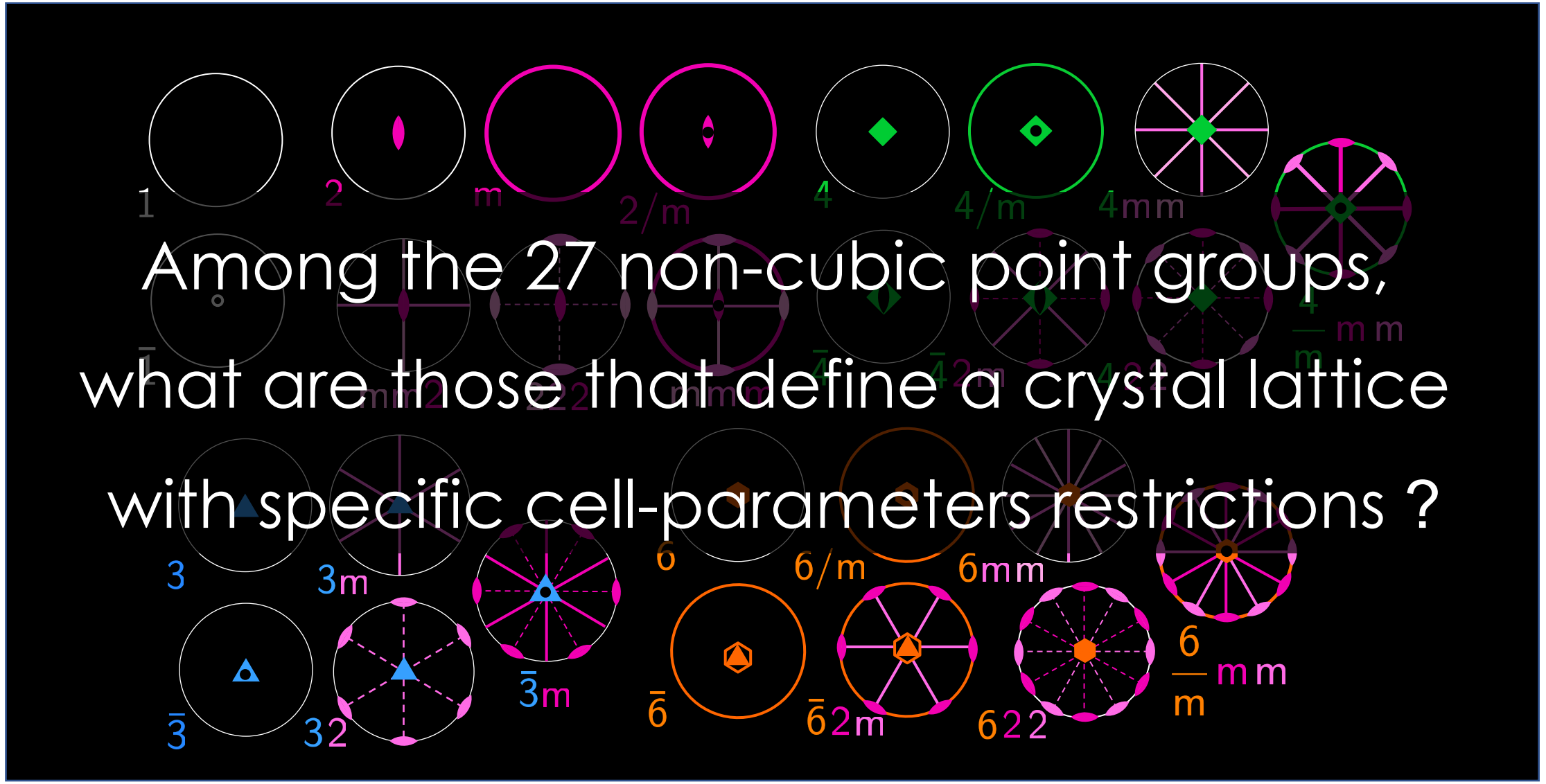
9 – The 7 crystal systems

We can classify the **32 crystallographic point groups** in **7 crystal systems**.

crystal symmetry ≤ lattice symmetry



9 – The 7 crystal systems



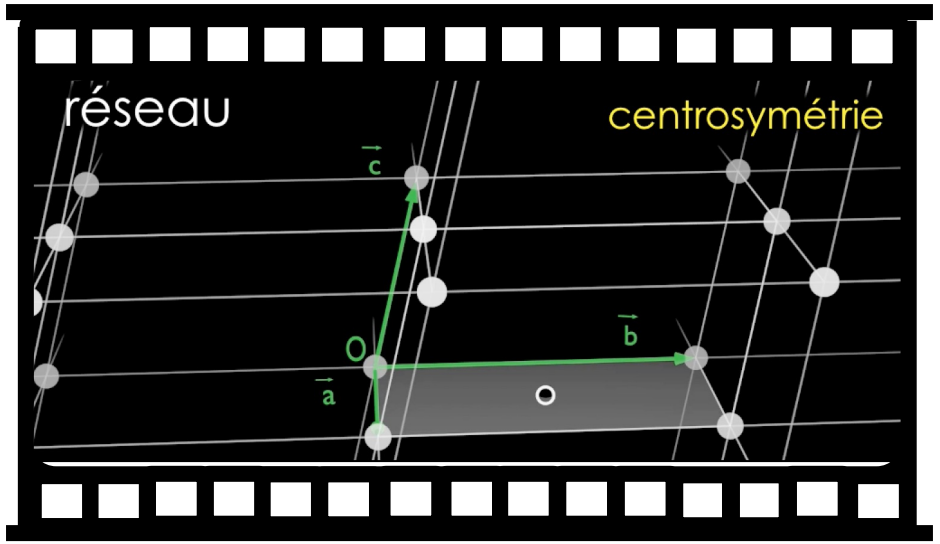
Among the 27 non-cubic point groups, what are those that define a crystal lattice with specific cell-parameters restrictions ?

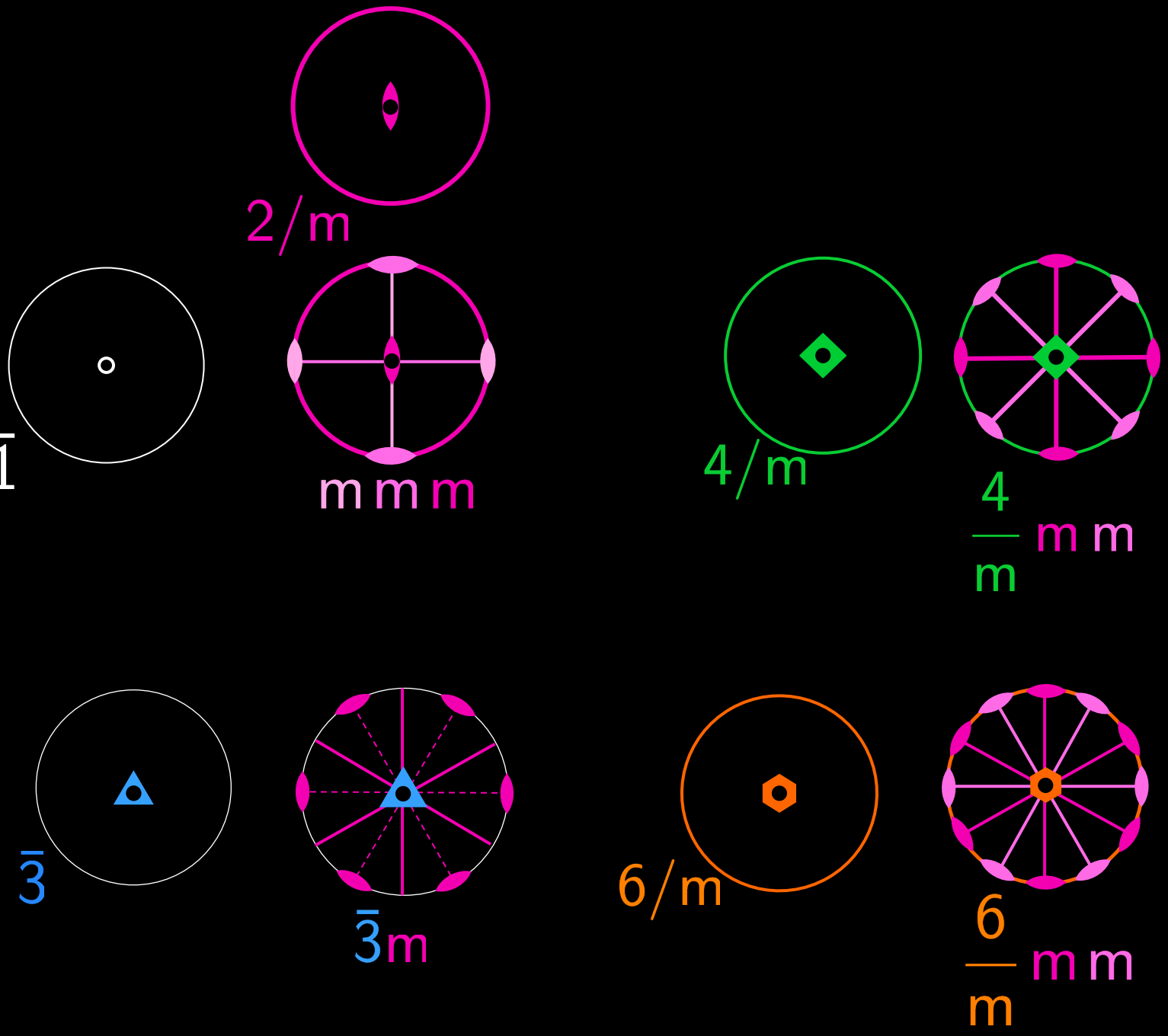
9 – The 7 crystal systems

We can classify the **32 crystallographic point groups** in **7 crystal systems**.

crystal symmetry ≤ lattice symmetry

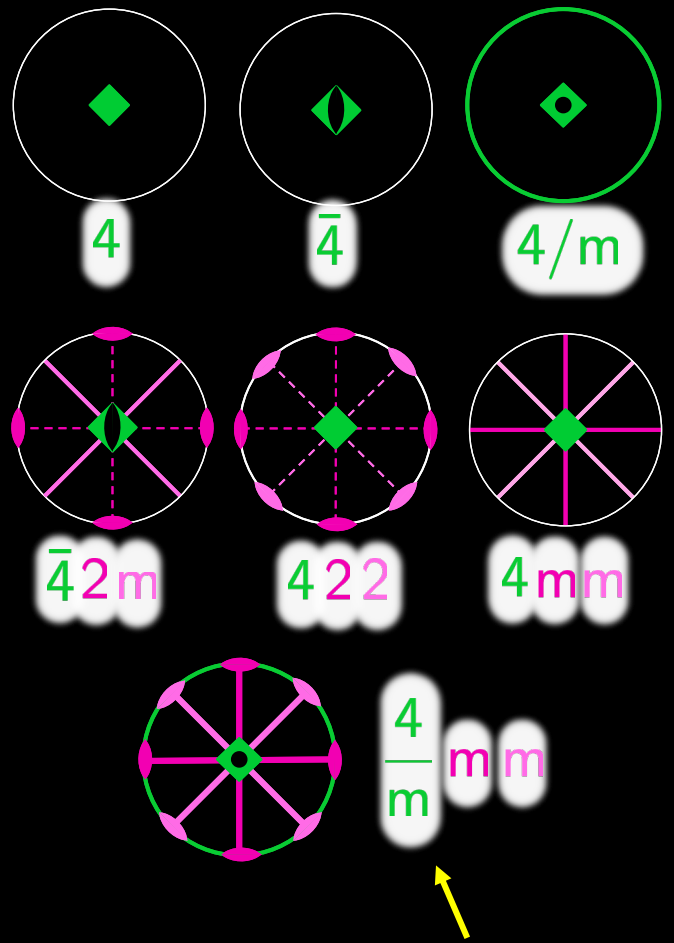
any lattice is centrosymmetric



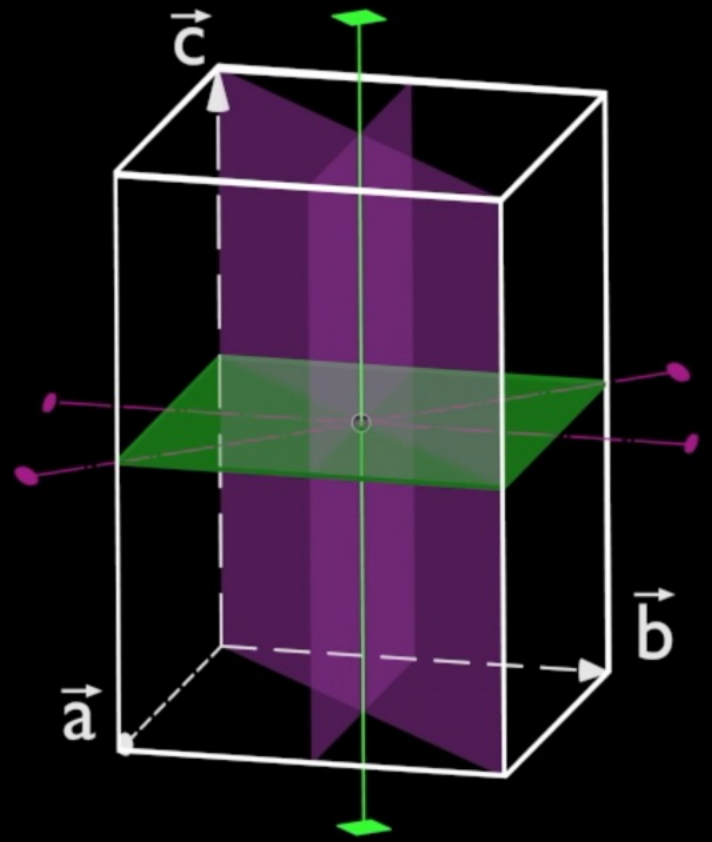


11 Laue classes

tetragonal system



holohedry



A_4 ➔ a = b $\gamma = 90°$

a = b

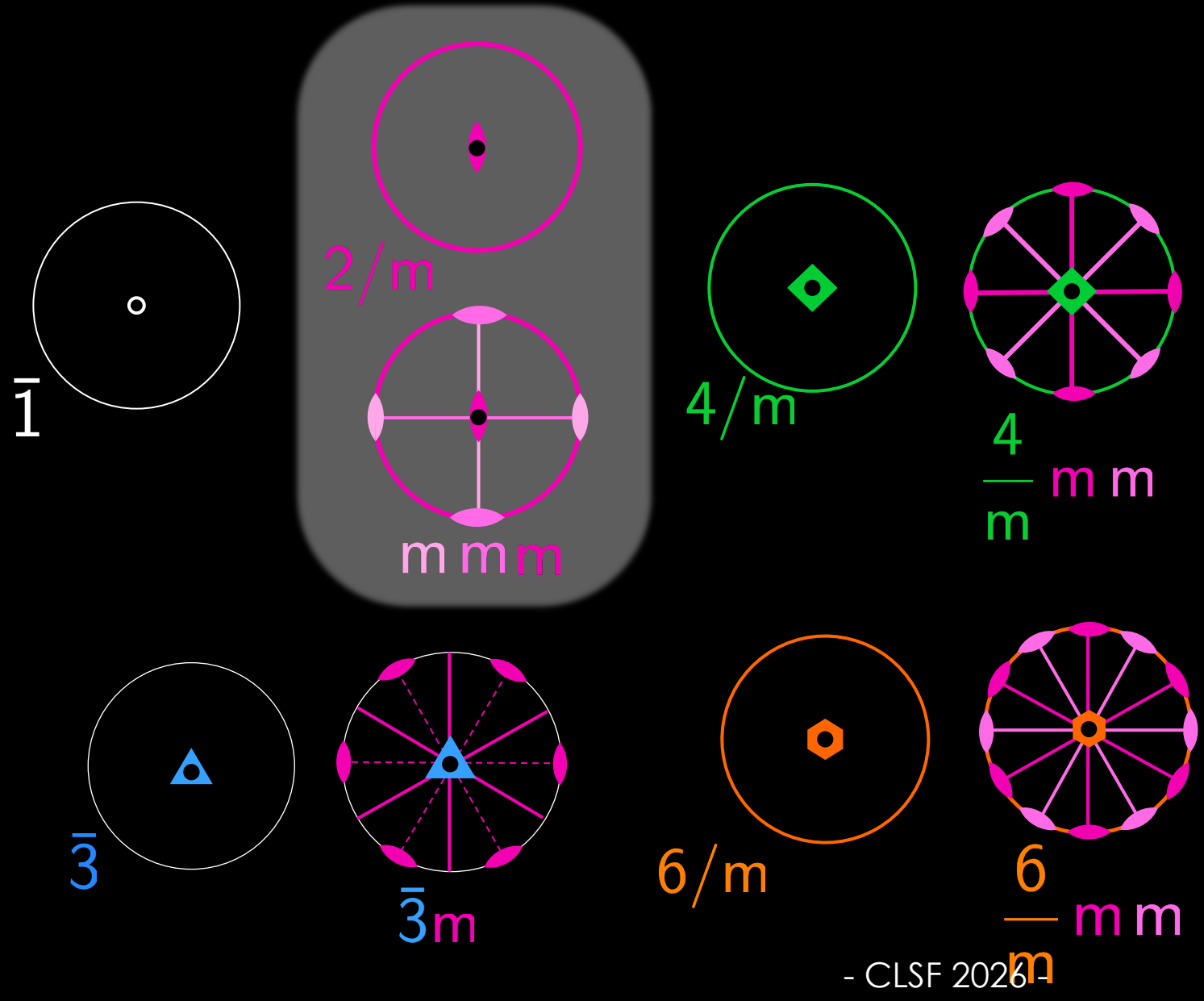
M ⊥ A_4 ➔ $\alpha = \beta = 90°$

$\alpha = \beta = \gamma = 90°$

direction [001]

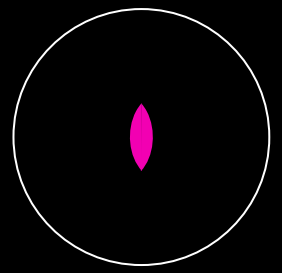
directions [100] & [010]

directions [110] & [$\bar{1}$10]

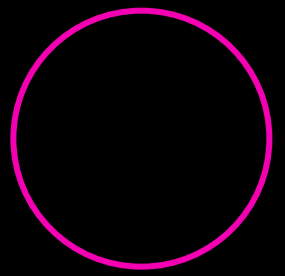


11 Laue Classes

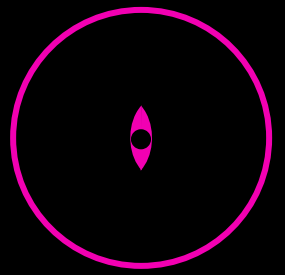
monoclinic system



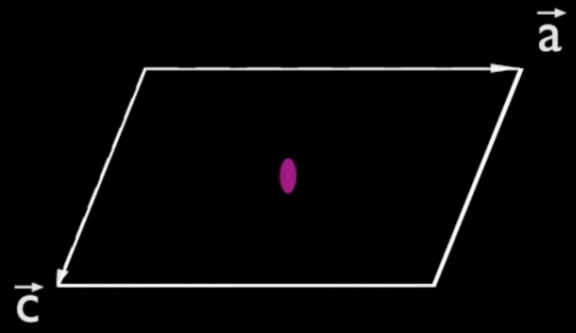
2

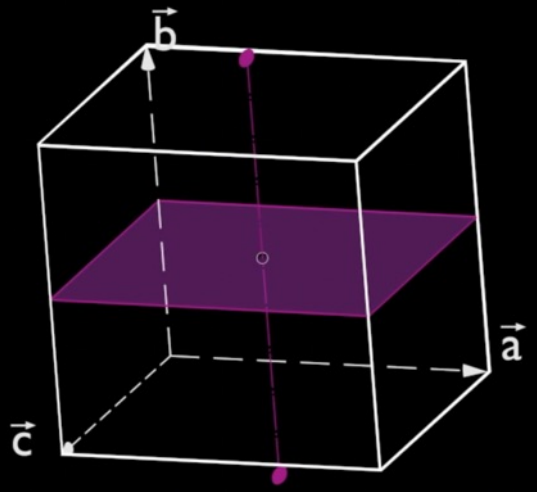


m



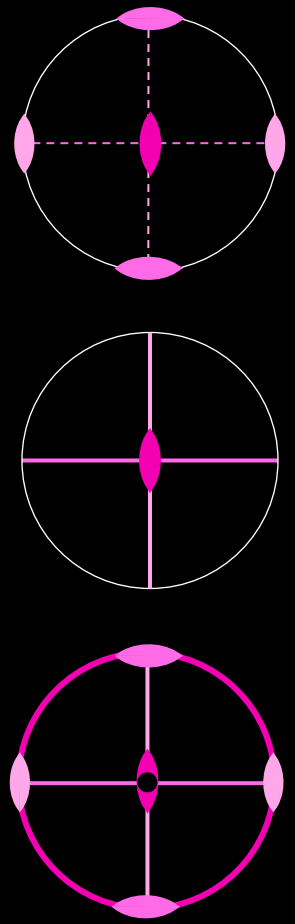
2/m





$\alpha = \gamma = 90°$

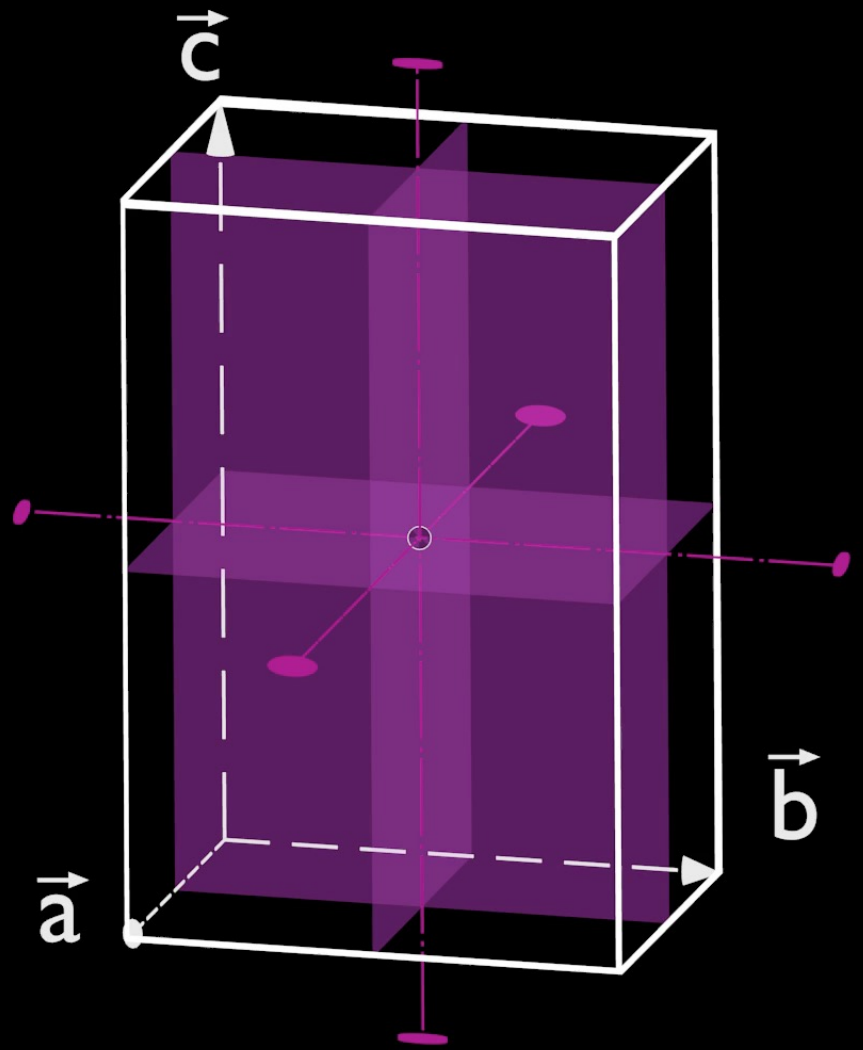
orthorhombic system



2 2 2

m m 2

m m m



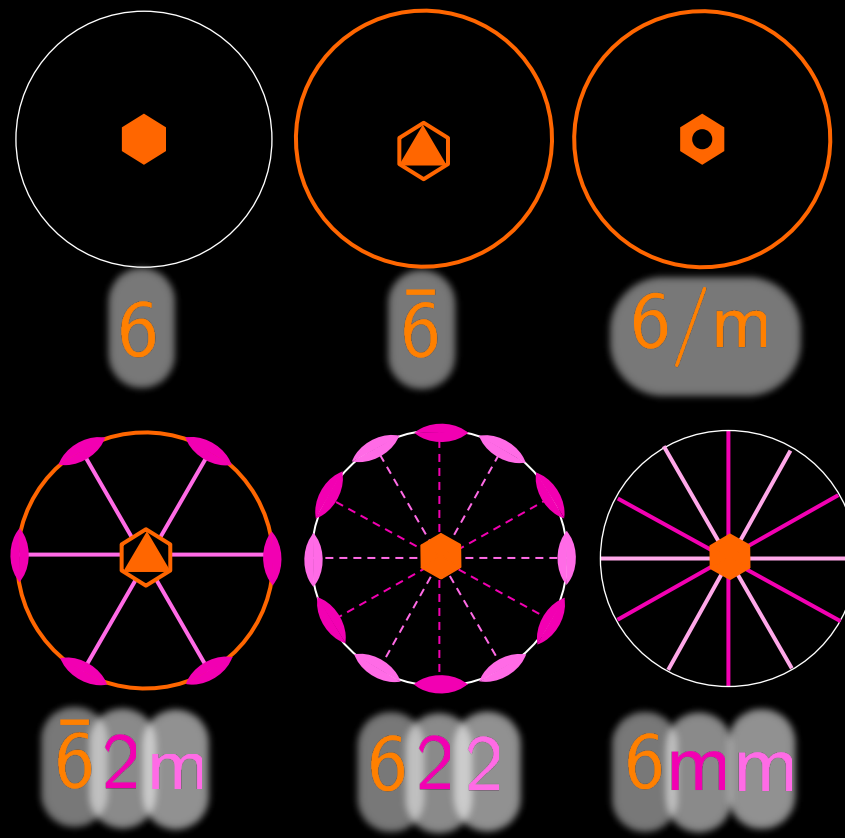
$\alpha = \beta = \gamma = 90°$

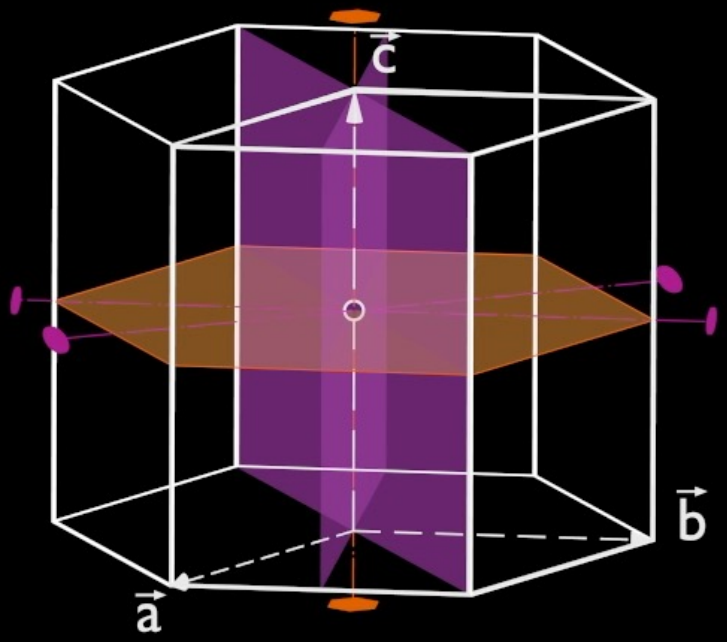
direction [100]

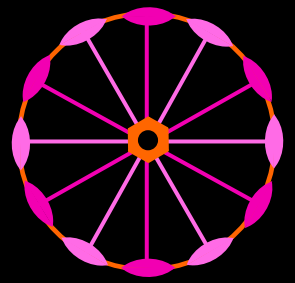
direction [010]

direction [001]

hexagonal system







$\frac{6}{m}\frac{m}{}\frac{m}{}$ ← holohedry

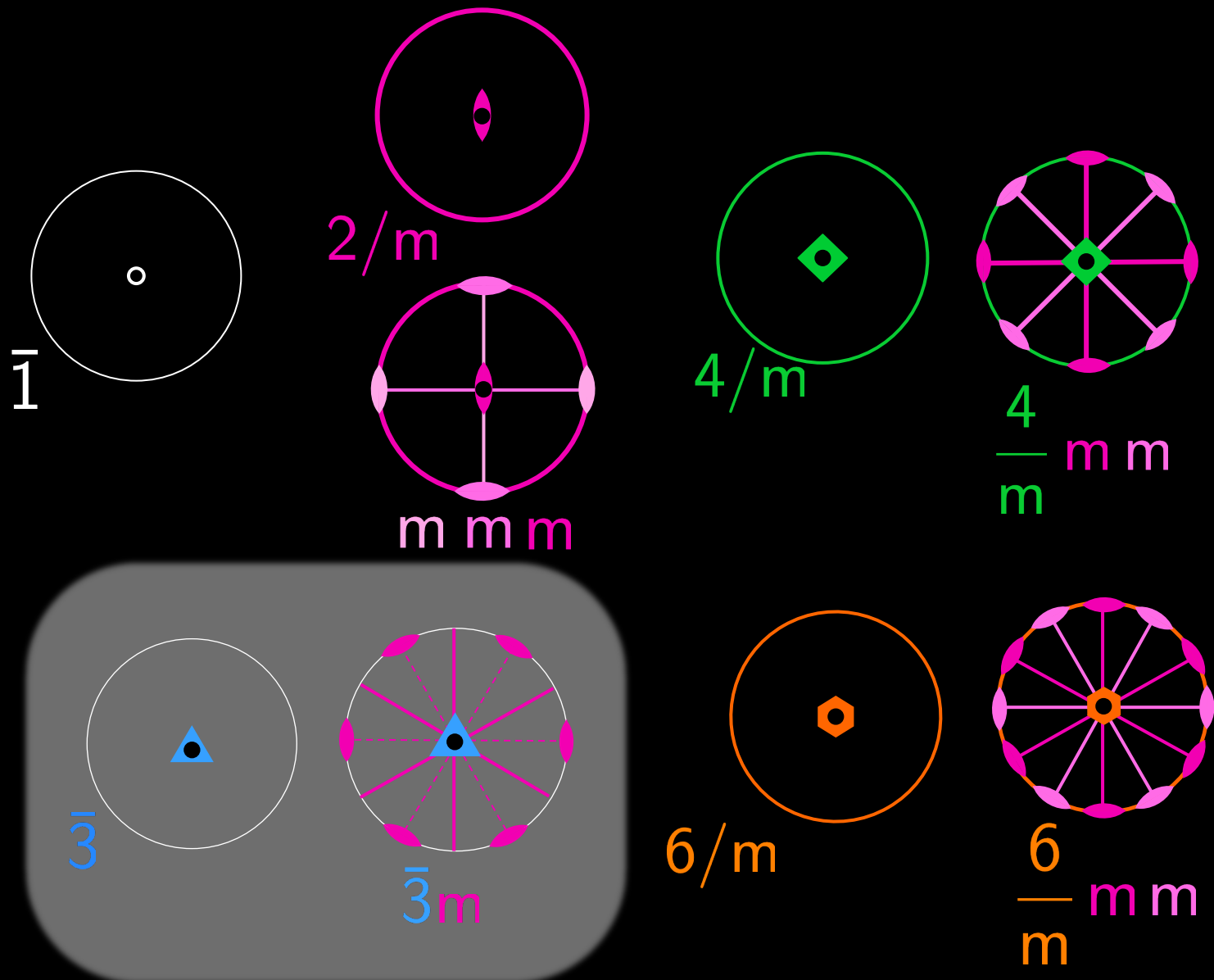
A_6 → a = b
γ = 120°

M ⊥ A_6 →
α = β = 90°

direction [001]

directions
[100], [010], [$\bar{1}\bar{1}$0]

directions
[1$\bar{1}$0], [120], [$\bar{2}\bar{1}$0]

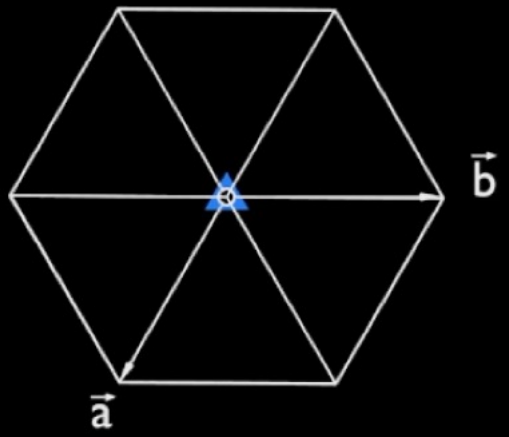


11 Laue Classes

trigonal system



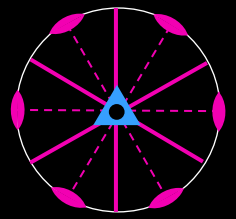
$\bar{3}$



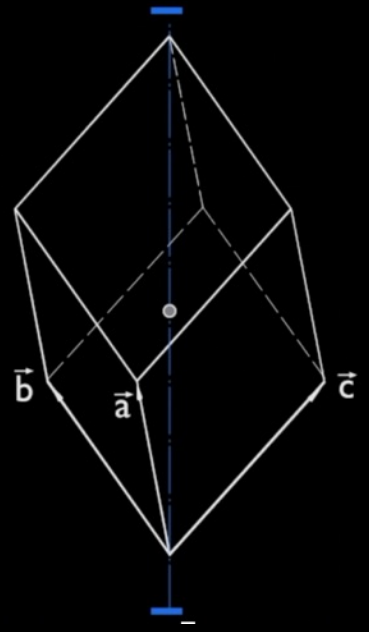
rhombohedral cell

$$a = b = c$$

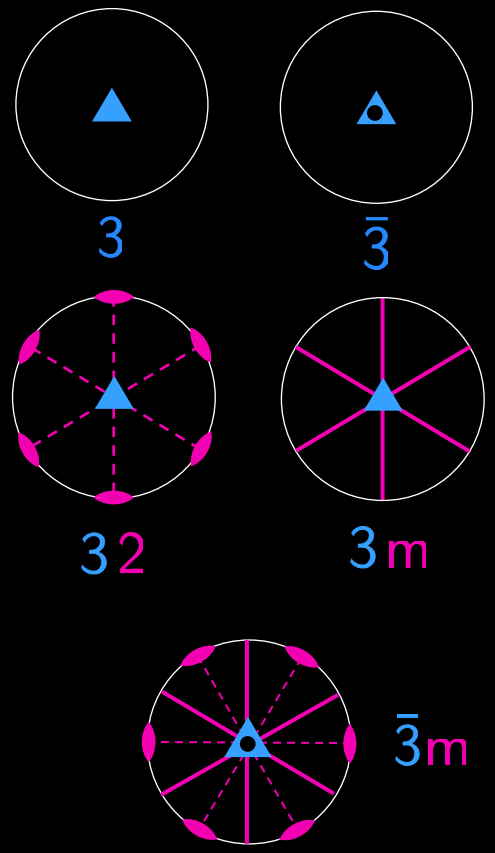
$$\alpha = \beta = \gamma$$



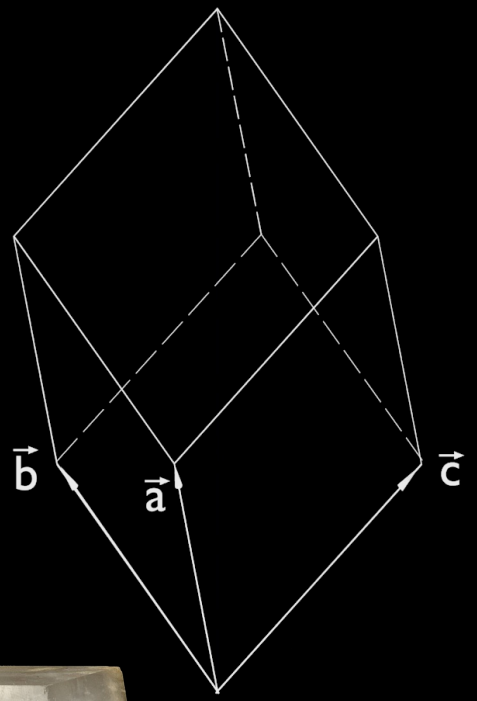
$\bar{3}m$



trigonal system



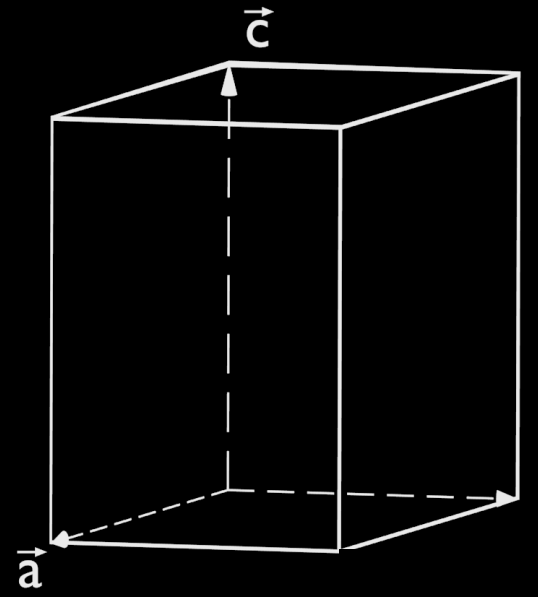
rhombohedral axes





calcite

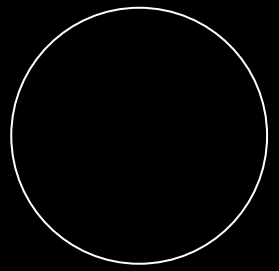
point groups compatible with hexagonal axes



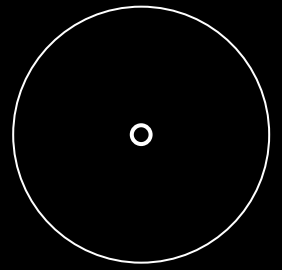


α-quartz

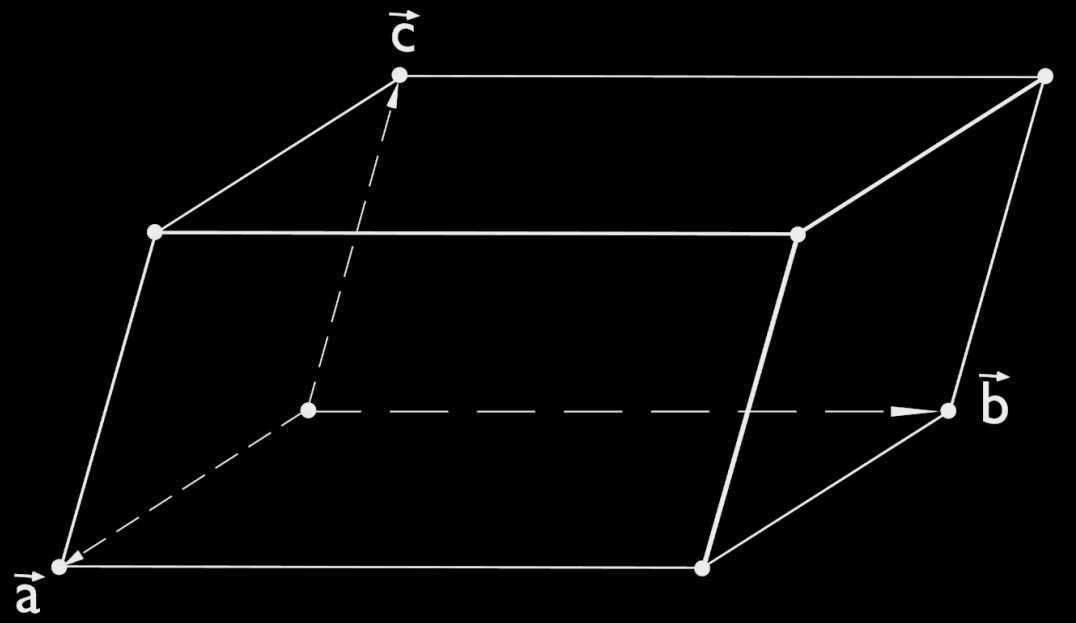
triclinic system



1



$\bar{1}$



Classification of the 32 point groups

crystal symmetry ≤ lattice symmetry

We have classified **the 32 point groups** according to the **3-dimensional lattice symmetry**, that defines 2 criteria:

1. Any lattice is centrosymmetric.
2. Any lattice that has a symmetry axis of order n>2 also presents n mirrors plane parallel to this axis.

➔ The 11 Laue classes (**criterion 1**) lead to 7 holohedries (criterion 2), which are each associated with one crystal system (with spectific restrictions on the cell parameters).

➔ The other 25 groups have lower symmetry. In order to find the symmetry of their lattice, just add to the symmetry elements of the group those which are necessary to satisfy criteria 1 and 2.

9 – The 7 crystal systems

Classification of the 32 point groups

Crystal system	*This course*	Hermann-Mauguin	Schoenflies
triclinic	A_1	1	C_1
1	C	$\bar{1}$	$C_i \equiv S_2$
monoclinic	A_2	2	C_2
2	$\mathrm{M} \equiv \bar{\mathrm{A}}_2$	m	$C_{1h} \equiv C_s$
	$\frac{\mathrm{A}_2}{\mathrm{M}}$ C	$2/m$	C_{2h}
orthorhombic	$\mathrm{A}_2\ \mathrm{M}'\ \mathrm{M}''$	$m\ m\ 2$	C_{2v}
3	$\mathrm{A}_2\ \mathrm{A}_2'\ \mathrm{A}_2''$	$2\ 2\ 2$	D_2
	$\frac{\mathrm{A}_2}{\mathrm{M}}\ \frac{\mathrm{A}_2'}{\mathrm{M}'}\ \frac{\mathrm{A}_2''}{\mathrm{M}''}$ C	$m\ m\ m$	D_{2h}
tetragonal	A_4	4	C_4
4	$\bar{\mathrm{A}}_4$	$\bar{4}$	S_4
	$\mathrm{A}_4\ 2\mathrm{M}'\ 2\mathrm{M}''$	$4\ m\ m$	C_{4v}
	$\frac{\mathrm{A}_4}{\mathrm{M}}$ C	$4/m$	C_{4h}
	$\bar{\mathrm{A}}_4\ 2\mathrm{A}_2'\ 2\mathrm{M}''$	$\bar{4}\ 2\ m$ (ou $\bar{4}\ m\ 2$)	D_{2d}
	$\mathrm{A}_4\ 2\mathrm{A}_2'\ 2\mathrm{A}_2''$	$4\ 2\ 2$	D_4
	$\frac{\mathrm{A}_4}{\mathrm{M}}\ \frac{2\mathrm{A}_2'}{2\mathrm{M}'}\ \frac{2\mathrm{A}_2''}{2\mathrm{M}''}$ C	$4/m\ m\ m$	D_{4h}
trigonal	A_3	3	C_3
5	$\bar{\mathrm{A}}_3$	$\bar{3}$	$C_{3i} \equiv S_6$
	$\mathrm{A}_3\ 3\mathrm{M}'$	$3\ m$	C_{3v}
	$\mathrm{A}_3\ 3\mathrm{A}_2'$	$3\ 2$	D_3
	$\bar{\mathrm{A}}_3\ \frac{3\mathrm{A}_2'}{3\mathrm{M}'}$ C	$\bar{3}\ m$	D_{3d}
hexagonal	A_6	6	C_6
6	$\bar{\mathrm{A}}_6$	$\bar{6}$	$C_{3h} \equiv S_3$
	$\mathrm{A}_6\ 3\mathrm{M}'\ 3\mathrm{M}''$	$6\ m\ m$	C_{6v}
	$\frac{\mathrm{A}_6}{\mathrm{M}}$ C	$6/m$	C_{6h}
	$\bar{\mathrm{A}}_6\ 3\mathrm{A}_2'\ 3\mathrm{M}''$	$\bar{6}\ 2\ m$	D_{3h}
	$\mathrm{A}_6\ 3\mathrm{A}_2'\ 3\mathrm{A}_2''$	$6\ 2\ 2$	D_6
	$\frac{\mathrm{A}_6}{\mathrm{M}}\ \frac{3\mathrm{A}_2'}{3\mathrm{M}'}\ \frac{3\mathrm{A}_2''}{3\mathrm{M}''}$ C	$6/m\ m\ m$	D_{6h}
cubic	$3\mathrm{A}_2\ 4\mathrm{A}_3$	$2\ 3$	T
7	$\frac{3\mathrm{A}_2}{3\mathrm{M}}\ 4\bar{\mathrm{A}}_3$ C	$m\ \bar{3}$	T_h
	$3\bar{\mathrm{A}}_4\ 4\mathrm{A}_3\ 6\mathrm{M}'$	$\bar{4}\ 3\ m$	T_d
	$3\mathrm{A}_4\ 4\mathrm{A}_3\ 6\mathrm{A}_2'$	$4\ 3\ 2$	O
	$\frac{3\mathrm{A}_4}{3\mathrm{M}}\ 4\bar{\mathrm{A}}_3\ \frac{6\mathrm{A}_2'}{6\mathrm{M}'}$ C	$m\ \bar{3}\ m$	O_h

Course outline

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2- Internal cause of the natural crystal shape

3 – Crystal lattice, cell, motif

4 – Lattice direction and planes

5 – Reciprocal lattice

6 – Crystal lattice & symmetries

7 – Conventional cell (unit cell)

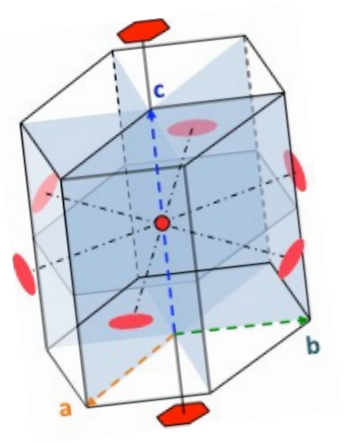
8 – The 32 crystallographic point groups

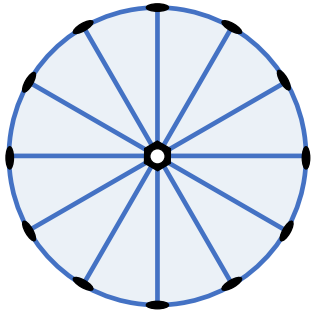
9 – The 7 crystal systems

10 – The 14 Bravais lattices

11 – The 230 space-groups



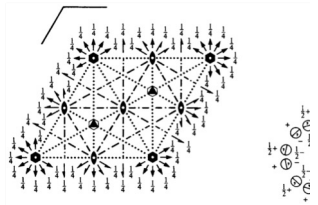




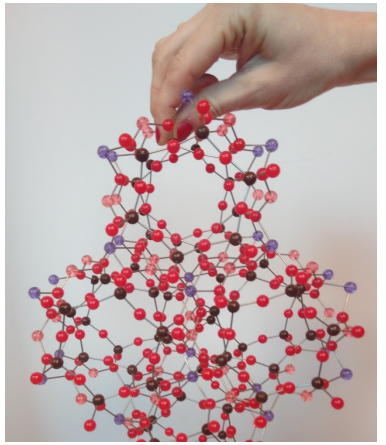
$$\frac{6}{m}mm$$

$P6/mcc$ D^2_{6h}

No. 192 $P\ 6/m\ 2/c\ 2/c$



Origin at centre $(6/m)$ at $6/mcc$



10 – The 14 Bravais lattices

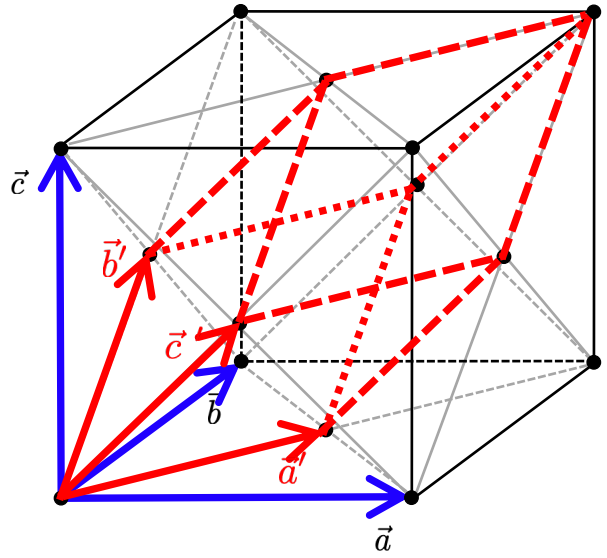
1 Bravais lattice ➔ 1 conventional cell = unit cell = holohedral cell

Conventional cell = unit cell (the cell chosen to define a crystal lattice):

smallest volume with the **same symmetry as the lattice**
and defined by 3 basis-vectors **a**, **b** and **c**.

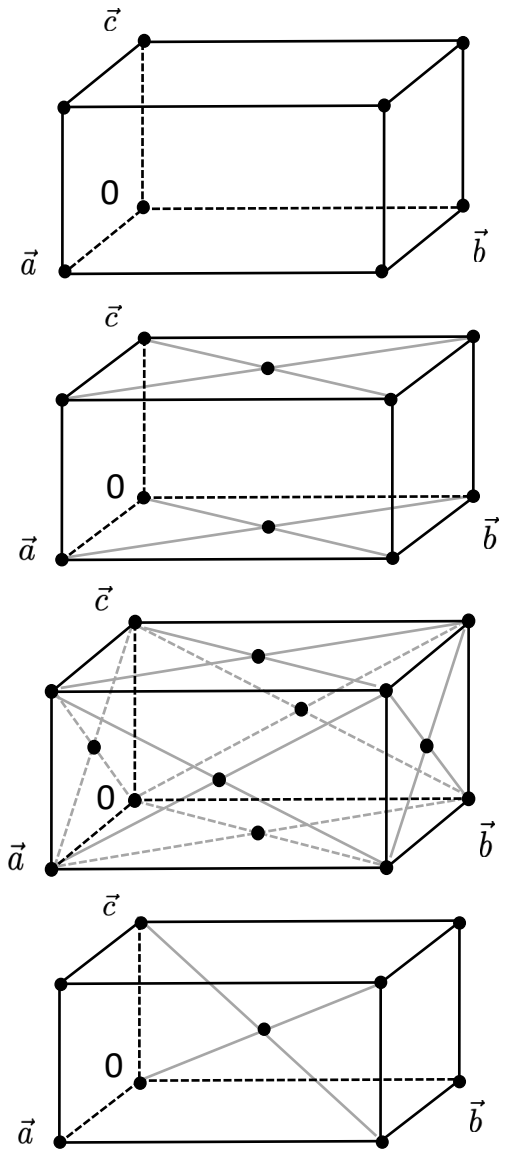
➔ When the most symmetric cell is the smallest, the conventional cell is **primitive**.

➔ When the most symmetric is not the smallest, the conventional cell is a **supercell**.



ex: fcc cell

10 – The 14 Bravais lattices



3D primitive cell and supercells

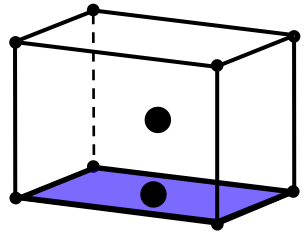
Translations	Cell	Lattice type	Cell Multiplicity
$\vec{a},\ \vec{b},\ \vec{c}$	primitive (*or simple*)	P	1
$\vec{a},\ \vec{b},\ \vec{c},\ \frac{\vec{b}+\vec{c}}{2}$	centred on face $(\vec{b},\ \vec{c})$	A	2
$\vec{a},\ \vec{b},\ \vec{c},\ \frac{\vec{a}+\vec{c}}{2}$	centred on face $(\vec{a},\ \vec{c})$	B	2
$\vec{a},\ \vec{b},\ \vec{c},\ \frac{\vec{a}+\vec{b}}{2}$	centred on face $(\vec{a},\ \vec{b})$	C	2
$\vec{a},\ \vec{b},\ \vec{c},\ \frac{\vec{a}+\vec{b}}{2},\ \frac{\vec{b}+\vec{c}}{2},\ \frac{\vec{a}+\vec{c}}{2}$	all-faces centred	F	4
$\vec{a},\ \vec{b},\ \vec{c},\ \frac{\vec{a}+\vec{b}+\vec{c}}{2}$	body centred	I	2

➔ **4 lattice types** (i.e. 4 translation groups)

Bravais lattice: associates a crystal system with a lattice type

7 crystal systems
4 lattice types
} 28 possibilities?

➔ only 14 Bravais lattices

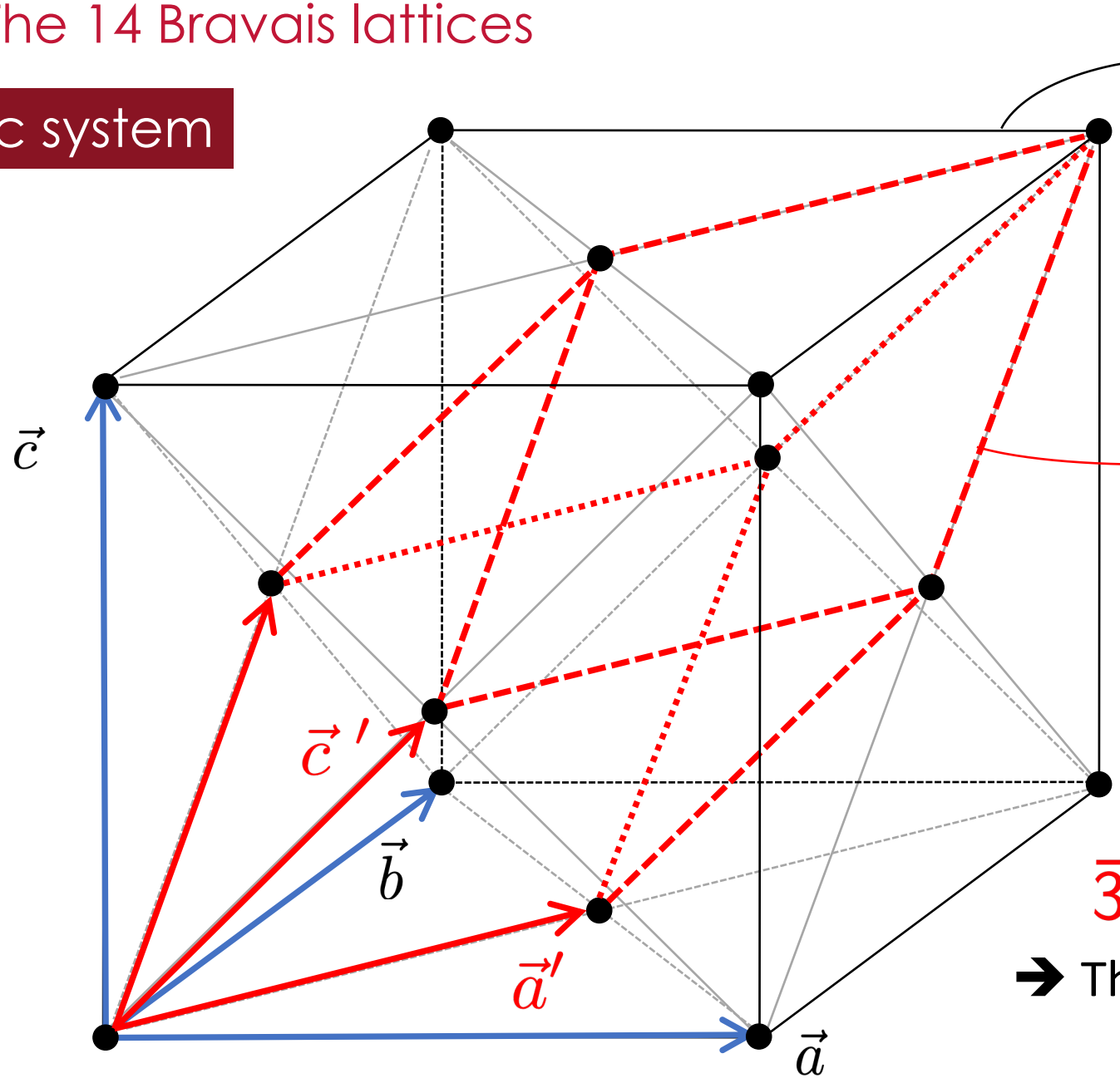


Is the starting holohedry conserved in the new primitive cell?

yes → Bravais lattice of **primitive cell**

no → Bravais lattice of **supercell**

Cubic system

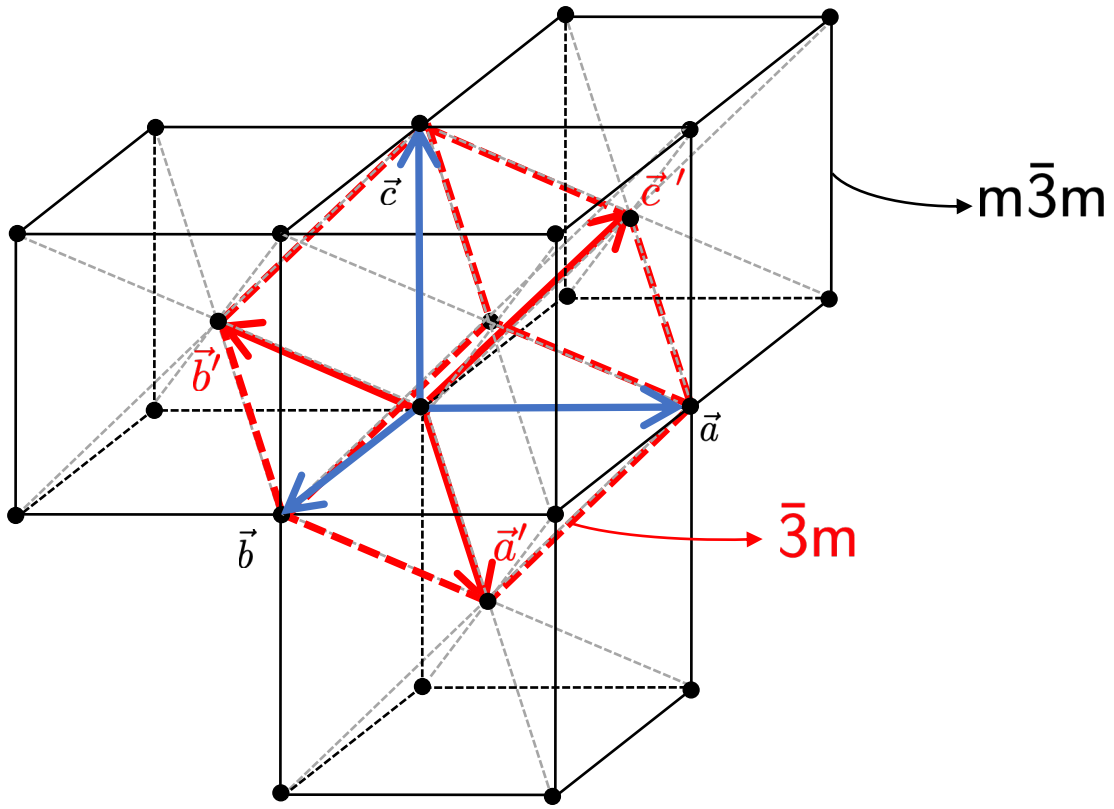


3̄m lower symmetry than m3̄m

➔ The face-centered cubic lattice exists!

10 – The 14 Bravais lattices

Cubic system



➡ 3 Bravais lattices

- cubic P (*cP*)
- cubic I (*cI*)
- cubic F (*cF*)

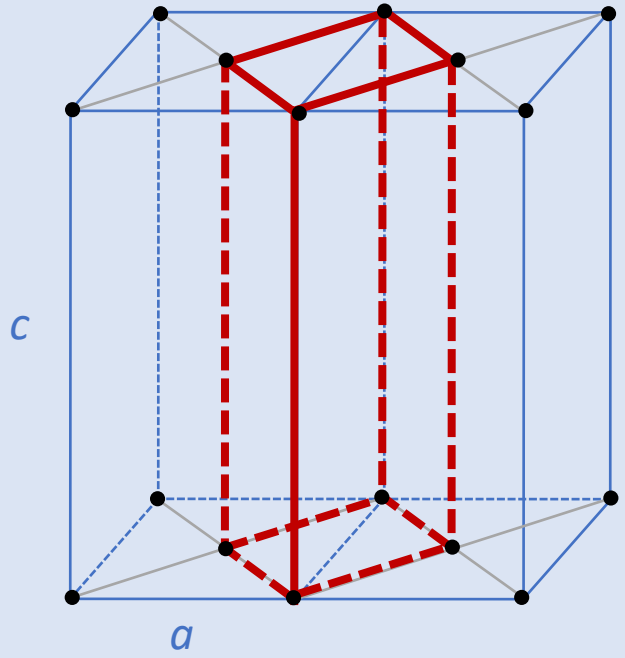
Tetragonal system

2 Bravais lattices

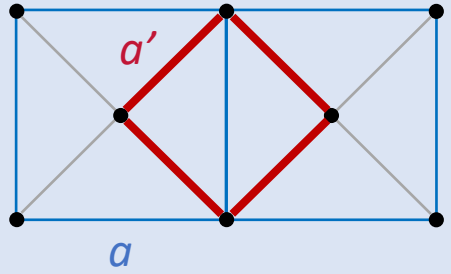
- tetragonal P (*tP*)
- tetragonal I (*tI*)

Exercize

Why doesn't the tetragonal C Bravais lattice exist?



It is possible to define a smaller tetragonal cell with parameters
a' = a / √2
c' = c



➔ It is equivalent to **tetragonal P** Bravais lattice

10 – The 14 Bravais lattices

Orthorhombic system

4 Bravais lattices

- orthorhombic P (*oP*) — 6
- orthorhombic I (*oI*) — 7
- orthorhombic with centred base (*oS*) — 8
  - *oA*
  - *oB*
  - *oC*
- orthorhombic F (*oF*) — 9

Monoclinic system

2 Bravais lattices

- monoclinic P (*mP*) — 10
- monoclinic with double cell (*mS*) — 11

unique axis $\vec{b}$

mC *mA* *mI*

Triclinic system

''anortic''

- triclinic P (*aP*) — 12

10 – The 14 Bravais lattices

Hexagonal system

1 Bravais lattice

➔ hexagonal primitive (*hP*) (13)

do not confuse with the **hcp** structure of some metals

Trigonal system

$\bar{3}$ m

hexagonal axes (hexagonal primitive cell)

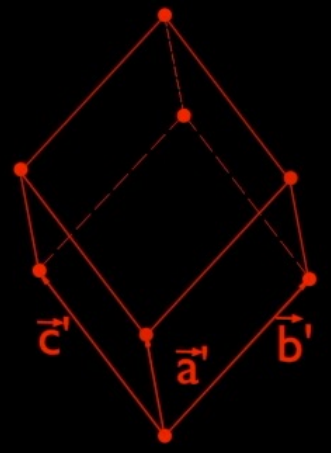
rhombohedral axes (rhombohedral cell)

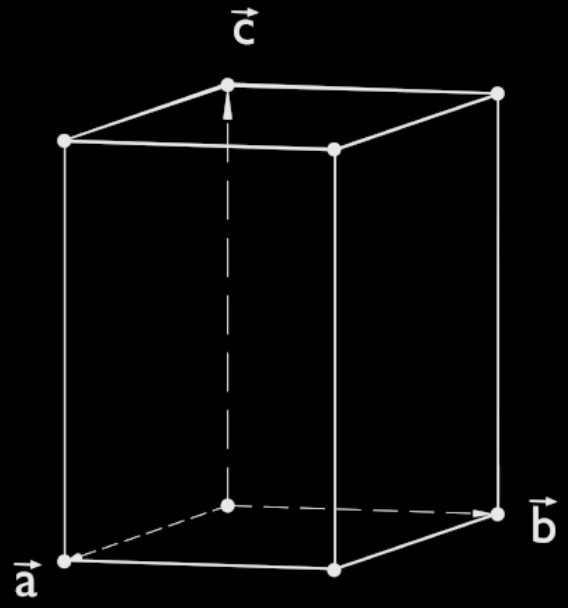
➔ Bravais lattice *hR (also primitive)* (14)

but in pratice, hR lattice are commonly described using a triple hexagonal cell

Bravais lattice *hR*

h R Bravais lattice





$$+\left(\frac{1}{3},\frac{2}{3},\frac{2}{3}\right)$$

$$+\left(\frac{2}{3},\frac{1}{3},\frac{1}{3}\right)$$

A_1	A_2		A_3	A_4	A_6	$3A_2 4A_3$
$\bar{A}_1$	$\bar{A}_2$		$\bar{A}_3$	$\bar{A}_4$	$\bar{A}_6$	$\frac{3A_2}{3M} 4\bar{A}_3 C$
		$MM'A_2''$	$A_3 3M'$	$A_4 2M' 2M''$	$A_6 3M' 3M''$	
	$\frac{A_2}{M} C$			$\frac{A_4}{M} C$	$\frac{A_6}{M} C$	
			$\bar{A}_3 \frac{3A_2'}{3M'} C$	$\bar{A}_4 2A_2' 2M''$	$\bar{A}_6 3A_2' 3M''$	$3\bar{A}_4 4A_3 6M'$
		$A_2 A_2' A_2''$	$A_3 3A_2'$	$A_4 2A_2' 2A_2''$	$A_6 3A_2' 3A_2''$	$3A_4 4A_3 6A_2'$
		$\frac{A_2}{M} \frac{A_2'}{M'} \frac{A_2''}{M''} C$		$\frac{A_4}{M} \frac{2A_2'}{2M'} \frac{2A_2''}{2M''} C$	$\frac{A_6}{M} \frac{3A_2'}{3M'} \frac{3A_2''}{3M''} C$	$\frac{3A_4}{3M} 4\bar{A}_3 \frac{6A_2'}{6M'} C$
triclinic	monoclinic	orthorhombic	trigonal	tetragonal	hexagonal	cubic
	$\alpha = \gamma = 90°$ or $\alpha = \beta = 90°$	$\alpha = \beta = \gamma = 90°$	rhombohedral cell $a = b = c$ $\alpha = \beta = \gamma$ hexagonal cell $a = b$ $\alpha = \beta = 90°$ $\gamma = 120°$	$a = b$ $\alpha = \beta = \gamma = 90°$	$a = b$ $\alpha = \beta = 90°$ $\gamma = 120°$	$a = b = c$ $\alpha = \beta = \gamma = 90°$
aP	mP, mS (S=A,B,C or I)	oP, oI, oF, oS (S=A, B or C)	hR ou hP	tP, tI	hP	cP, cI, cF

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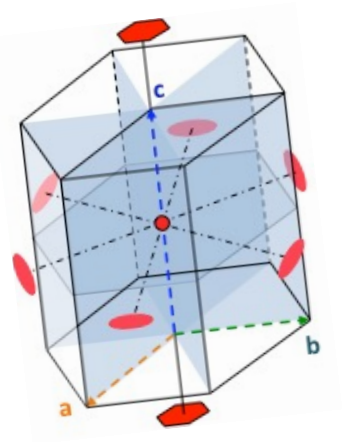
8 – The 32 crystallographic point groups

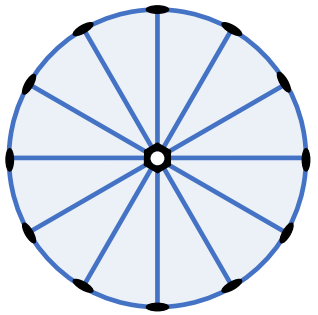
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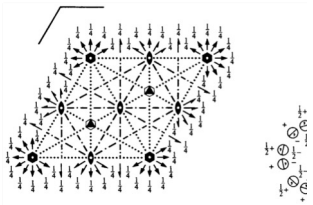




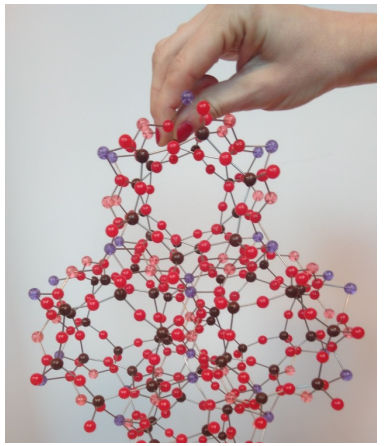
$$\frac{6}{m}mm$$

$P6/mcc$ D^2_{6h}

No. 192 $P\ 6/m\ 2/c\ 2/c$



Origin at centre $(6/m)$ at $6/mcc$



11 – Space groups

Orientation symmetry ➔ 32 crystallographic point groups

set of the symmetry operations that let invariant crystal morphology and its physical properties

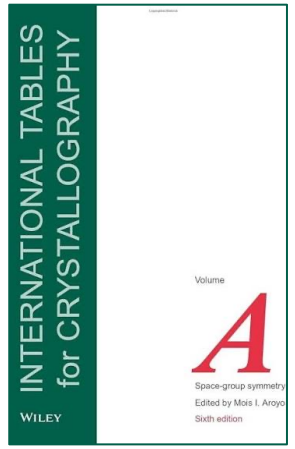
7 crystal systems (6 crystal families)

+ 4 lattice types
(translation groups)

14 Bravais lattices

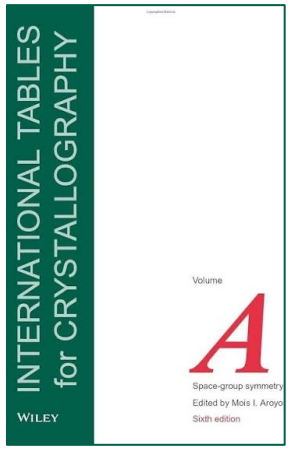
Position symmetry ➔ the 230 space groups

set of the symmetry operations that let invariant the atomic structure



11 – Space groups

International Tables of Crystallography: an example of space group



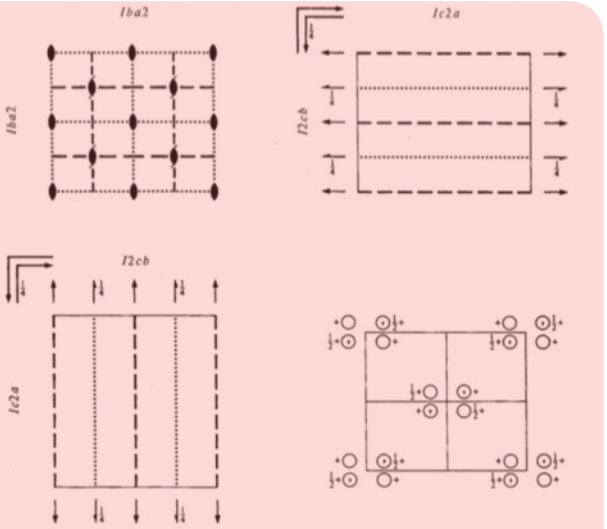
International Tables for Crystallography (2006). Vol. A, Space group 45, pp. 258–259.

$Iba2$?
No. 45

C_{2v}^{21}
$Iba2$

$mm2$ Orthorhombic

Patterson symmetry $Immm$



?

Origin on $cc2$

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

Symmetry operations

For $(0,0,0)+$ set
(1) 1 (2) 2 $0,0,z$ (3) a $x,\frac{1}{4},z$ (4) b $\frac{1}{4},y,z$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set
(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ (2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$ (3) c $x,0,z$ (4) c $0,y,z$

CONTINUED No. 45 $Iba2$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$			General:
8	c	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(4) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	hkl : $h+k+l=2n$ $0kl$: $k,l=2n$ $h0l$: $h,l=2n$ $hk0$: $h+k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
4	b	$..2$	$0,\frac{1}{4},z$		$\frac{1}{2},0,z$		hkl : $l=2n$
4	a	$..2$	$0,0,z$		$\frac{1}{2},\frac{1}{4},z$		hkl : $l=2n$

to know how to use this section

?

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [010] $p11m$
$\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I	[2] $I1a1$ (Cc, 9)	(1; 3)+
	[2] $Ib11$ (Cc, 9)	(1; 4)+
	[2] $I112$ ($C2$, 5)	(1; 2)+
IIa	[2] $Pba2$ (32)	1; 2; 3; 4
	[2] $Pca2_1$ (29)	1; 3; (2; 4) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $Pbc2_1$ ($Pca2_1$, 29)	1; 4; (2; 3) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	[2] $Pcc2$ (27)	1; 2; (3; 4) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
IIb	none	

Maximal isomorphic subgroups of lowest index

IIc [3] $Iba2$ ($\mathbf{a}' = 3\mathbf{a}$ or $\mathbf{b}' = 3\mathbf{b}$) (45); [3] $Iba2$ ($\mathbf{c}' = 3\mathbf{c}$) (45)

Minimal non-isomorphic supergroups

I [2] $Ibam$ (72); [2] $Ibca$ (73); [2] $I4cm$ (108); [2] $I4_1cd$ (110); [2] $I\bar{4}c2$ (120)

II [2] $Cmm2$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) (35); [2] $Aem2$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) (39); [2] $Bme2$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) ($Aem2$, 39)

The symmorphic groups (73)

*Association of the symmetry elements of the crystallographic point groups with the Bravais lattice translation groups: the generators **are neither** screw axes **nor** glide planes)*

Hermann-Mauguin symbols: Lattice-type letter (P, A, B, C, I, F, R) followed by the Hermann-Mauguin symbol of the crystallographic point group

examples : *P m m m*, *F m m m*, *P 4 m m*, *I 4 m m*

The non-symmorphic groups(157)

Space groups whose generators are screw axes and/or glide planes.

examples : *I b a* 2, *P* 4_1, *P* 4_2 *c m*

position symmetry elements

- The 10 symmetry elements of the crystallographic point groups
- New symmetry elements resulting from products:
  - $m \times \vec{t}$ → **glide planes**
  - $\mathrm{A}_n \times \vec{t}$ → **screw axes**

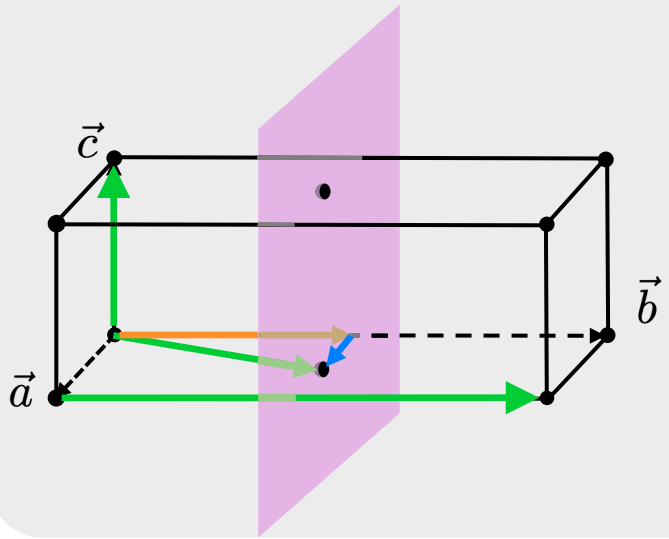
Glide plane

mirror plane m × $\vec{t}$

case 1: $\vec{t} \parallel$ mirror $\quad \vec{t} = \vec{c}$

case 2: $\vec{t} \perp$ mirror $\quad \vec{t} = \vec{b}$

case 3: $\vec{t}$ oblique / mirror $\quad \vec{t} = \frac{\vec{a}+\vec{b}}{2} \quad \vec{t} = \vec{t}_{\perp} + \vec{t}_{\parallel}$

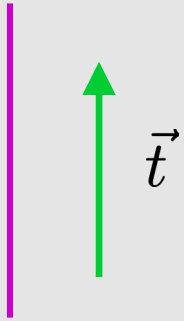


$\vec{t}_{\perp}$ & $\vec{t}_{\parallel}$ *are not lattice translation*

Glide plane

case 1: $m \times \vec{t}$ with $\vec{t} \parallel m$

m *perpendicular to the screen*

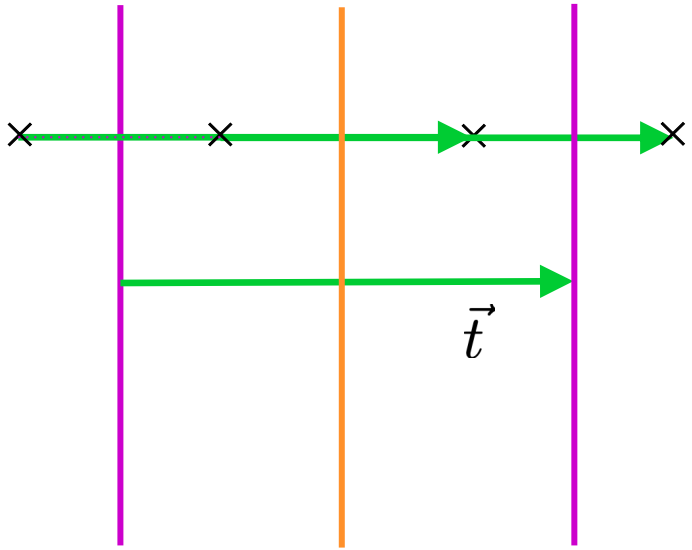


any mirror plane m is infinite

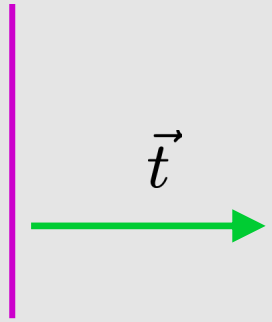
Any translation $\vec{t} \parallel m$
has no effect on it

Glide plane

case 2: $m \times \vec{t}$ with $\vec{t} \perp m$



m *perpendicular to the screen*



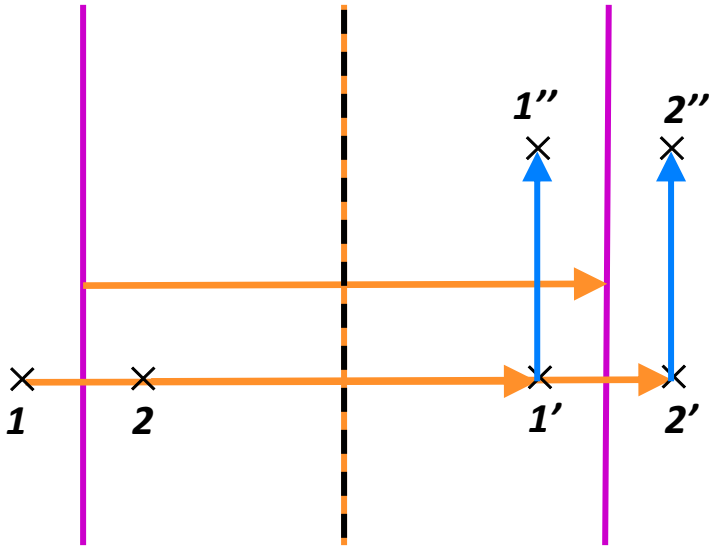
→ new mirror plane m at $\frac{\vec{t}}{2}$ from the first one

Glide plane

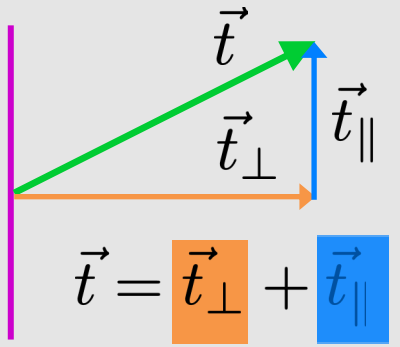
case 3: $m \times \vec{t}$ with $\vec{t}$ oblique / m

Decomposition $\vec{t} = \vec{t}_{\perp} + \vec{t}_{\parallel}$

where $\vec{t}_{\perp}$ & $\vec{t}_{\parallel}$ are the components $\perp$ & $\parallel$ to m.

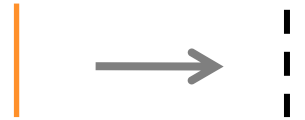


m perpendicular to the screen



$\vec{t}_{\parallel}$ changes the nature of the **mirror** obtained by considering $\vec{t}_{\perp}$, but only if $\vec{t}_{\parallel}$ **is not** a lattice translation.

glide plane



Glide plane

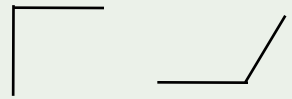
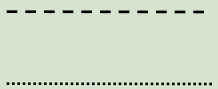
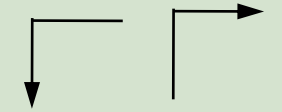
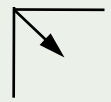
- Mirror m combined with a translation $\vec{t}_{\parallel}$ parallel to m
  ($\vec{t}_{\parallel}$ **is not** a lattice translation)
- Symmetry element of order 2; associated operation noted $\left(m, \vec{t}_{\parallel}\right)$

$$\left(m, \vec{t}_{\parallel}\right)^2 = \left(2\,m, 2\,\vec{t}_{\parallel}\right)$$ = identity thus $2\vec{t}_{\parallel} = p\,\vec{t}$ with p = 0 or 1

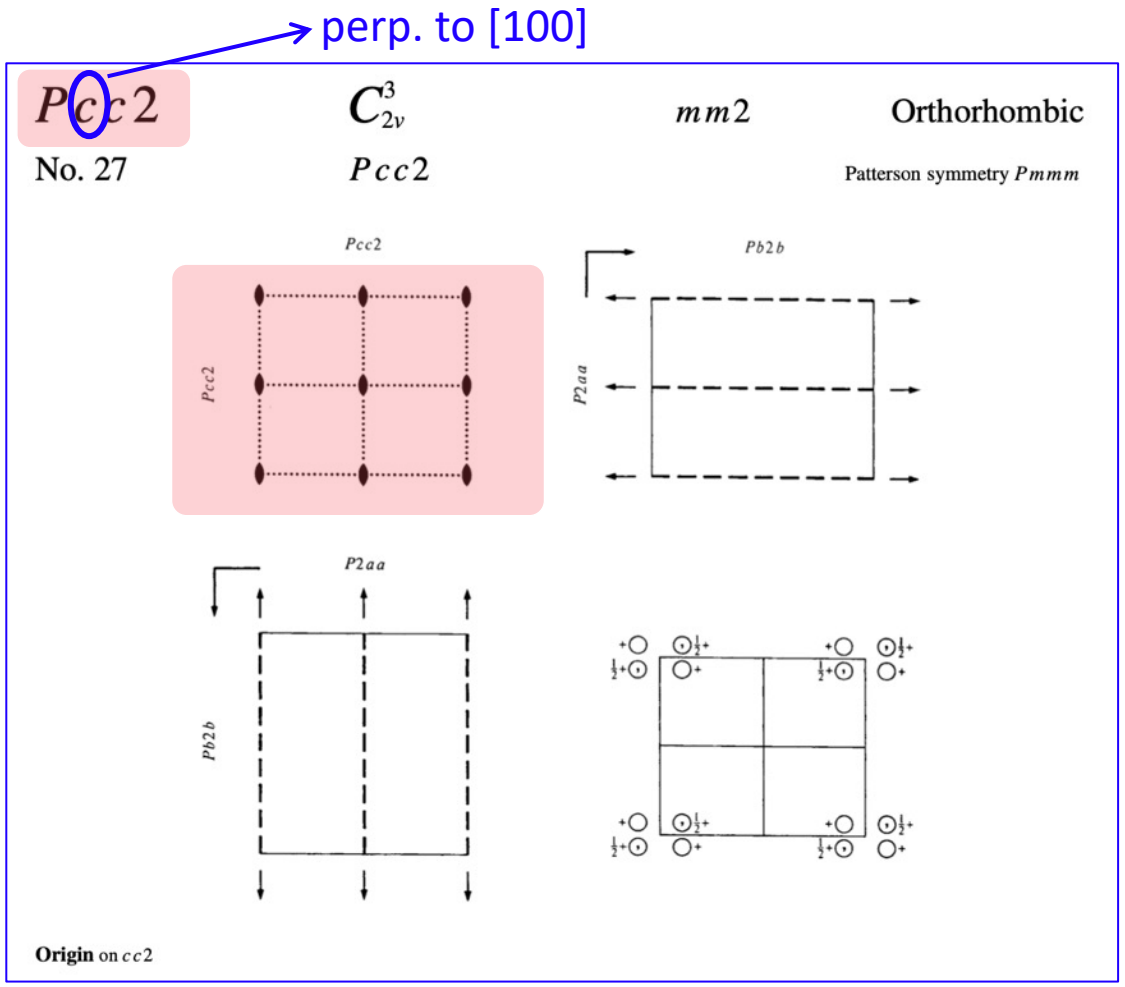
Axial glide planes

lattice translation	glide	symbol
$\vec{t} = \vec{a}$	$\vec{t}_{\parallel} = \frac{\vec{a}}{2}$	a
$\vec{t} = \vec{b}$	$\vec{t}_{\parallel} = \frac{\vec{b}}{2}$	b
$\vec{t} = \vec{c}$	$\vec{t}_{\parallel} = \frac{\vec{c}}{2}$	c

Glide plane

Type of plane	Symbol	Translation	Representation	
			normal to the plane of the figure	parallel to the plane of the figure
mirror plane	m	0		
axial glide plane	a or b c	$\vec{a}/2$ or $\vec{b}/2$ $\vec{c}/2$		
diagonal glide plane	n	$(\vec{a} \pm \vec{b})/2$ $(\vec{a} \pm \vec{c})/2$ $(\vec{b} \pm \vec{c})/2$		
diamond-type glide plane	d	$(\vec{a} \pm \vec{b})/4$ $(\vec{a} \pm \vec{c})/4$ $(\vec{b} \pm \vec{c})/4$		

glide planes as space group generators



The spacegroup symbol contains
2 glide planes *c*
that we can see on the schemes.

glide planes generated by lattice type I

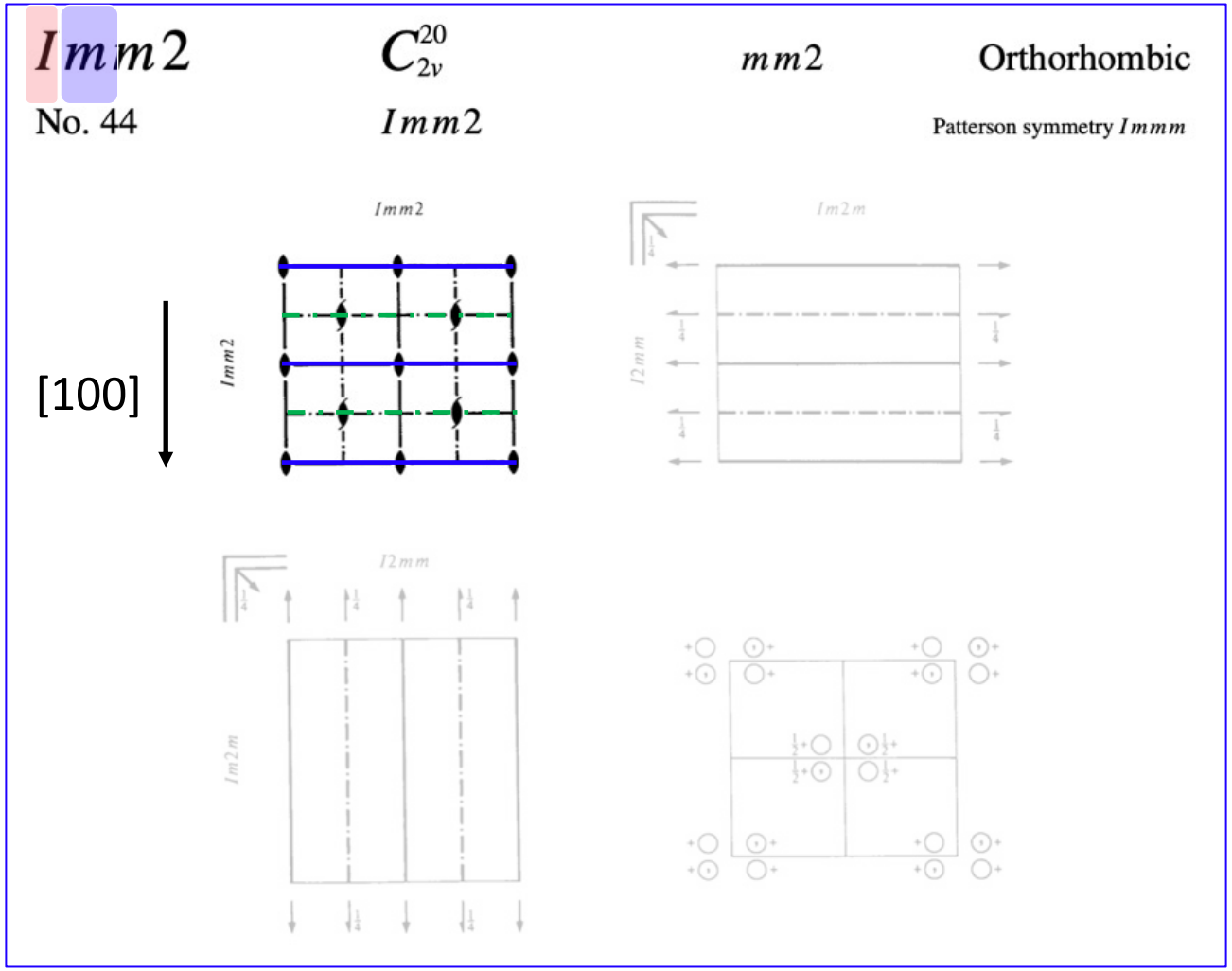
$m \perp [100]$

I lattice $\quad \vec{t} = \dfrac{\vec{a}+\vec{b}+\vec{c}}{2}$

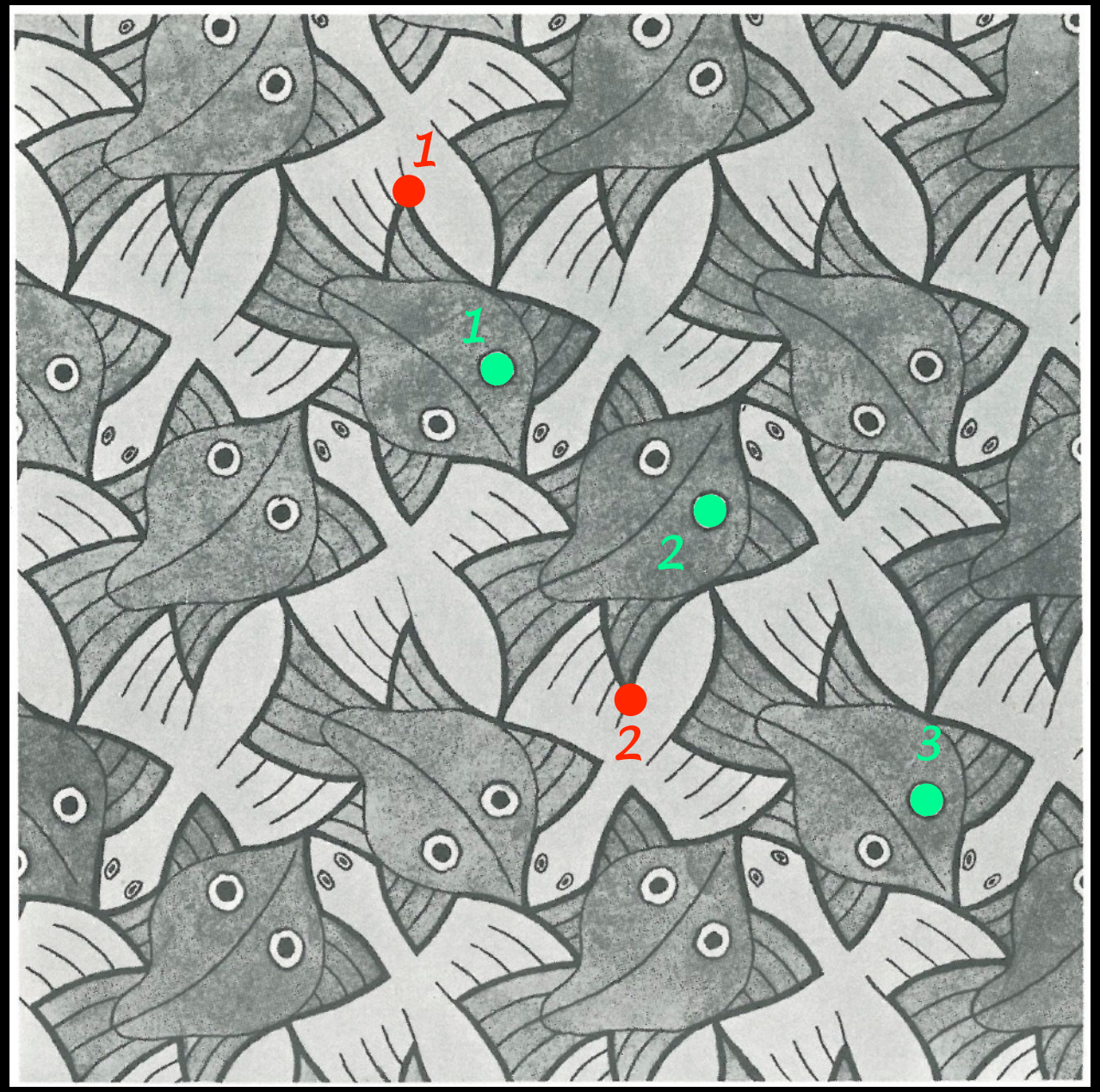
$\vec{t}_{\perp} = \dfrac{\vec{a}}{2}$

$\vec{t}_{\parallel} = \dfrac{\vec{b}+\vec{c}}{2}$

➔ Glide plane of type n (diagonal glide) at $\dfrac{\vec{t}_{\perp}}{2}$



Exercize



motif = 2 birds and 2 fishes

asymmetric unit
=
1 bird and 1 fish

Determine the symmetry element that permits to go from a point of the asymmetric unit to an equivalent one

reproduction of periodic drawing n°110
by Escher
(ink and watercolor, 1961)

screw axis

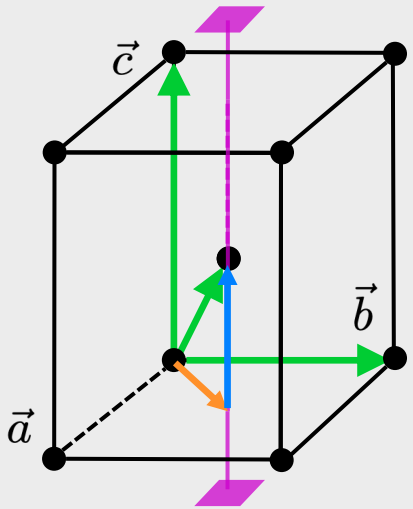
axis A_n × $\vec{t}$

casse 1: $\vec{t} \parallel$ axis $\quad \vec{t} = \vec{c}$

case 2: $\vec{t} \perp$ axis $\quad \vec{t} = \vec{b}$

case 3: $\vec{t}$ oblique / axis $\quad \vec{t} = \frac{\vec{a}+\vec{b}+\vec{c}}{2} \quad \vec{t} = \vec{t}_{\perp} + \vec{t}_{\parallel}$

$\vec{t}_{\perp}$ & $\vec{t}_{\parallel}$ *are not lattice translations*



screw axis

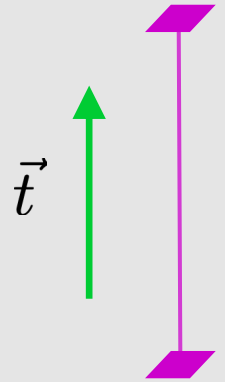
case 1: $\mathrm{A}_n \times \vec{t}$ with $\vec{t} \parallel \mathrm{A}_n$

Any axis A_n is infinite

$\vec{t}$ has no effect on it

wether $\vec{t}$ is a lattice translation or not

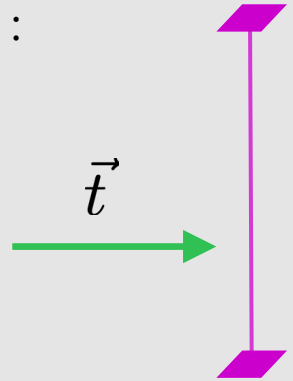
example :
$n = 4$

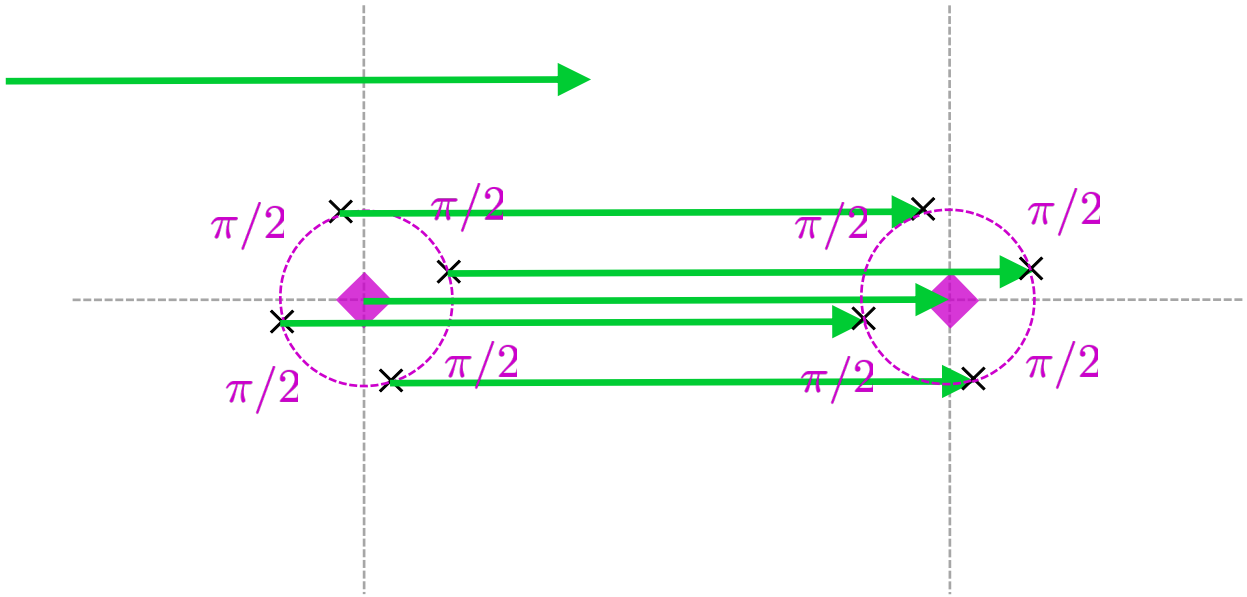


screw axis

case 2: $\mathrm{A}_n \times \vec{t}$ with $\vec{t} \perp \mathrm{A}_n$

example :
$n = 4$

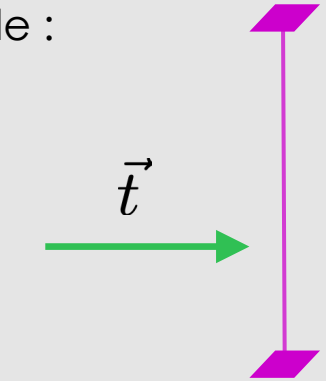


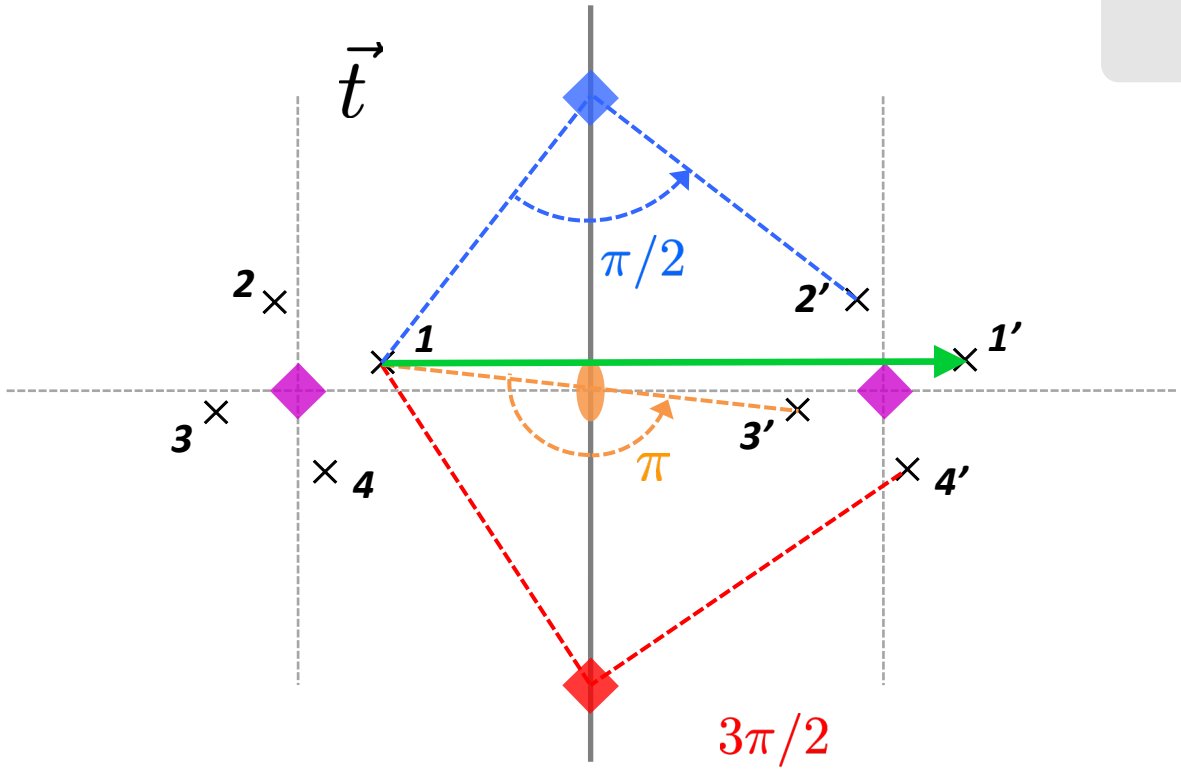


screw axis

case 2: $\mathrm{A}_n \times \vec{t}$ with $\vec{t} \perp \mathrm{A}_n$

example :
$n = 4$





$1 \longrightarrow 1' : \vec{t}$

$1 \longrightarrow 2' : \mathrm{A}_4$

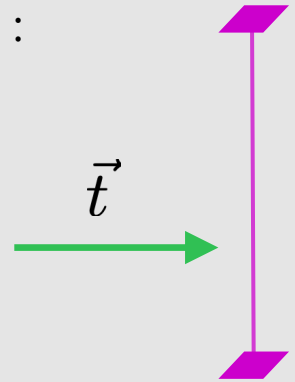
$1 \longrightarrow 3' : \mathrm{A}_2$

$1 \longrightarrow 4' : \mathrm{A}_4$

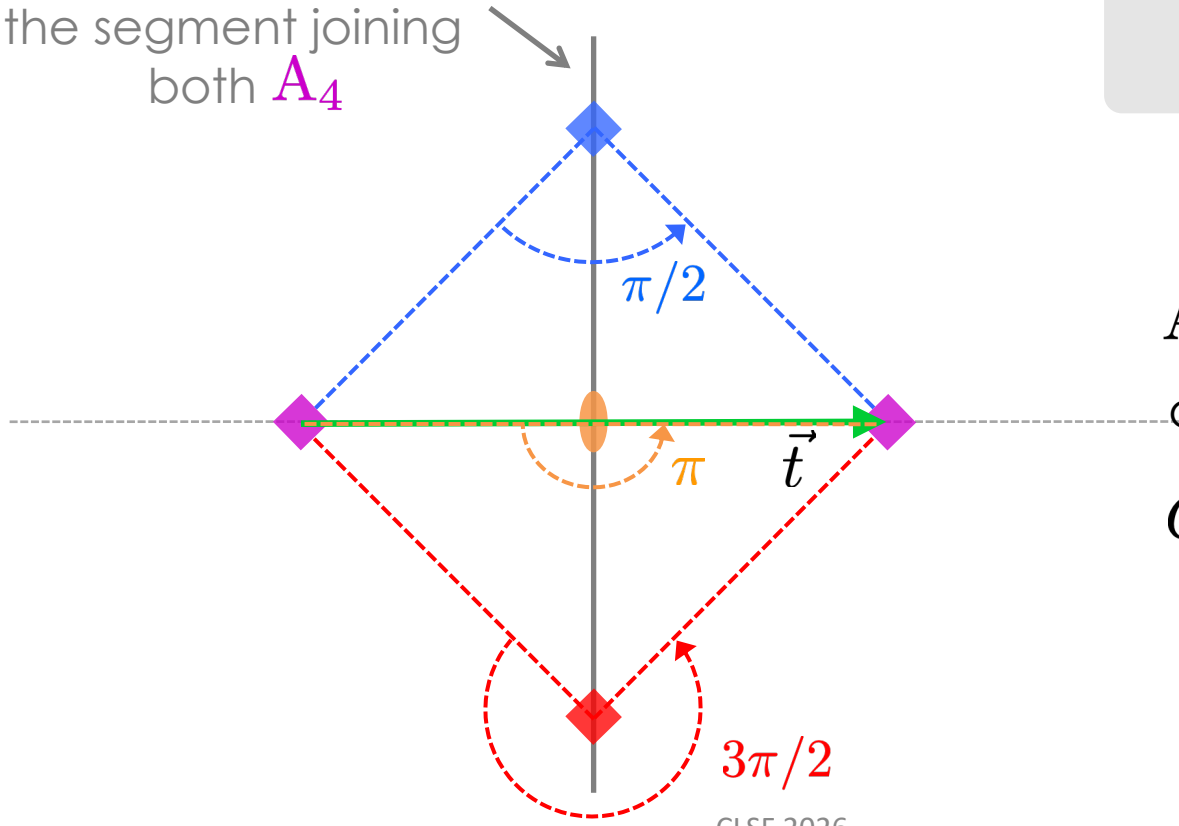
screw axis

case 2: $\mathrm{A}_n \times \vec{t}$ with $\vec{t} \perp \mathrm{A}_n$

example :
$n = 4$



bisecting plane perpendicular to the segment joining both A_4



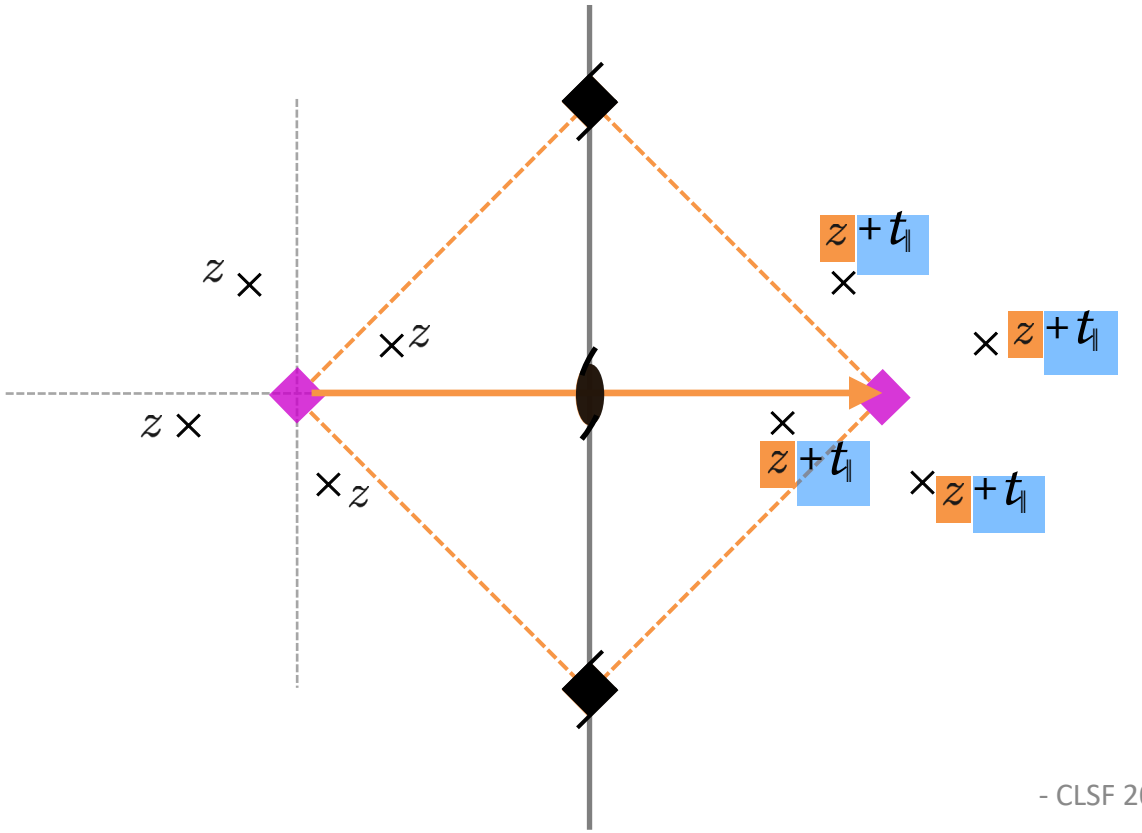
A_4 = representation of cyclic group

$C_4 = (a, a^2, a^3, e)$

case 3: $\mathrm{A}_n \times \vec{t}$ with $\vec{t}$ oblique / A_n

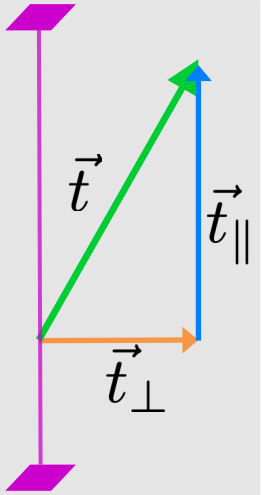
Taking $\vec{t}_{\parallel}$ into account

➔ a component $t_{\parallel}$ to z is added



example :
$n = 4$

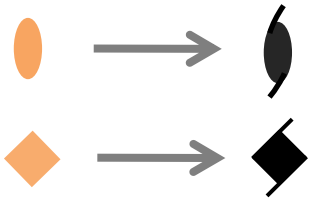
$\vec{t} = \vec{t}_{\perp} + \vec{t}_{\parallel}$



screw axis

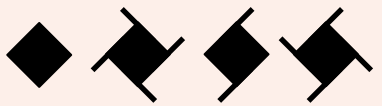
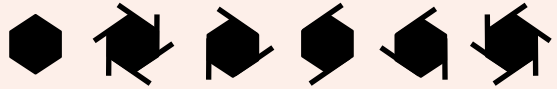
Adding $\vec{t}_{\parallel}$ changes the nature of axes A_4 & A_2 obtained by considering $\vec{t}_{\perp}$, if $\vec{t}_{\parallel}$ **is not** a lattice translation.

screw axes



screw axis

- Rotation axis A_n of order n combined with translation $\vec{t}_{\parallel}$ parallel to A_n ($\vec{t}_{\parallel}$ **is not** lattice translation)
- Associate operation noted $\left(\frac{2\pi}{n}, \vec{t}_{\parallel}\right)$

A_n order	1	2		3			4				6					
Translation	0	0	$\frac{\vec{c}}{2}$	0	$\frac{\vec{c}}{3}$	$\frac{2\vec{c}}{3}$	0	$\frac{\vec{c}}{4}$	$\frac{2\vec{c}}{4}$	$\frac{3\vec{c}}{4}$	0	$\frac{\vec{c}}{6}$	$\frac{2\vec{c}}{6}$	$\frac{3\vec{c}}{6}$	$\frac{4\vec{c}}{6}$	$\frac{5\vec{c}}{6}$
Hermann-Mauguin symbol	1	2	2_1	3	3_1	3_2	4	4_1	4_2	4_3	6	6_1	6_2	6_3	6_4	6_5
Representation																

screw axis

axis A_n × $\vec{t}$

case 1: $\vec{t} \parallel$ axis → no effect

case 2: $\vec{t} \perp$ axis → **new rotation axes** in the bisecting plane perpendicular to the segment joining axis A_n and its image by application of $\vec{t}$

case 3: $\vec{t}$ oblique / axis $\quad \vec{t} = \vec{t}_{\perp} + \vec{t}_{\parallel}$

→ **Change of the new axes nature** if $\vec{t}_{\parallel}$ is not a lattice translation

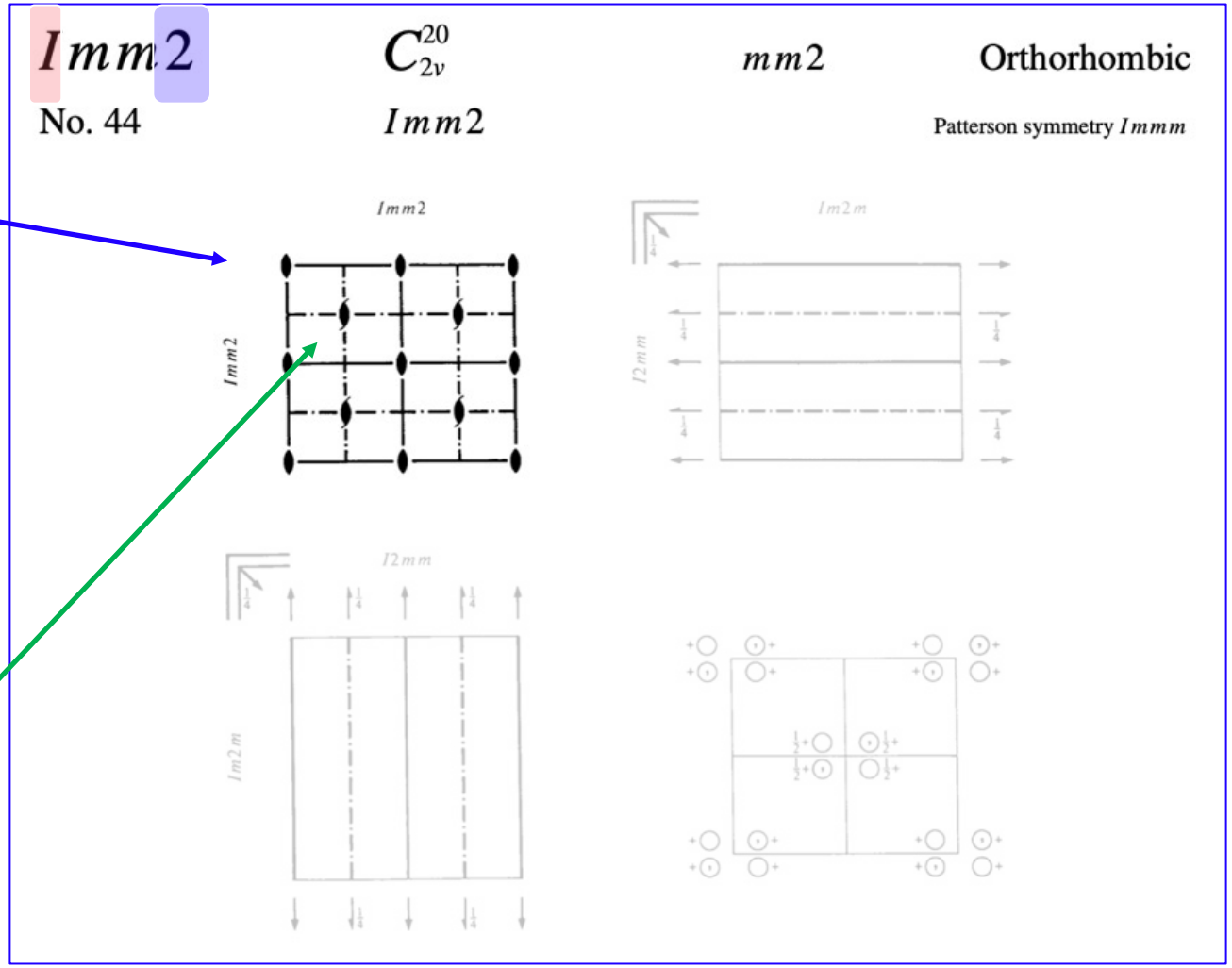
screw axis generated by lattice type I

$A_2 \parallel [001]$

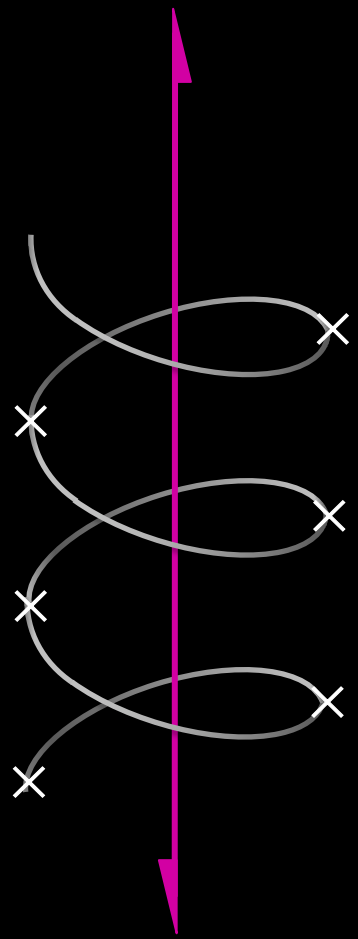
I lattice $\quad \vec{t} = \dfrac{\vec{a}+\vec{b}+\vec{c}}{2}$

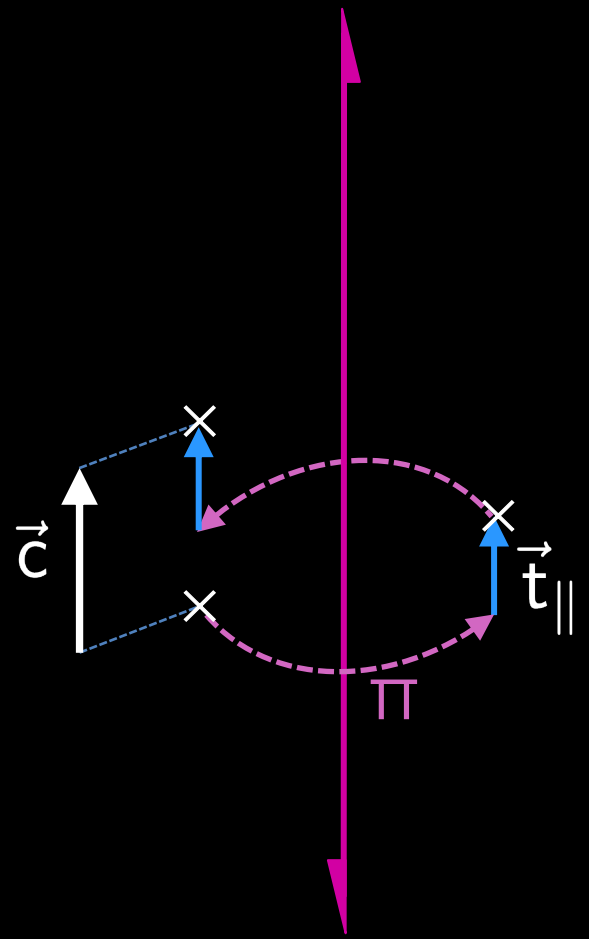
$\vec{t}_{\parallel} = \dfrac{\vec{c}}{2} \qquad \vec{t}_{\perp} = \dfrac{\vec{a}+\vec{b}}{2}$

➔ Screw axis 2_1 at $\dfrac{\vec{t}_{\perp}}{2}$

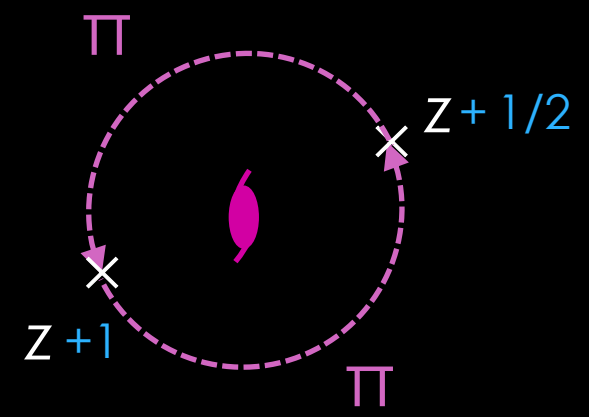


Screw axis $2_1 \parallel \vec{c}$





in the plane of the screen





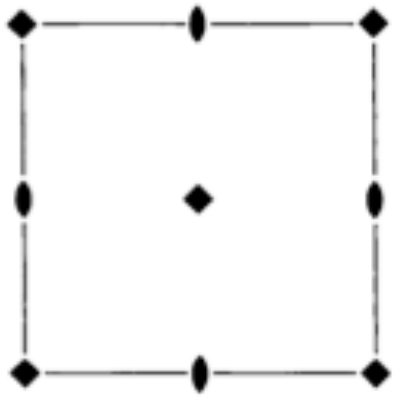
normal to the plane of the screen

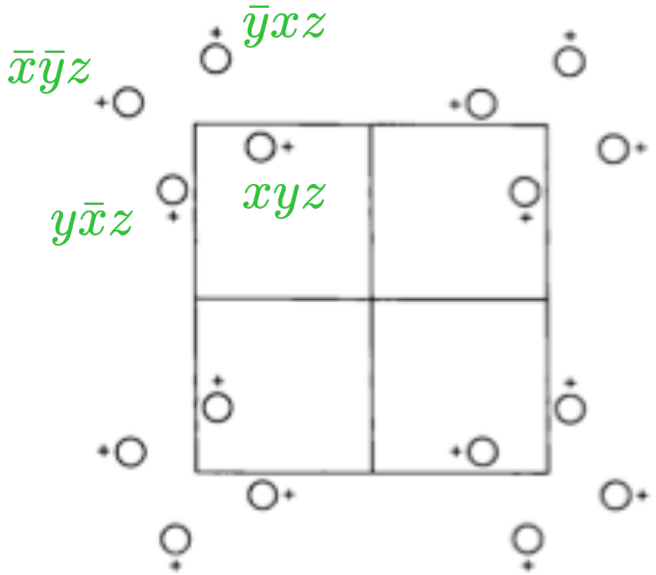
example of 1-generator point group

1st space group of point group C_4

International Tables for Crystallography (2006). Vol. A, Space group 75, p. 332.

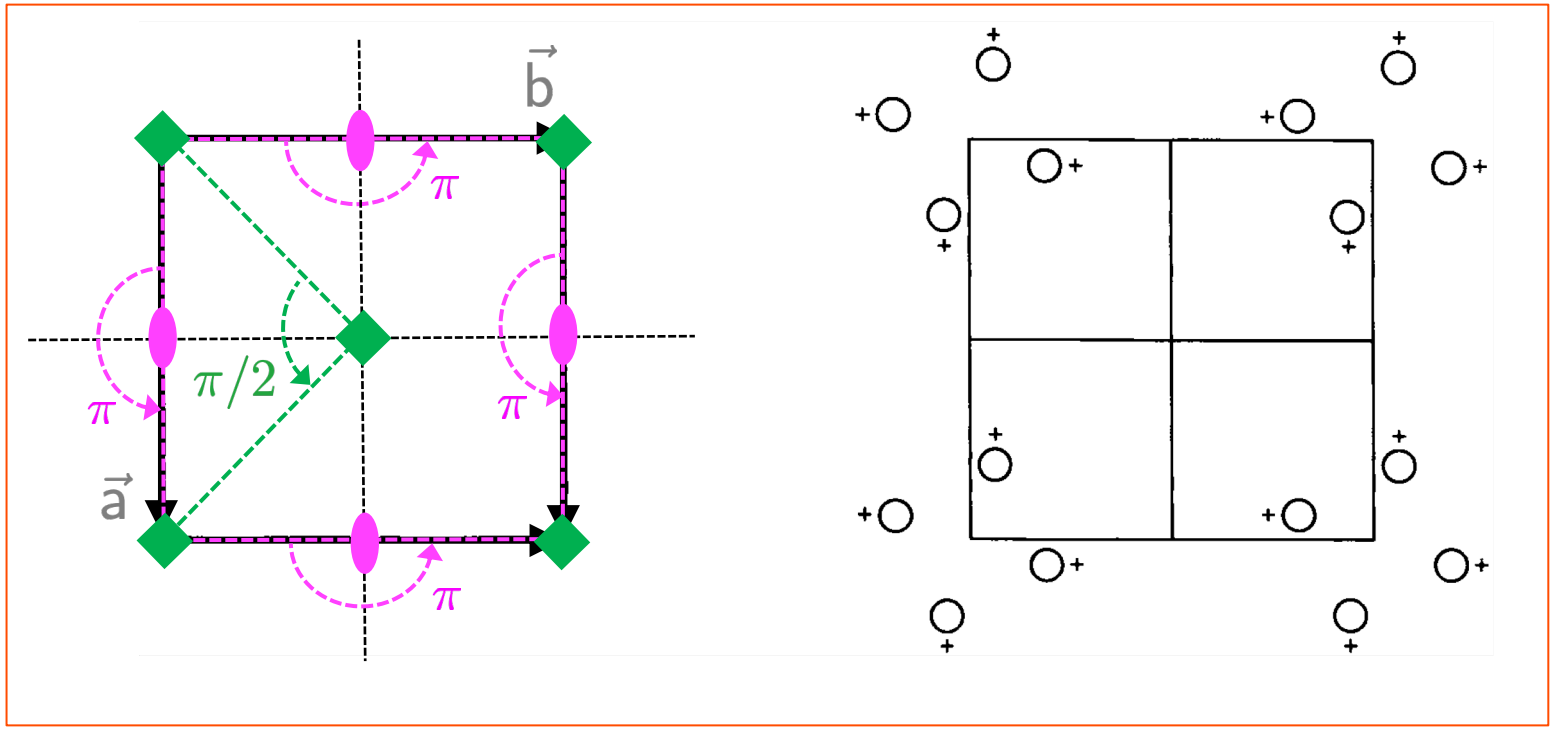
***P*4**	C_4^1	4	Tetragonal
No. 75	***P*4**		Patterson symmetry $P4/m$





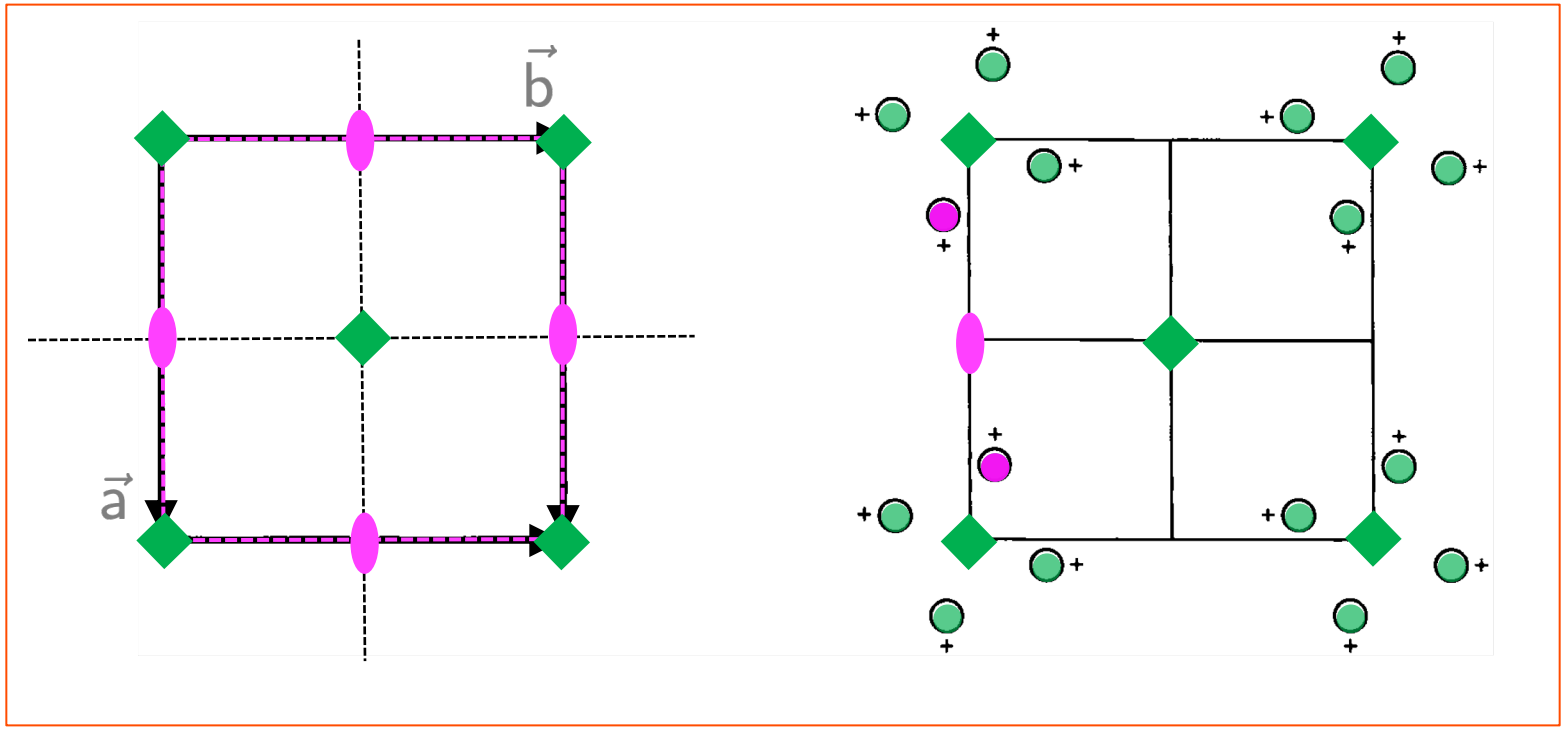
example of 1-generator point group

P4



example of 1-generator point group

P4



11 – Space groups

name (symbol) & number of the space group

Schönflies symbol

crystal system

corresponding point group

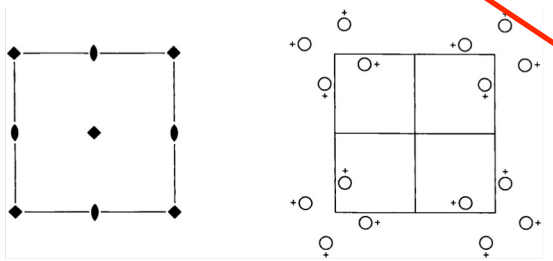
origin choice (drawings and positions)

≡ motif
- The symmetry-independent part of the structure
- A rational fraction of the unit cell (related to the other part of the unit cell by space group symmetry operations)

International Tables for Crystallography (2006). Vol. A, Space group 75, p. 332.

$P4$ No. 75 — C_4^1 $P4$ — 4 — Tetragonal

Patterson symmetry $P4/m$



Origin on 4

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

Symmetry operations

(1) 1 (2) 2 0,0,z (3) 4^+ 0,0,z (4) 4^- 0,0,z

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	d	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$	no conditions
							Special:
2	c	2 . .	0, $\frac{1}{2}$, z		$\frac{1}{2}$,0,z		hkl : $h+k=2n$
1	b	4 . .	$\frac{1}{2}$, $\frac{1}{2}$, z				no extra conditions
1	a	4 . .	0,0,z				no extra conditions

Symmetry of special projections

Along [001] $p4$ — $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$ — Origin at 0,0,z

Along [100] $p1m1$ — $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$ — Origin at x,0,0

Along [110] $p1m1$ — $\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$ — Origin at x,x,0

Maximal non-isomorphic subgroups

I [2] $P2$ (3) 1; 2

IIa none

IIb [2] $P4_2$ ($\mathbf{c}' = 2\mathbf{c}$) (77); [2] $F4$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($I4$, 79)

Maximal isomorphic subgroups of lowest index

IIc [2] $P4$ ($\mathbf{c}' = 2\mathbf{c}$) (75); [2] $C4$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P4$, 75)

Minimal non-isomorphic supergroups

I [2] $P4/m$ (83); [2] $P4/n$ (85); [2] $P422$ (89); [2] $P42_12$ (90); [2] $P4mm$ (99); [2] $P4bm$ (100); [2] $P4cc$ (103); [2] $P4nc$ (104)

II [2] $I4$ (79)

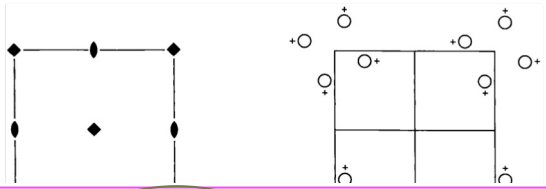
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11 – Space groups

International Tables for Crystallography (2006). Vol. A, Space group 75, p. 332.

$P4$ C_4^1 4 Tetragonal

No. 75 $P4$ Patterson symmetry $P4/m$



Positions

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

Reflection conditions

General:

no conditions

Special:

hkl : $h+k=2n$

no extra conditions

no extra conditions

cf. diffraction course

Symmetry of special projections

Along [001] $p4$ $\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$

Along [100] $p1m1$ $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$

Along [110] $p1m1$ $\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$

Maximal non-isomorphic subgroups

I [2] $P2$ (3) 1; 2

IIa none

multiplicity: number of equivalent positions équivalentes within the unit cell for a given Wyckoff position

Wyckoff letter: identifies the atomic positions, in alphabetic order,
from the most symmetric (bottom) to the general position without symmetry (top)

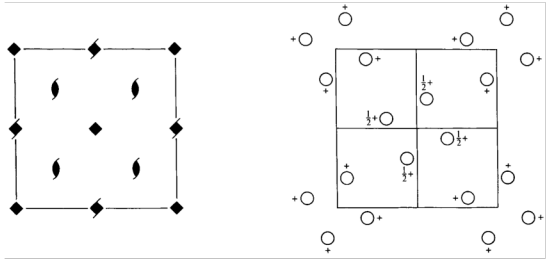
point group of the site (sub-group of the crystal point group)

11 – Space groups

International Tables for Crystallography (2006). Vol. A, Space group 79, pp. 336–337.

$I4$ C_4^5 4 Tetragonal

No. 79 $I4$ Patterson symmetry $I4/m$



Origin on 4

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

Symmetry operations

For $(0,0,0)+$ set

(1) 1 (2) 2 $0,0,z$

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

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ (2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3)

Positions

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

Reflection conditions

General:

hkl : $h+k+l=2n$
$hk0$: $h+k=2n$
$0kl$: $k+l=2n$
hhl : $l=2n$
$00l$: $l=2n$
$h00$: $h=2n$

Special: as above, plus

hkl : $l=2n$

no extra conditions

Symmetry of special projections

Along [001] $p4$

Along [100] $c1m1$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [110] $p1m1$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

$\frac{1}{2},\frac{1}{2}$)

west index

$-2\mathbf{b},\mathbf{b}' = -2\mathbf{a}+\mathbf{b}$ or $\mathbf{a}' = \mathbf{a}-2\mathbf{b},\mathbf{b}' = 2\mathbf{a}+\mathbf{b}$) (79)

s

mm (107); [2] $I4cm$ (108)

Positions

Multiplicity, Wyckoff letter, Site symmetry — Coordinates: $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$

8 c 1 (1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $\bar{y},x,z$ (4) $y,\bar{x},z$

4 b 2 . . $0,\frac{1}{2},z$ $\frac{1}{2},0,z$

2 a 4 . . $0,0,z$

To take a fresh look at all these concepts…

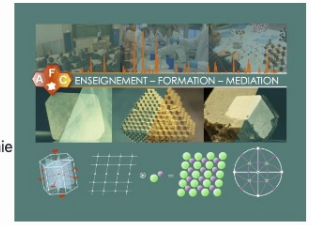
Association Française de Cristallographie

Association ▾ Adhésion Connexion Cristallographie

L'axe transverse Enseignement de la Cristallographie

L'objectif de cet axe est multiple :

- Promouvoir l'enseignement de la cristallographie en France
- Diffuser auprès d'un large public des ressources pédagogiques
- Informer sur les différentes événements en lien avec l'enseignement de la cristallographie



Vous êtes

étudiant-e de licence et master

et vous cherchez

des cours
des ouvrages
des conférences
des logiciels

doctorant-e, ingénieur-e, chercheur-e, enseignant-e du supérieur

et vous cherchez

une formation
une école
un manuel
un logiciel

élève ou enseignant-e du secondaire

et vous cherchez

une vidéo pédagogique
de la documentation

curieux de découvrir le monde des cristaux et la cristallographie

et vous cherchez

de la documentation et des vidéos accesibles à tous

Les cours en ligne

- Les capsules éducatives de Michel Evain (Université de Nantes)
  Développées en trois thèmes (cristallographie géométrique, solide cristallin et diffraction), ces capsules vidéo de 3 à 19 minutes chacune const complète et idéale pour comprendre l'organisation de la matière cristalline et des notions élémentaires de cristallographie.
- Les capsules éducatives en anglais de Frank Hoffmann (Université d'Hambourg)
  Développées en sept chapitres, ces capsules vidéo de 1 à 14 minutes chacune, constitue une ressource visuelle, didactique, complète et idéale cristalline et des notions élémentaires de cristallographie.
- Les vidéos du cours en ligne de cristallographie géométrique SYMCRIS de Delphine Cabaret (Sorbonne Université) è créer une nouvelle page
  Un ensemble de 24 vidéos réparties en 6 chapitres, pour comprendre la structure interne des cristaux, apprendre les différentes notions qui per de symétrie.
- Autres vidéos courtes
  Ces capsules vidéo ont été conçues de manière isolée, notamment à l'occasion de l'année internationale de la cristallographie en 2014. Elles ne décliné en une succession de vidéos courtes.
- MOOC (Massive Open Online Courses)
  Cours séquencés, ouverts à tous, qui demandent un travail régulier sur plusieurs semaines
- Cours en ligne sur la solidification
  Mis au point par Marie Danielle Dupouy, Thierry Duffar et Kader Zaidat, avec l'aide de plusieurs générations d'étudiants de Grenoble INP. Le site en anglais.
- Cours écrits



To take a fresh look at all these concepts…

Les capsules éducatives de Frank Hoffmann

Il s'agit d'un ensemble de 54 vidéos, en langue anglaise, conçu dans le cadre d'un MOOC, intitulé "The fascination and Crystals and Symmetry", qui a été diffusé sur la plateforme Iversity.
Elles sont désormais accessibles sur la chaîne YouTube de Frank Hoffmann. Nous en donnons ici une liste, classés par chapitre, qui sont au nombre de 7 :

Chapitre 1 : Introduction to Crystals and Crystal Systems

Chapitre 2 : Crystal Systems, Fractional Coordinates, and Morphology of Crystals

Chapitre 3 : The World of Symmetry, Crystal classes and Plane groups

Chapitre 4 : Glide planes, Screw axes and Space groups

Chapitre 5 : Quasicrystals and Real Crystal Structures (in 3D)

Chapitre 6 : Metal-Organic Frameworks (MOF) and Networks

Chapitre 7 : Practising Topology Determination, Tilings

Chapter 1: Introduction to Crystals and Crystal Systems		
Trailer	Unit 1.0	1 min
Crystal and Structures - Powers of Ten	Unit 1.1	7 min
Crystallographic poetry	Unit 1.2a	3 min
Systematization and course overview	Unit 1.2b	5 min
Definition of Crystals and Anisotropy	Unit 1.3	8 min
The Correspondence Principle (I)	Unit 1.4	6 min
The Correspondence Principle (II)	Unit 1.5	4 min
The formation of Snowflakes	Unit 1.6	3 min
The concept of Unit Cell	Unit 1.7	7 min
The seven Crystal Systems	Unit 1.8	10 min
Crystal = lattice + motif	Unit 1.9	5 min
Chapter 2: Crystal Systems, Fractional Coordinates, and Morphology of Crystals	Back to Chapter list	
Visiting the Mineralogical Museum of Hamburg	Unit 2.1	4 min

Les capsules éducatives de Michel Evain

Développées en trois thèmes (cristallographie géométrique, solide cristallin et diffraction), ces capsules vidéo de 3 à 19 minutes chacune constitue une ressource visuelle, didactique, complète et idéale pour comprendre l'organisation de la matière cristalline et des notions élémentaires de cristallographie.



Les vidéos du cours en ligne de cristallographie géométrique SYMCRIS de Delphine Cabaret

SYMCRIS est le nom d'un projet numérique de cours en ligne proposant "*Un voyage au cœur des cristaux et de leur symétrie*". Ce cours en ligne a pour objectif principal d'initier les étudiants aux notions de symétrie qui sont un aspect fondamental de la cristallographie.
Vous découvrirez, dans une approche pas-à-pas, les éléments de symétrie qu'on peut facilement observer dans certains minéraux, le réseau cristallin, puis les groupes ponctuels cristallographiques, les systèmes cristallins et les réseaux de Bravais, pour finir avec les groupes d'espace.
Ce cours peut être suivi à partir de la L1, les prérequis ayant été réduits au minimum.







Tutorial

The crystal structure of corundum α-Al_2O_3

1. What is the space group of corundum?
2. Using the table of the space group, deduce the Bravais lattice of corundum, its crystal system and its crystallographic point group.
   Note that there are two crystal axes settings to describe the structure. In the following, use the conventionel (usual) one.
3. What are the cell parameter values at 300 K?
4. In which Wyckoff sites are located the atoms? Give associated multiplicity and local point groups.
5. Deduce from the latter question the number of Al_2O_3 formula units in the chosen-setting cell.
6. Represent the 300 K structure using the Vesta software.
   Visualize it in both ball-and-stick model and polyhedral model.
   Switch from one setting to another.
   Check that the Al-O distances given in the software are equal to those given in the paper.
   Generate the X-ray powder diagram.

Acta Cryst. (1980). B**36**, 228–230

A Structural Investigation of α-Al_2O_3 at 2170 K

By N. Ishizawa, T. Miyata, I. Minato, F. Marumo and S. Iwai

Introduction

In corundum-type structures, the O atom is located at $(x,0,\frac{1}{4})$ and the Al atom at $(0,0,z)$ in the hexagonal setting of $R\bar{3}c$.

Table 1. *Cell dimensions and atomic parameters for* α-Al_2O_3

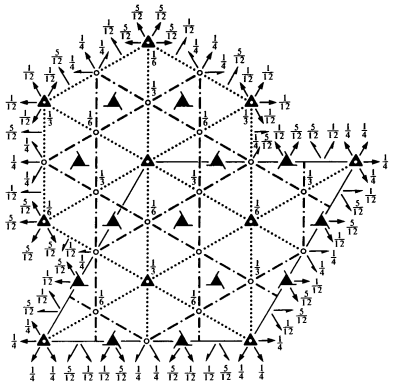
	300 K	2170 K
a	4·754 (1) Å	4·844 (2) Å
c	12·99 (2)	13·27 (2)
z	0·35228 (5)	0·3533 (2)
U_{11}	0·0051 (2) Å²	0·0299 (22) Å²
U_{33}	0·0019 (2)	0·0255 (22)
B_{iso}	0·32	2·25
x	0·3064 (3)	0·307 (1)
U_{11}	0·0051 (3) Å²	0·0282 (28) Å²
U_{22}	0·0051 (4)	0·0290 (37)
U_{33}	0·0025 (3)	0·0275 (33)
U_{23}	0·0007 (2)	0·0046 (24)
B_{iso}	0·33	2·22

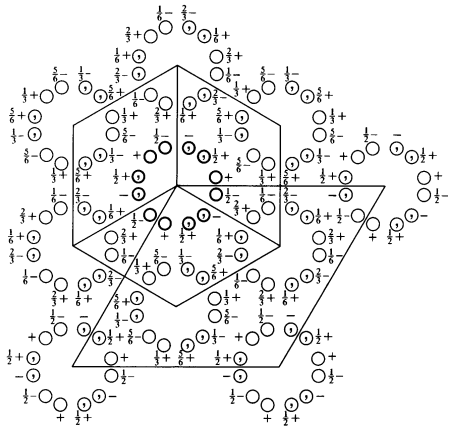
Tutorial

$R\bar{3}c$ D_{3d}^6 $\bar{3}m$ Trigonal

No. 167 $R\bar{3}2/c$ Patterson symmetry $R\bar{3}m$

HEXAGONAL AXES





Origin at centre $(\bar{3})$ at $\bar{3}c$

Asymmetric unit $0\le x\le\frac{1}{3}$; $0\le y\le\frac{2}{3}$; $0\le z\le\frac{1}{12}$; $x\le(1+y)/2$; $y\le\min(1-x,(1+x)/2)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{2}{3},\frac{1}{3},0$ $\frac{1}{3},\frac{2}{3},0$ $0,\frac{1}{2},0$
$0,0,\frac{1}{12}$ $\frac{1}{2},0,\frac{1}{12}$ $\frac{2}{3},\frac{1}{3},\frac{1}{12}$ $\frac{1}{3},\frac{2}{3},\frac{1}{12}$ $0,\frac{1}{2},\frac{1}{12}$

CONTINUED No. 167 $R\bar{3}c$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 (2) 3^+ $0,0,z$ (3) 3^- $0,0,z$
(4) 2 $x,x,\frac{1}{4}$ (5) 2 $x,0,\frac{1}{4}$ (6) 2 $0,y,\frac{1}{4}$
(7) $\bar{1}$ $0,0,0$ (8) $\bar{3}^+$ $0,0,z$; $0,0,0$ (9) $\bar{3}^-$ $0,0,z$; $0,0,0$
(10) c $x,\bar{x},z$ (11) c $x,2x,z$ (12) c $2x,x,z$

For $(\frac{2}{3},\frac{1}{3},\frac{1}{3})+$ set

(1) $t(\frac{2}{3},\frac{1}{3},\frac{1}{3})$ (2) $3^+(0,0,\frac{1}{3})$ $\frac{2}{3},\frac{1}{3},z$ (3) $3^-(0,0,\frac{1}{3})$ $\frac{2}{3},0,z$
(4) $2(\frac{2}{3},\frac{1}{3},0)$ $x,x-\frac{1}{6},\frac{1}{12}$ (5) $2(\frac{2}{3},0,0)$ $x,\frac{1}{3},\frac{1}{12}$ (6) 2 $\frac{2}{3},y,\frac{1}{12}$
(7) $\bar{1}$ $\frac{1}{3},\frac{2}{3},\frac{1}{6}$ (8) $\bar{3}^+$ $\frac{1}{3},-\frac{1}{3},z$; $\frac{1}{3},-\frac{1}{3},\frac{1}{6}$ (9) $\bar{3}^-$ $\frac{1}{3},\frac{2}{3},z$; $\frac{1}{3},\frac{2}{3},\frac{1}{6}$
(10) $g(\frac{1}{3},-\frac{1}{3},\frac{1}{6})$ $x+\frac{1}{3},\bar{x},z$ (11) $g(\frac{1}{3},\frac{2}{3},\frac{1}{6})$ $x+\frac{1}{3},2x,z$ (12) $g(\frac{2}{3},\frac{1}{3},\frac{1}{6})$ $2x,x,z$

For $(\frac{1}{3},\frac{2}{3},\frac{2}{3})+$ set

(1) $t(\frac{1}{3},\frac{2}{3},\frac{2}{3})$ (2) $3^+(0,0,\frac{2}{3})$ $0,\frac{1}{3},z$ (3) $3^-(0,0,\frac{2}{3})$ $\frac{1}{3},\frac{2}{3},z$
(4) $2(\frac{1}{3},\frac{2}{3},0)$ $x,x+\frac{1}{6},\frac{1}{12}$ (5) 2 $x,\frac{2}{3},\frac{1}{12}$ (6) $2(0,\frac{1}{3},0)$ $\frac{1}{3},y,\frac{1}{12}$
(7) $\bar{1}$ $\frac{2}{3},\frac{1}{3},\frac{1}{6}$ (8) $\bar{3}^+$ $\frac{2}{3},\frac{1}{3},z$; $\frac{2}{3},\frac{1}{3},\frac{1}{6}$ (9) $\bar{3}^-$ $-\frac{1}{3},\frac{1}{3},z$; $-\frac{1}{3},\frac{1}{3},\frac{1}{6}$
(10) $g(-\frac{1}{3},\frac{1}{3},\frac{1}{6})$ $x+\frac{1}{3},\bar{x},z$ (11) $g(\frac{1}{3},\frac{2}{3},\frac{1}{6})$ $x,2x,z$ (12) $g(\frac{2}{3},\frac{1}{3},\frac{1}{6})$ $2x-\frac{1}{3},x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{2}{3},\frac{1}{3},\frac{1}{3})$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
			$(0,0,0)+$	$(\frac{2}{3},\frac{1}{3},\frac{1}{3})+$	$(\frac{1}{3},\frac{2}{3},\frac{2}{3})+$	
						General:
36	f	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	$hkil$: $-h+k+l=3n$
			(4) $y,x,\bar{z}+\frac{1}{2}$	(5) $x-y,\bar{y},\bar{z}+\frac{1}{2}$	(6) $\bar{x},\bar{x}+y,\bar{z}+\frac{1}{2}$	$hki\bar{0}$: $-h+k=3n$
			(7) $\bar{x},\bar{y},\bar{z}$	(8) $y,\bar{x}+y,\bar{z}$	(9) $x-y,x,\bar{z}$	$hh\bar{2}hl$: $l=3n$
			(10) $\bar{y},\bar{x},z+\frac{1}{2}$	(11) $\bar{x}+y,y,z+\frac{1}{2}$	(12) $x,x-y,z+\frac{1}{2}$	$hh\bar{0}l$: $h+l=3n$, $l=2n$
						$000l$: $l=6n$
						$hh\bar{0}0$: $h=3n$
						Special: as above, plus
18	e	. 2	$x,0,\frac{1}{4}$	$0,x,\frac{1}{4}$	$\bar{x},\bar{x},\frac{1}{4}$	$\bar{x},0,\frac{1}{4}$ $0,\bar{x},\frac{1}{4}$ $x,x,\frac{1}{4}$ no extra conditions
18	d	$\bar{1}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$ $\frac{1}{2},0,\frac{1}{2}$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$ $hkil$: $l=2n$
12	c	3 .	$0,0,z$	$0,0,\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,z+\frac{1}{2}$ $hkil$: $l=2n$
6	b	3 .	$0,0,0$	$0,0,\frac{1}{2}$		$hkil$: $l=2n$
6	a	3 2	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$		$hkil$: $l=2n$

Symmetry of special projections

Along [001] $p6mm$ $\mathbf{a}'=\frac{1}{3}(2\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+\mathbf{b})$ Origin at $0,0,z$

Along [100] $p2$ $\mathbf{a}'=\frac{1}{3}(2\mathbf{a}+4\mathbf{b}+\mathbf{c})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}-2\mathbf{b}+\mathbf{c})$ Origin at $x,0,0$

Along [210] $p2gm$ $\mathbf{a}'=\frac{1}{3}\mathbf{b}$ $\mathbf{b}'=\frac{1}{6}\mathbf{c}$ Origin at $x,\frac{1}{2}x,0$

$R\bar{3}c$ No. 167 CONTINUED

HEXAGONAL AXES

Maximal non-isomorphic subgroups

I
[2] $R3c$ (161) (1; 2; 3; 10; 11; 12)+
[2] $R32$ (155) (1; 2; 3; 4; 5; 6)+
[2] $R\bar{3}1$ ($R\bar{3}$, 148) (1; 2; 3; 7; 8; 9)+
{ [3] $R12/c$ ($C2/c$, 15) (1; 4; 7; 10)+
[3] $R12/c$ ($C2/c$, 15) (1; 5; 7; 11)+
[3] $R12/c$ ($C2/c$, 15) (1; 6; 7; 12)+

IIa
{ [3] $P\bar{3}c1$ (165) 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12
[3] $P\bar{3}c1$ (165) 1; 2; 3; 10; 11; 12; (4; 5; 6; 7; 8; 9)+$(\frac{2}{3},\frac{1}{3},\frac{1}{3})$
[3] $P\bar{3}c1$ (165) 1; 2; 3; 10; 11; 12; (4; 5; 6; 7; 8; 9)+$(\frac{1}{3},\frac{2}{3},\frac{2}{3})$

IIb none

Maximal isomorphic subgroups of lowest index

IIc [4] $R\bar{3}c$ ($\mathbf{a}'=-2\mathbf{a},\mathbf{b}'=-2\mathbf{b}$) (167); [5] $R\bar{3}c$ ($\mathbf{a}'=-\mathbf{a},\mathbf{b}'=-\mathbf{b},\mathbf{c}'=5\mathbf{c}$) (167)

Minimal non-isomorphic supergroups

I [4] $Pn\bar{3}n$ (222); [4] $Pm\bar{3}n$ (223); [4] $Fm\bar{3}c$ (226); [4] $Fd\bar{3}c$ (228); [4] $Ia\bar{3}d$ (230)

II [2] $R\bar{3}m$ ($\mathbf{a}'=-\mathbf{a},\mathbf{b}'=-\mathbf{b},\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (166); [3] $P\bar{3}1c$ ($\mathbf{a}'=\frac{1}{2}(2\mathbf{a}+\mathbf{b}),\mathbf{b}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b}),\mathbf{c}'=\frac{1}{2}\mathbf{c}$) (163)

RHOMBOHEDRAL AXES

Maximal non-isomorphic subgroups

I
[2] $R3c$ (161) 1; 2; 3; 10; 11; 12
[2] $R32$ (155) 1; 2; 3; 4; 5; 6
[2] $R\bar{3}1$ ($R\bar{3}$, 148) 1; 2; 3; 7; 8; 9
{ [3] $R12/c$ ($C2/c$, 15) 1; 4; 7; 10
[3] $R12/c$ ($C2/c$, 15) 1; 5; 7; 11
[3] $R12/c$ ($C2/c$, 15) 1; 6; 7; 12

IIa none

IIb [3] $P\bar{3}c1$ ($\mathbf{a}'=\mathbf{a}-\mathbf{b},\mathbf{b}'=\mathbf{b}-\mathbf{c},\mathbf{c}'=\mathbf{a}+\mathbf{b}+\mathbf{c}$) (165)

Maximal isomorphic subgroups of lowest index

IIc [4] $R\bar{3}c$ ($\mathbf{a}'=-\mathbf{a}+\mathbf{b}+\mathbf{c},\mathbf{b}'=\mathbf{a}-\mathbf{b}+\mathbf{c},\mathbf{c}'=\mathbf{a}+\mathbf{b}-\mathbf{c}$) (167); [5] $R\bar{3}c$ ($\mathbf{a}'=\mathbf{a}+2\mathbf{b}+2\mathbf{c},\mathbf{b}'=2\mathbf{a}+\mathbf{b}+2\mathbf{c},\mathbf{c}'=2\mathbf{a}+2\mathbf{b}+\mathbf{c}$) (167)

Minimal non-isomorphic supergroups

I [4] $Pn\bar{3}n$ (222); [4] $Pm\bar{3}n$ (223); [4] $Fm\bar{3}c$ (226); [4] $Fd\bar{3}c$ (228); [4] $Ia\bar{3}d$ (230)

II [2] $R\bar{3}m$ ($\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b}+\mathbf{c}),\mathbf{b}'=\frac{1}{2}(\mathbf{a}-\mathbf{b}+\mathbf{c}),\mathbf{c}'=\frac{1}{2}(\mathbf{a}+\mathbf{b}-\mathbf{c})$) (166);
[3] $P\bar{3}1c$ ($\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c}),\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c}),\mathbf{c}'=\frac{1}{3}(\mathbf{a}+\mathbf{b}+\mathbf{c})$) (163)

Trigonal $\bar{3}m$ D_{3d}^6 $R\bar{3}c$

Patterson symmetry $R\bar{3}m$ $R\bar{3}2/c$ No. 167

RHOMBOHEDRAL AXES
(For drawings see hexagonal axes)

Origin at centre $(\bar{3})$ at $\bar{3}c$

Asymmetric unit $\frac{1}{4}\le x\le\frac{1}{2}$; $\frac{1}{4}\le y\le\frac{1}{2}$; $\frac{1}{4}\le z\le\frac{1}{2}$; $y\le x$; $z\le\min(y,\frac{1}{2}-x)$

Vertices $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ $\frac{1}{2},\frac{1}{4},\frac{1}{4}$ $\frac{1}{4},\frac{1}{2},\frac{1}{4}$ $\frac{1}{4},\frac{1}{4},\frac{1}{2}$

Symmetry operations

(1) 1 (2) 3^+ x,x,x (3) 3^- x,x,x
(4) 2 $\bar{x}+\frac{1}{2},\frac{1}{2},x$ (5) 2 $x,\bar{x}+\frac{1}{2},\frac{1}{2}$ (6) 2 $\frac{1}{2},y+\frac{1}{2},\bar{y}$
(7) $\bar{1}$ $0,0,0$ (8) $\bar{3}^+$ x,x,x; $0,0,0$ (9) $\bar{3}^-$ x,x,x; $0,0,0$
(10) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,y,x (11) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,z (12) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,y,y

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
12	f	1	(1) x,y,z	(2) z,x,y	(3) y,z,x	hhl : $l=2n$
			(4) $\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2},x+\frac{1}{2}$	(5) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(6) $\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},y+\frac{1}{2}$	hhh : $h=2n$
			(7) $\bar{x},\bar{y},\bar{z}$	(8) $\bar{y},\bar{z},\bar{x}$	(9) $\bar{y},\bar{z},x$	
			(10) $z+\frac{1}{2},y+\frac{1}{2},x+\frac{1}{2}$	(11) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(12) $x+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$	
						Special: as above, plus
6	e	. 2	$x,\bar{x}+\frac{1}{2},\frac{1}{4}$	$\frac{1}{4},x,\bar{x}+\frac{1}{2}$	$\bar{x}+\frac{1}{2},\frac{1}{4},x$	no extra conditions
			$\bar{x},x+\frac{1}{2},\frac{3}{4}$	$\frac{3}{4},\bar{x},x+\frac{1}{2}$	$x+\frac{1}{2},\frac{3}{4},\bar{x}$	
6	d	$\bar{1}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$ $\frac{1}{2},0,\frac{1}{2}$ $0,\frac{1}{2},\frac{1}{2}$ hkl : $h+k+l=2n$
4	c	3 .	x,x,x	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x+\frac{1}{2}$	$\bar{x},\bar{x},\bar{x}$	$x+\frac{1}{2},x+\frac{1}{2},x+\frac{1}{2}$ hkl : $h+k+l=2n$
2	b	$\bar{3}$.	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$		hkl : $h+k+l=2n$
2	a	3 2	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$		hkl : $h+k+l=2n$

Symmetry of special projections

Along [111] $p6mm$ $\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$ Origin at x,x,x

Along [1$\bar{1}$0] $p2$ $\mathbf{a}'=\frac{1}{2}(\mathbf{a}+\mathbf{b}-2\mathbf{c})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$ Origin at $x,\bar{x},0$

Along [2$\bar{1}\bar{1}$] $p2gm$ $\mathbf{a}'=\frac{1}{2}(\mathbf{b}-\mathbf{c})$ $\mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b}+\mathbf{c})$ Origin at $2x,\bar{x},\bar{x}$

(*Continued on preceding page*)