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Commission on Mathematical and Theoretical Crystallography

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Facultad de Ciencias

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Workshop on the Applications of Group Theory in the Study of Phase Transitions

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CRYSTALLOGRAPHIC POINT GROUPS II (further developments)

Mois I. Aroyo
Universidad del Pais Vasco, Bilbao, Spain

eman ta zabal zazu
Universidad del País Vasco
Euskal Herriko Unibertsitatea

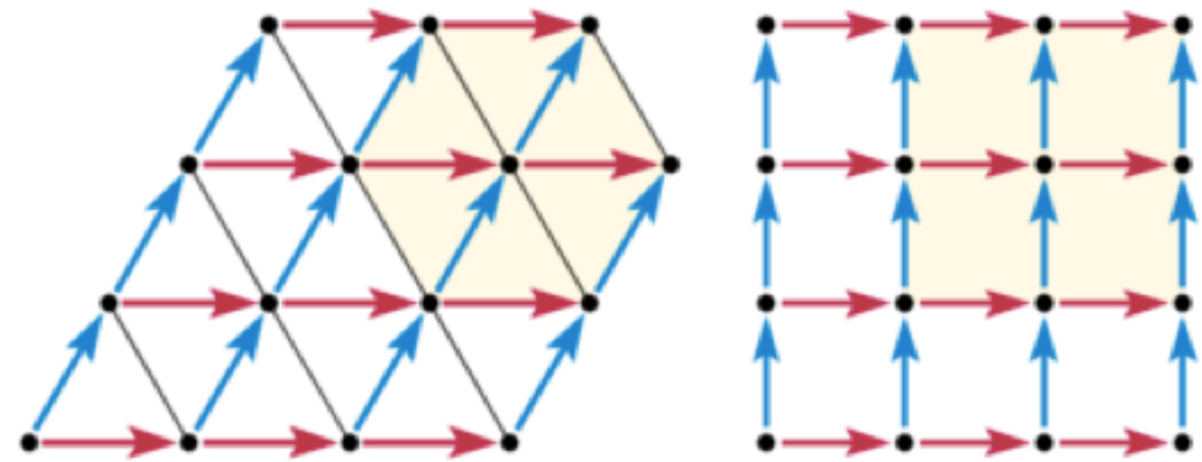
CRYSTALLOGRAPHIC POINT GROUPS IN THE PLANE

Crystallographic symmetry operations

Crystallographic restriction theorem

The rotational symmetries of a crystal pattern are limited to 2-fold, 3-fold, 4-fold, and 6-fold.

Matrix proof:



Rotation with respect to orthonormal basis

$$R = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}$$

Rotation with respect to lattice basis

R: integer matrix

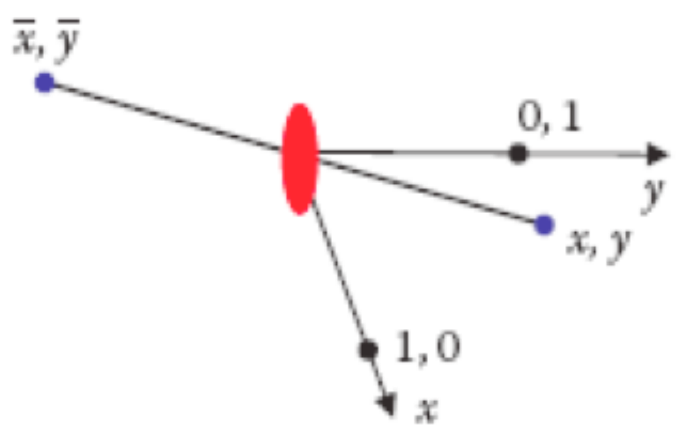
In a lattice basis, because the rotation must map lattice points to lattice points, each matrix entry — and hence the trace — must be an integer.

$\mathrm{Tr}\,R = 2\cos\theta = \text{integer}$

m	$m/2 = \cos\theta$	θ (°)	$n = 360°/\theta$
0	0	90	Fourfold
1	1/2	60	Sixfold
2	1	0 = 360	Identity (onefold)
−1	−1/2	120	Threefold
−2	−1	180	Twofold

Symmetry operations in the plane
Matrix representations

2-fold rotation

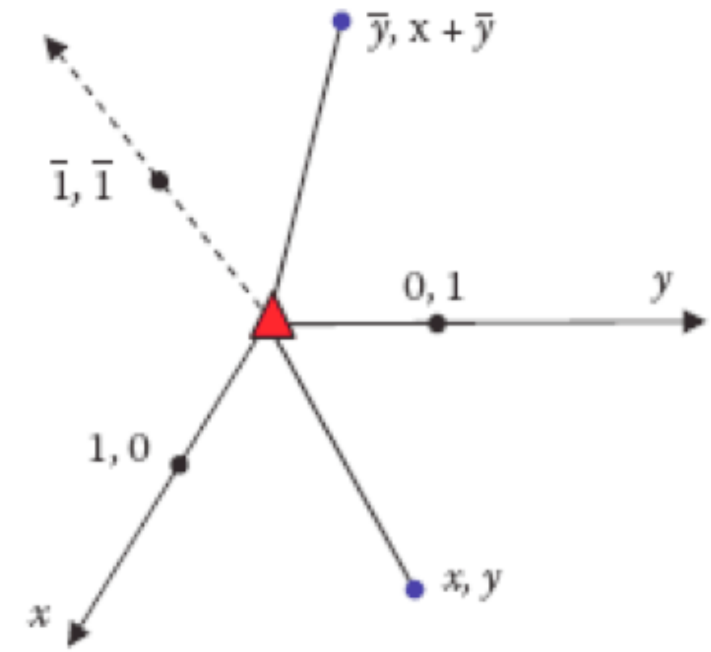


$$2_z \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} -x \\ -y \end{pmatrix} = \begin{pmatrix} -1 & \\ & -1 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}$$

$$\det \begin{pmatrix} -1 & \\ & -1 \end{pmatrix} = ?$$

$$\mathrm{tr} \begin{pmatrix} -1 & \\ & -1 \end{pmatrix} = ?$$

3-fold rotation



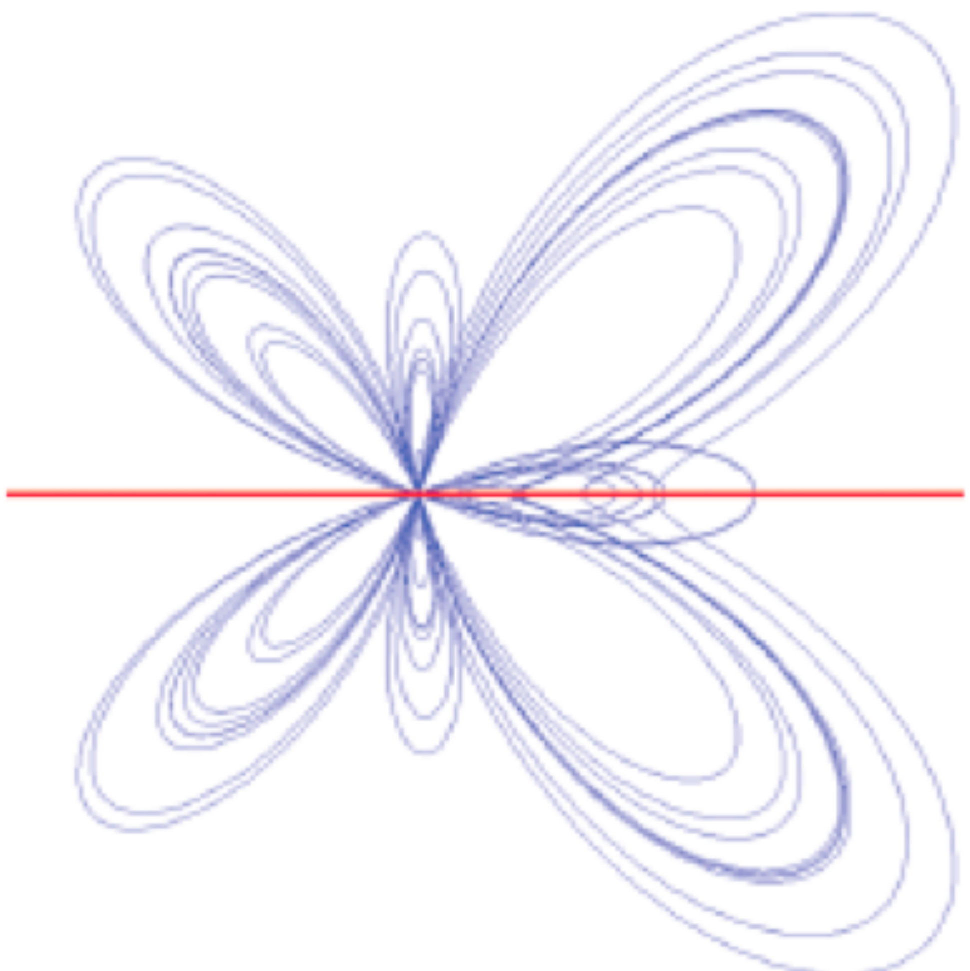
$$3^+ \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} -y \\ x-y \end{pmatrix} = \begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}$$

$$\det \begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix} = ?$$

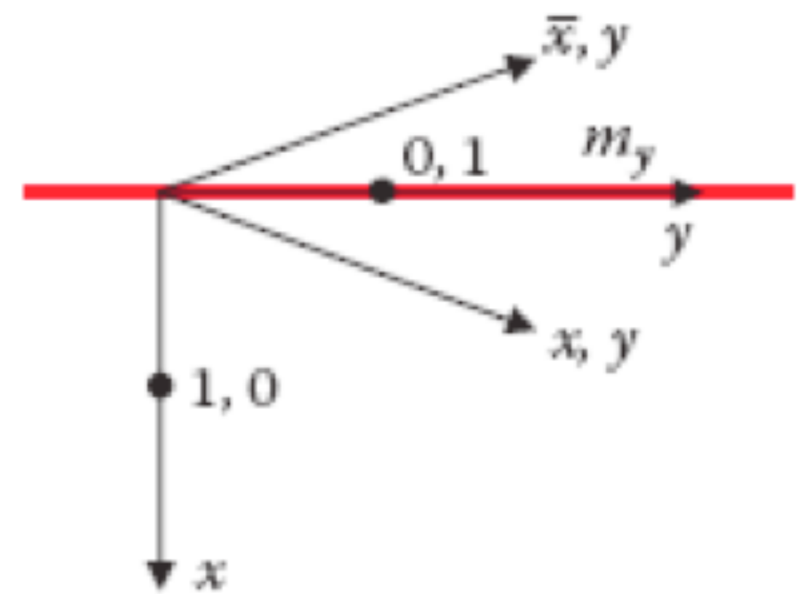
$$\mathrm{tr} \begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix} = ?$$

Crystallographic symmetry operations in the plane

Mirror symmetry operation



Mirror line m_y at 0,y



Matrix representation

$$m_y \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} -x \\ y \end{pmatrix} = \begin{pmatrix} -1 & \\ & 1 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}$$

$$\det \begin{pmatrix} -1 & \\ & 1 \end{pmatrix} = ? \quad \mathrm{tr} \begin{pmatrix} -1 & \\ & 1 \end{pmatrix} = ?$$

Fixed points

$$m_y \begin{pmatrix} x_f \\ y_f \end{pmatrix} = \begin{pmatrix} x_f \\ y_f \end{pmatrix}$$

Crystallographic symmetry operations in 2D

Operations of the first kind (no change of handedness)		Operations of the second kind (change of handedness)	
Element	**Operation**	**Element**	**Operation**
Rotation point	*Rotation*	*Reflection line (mirror)*	
1	$2\pi/1$	*m*	*m*
2	$2\pi/2$		
3	$2\pi/3$		
4	$2\pi/4$		
6	$2\pi/6$		

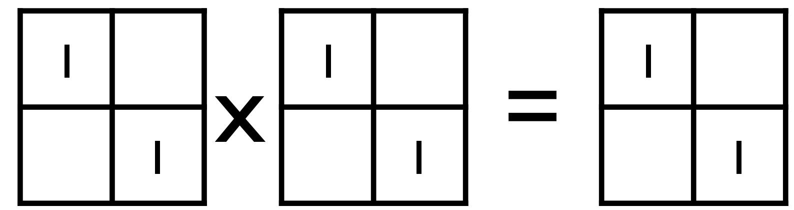
Crystallographic point groups in 2D?

Crystallographic Point Groups in 2D

Point group **1** = {1}

Motif with symmetry of **1**

-group axioms?

I x I = 

-order of **1**?

-multiplication table

×	1
1	1

-generators of **1**?

Crystallographic Point Groups in 2D

Point group **2** = {1,2}

Motif with symmetry of **2**

Where is the two-fold point?

-group axioms?

$$2 \times 2 = \begin{bmatrix} -1 & \\ & -1 \end{bmatrix} \times \begin{bmatrix} -1 & \\ & -1 \end{bmatrix} = \begin{bmatrix} 1 & \\ & 1 \end{bmatrix}$$

-order of **2**?

-multiplication table

×	1	2
1	1	2
2	2	1

-generators of **2**?

Crystallographic Point Groups in 2D

Point group **m** = {1,m}

Motif with symmetry of **m**

Where is the mirror line?

-group axioms?

$$m \times m = \begin{bmatrix} -1 & \\ & 1 \end{bmatrix} \times \begin{bmatrix} -1 & \\ & 1 \end{bmatrix} = \begin{bmatrix} 1 & \\ & 1 \end{bmatrix}$$

-order of **m**?

-multiplication table

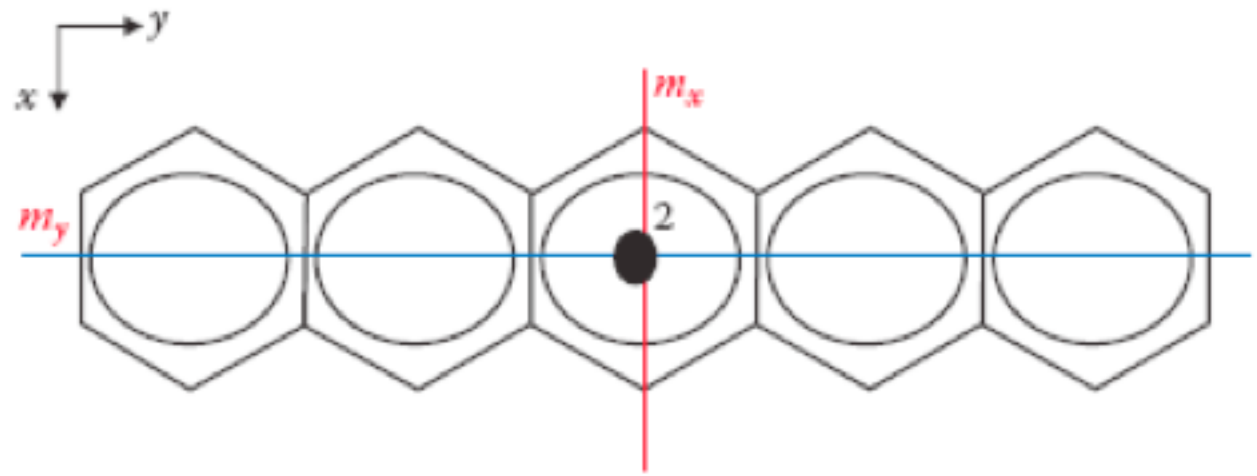
×	1	m_y
1	1	m_y
m_y	m_y	1

-generators of **m**?

Crystallographic Point Groups in 2D

Point group **mm2** = $\{1, 2_z, m_x, m_y\}$

Molecule of pentacene



-order of **mm2**?

-group axioms?

$$m_y \times 2 = \begin{pmatrix} -1 & \\ & 1 \end{pmatrix} \times \begin{pmatrix} -1 & \\ & -1 \end{pmatrix} = \begin{pmatrix} 1 & \\ & -1 \end{pmatrix} = m_x$$

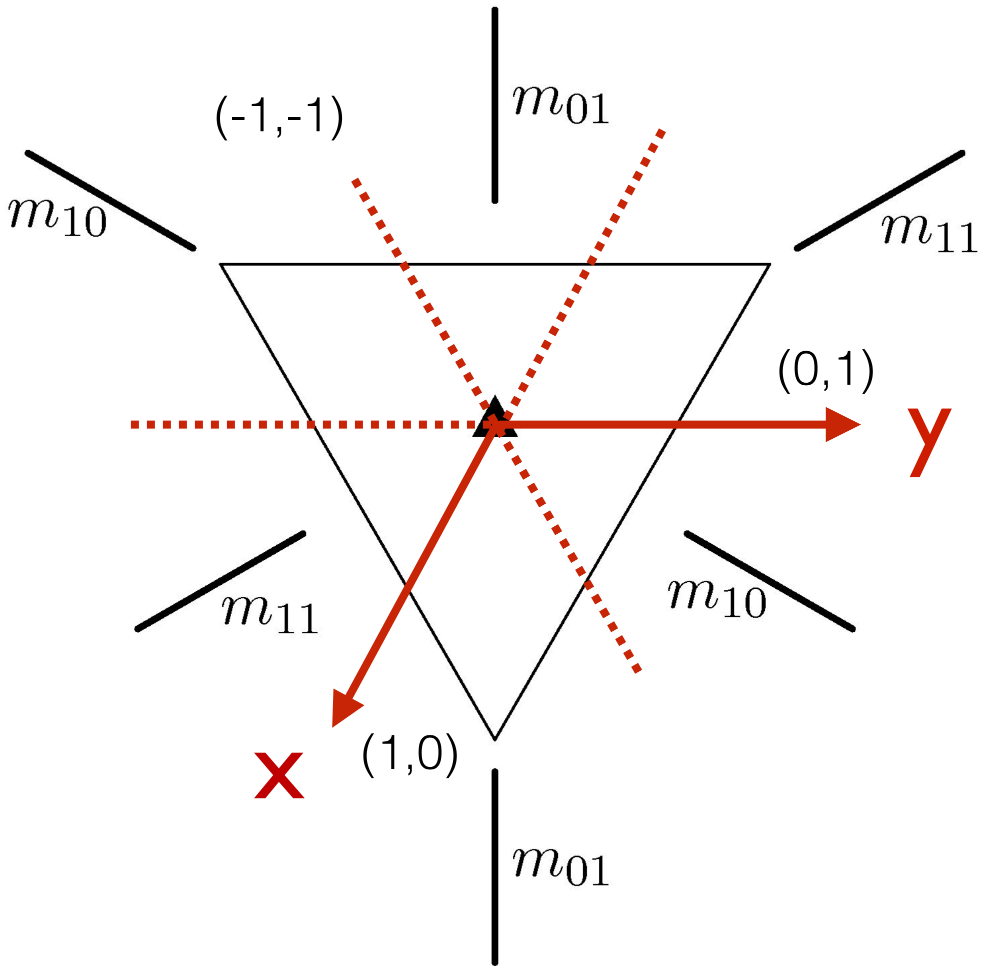
-multiplication table

×	1	2	m_x	m_y
1	1	2	m_x	m_y
2	2	1	m_y	m_x
m_x	m_x	m_y	1	2
m_y	m_y	m_x	2	1

-generators of **mm2**?

EXAMPLE

Stereographic Projections of *3m*

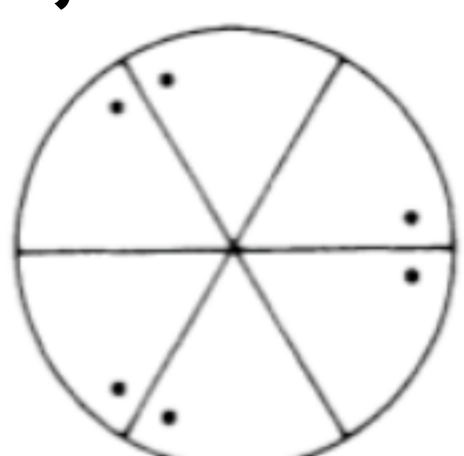


Point group **3m** =

$\{1, 3^+, 3^-, m_{10}, m_{01}, m_{11}\}$

Stereographic projections diagrams

general position



symmetry elements

Example

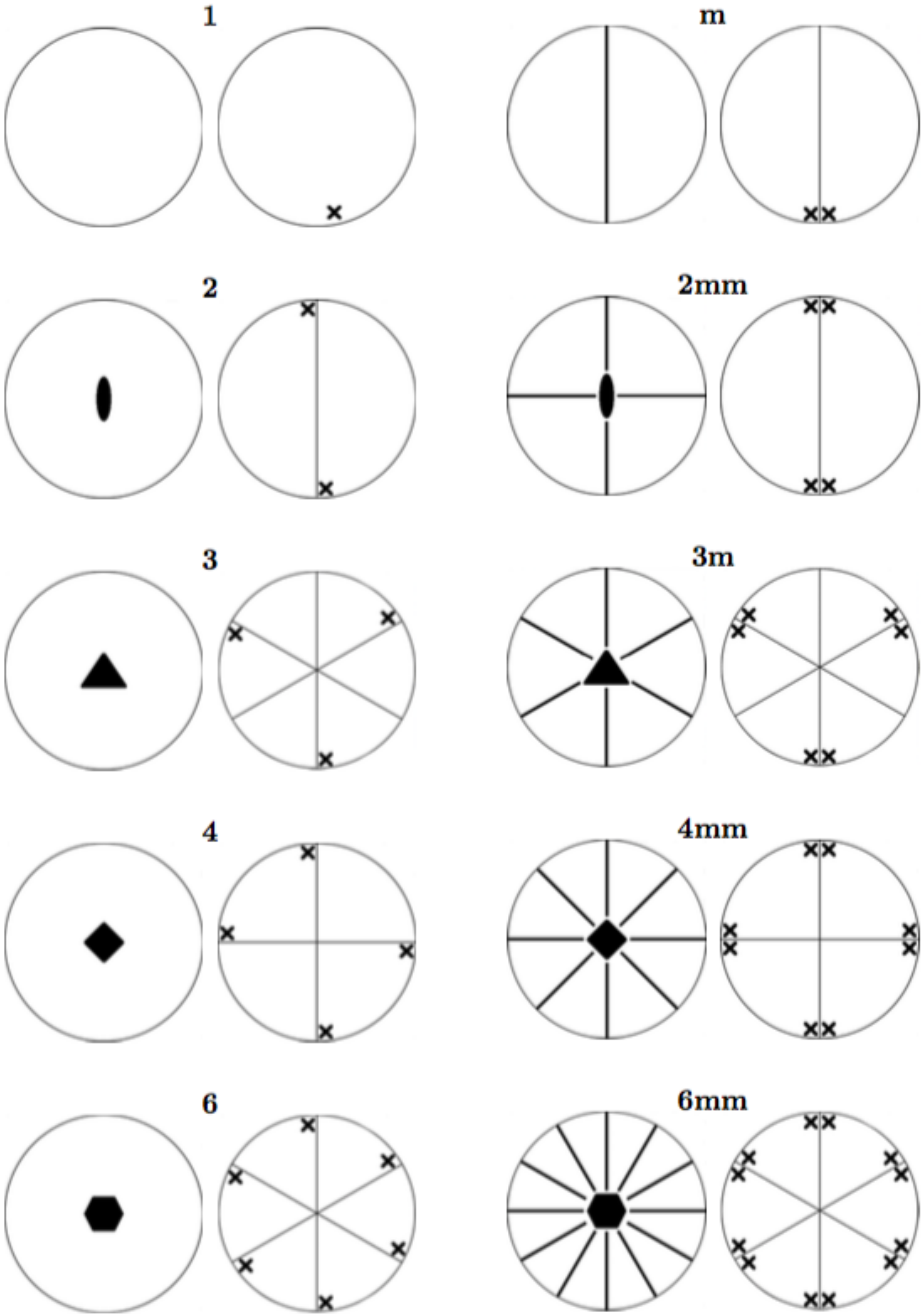
Symmetry-elements diagrams

and

General-positions diagrams

of the

plane point groups.



Hermann-Mauguin symbolism (International Tables A)

-symmetry elements along *primary*, *secondary* and *ternary* symmetry directions

rotations: by the axes of rotation
reflections: by the normals to the planes

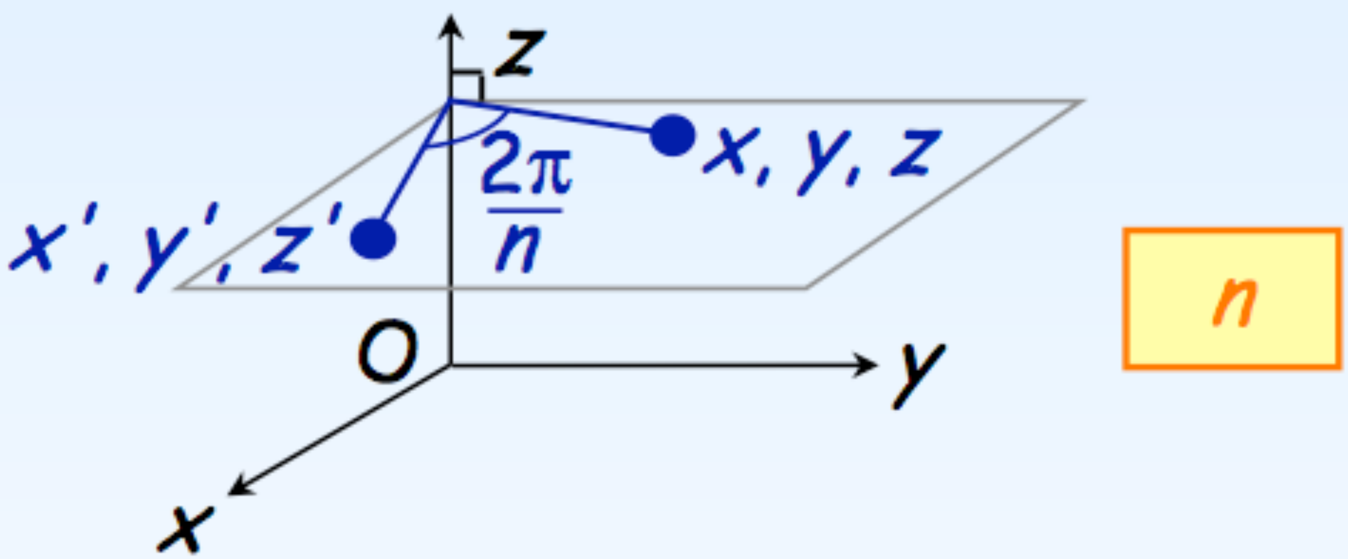
Lattice	Symmetry direction (position in Hermann–Mauguin symbol)		
	Primary	Secondary	Tertiary
Two dimensions			
Oblique	Rotation point in plane		
Rectangular		[10]	[01]
Square		{ [10] [01] }	{ $[1\bar{1}]$ [11] }
Hexagonal		{ [10] [01] $[\bar{1}\bar{1}]$ }	{ $[1\bar{1}]$ [12] $[\bar{2}\bar{1}]$ }

CRYSTALLOGRAPHIC POINT GROUPS IN 3D (brief overview)

Symmetry operations in 3D
Rotations

Rotation (around an axis)

Rotation of order n = *rotation by* $\varphi = \dfrac{2\pi}{n}$

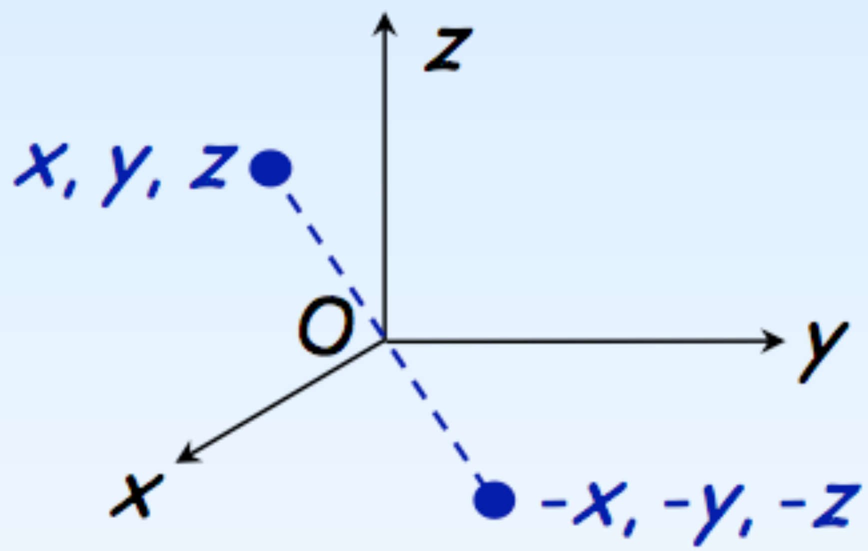


$$\alpha(n) = \begin{pmatrix} \cos\varphi & -\sin\varphi & 0 \\ \sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Det = +1

Symmetry operations in 3D
Rotoinvertions

Inversion (through a point)



$\bar{1}$

a crystal which has the inversion symmetry is called centrosymmetrical.

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

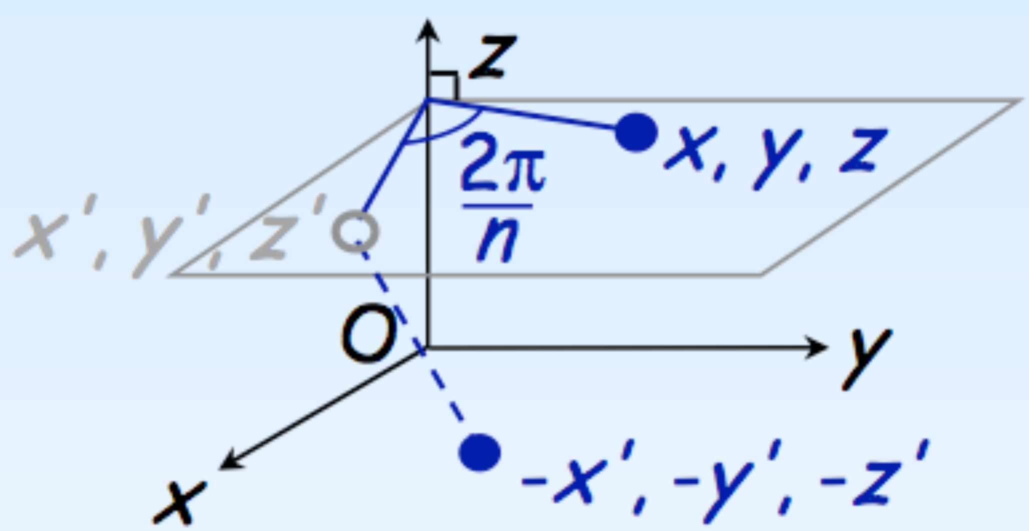
Det = -1

Symmetry operations in 3D
Rotoinversions

Roto-inversion

(around an axis and through a point)

Rotation followed by an inversion



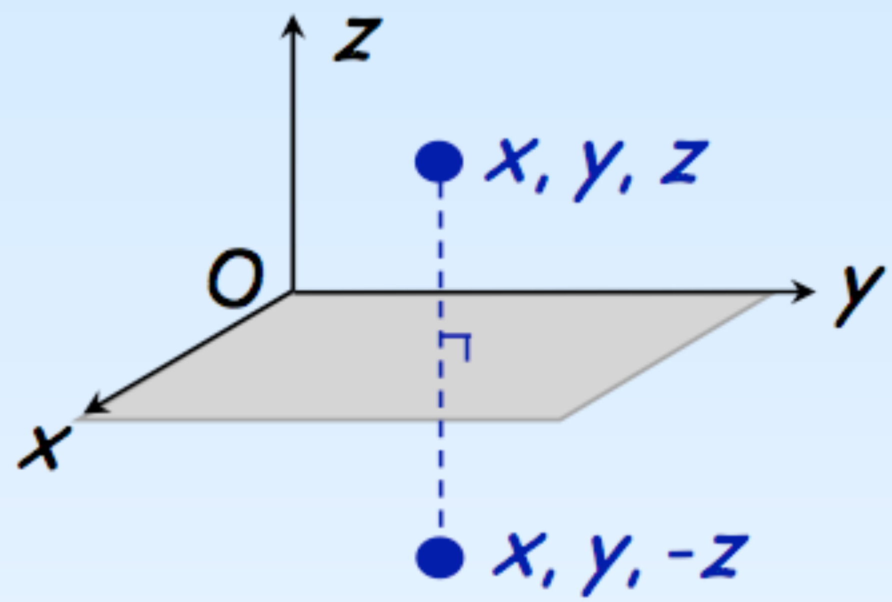
$\bar{n}$

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

Det = -1

Symmetry operations in 3D
Rotoinvertions

Reflection (through a mirror plane)



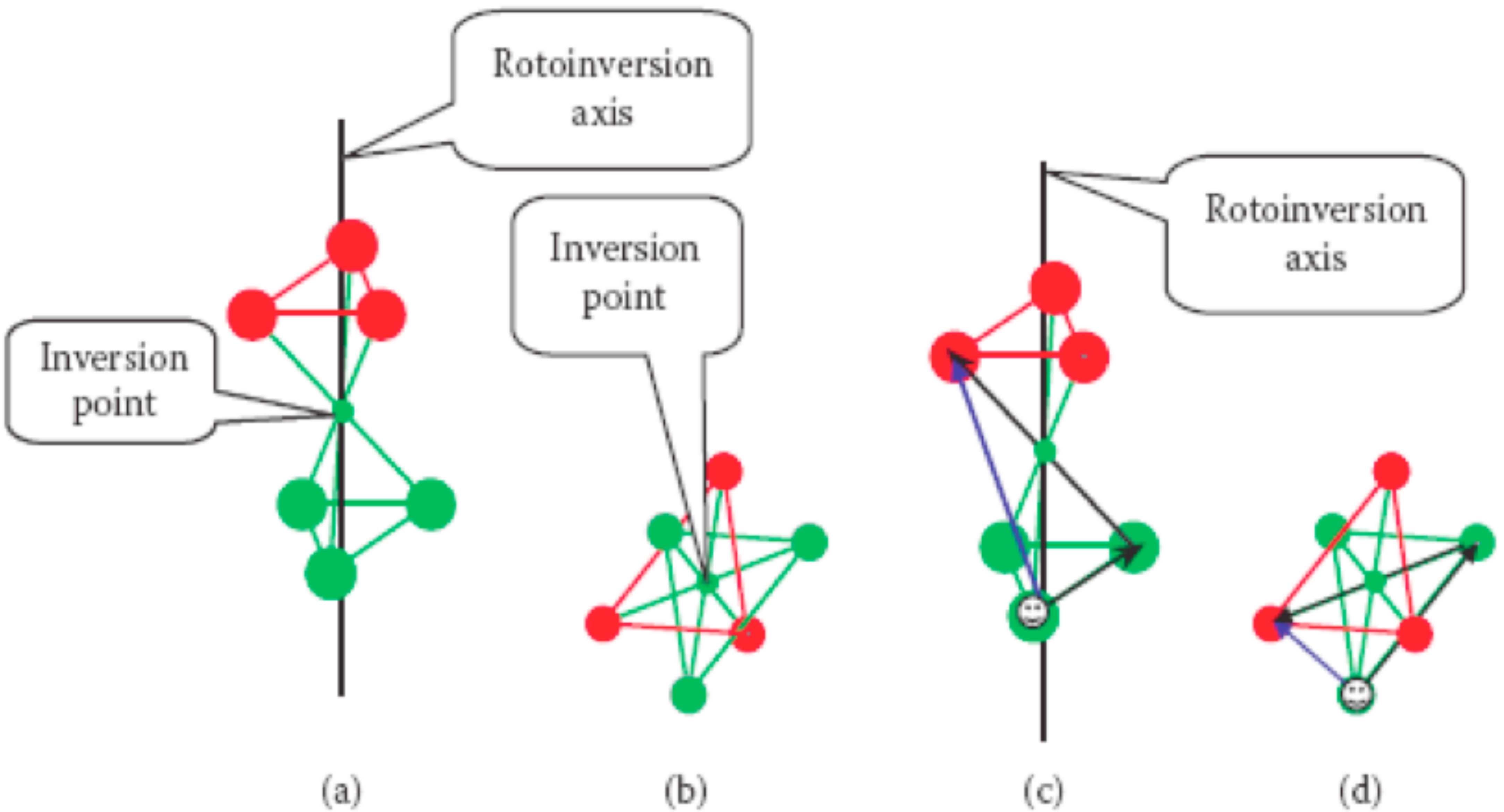
m

Note that: $m = \bar{2}$!

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

Det = -1

Symmetry operations in 3D
$\bar{3}$ Roto-inversion



general view | down the symmetry axis | $\bar{3}^{+}$ general view | $\bar{3}^{+}$ down the symmetry axis

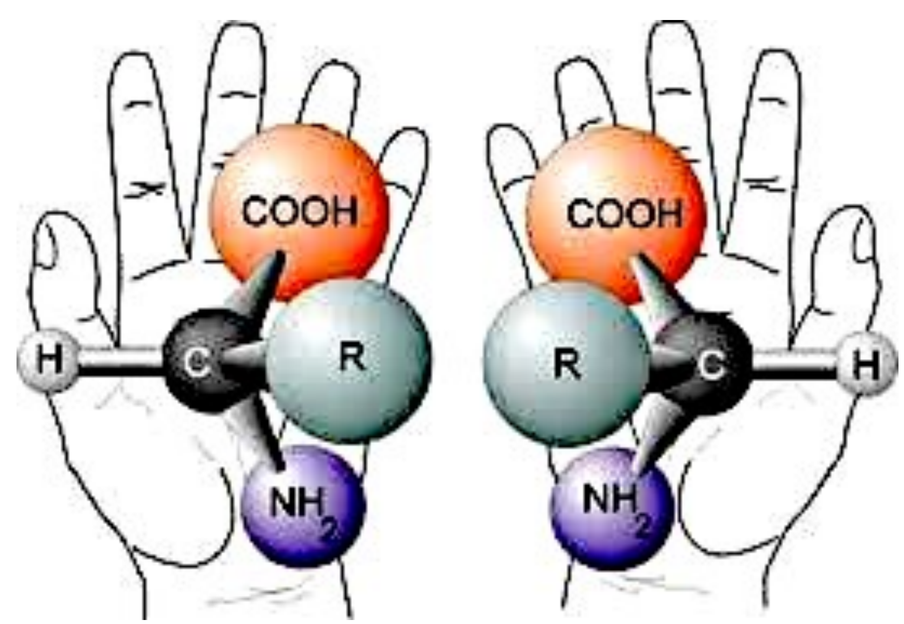
Crystallographic Point Groups in 3D

Proper rotations: det =+1: 1 2 3 4 6

chirality preserving

Improper rotations: det =-1: $\bar{1}$ $\bar{2}$=m $\bar{3}$ $\bar{4}$ $\bar{6}$

chirality non-preserving



Crystallographic Point Groups in 3D

System used in this volume	Point group: International symbol, Short	Point group: International symbol, Full	Schoenflies symbol
Triclinic	1 $\bar{1}$	1 $\bar{1}$	C_1 $C_i(S_2)$
Monoclinic	2 m $2/m$	2 m $\frac{2}{m}$	C_2 $C_s(C_{1h})$ C_{2h}
Orthorhombic	222 $mm2$ mmm	222 $mm2$ $\frac{2}{m}\frac{2}{m}\frac{2}{m}$	$D_2(V)$ C_{2v} $D_{2h}(V_h)$
Tetragonal	4 $\bar{4}$ $4/m$ 422 $4mm$ $\bar{4}2m$ $4/mmm$	4 $\bar{4}$ $\frac{4}{m}$ 422 $4mm$ $\bar{4}2m$ $\frac{4}{m}\frac{2}{m}\frac{2}{m}$	C_4 S_4 C_{4h} D_4 C_{4v} $D_{2d}(V_d)$ D_{4h}
Trigonal	3 $\bar{3}$ 32 $3m$ $\bar{3}m$	3 $\bar{3}$ 32 $3m$ $\bar{3}\frac{2}{m}$	C_3 $C_{3i}(S_6)$ D_3 C_{3v} D_{3d}
Hexagonal	6 $\bar{6}$ $6/m$ 622 $6mm$ $\bar{6}2m$ $6/mmm$	6 $\bar{6}$ $\frac{6}{m}$ 622 $6mm$ $\bar{6}2m$ $\frac{6}{m}\frac{2}{m}\frac{2}{m}$	C_6 C_{3h} C_{6h} D_6 C_{6v} D_{3h} D_{6h}
Cubic	23 $m\bar{3}$ 432 $\bar{4}3m$ $m\bar{3}m$	23 $\frac{2}{m}\bar{3}$ 432 $\bar{4}3m$ $\frac{4}{m}\bar{3}\frac{2}{m}$	T T_h O T_d O_h

International Tables for Crystallography, Vol. A

Hermann-Mauguin symbolism (International Tables A)

-symmetry elements along *primary*, *secondary* and *ternary* symmetry directions

rotations: by the axes of rotation

planes: by the normals to the planes

- rotations/planes along the same direction
- full/short Hermann-Mauguin symbols

-symmetry elements in decreasing order of symmetry (except for two cubic groups: 23 and m$\bar{3}$)

Crystal systems and Crystallographic point groups

Crystal system	Crystallographic point groups†	Restrictions on cell parameters	primary	secondary	ternary
Triclinic	1, $\bar{1}$	None	None		
Monoclinic	2, m, $2/m$	b-unique setting $\alpha = \gamma = 90°$	[010] ('unique axis b')		
		c-unique setting $\alpha = \beta = 90°$	[001] ('unique axis c')		
Orthorhombic	222, $mm2$, mmm	$\alpha = \beta = \gamma = 90°$	[100]	[010]	[001]
Tetragonal	4, $\bar{4}$, $4/m$, 422, $4mm$, $\bar{4}2m$, $4/mmm$	$a = b$, $\alpha = \beta = \gamma = 90°$	[001]	$\left\{ \begin{matrix} [100] \\ [010] \end{matrix} \right\}$	$\left\{ \begin{matrix} [1\bar{1}0] \\ [110] \end{matrix} \right\}$

Crystal systems and Crystallographic point groups

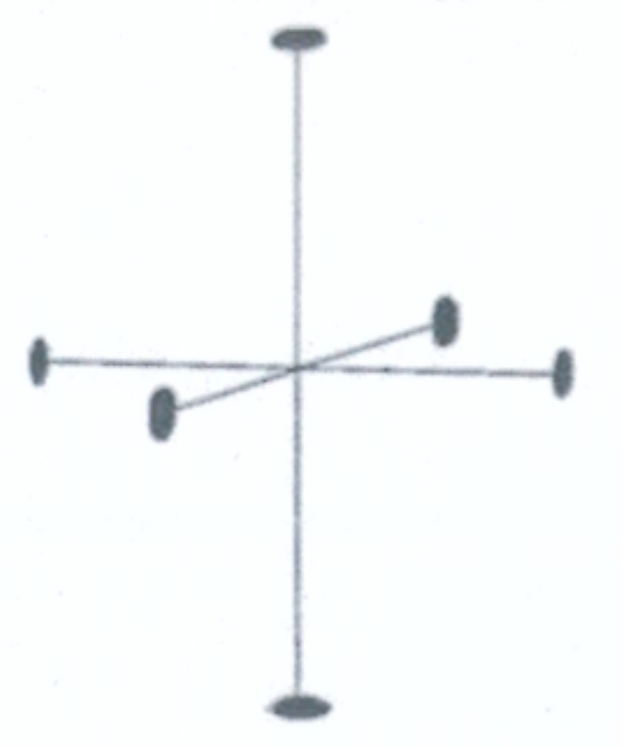
Crystal system	Crystallographic point groups†	Restrictions on cell parameters	primary	secondary	ternary
Trigonal	3, $\bar{3}$ 32, $3m$, $\bar{3}m$	$a = b$ $\alpha = \beta = 90°,\ \gamma = 120°$			
		$a = b = c$ $\alpha = \beta = \gamma$ (rhombohedral axes, primitive cell)	[111]	$\{[1\bar{1}0], [01\bar{1}], [\bar{1}01]\}$	
		$a = b$ $\alpha = \beta = 90°, \gamma = 120°$ (hexagonal axes, triple obverse cell)	[001]	$\{[100], [010], [\bar{1}\bar{1}0]\}$	
Hexagonal	$6, \bar{6}$, $6/m$ $622, 6mm, \bar{6}2m$, $6/mmm$	$a = b$ $\alpha = \beta = 90°, \gamma = 120°$	[001]	$\{[100], [010], [\bar{1}\bar{1}0]\}$	$\{[1\bar{1}0], [120], [\bar{2}\bar{1}0]\}$
Cubic	23, $m\bar{3}$ $432, \bar{4}3m$, $m\bar{3}m$	$a = b = c$ $\alpha = \beta = \gamma = 90°$	$\{[100], [010], [001]\}$	$\{[111], [1\bar{1}\bar{1}], [\bar{1}1\bar{1}], [\bar{1}\bar{1}1]\}$	$\{[1\bar{1}0]\ [110], [01\bar{1}]\ [011], [\bar{1}01]\ [101]\}$

Rotation Crystallographic Point Groups in 3D

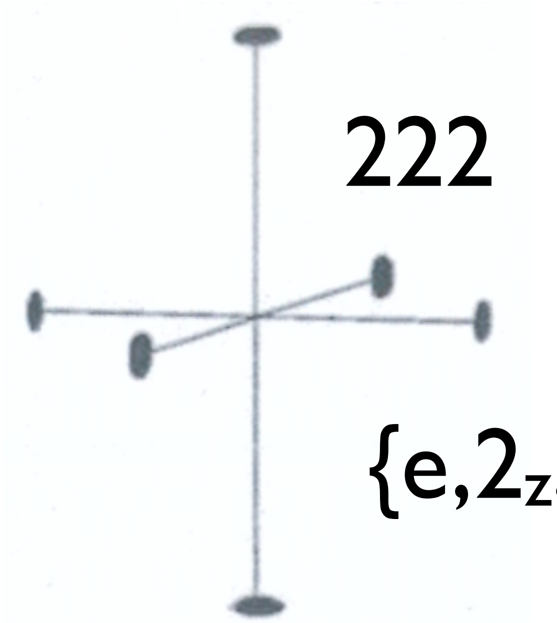
Cyclic: 1(C_1), 2(C_2), 3(C_3), 4(C_4), 6(C_6)

Dihedral: 222(D_2), 32(D_3), 422(D_4), 622(D_6)

Cubic: 23 (T), 432 (O)

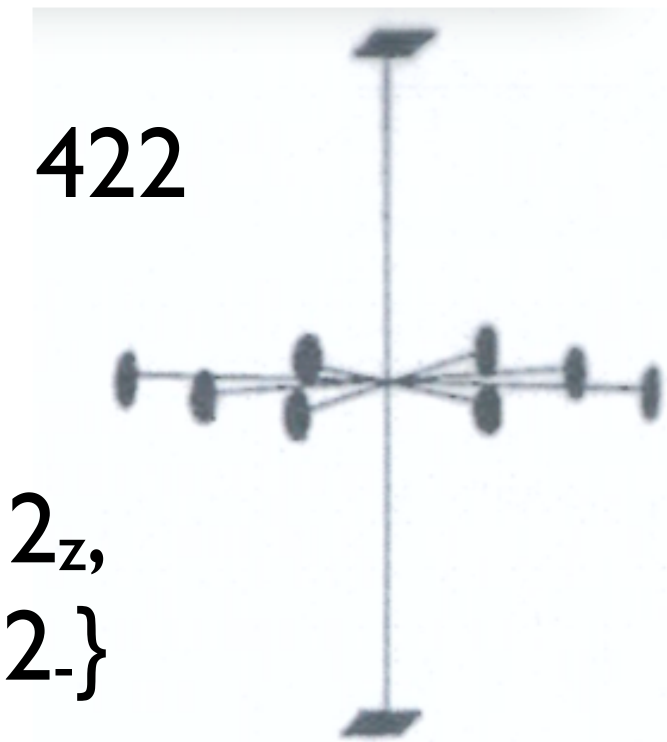


Dihedral Point Groups



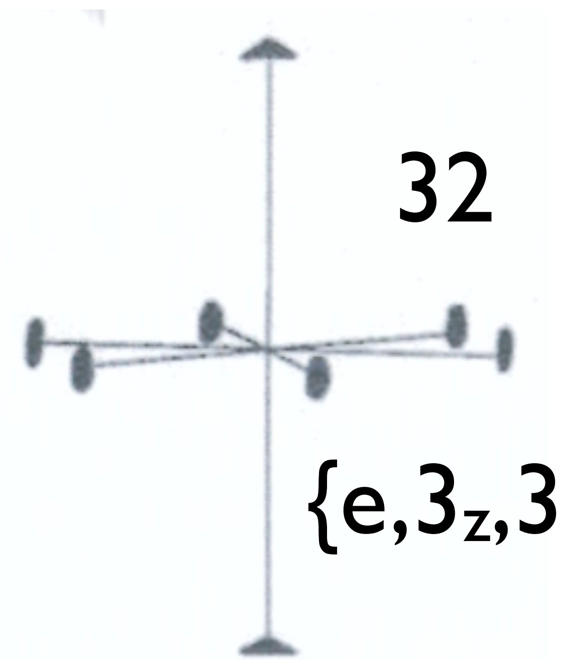
222

$\{e, 2_z, 2_y, 2_x\}$



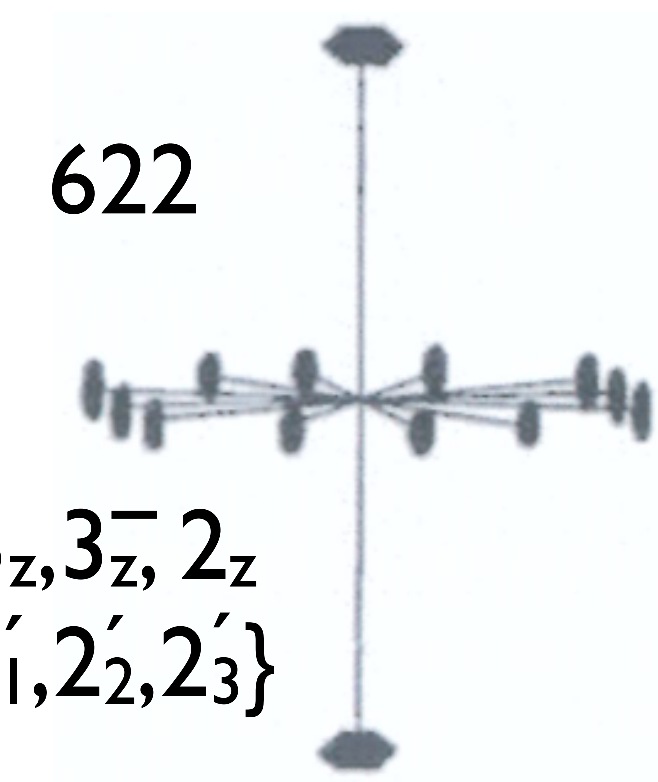
422

$\{e, 4_z, 4_{\bar{z}}, 2_z,$
$2_y, 2_x, 2_+, 2_-\}$



32

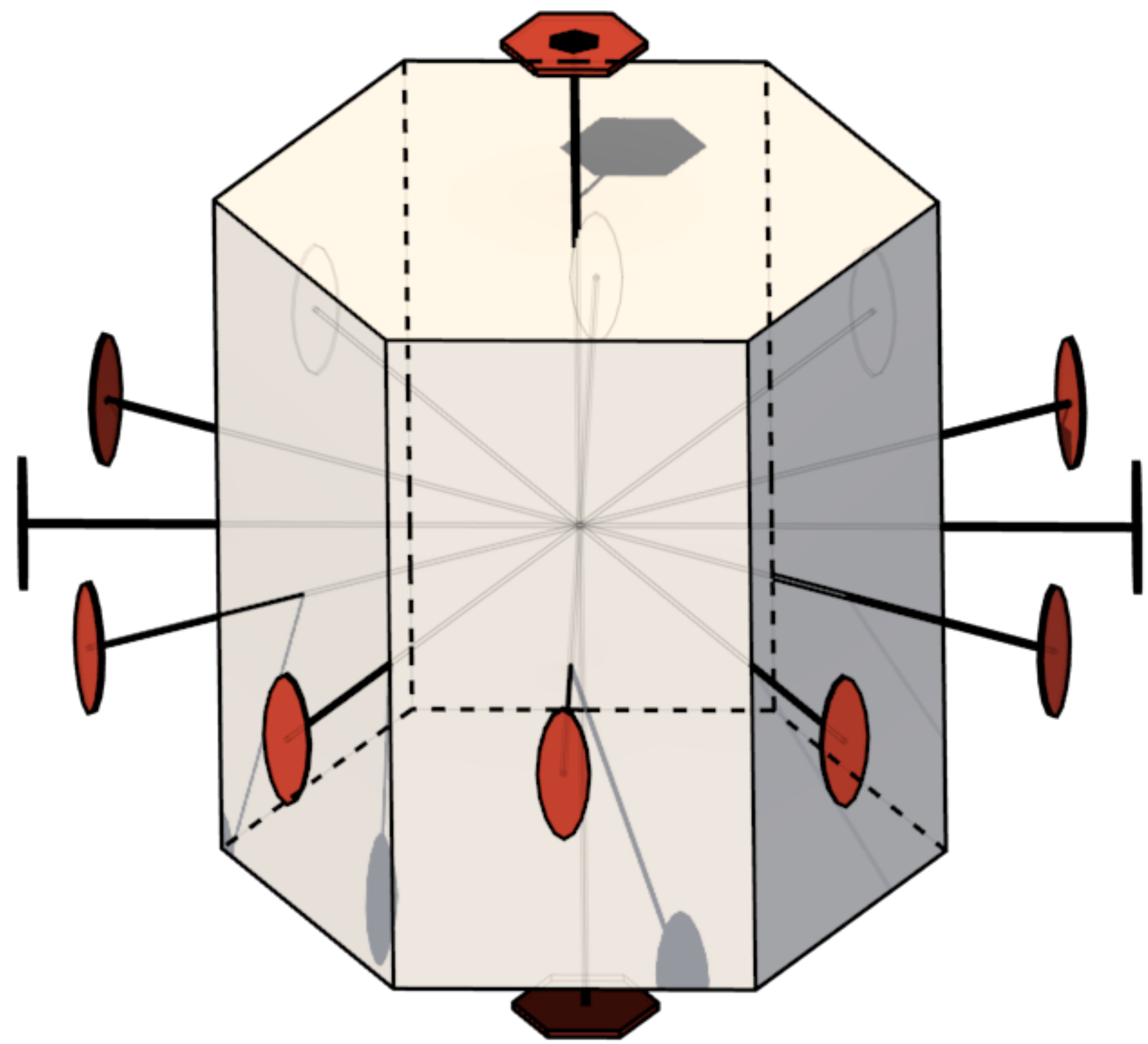
$\{e, 3_z, 3_{\bar{z}}, 2_1, 2_2, 2_3\}$



622

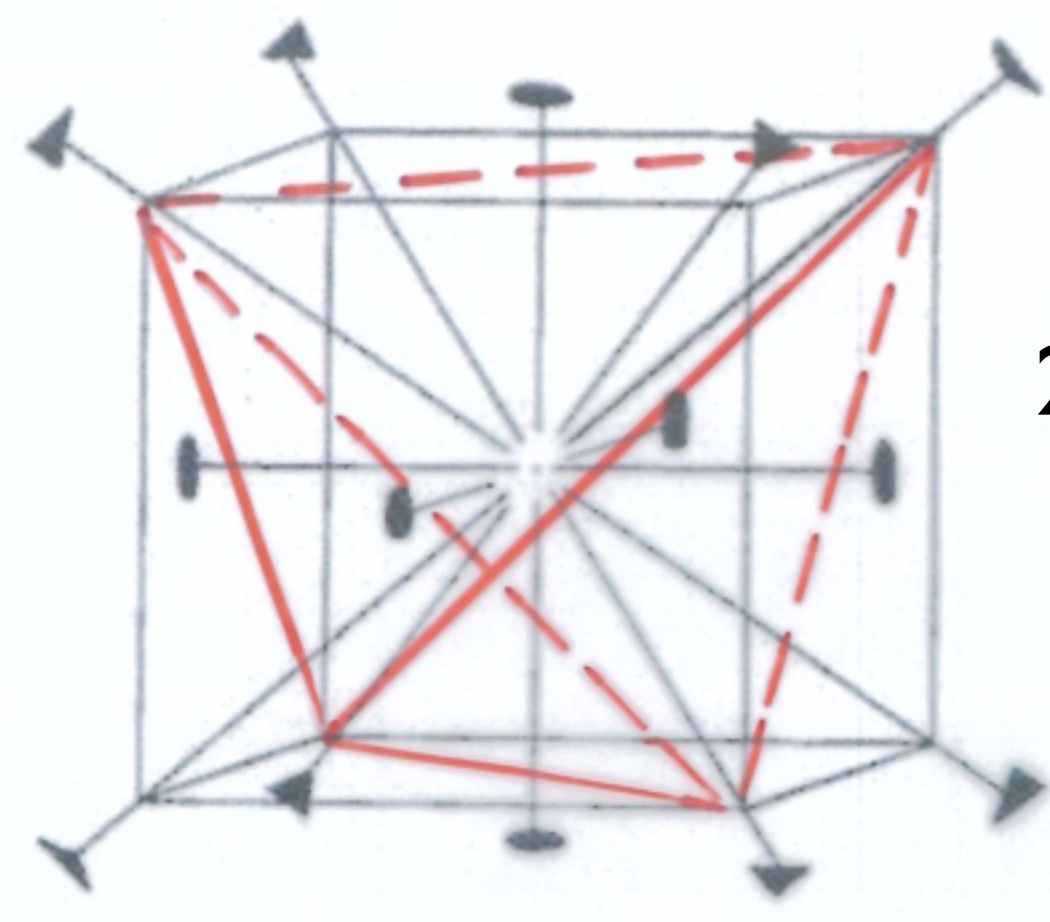
$\{e, 6_z, 6_{\bar{z}}, 3_z, 3_{\bar{z}}, 2_z$
$2_1, 2_2, 2_3, 2_1', 2_2', 2_3'\}$

622 (D_6)



$\{e, 6_z, 6_{\bar{z}}, 3_z, 3_{\bar{z}}, 2_z, 2_1, 2_2, 2_3, 2_1, 2_2, 2_3\}$

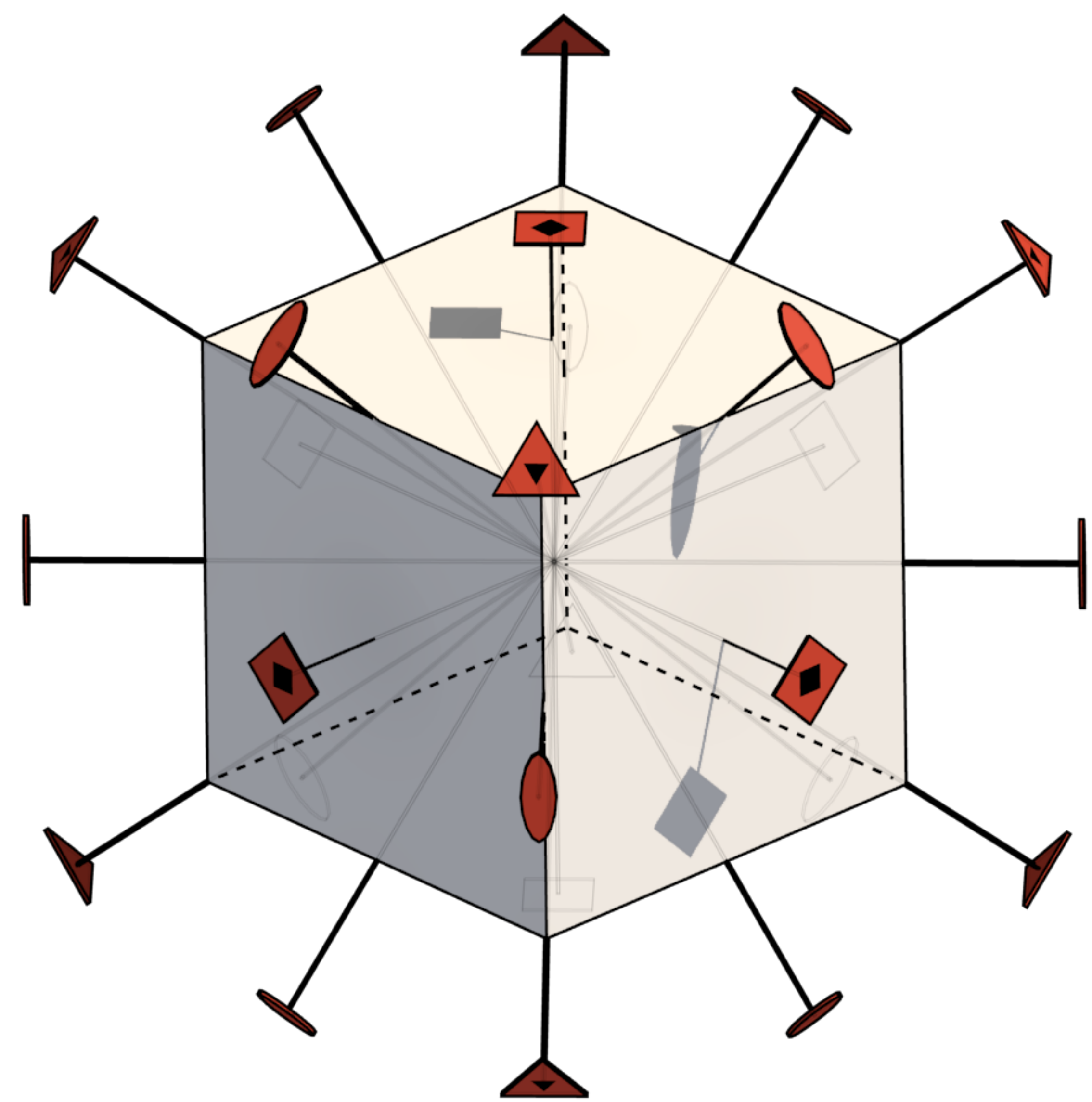
Cubic Rotational Point Groups



23 (T)

$\{e, 2_x, 2_y, 2_z,$
$3_1, 3_{\bar{1}}, 3_2, 3_{\bar{2}}, 3_3, 3_{\bar{3}}, 3_4, 3_{\bar{4}}\}$

432(O)



$\{e, 2_x, 2_y, 2_z,$
$4x, 4\bar{x}, 4y, 4\bar{y}, 4z, 4\bar{z}$
$3_1, 3_{\bar{1}}, 3_2, 3_{\bar{2}}, 3_3, 3_{\bar{3}}, 3_4, 3_{\bar{4}}$
$2_1, 2_2, 2_3, 2_4, 2_5, 2_6\}$

Direct-product groups

Let G_1 and G_2 are two groups. The set of all pairs $\{(g_1,g_2), g_1 \in G_1, g_2 \in G_2\}$ forms a group $G_1 \otimes G_2$ with respect to the product: $(g_1,g_2)(g'_1,g'_2) = (g_1g'_1, g_2g'_2)$.

The group $G = G_1 \otimes G_2$ is called a **direct-product** group

Point group mm2 $= \{1, 2_{001}, m_{100}, m_{010}\}$

$G_1 = \{1, 2_{001}\}$ $G_2 = \{1, m_{100}\}$

$G_1 \otimes G_2 = \{1.1,\ 2_{001}.1,\ 1.m_{100},\ 2_{001}m_{100} = m_{010}\}$

Centro-symmetrical groups

G_1: rotational groups $G_2 = \{1, \bar{1}\}$ group of inversion

$G_1 \otimes \{1, \bar{1}\} = G_1 + \bar{1}.G_1$

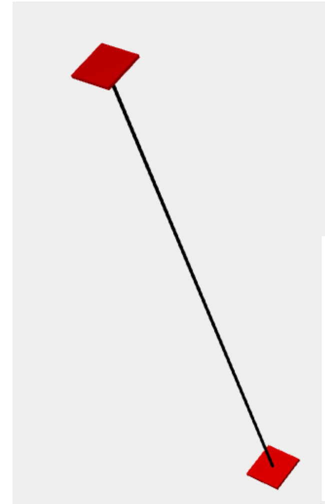
$\{1, 2_{001}, m_{100}, m_{010}\} \otimes \{1, \bar{1}\} =$

$\{1.1,\ 2_{001}.1,\ m_{100}.1, m_{010}.1,\ 1.\bar{1},\ 2_{001}.\bar{1},\ m_{100}.\bar{1}, m_y.\bar{1}\}$

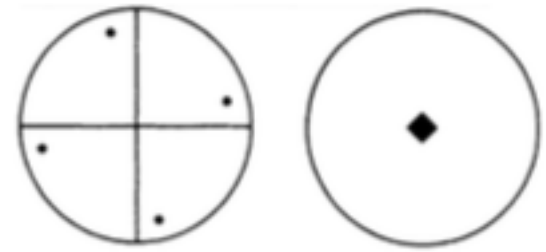
$\{1, 2_{001}, m_{100}, m_{010}, \bar{1}, m_{001}, 2_{100}, 2_{010}\} = 2/m2/m2/m$ or mmm

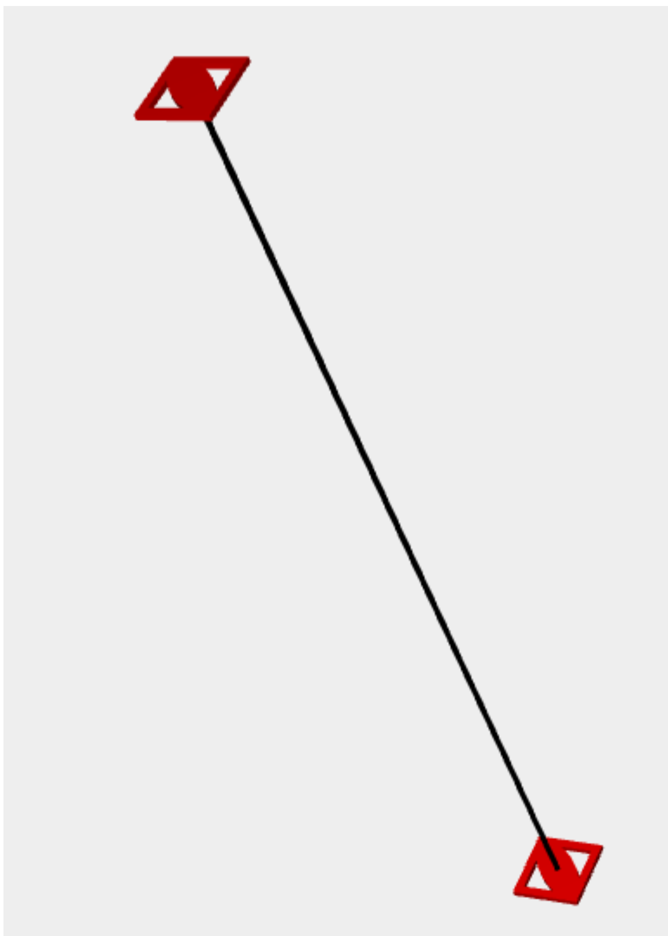
Crystallographic Point Groups

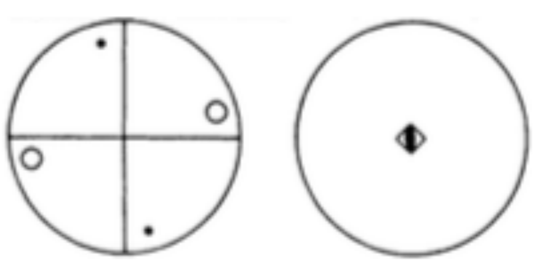
G	$G+\bar{1}G$	G(G')	$G'+\bar{1}(G-G')$
1 (C_1)	$1+\bar{1}.1=\bar{1}$ (C_i)	----	-----
2 (C_2)	$2+\bar{1}.2=2/m$ (C_{2h})	2(1)	m (C_s)
3 (C_3)	$3+\bar{1}.3=\bar{3}$ (C_{3i} or S_6)	----	----
4 (C_4)	$4+\bar{1}.4=4/m$ (C_{4h})	4(2)	$\bar{4}$ (S_4)
6 (C_6)	$6+\bar{1}.6=6/m$ (C_{6h})	6(3)	$\bar{6}$ (C_{3h})



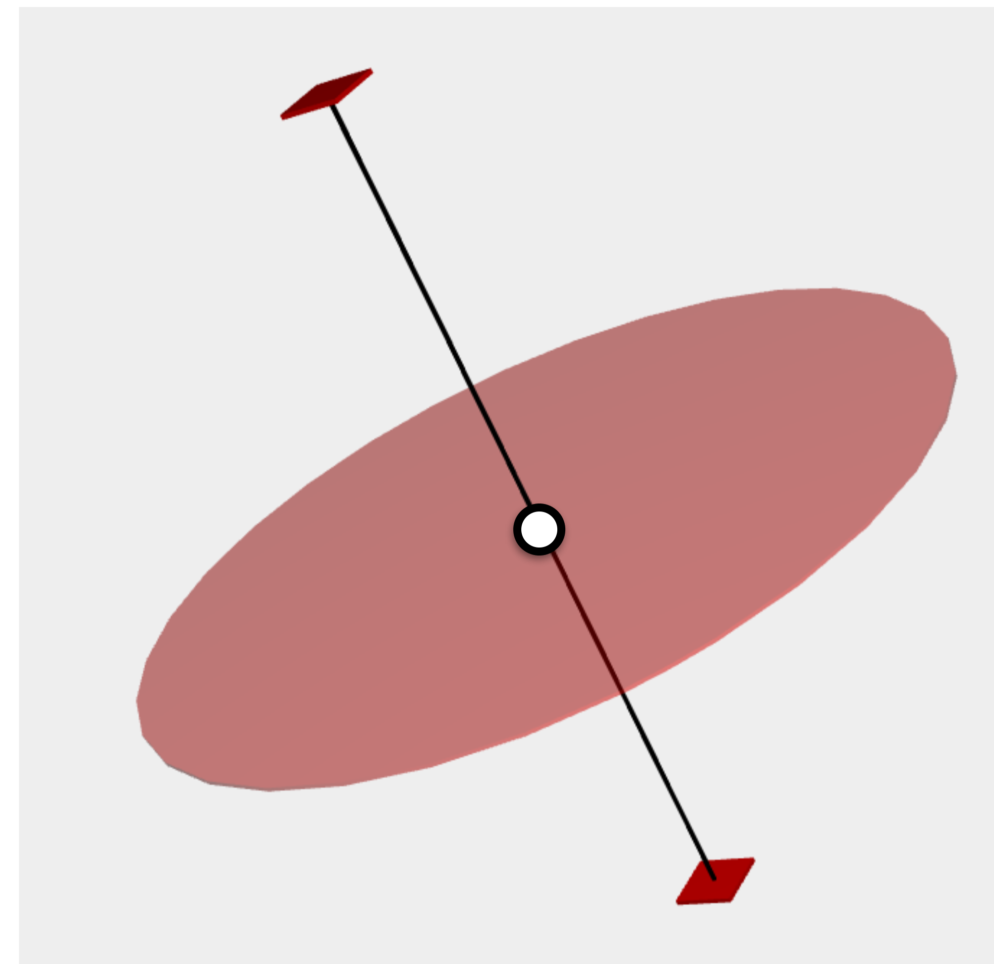
4 (C_4)

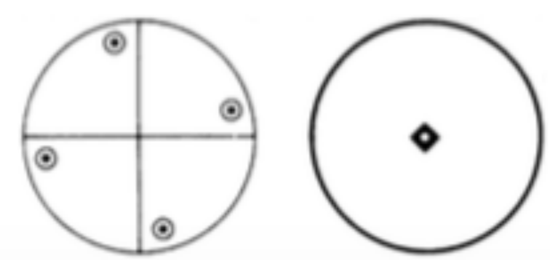






4(2) 4 (S_4)



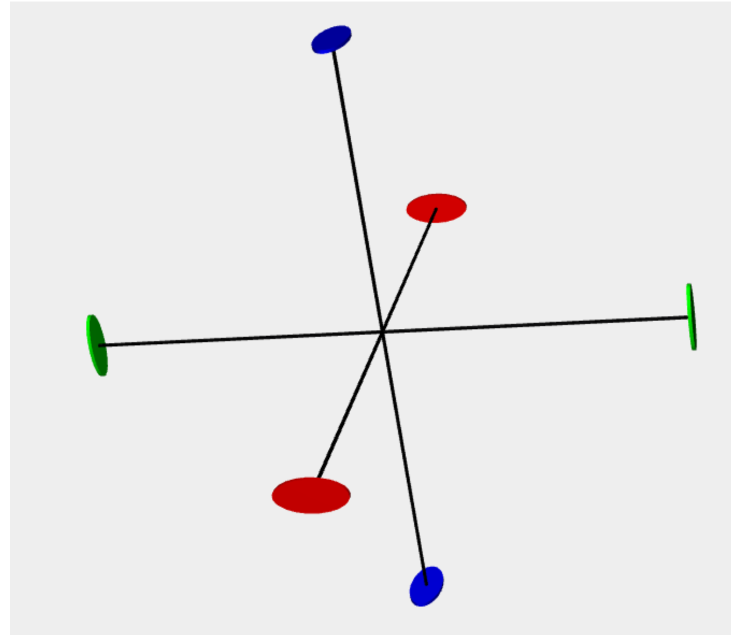


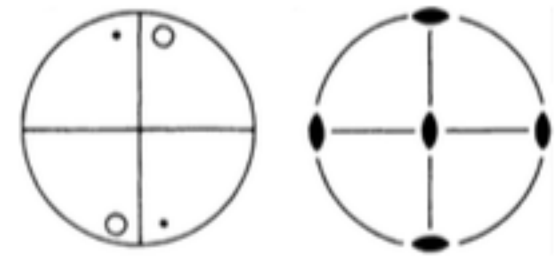
$4+\bar{1}.4=4/m$ (C_{4h})

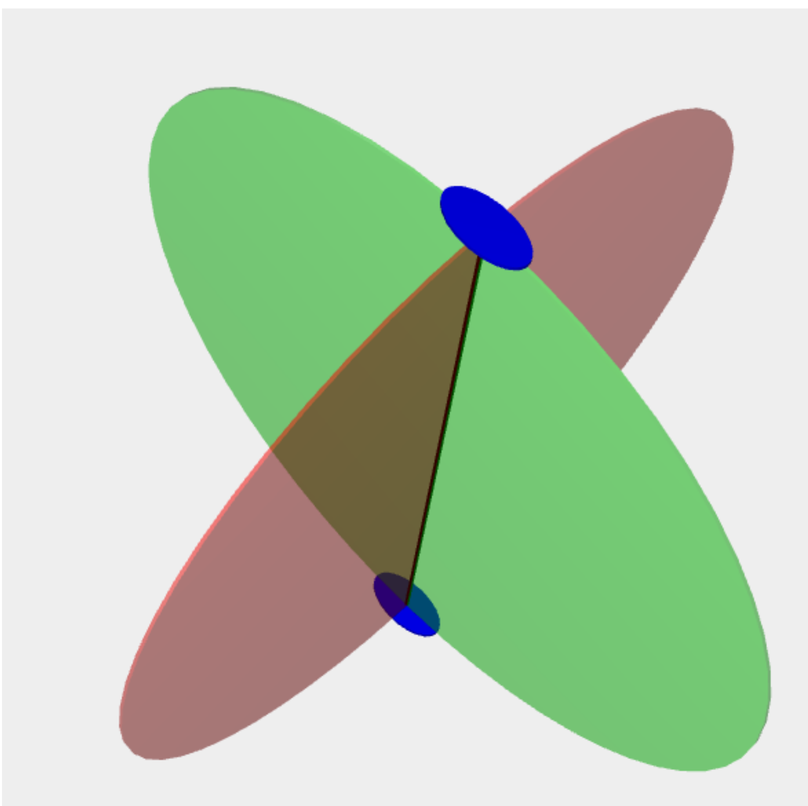
Crystallographic Point Groups

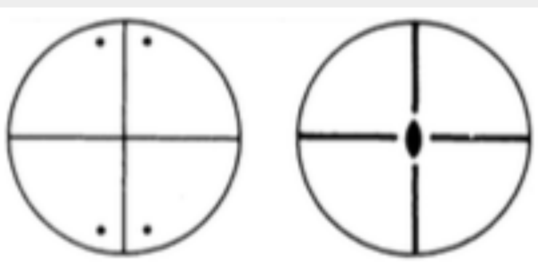
G	$G+\bar{1}G$	G(G')	$G'+\bar{1}(G-G')$
222 (D_2)	$222+\bar{1}.222=2/m2/m2/m$ mmm (D_{2h})	222(2)	2mm (C_{2v})
32 (D_3)	$32+\bar{1}.32=\bar{3}2/m$ $\bar{3}m(D_{3d})$	32(3)	3m (C_{3v})
422 (D_4)	$422+\bar{1}.422=4/m2/m2/m$ 4/mmm(D_{4h})	422(4) 422(222)	4mm (C_{4v}) $\bar{4}2m$ (D_{2d})
622 (D_6)	$622+\bar{1}.622=6/m2/m2/m$ 6/mmm(D_{6h})	622(6) 622(32)	6mm (C_{6v}) $\bar{6}2m$ (D_{3h})
23 (T)	$23+\bar{1}.23=2/m3$ $m\bar{3}$ (T_h)	----	-----
432 (O)	$432+\bar{1}.432=4/m\bar{3}2/m$ $m\bar{3}m(O_h)$	432(23)	$\bar{4}3m$ (Td)

222 (D_2)

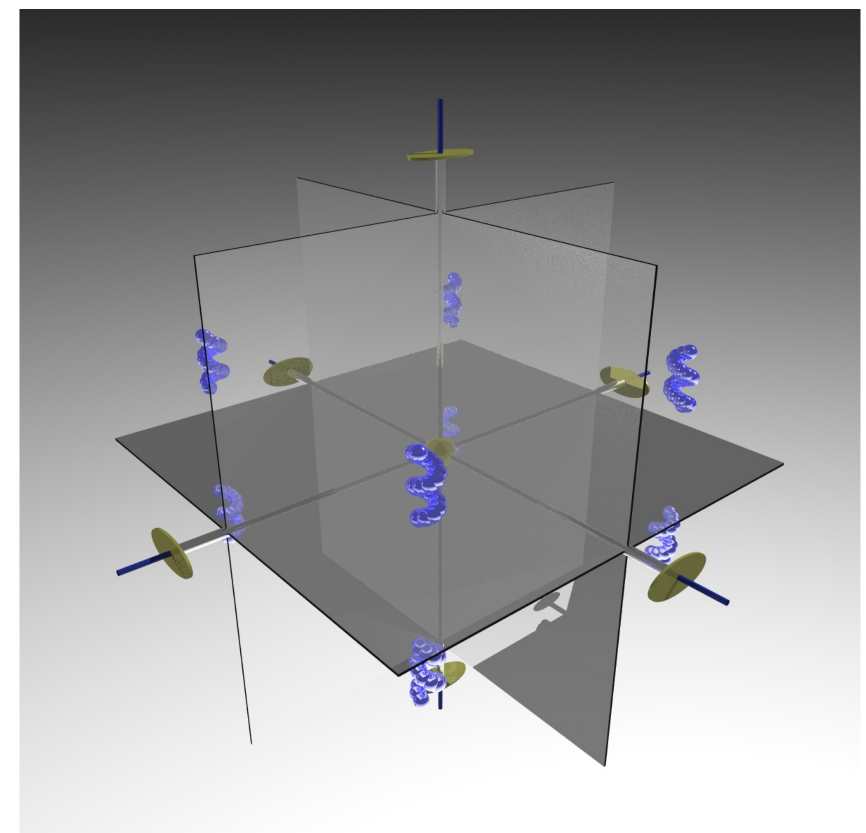


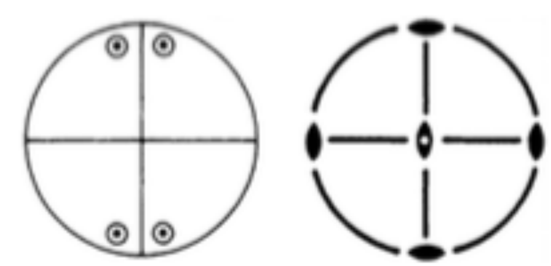






222(2)   2mm (C_{2v})





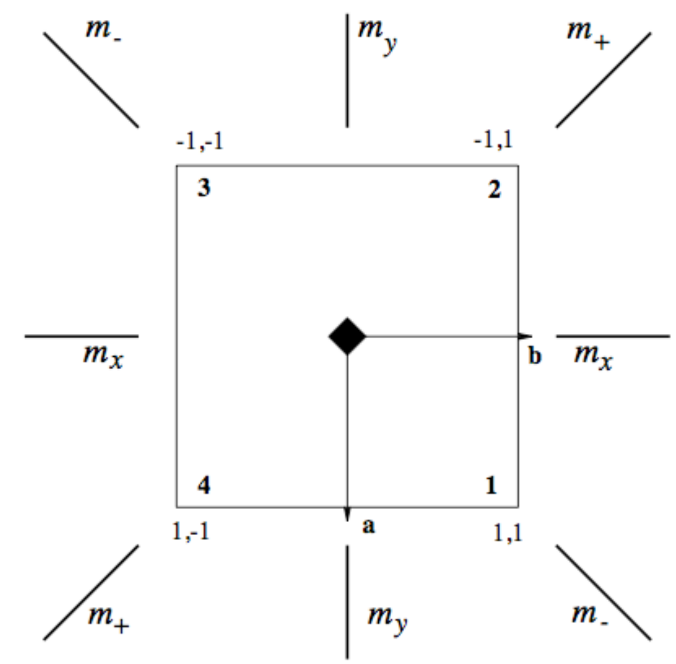
$222+\bar{1}.222=2/m2/m2/m$

mmm (D_{2h})

Crystallographic Point Groups

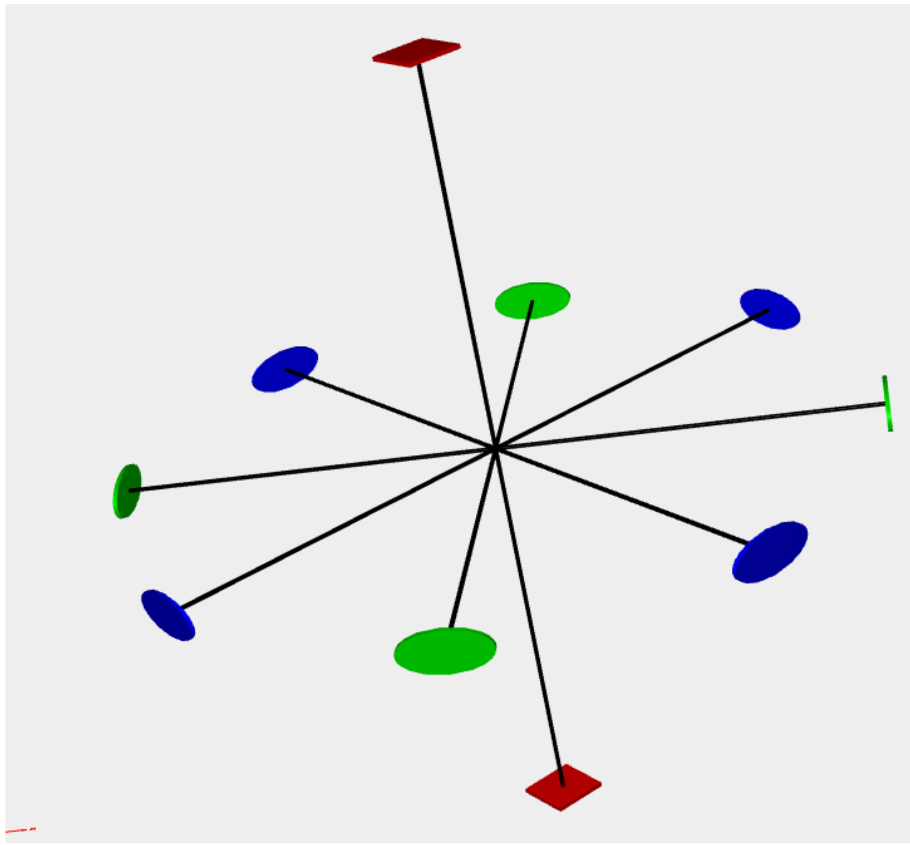
Groups isomorphic to 422

422	e	4_z 4_z^-	2_z	2_x 2_y	2_+ 2_-
4mm	e	4_z 4_z^-	2_z	m_x m_y	m_+ m_-
$\bar{4}2m$	e	$\bar{4}_z$ $\bar{4}_z^-$	2_z	2_x 2_y	m_+ m_-
$\bar{4}m2$	e	$\bar{4}_z$ $\bar{4}_z^-$	2_z	m_x m_y	2_+ 2_-

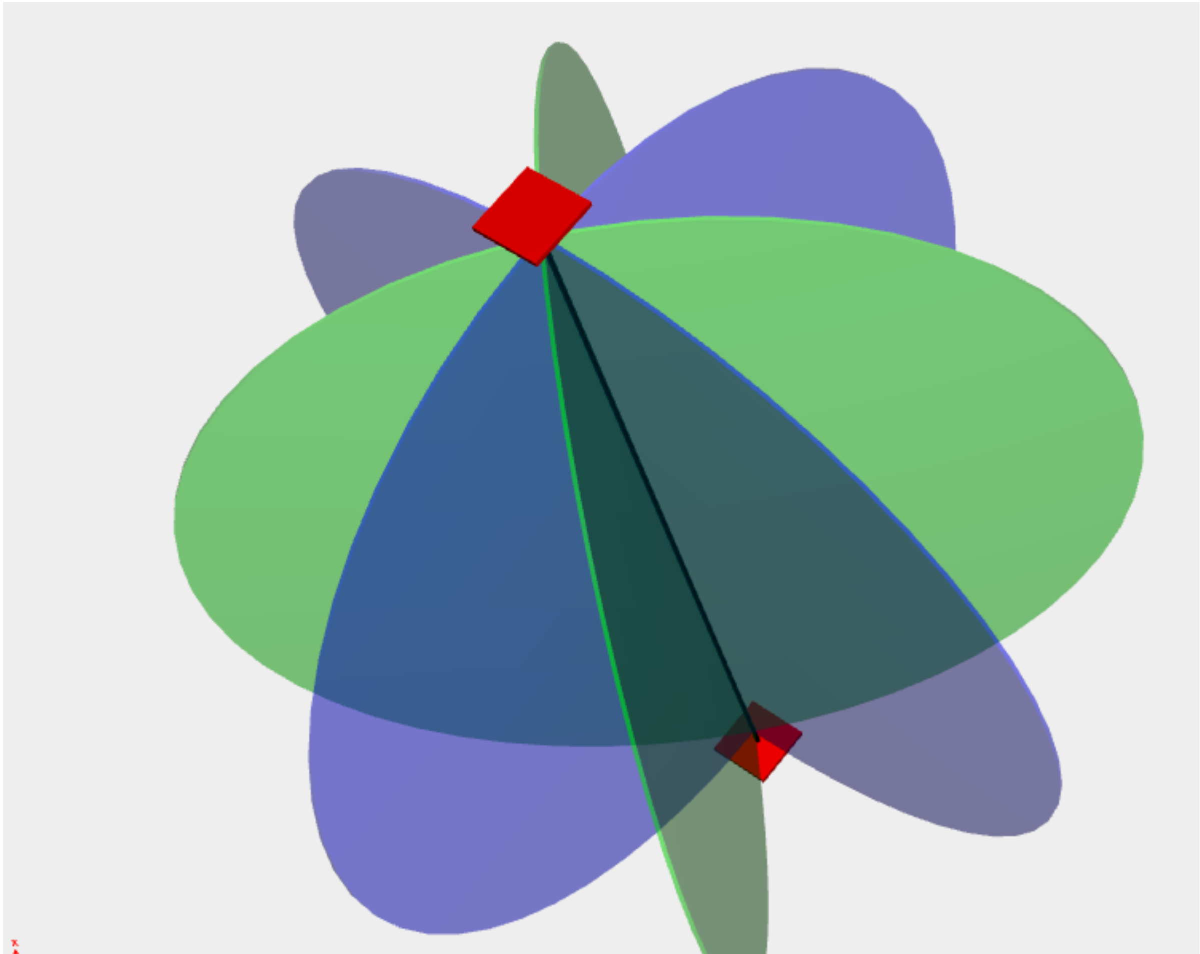


Groups isomorphic to 622

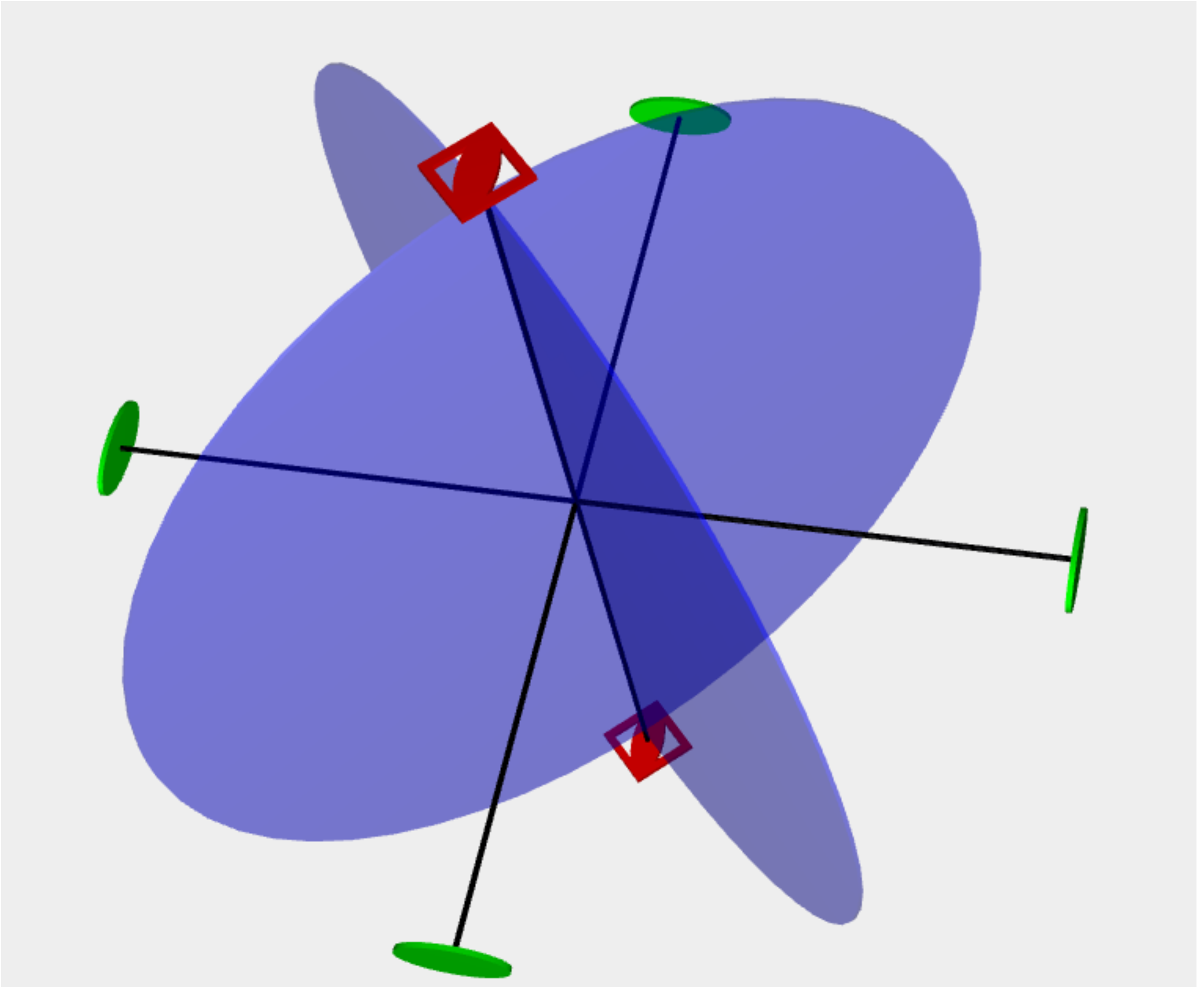
622	e	$6_z 6_z^-$	$3_z 3_z^-$	2_z	$2_1 2_2 2_3$	$2'_1 2'_2 2'_3$
6mm	e	$6_z 6_z^-$	$3_z 3_z^-$	2_z	$m_1 m_2 m_3$	$m'_1 m'_2 m'_3$
$\bar{6}2m$	e	$\bar{6}_z \bar{6}_z^-$	$3_z 3_z^-$	m_z	$2_1 2_2 2_3$	$m'_1 m'_2 m'_3$
$\bar{6}m2$	e	$\bar{6}_z \bar{6}_z^-$	$3_z 3_z^-$	m_z	$m_1 m_2 m_3$	$2'_1 2'_2 2'_3$



422 (D_4)

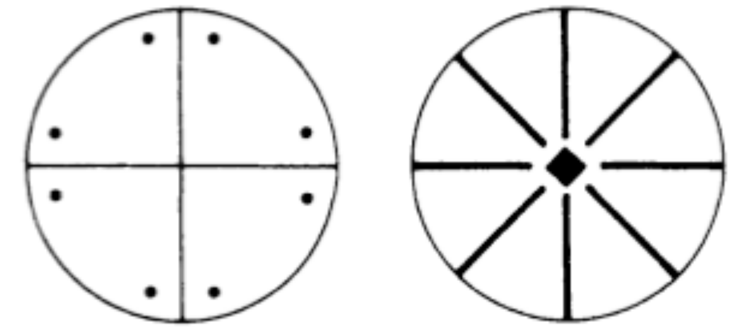


422(4) 4mm (C_{4v})

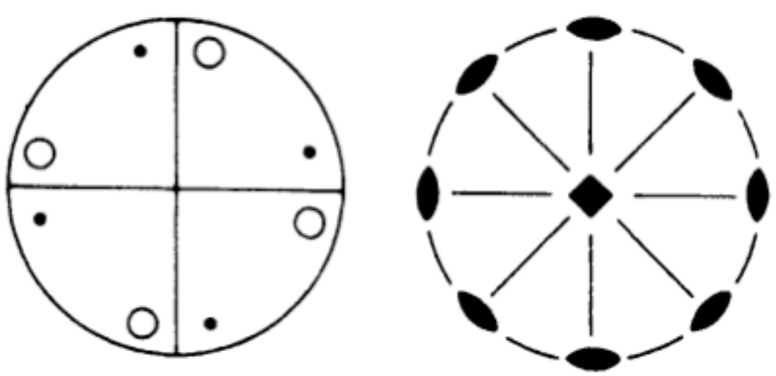
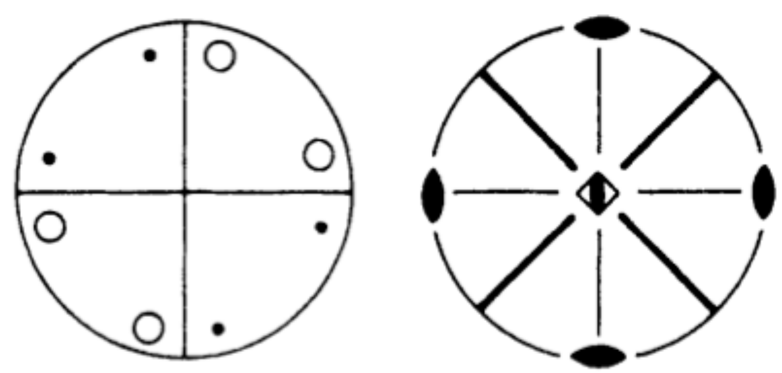
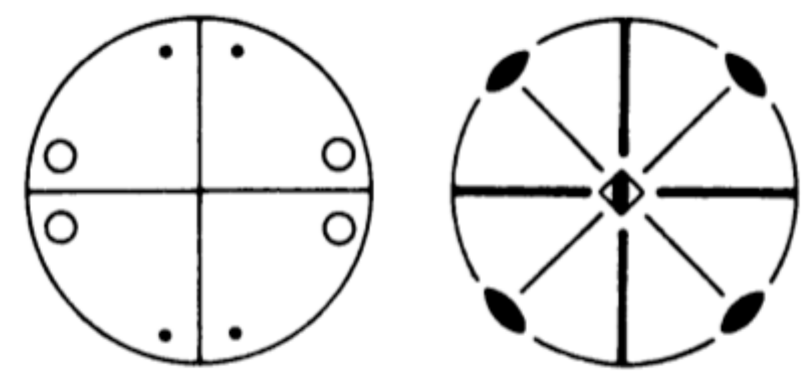


422(222) $\bar{4}2m$ (D_{2d})

Problem 2.11

_4mm_ 

Consider the following three pairs of stereographic projections. Each of them correspond to a crystallographic point group isomorphic to ***4mm***:

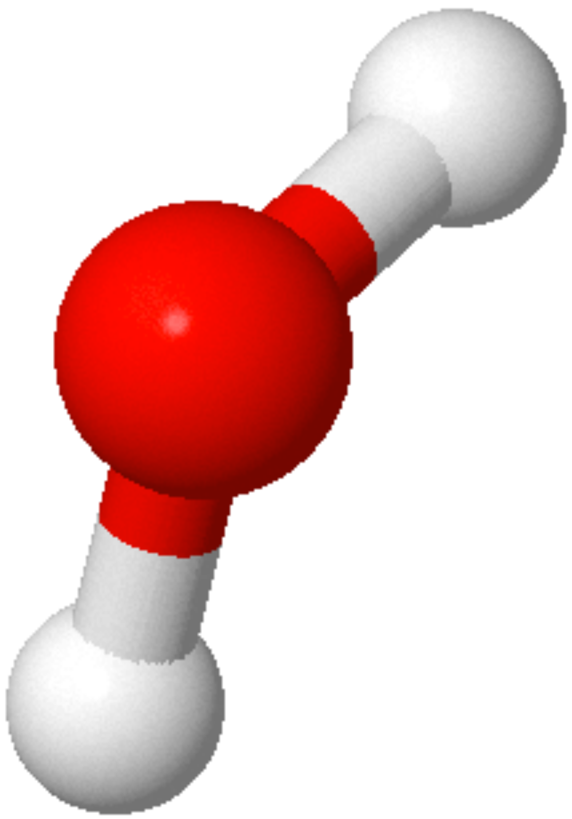
(i) Determine those point groups by indicating their symbols, symmetry operations and possible sets of generators;
(ii) For each of the isomorphic point groups indicate the one-to-one correspondence with the symmetry operations of ***4mm***.

MOLECULAR POINT-GROUP SYMMETRY

Molecular Point-group Symmetry

Example

Determine the symmetry elements and the corresponding point groups for the molecule of water

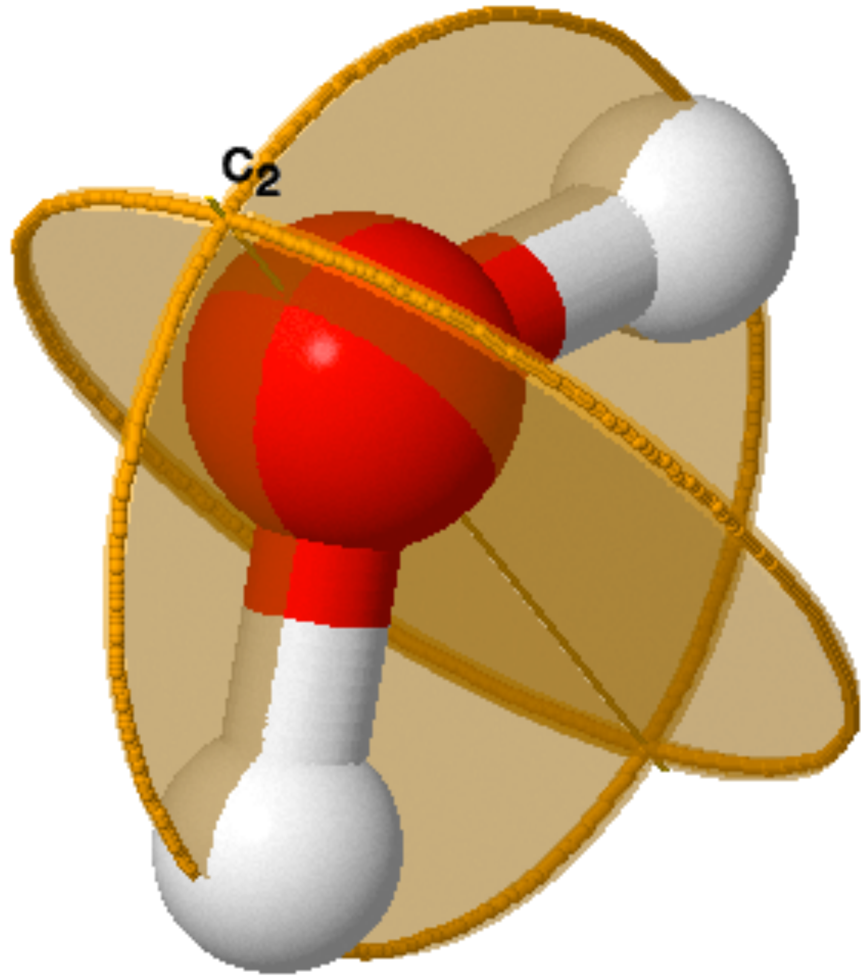


molecule of water

Example

SOLUTION

Molecular Point-group Symmetry



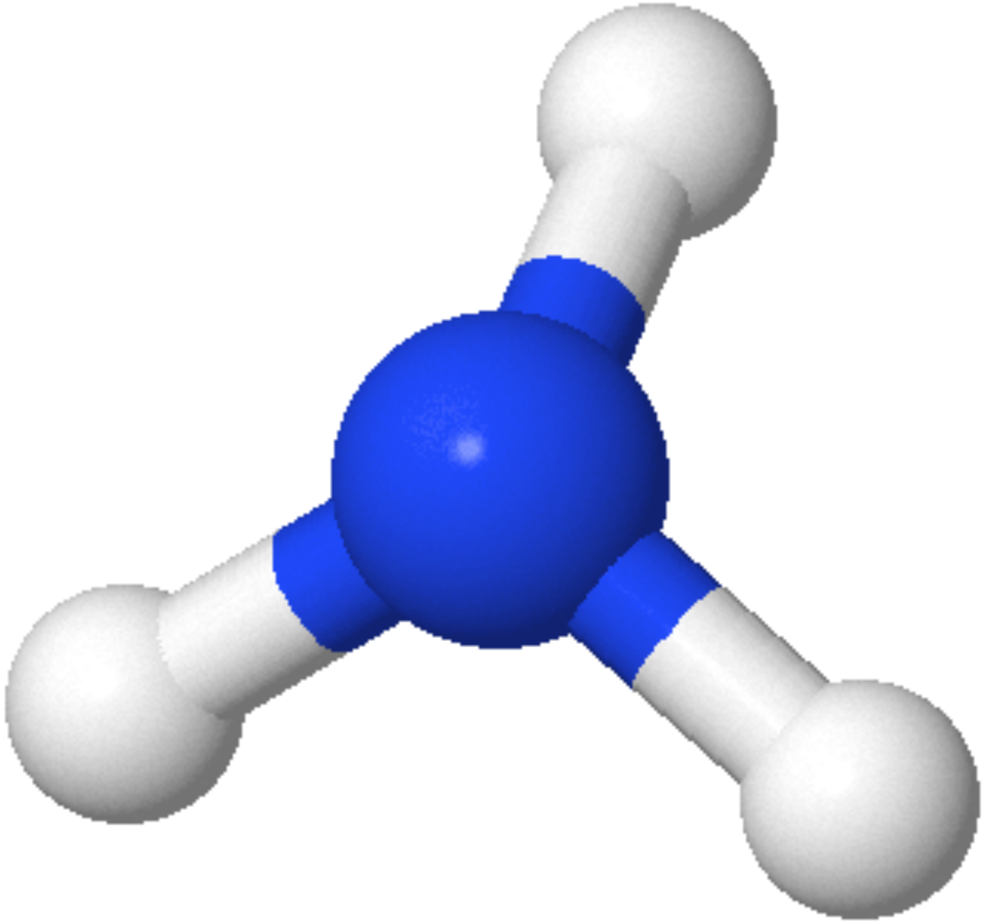
molecule of water

symmetry group: mm2

Molecular Point-group Symmetry

Example

Determine the symmetry elements and the corresponding point groups for the molecule of ammonia

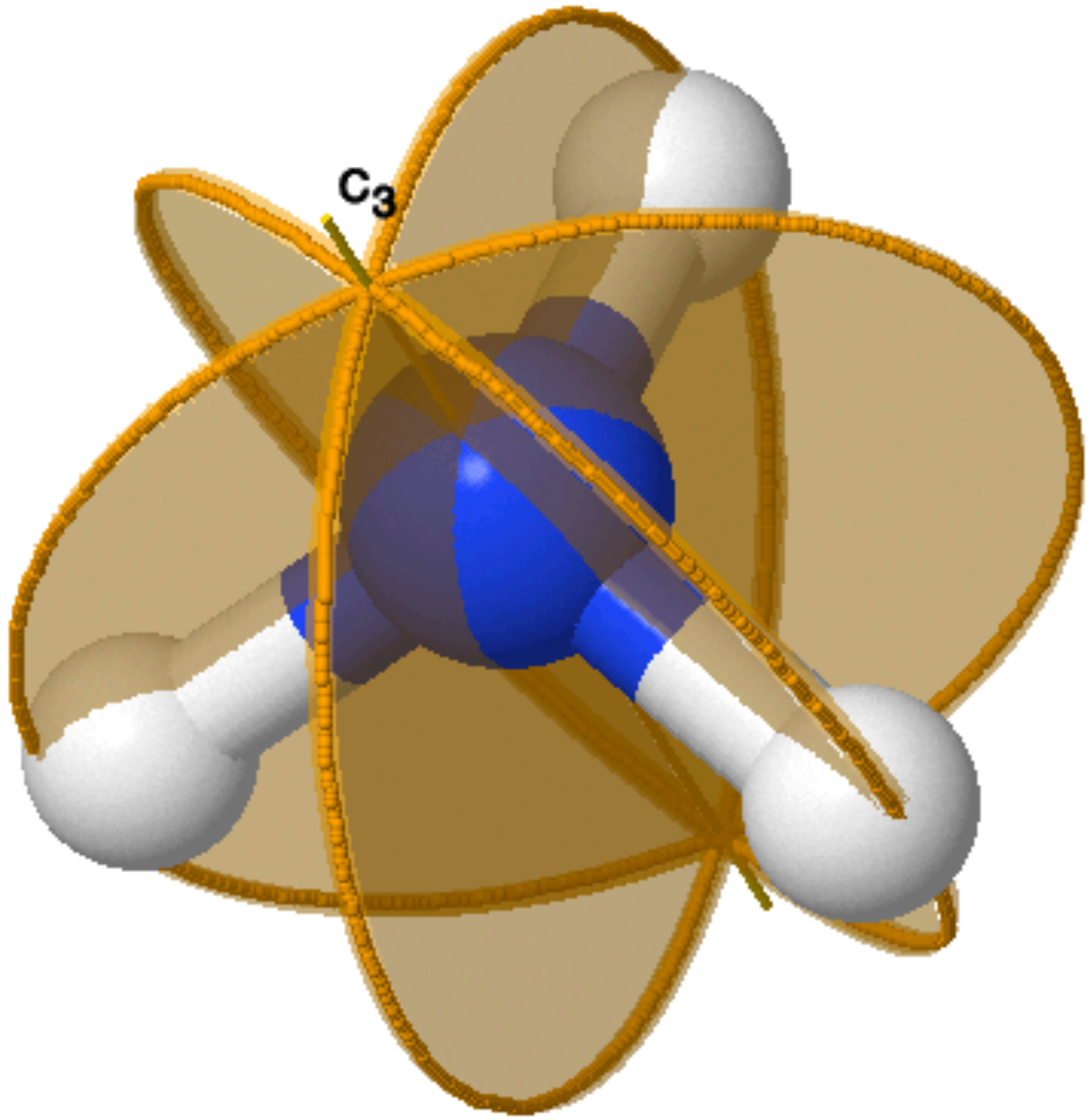


ammonia molecule

Example

SOLUTION

Molecular Point-group Symmetry

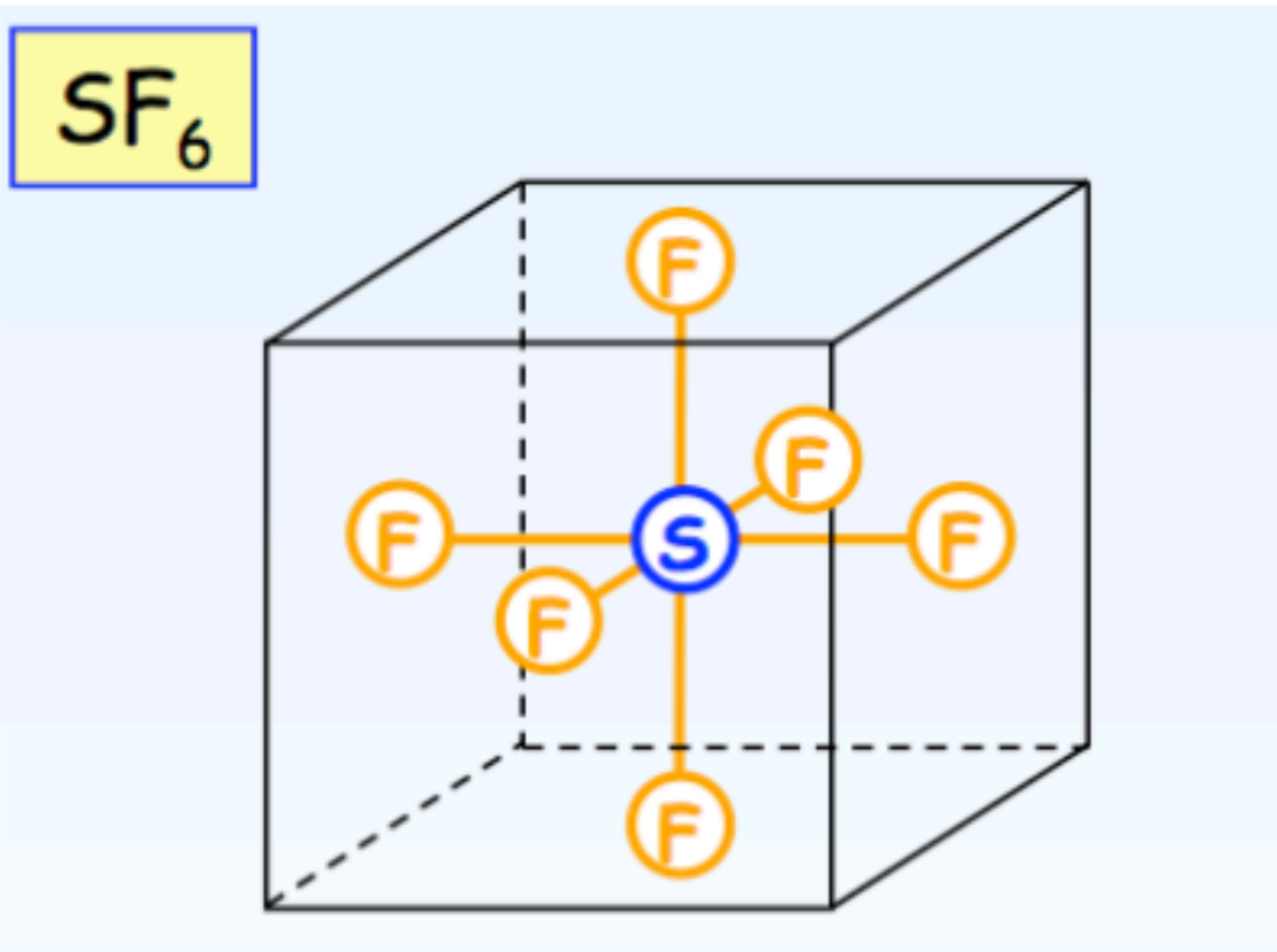


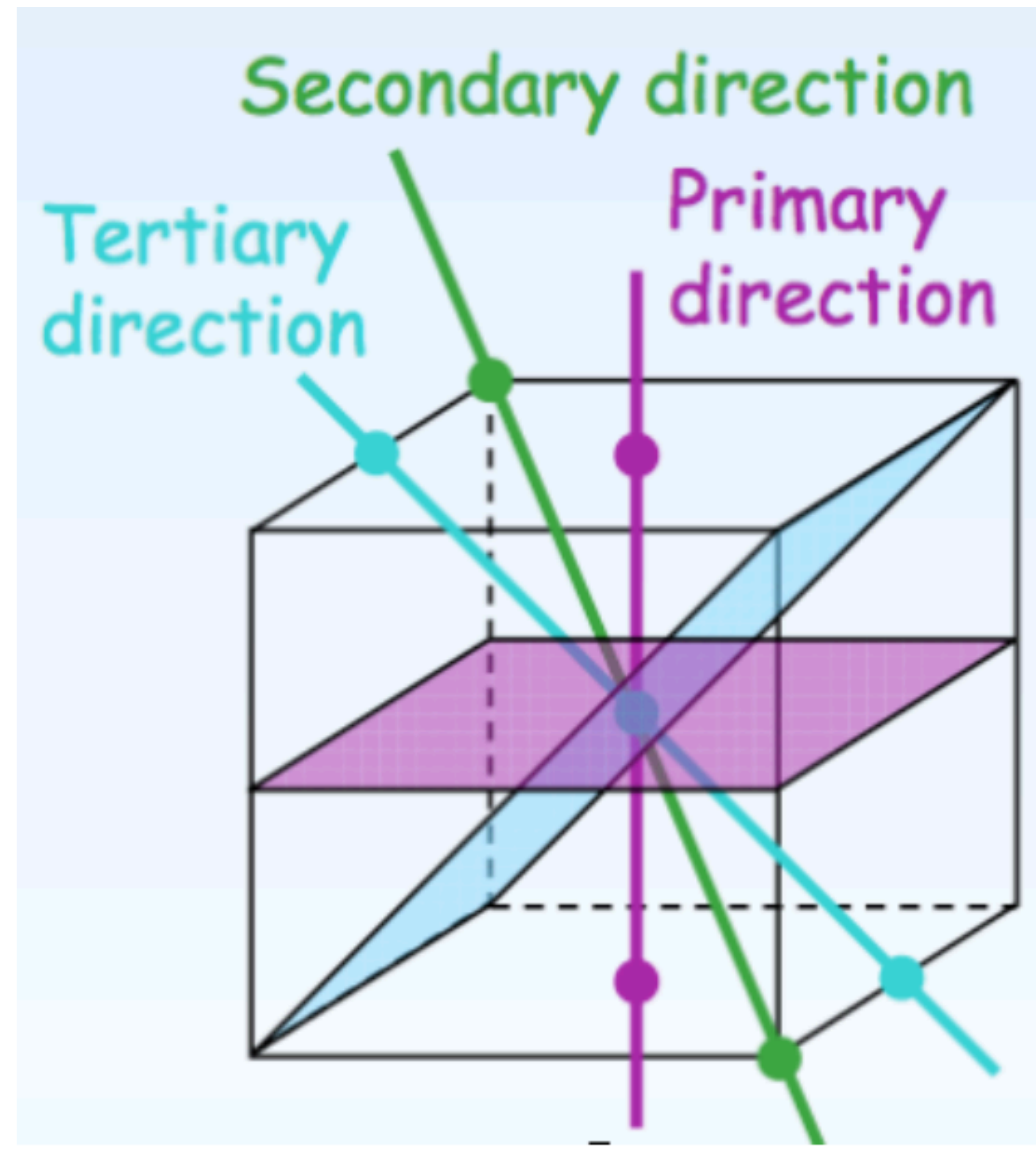
ammonia molecule

symmetry group: 3m

Molecular Point-group Symmetry

Example Determine the symmetry elements and the corresponding point groups for the molecule of SF_6

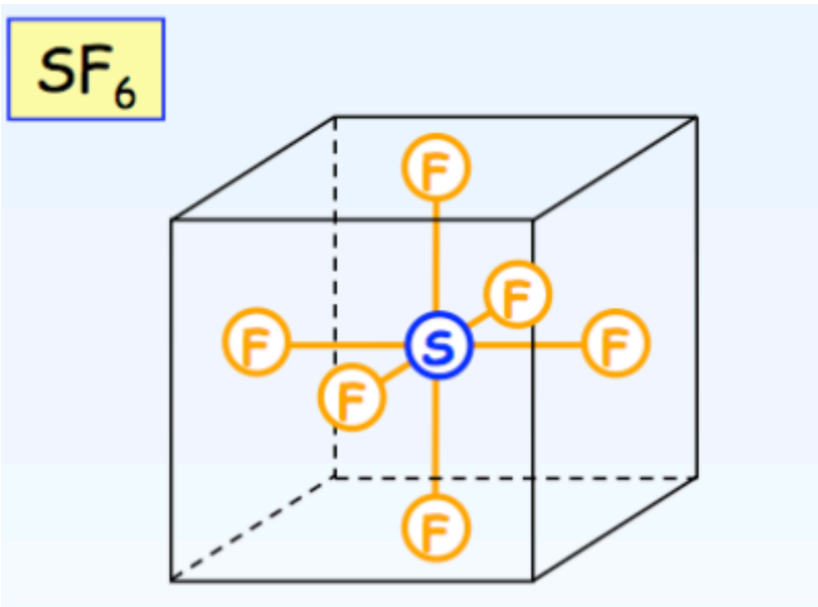


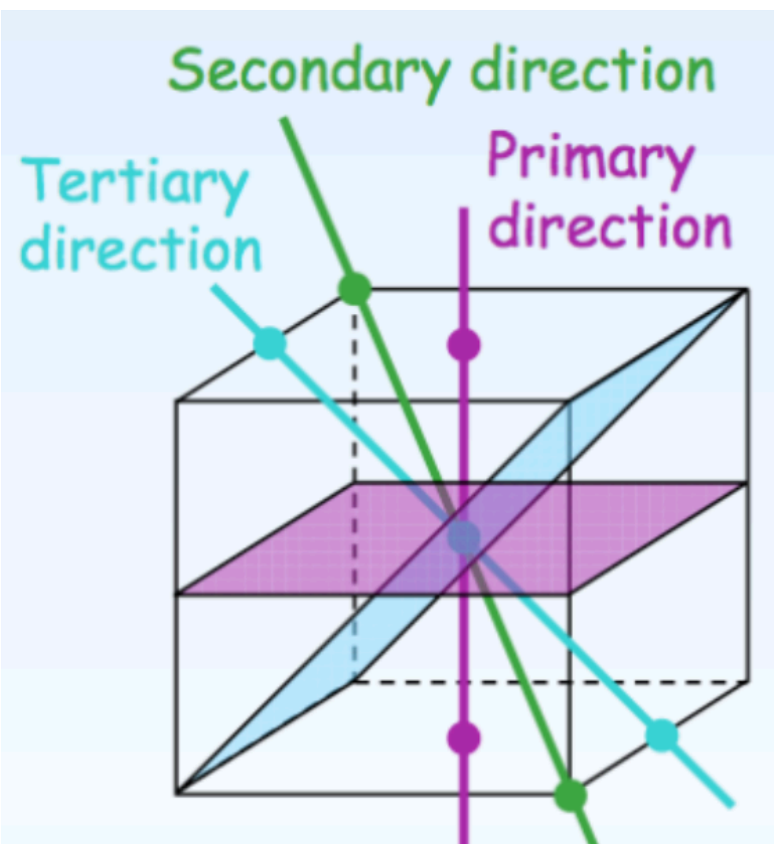


Example

Molecular Point-group Symmetry

SOLUTION





axis 4 and mirrors

axis $\bar{3}$

axis 2 and mirror

⇓

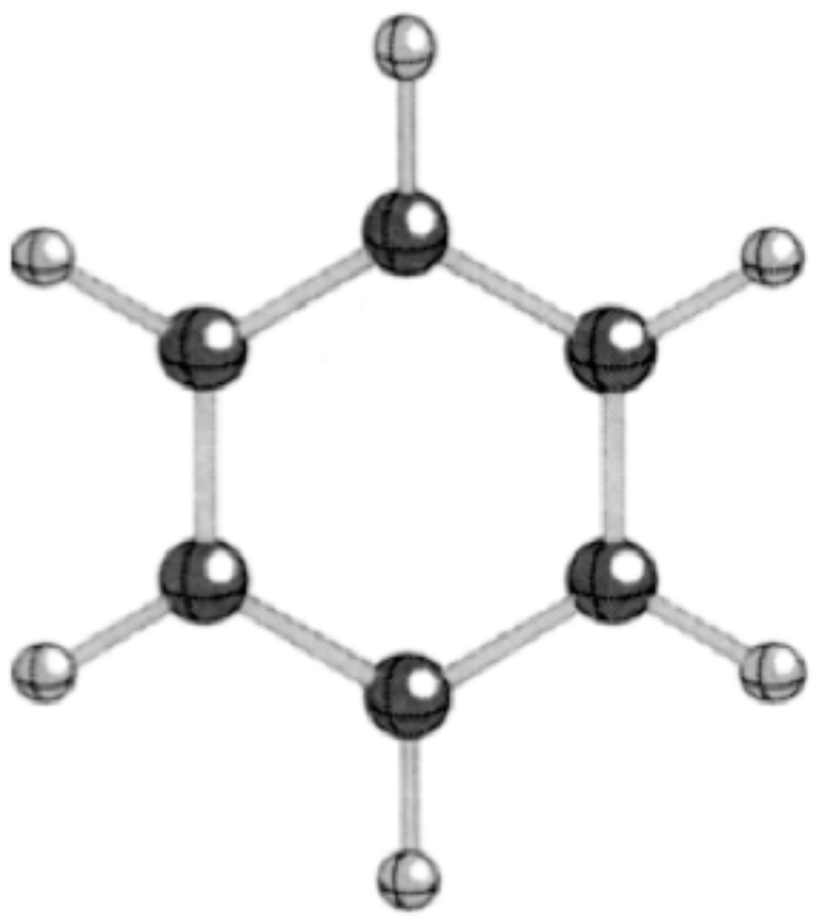
Point group: $\frac{4}{m}\bar{3}\frac{2}{m}$

$\longrightarrow m\bar{3}m$

Problem 2.12

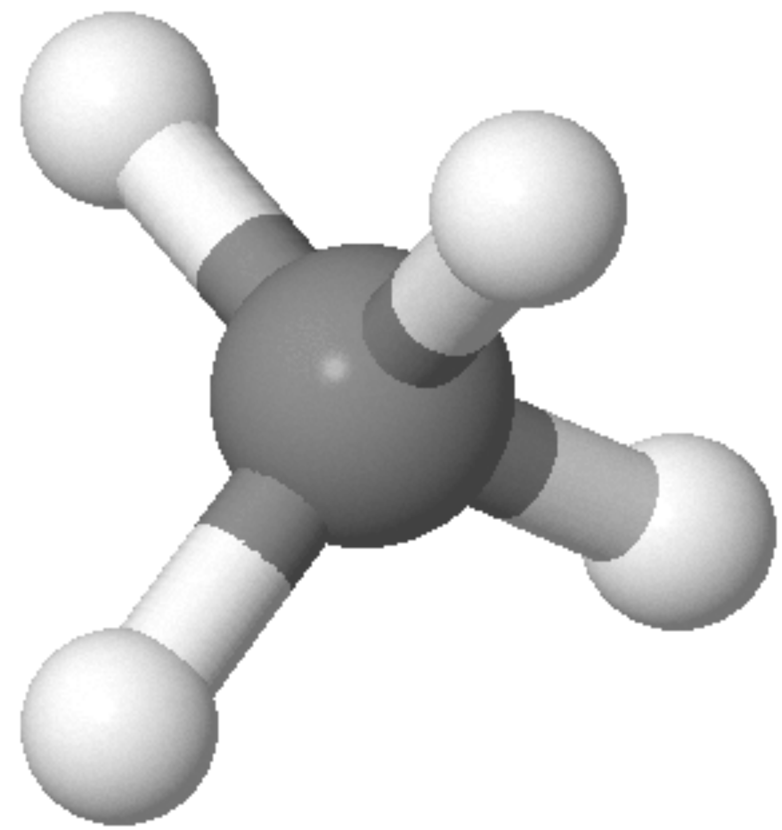
Determine the symmetry elements and the corresponding point groups for each of the following models of molecules:

Benzene C_6H_6



(a)

(CH_4 methane)



(b)

GENERATION OF CRYSTALLOGRAPHIC POINT GROUPS

Generation of point groups

Crystallographic groups are **solvable** groups

Composition series: $1 \lhd Z_2 \lhd Z_3 \lhd \ldots \lhd G$

index 2 or 3

Set of generators of a group is a set of group elements such that each element of the group can be obtained as an ordered product of the generators

$$W = (g_h)^{k_h} * (g_{h-1})^{k_{h-1}} * \ldots * (g_2)^{k_2} * g_1$$

g_1 - identity

$g_2, g_3, \ldots$ - generate the rest of elements

Example

Generation of the group of the square

Composition series: $\boldsymbol{1} \overset{2_z}{\underset{[2]}{\lhd}} \boldsymbol{2} \overset{4_z}{\underset{[2]}{\lhd}} \boldsymbol{4} \overset{m_{10}}{\underset{[2]}{\lhd}} \boldsymbol{4mm}$

Step 1:

$\boldsymbol{1} = \{1\}$

Step 2:

$\boldsymbol{2} = \{1\} + 2_z \{1\}$

Step 3:

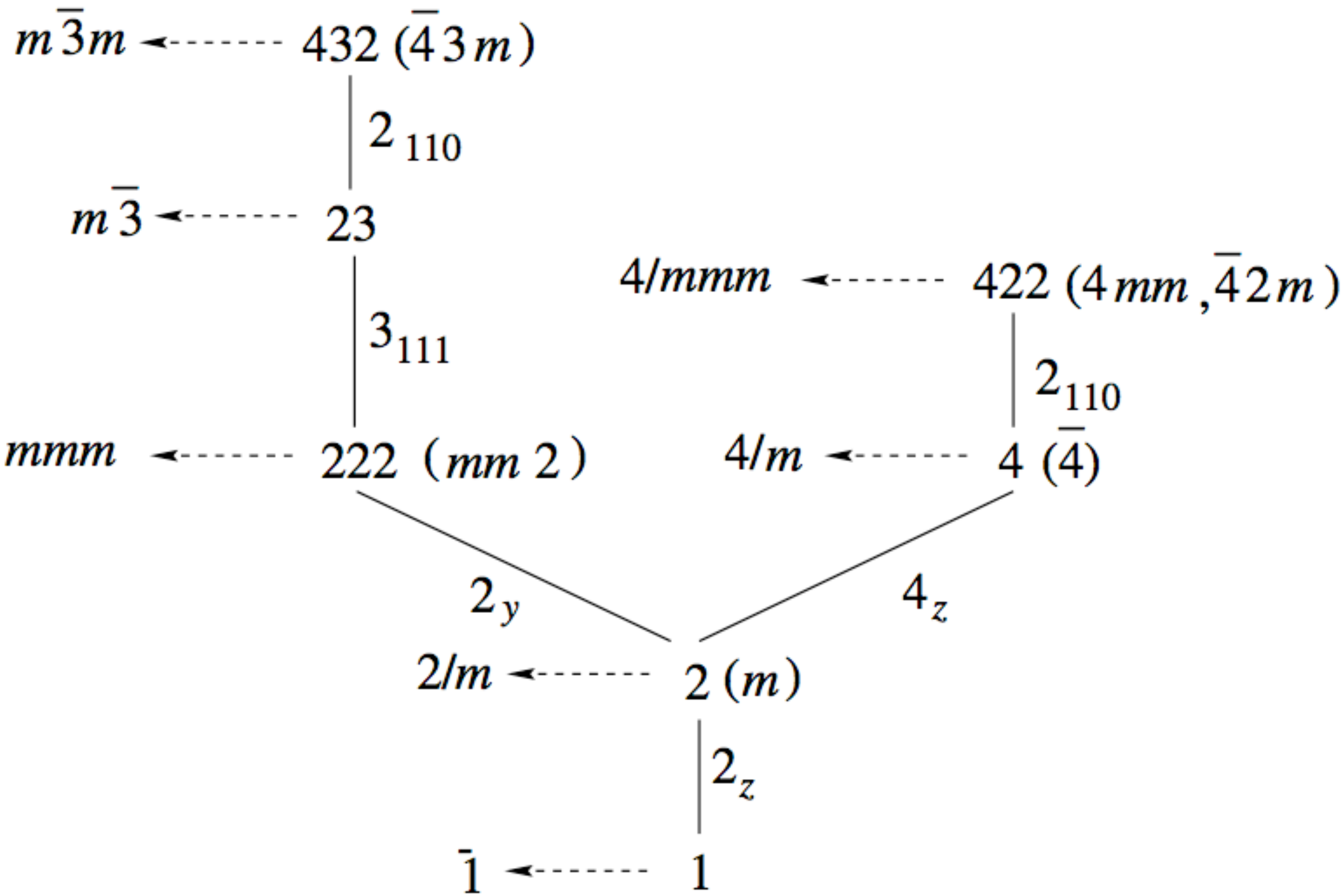
$\boldsymbol{4} = \{1,2\} + 4_z \{1,2\}$

Step 4:

$\boldsymbol{4mm} = \boldsymbol{4} + m_{10}\, \boldsymbol{4}$

	1	2	4^+	4^-	m_{10}	m_{01}	m_{11}	$m_{1\bar{1}}$
1	1	2	4^+	4^-	m_{10}	m_{01}	m_{11}	$m_{1\bar{1}}$
2	2	1	4^-	4^+	m_{01}	m_{10}	$m_{1\bar{1}}$	m_{11}
4^+	4^+	4^-	2	1	m_{11}	$m_{1\bar{1}}$	m_{01}	m_{10}
4^-	4^-	4^+	1	2	$m_{1\bar{1}}$	m_{11}	m_{10}	m_{01}
m_{10}	m_{10}	m_{01}	$m_{1\bar{1}}$	m_{11}	1	2	4^-	4^+
m_{01}	m_{01}	m_{10}	m_{11}	$m_{1\bar{1}}$	2	1	4^+	4^-
m_{11}	m_{11}	$m_{1\bar{1}}$	m_{10}	m_{01}	4^+	4^-	1	2
$m_{1\bar{1}}$	$m_{1\bar{1}}$	m_{11}	m_{01}	m_{10}	4^-	4^+	2	1

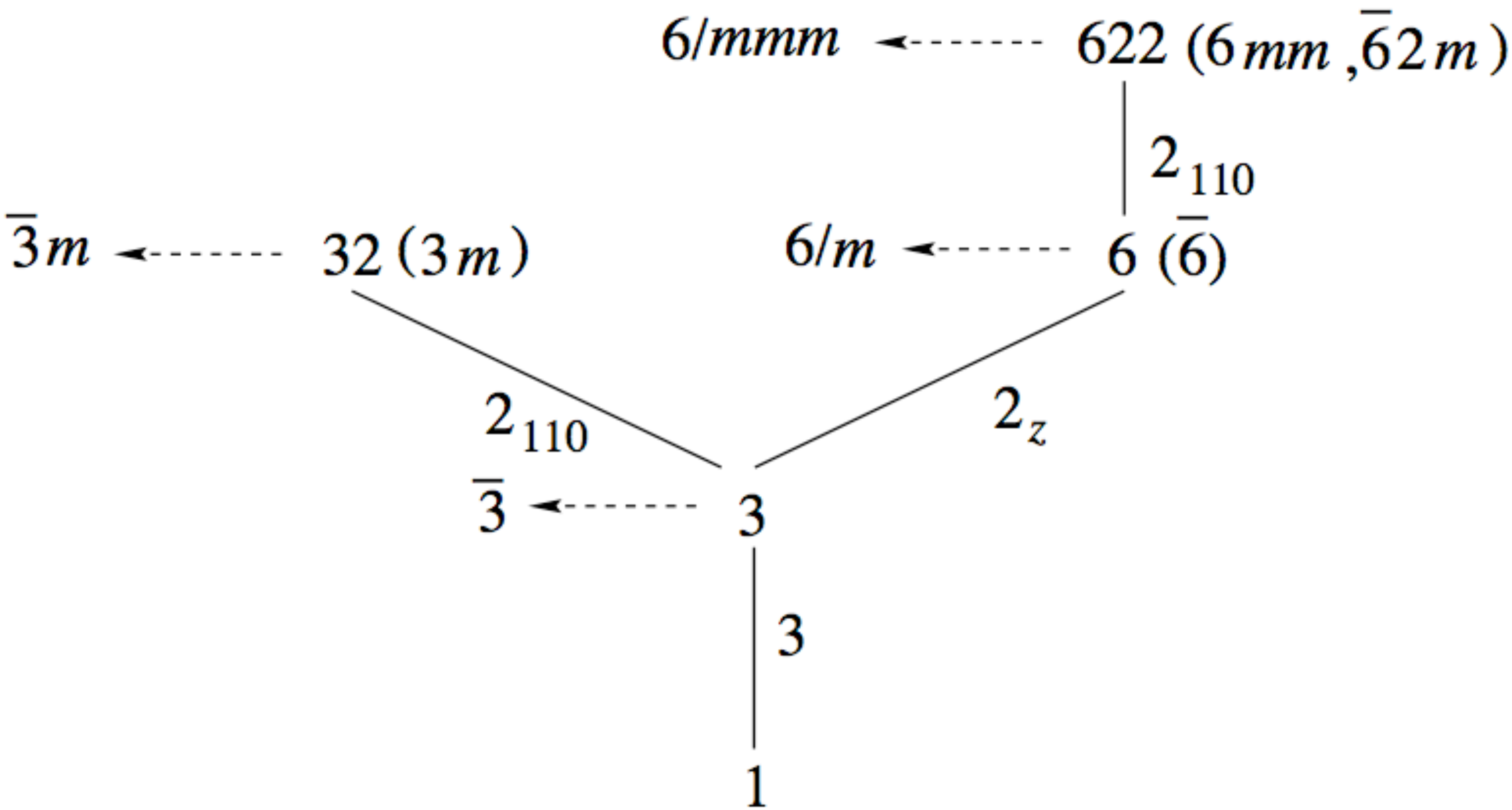
Generation of sub-cubic point groups



Composition series of cubic point groups and their subgroups

HM Symbol	SchoeSy	generators	compos. series
1	$\mathcal{C}_1$	1	1
$\bar{1}$	$\mathcal{C}_i$	$1, \bar{1}$	$\bar{1} \triangleright 1$
2	$\mathcal{C}_2$	$1, 2$	$2 \triangleright 1$
m	$\mathcal{C}_s$	$1, m$	$m \triangleright 1$
$2/m$	$\mathcal{C}_{2h}$	$1, 2, \bar{1}$	$2/m \triangleright 2 \triangleright 1$
222	$\mathcal{D}_2$	$1, 2_z, 2_y$	$222 \triangleright 2 \triangleright 1$
$mm2$	$\mathcal{C}_{2v}$	$1, 2_z, m_y$	$mm2 \triangleright 2 \triangleright 1$
mmm	$\mathcal{D}_{2h}$	$1, 2_z, 2_y, \bar{1}$	$mmm \triangleright 222 \triangleright \ldots$
4	$\mathcal{C}_4$	$1, 2_z, 4$	$4 \triangleright 2 \triangleright 1$
$\bar{4}$	$\mathcal{S}_4$	$1, 2_z, \bar{4}$	$\bar{4} \triangleright 2 \triangleright 1$
$4/m$	$\mathcal{C}_{4h}$	$1, 2_z, 4, \bar{1}$	$4/m \triangleright 4 \triangleright \ldots$
422	$\mathcal{D}_4$	$1, 2_z, 4, 2_y$	$422 \triangleright 4 \triangleright \ldots$
$4mm$	$\mathcal{C}_{4v}$	$1, 2_z, 4, m_y$	$4mm \triangleright 4 \triangleright \ldots$
$\bar{4}2m$	$\mathcal{D}_{2d}$	$1, 2_z, \bar{4}, 2_y$	$\bar{4}2m \triangleright \bar{4} \triangleright \ldots$
$4/mmm$	$\mathcal{D}_{4h}$	$1, 2_z, 4, 2_y, \bar{1}$	$4/mmm \triangleright 422 \triangleright \ldots$
23	$\mathcal{T}$	$1, 2_z, 2_y, 3_{111}$	$23 \triangleright 222 \triangleright \ldots$
$m\bar{3}$	$\mathcal{T}_h$	$1, 2_z, 2_y, 3_{111}, \bar{1}$	$m\bar{3} \triangleright 23 \triangleright \ldots$
432	$\mathcal{O}$	$1, 2_z, 2_y, 3_{111}, 2_{110}$	$432 \triangleright 23 \triangleright \ldots$
$\bar{4}3m$	$\mathcal{T}_d$	$1, 2_z, 2_y, 3_{111}, m_{1\bar{1}0}$	$\bar{4}3m \triangleright 23 \triangleright \ldots$
$m\bar{3}m$	$\mathcal{O}_h$	$1, 2_z, 2_y, 3_{111}, 2_{110}, \bar{1}$	$m\bar{3}m \triangleright 432 \triangleright \ldots$

Generation of sub-hexagonal point groups



Composition series of hexagonal point groups and their subgroups

HM Symbol	SchoeSy	generators	compos. series
1	$\mathcal{C}_1$	1	1
3	$\mathcal{C}_3$	$1, 3$	$3 \triangleright 1$
$\overline{3}$	$\mathcal{S}_6$	$1, 3, \overline{1}$	$\overline{3} \triangleright 3 \triangleright 1$
32	$\mathcal{D}_3$	$1, 3, 2_{110}$	$32 \triangleright 3 \triangleright 1$
$3m$	$\mathcal{C}_{3v}$	$1, 3, m_{110}$	$3m \triangleright 3 \triangleright 1$
$\overline{3}m$	$\mathcal{D}_{3d}$	$1, 3, 2_{110}, \overline{1}$	$\overline{3}m \triangleright 32 \triangleright \ldots$
6	$\mathcal{C}_6$	$1, 3, 2_z$	$6 \triangleright 3 \triangleright 1$
$\overline{6}$	$\mathcal{C}_{3h}$	$1, 3, m_z$	$\overline{6} \triangleright 3 \triangleright 1$
$6/m$	$\mathcal{C}_{6h}$	$1, 2, 2_z, \overline{1}$	$6/m \triangleright 6 \triangleright \ldots$
622	$\mathcal{D}_6$	$1, 3, 2_z, 2_{110}$	$622 \triangleright 6 \triangleright \ldots$
$6mm$	$\mathcal{C}_{6v}$	$1, 3, 2_z, m_{110}$	$6mm \triangleright 6 \triangleright \ldots$
$\overline{6}2m$	$\mathcal{D}_{3h}$	$1, 3, m_z, 2_{110}$	$\overline{6}2m \triangleright \overline{6} \triangleright \ldots$
$6/mmm$	$\mathcal{D}_{6h}$	$1, 3, 2_z, 2_{110}, \overline{1}$	$6/mmm \triangleright 622 \triangleright \ldots$

Problem 2.13

Generate the symmetry operations of the group ***4/mmm*** following its composition series.

Generate the symmetry operations of the group $\bar{3}m$ following its composition series.

GROUP-SUPERGROUP RELATIONS

Supergroups: Some basic results (summary)

Supergroup G>H

$H=\{e,h_1,h_2,\ldots,h_k\} \subset G$

Proper supergroups G>H, and
trivial supergroup: H

Index of the group H in supergroup G: $[i]=|G|/|H|$
(order of G)/(order of H)

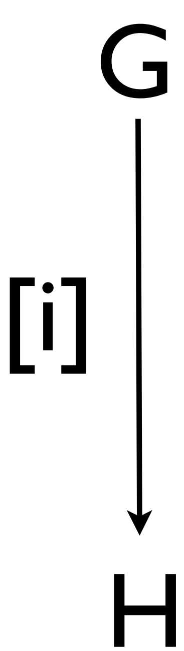
Minimal supergroups G of H

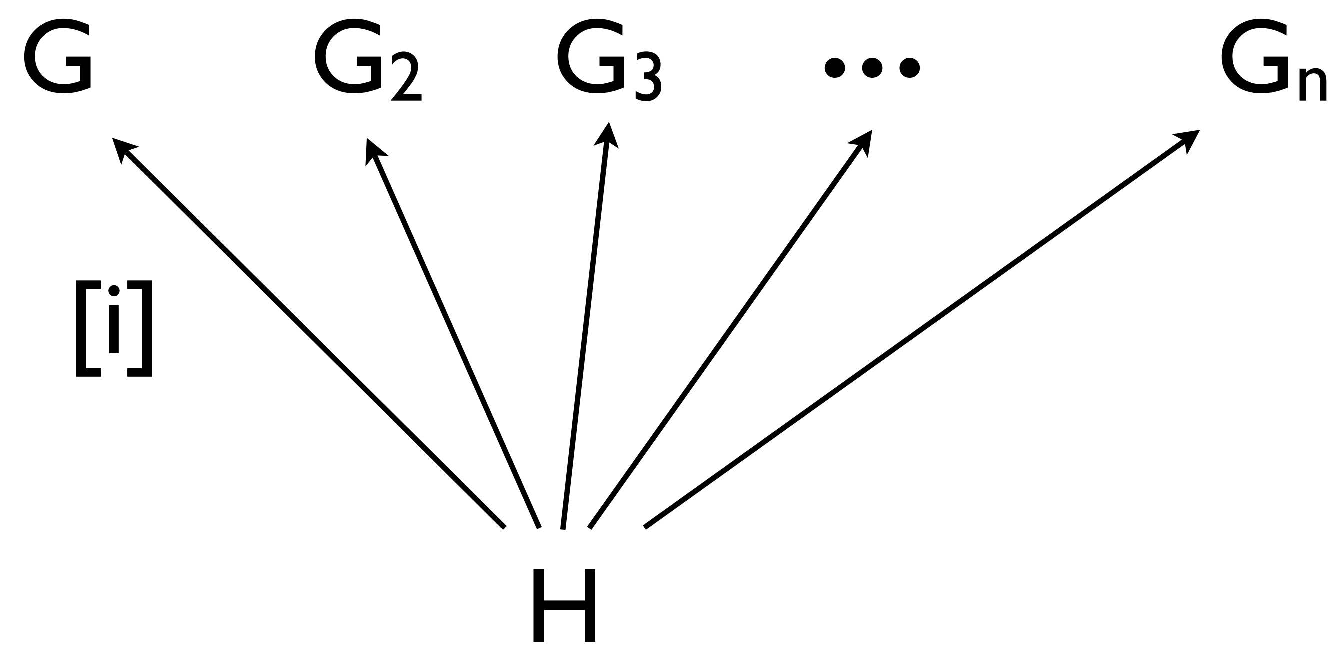
NO subgroup Z exists such that:
$H < Z < G$

The Supergroup Problem

Given a group-subgroup pair G>H of index [i]

Determine: all G_k>H of index [i], $G_i \simeq G$



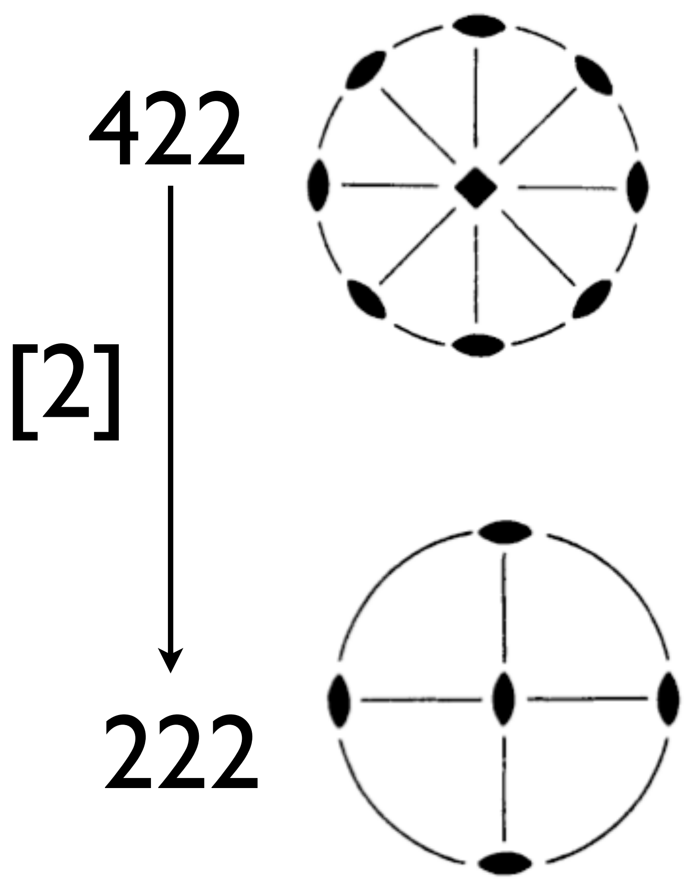


all G_k>H contain H as subgroup

$G_k = H + g_2H + \ldots + g_{ik}H$

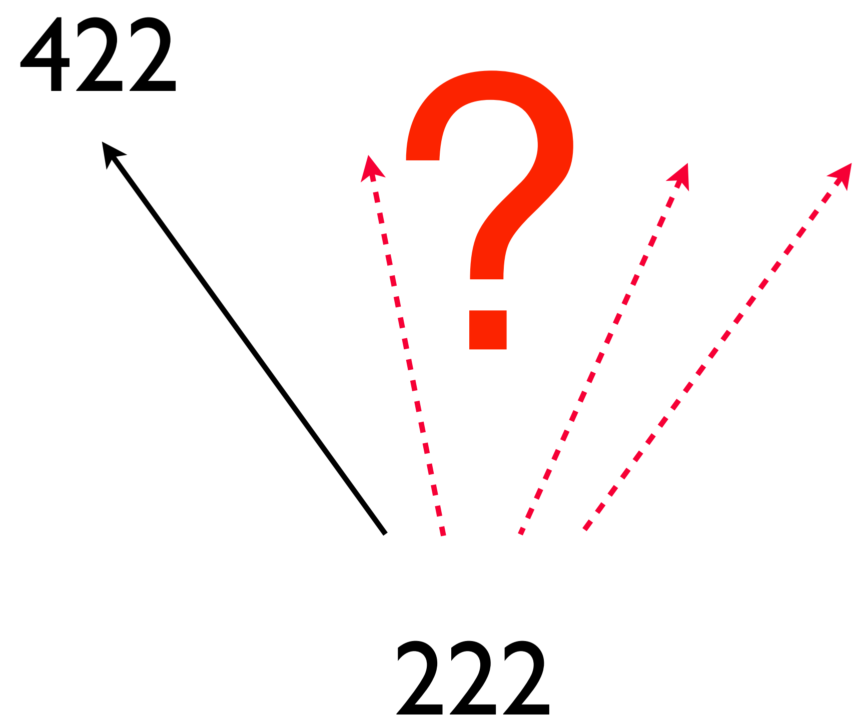
Example: Supergroup problem

Group-subgroup pair 422>222



How many are the subgroups 222 of 422?

Supergroups 422 of the group 222

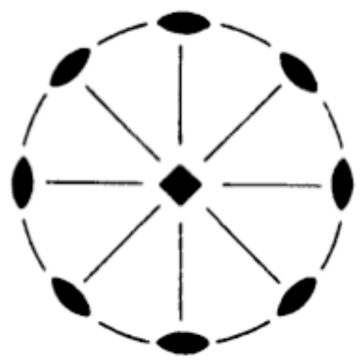


How many are the supergroups 422 of 222?

Example: Supergroup problem

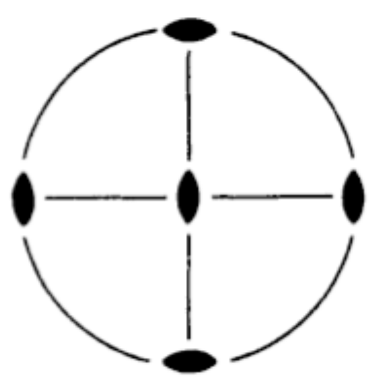
Group-subgroup pair 422>222

422



[2]

$2_z2_x2_y$ $\quad$ $2_z2_+2_-$



$$4_z22 = 2_z2_x2_y + 4_z(2_z2_x2_y)$$

$$4_z22 = 2_z2_+2_- + 4_z(2_z2_+2_-)$$

Supergroups 422 of the group 222

4_z22 $\quad$ 4_x22 $\quad$ 4_y22

[2]

222

$$4_z22=222+4_z222$$

$$4_y22=222+4_y222$$

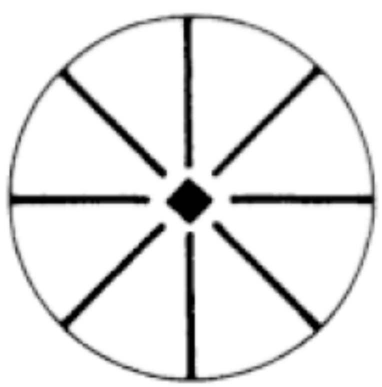
$$4_x22=222+4_x222$$

NORMALIZERS

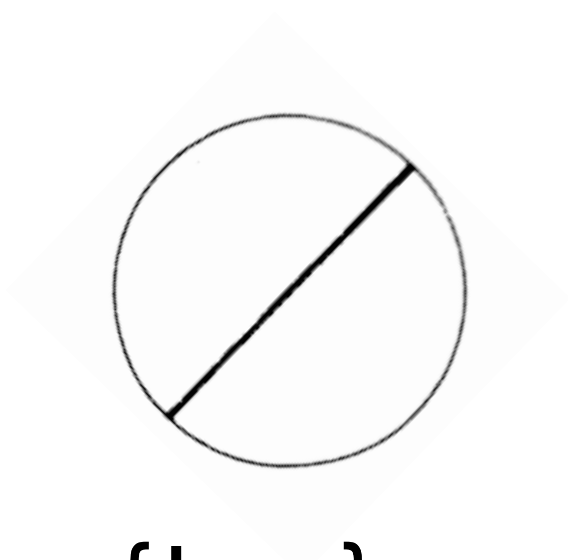
Normalizer of H < G

$\{e,2,4,4^{-1},m_x,m_y,m_+,m_-\}$

4*mm*

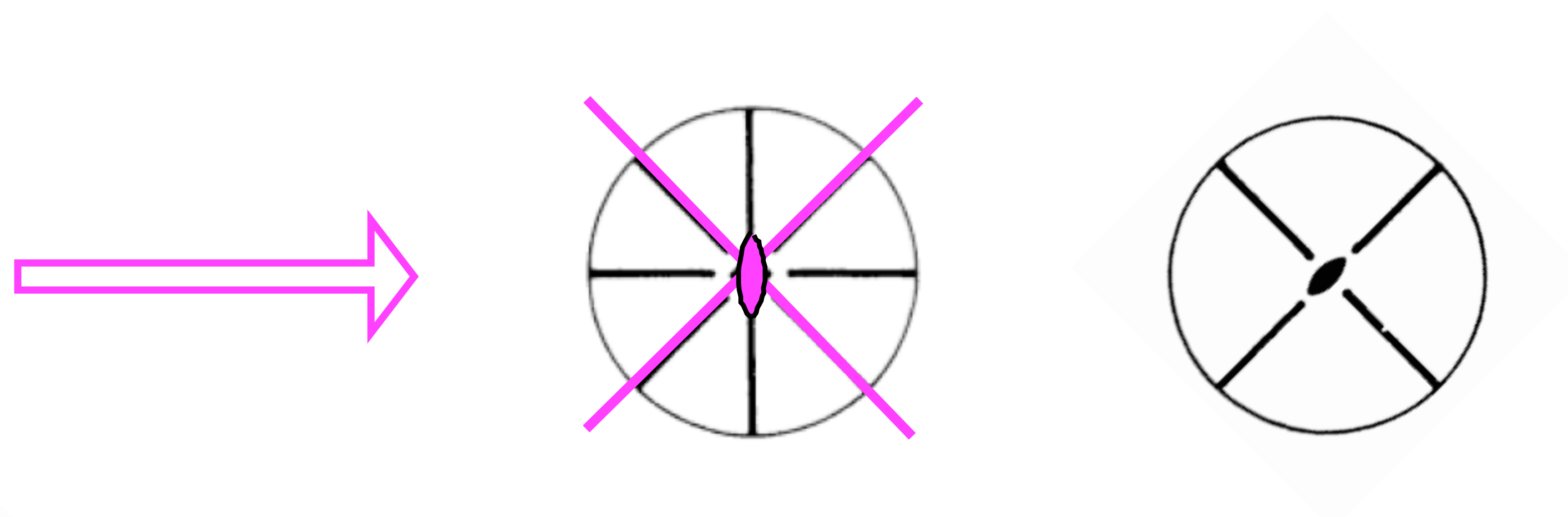


m



$\{1,m_+\}$

Normalizer of $\{1,m_+\}$ in 4*mm*



2*mm*$=\{e,2,m_+,m_-\}$

Normalizer of H in G

Normal subgroup

$H \lhd G$, if $g^{-1} H g = H$, for $\forall g \in G$

Normalizer of H in G, H<G

$N_G(H) = \{g \in G, \text{ if } g^{-1} H g = H\}$

$G \geq N_G(H) \geq H$

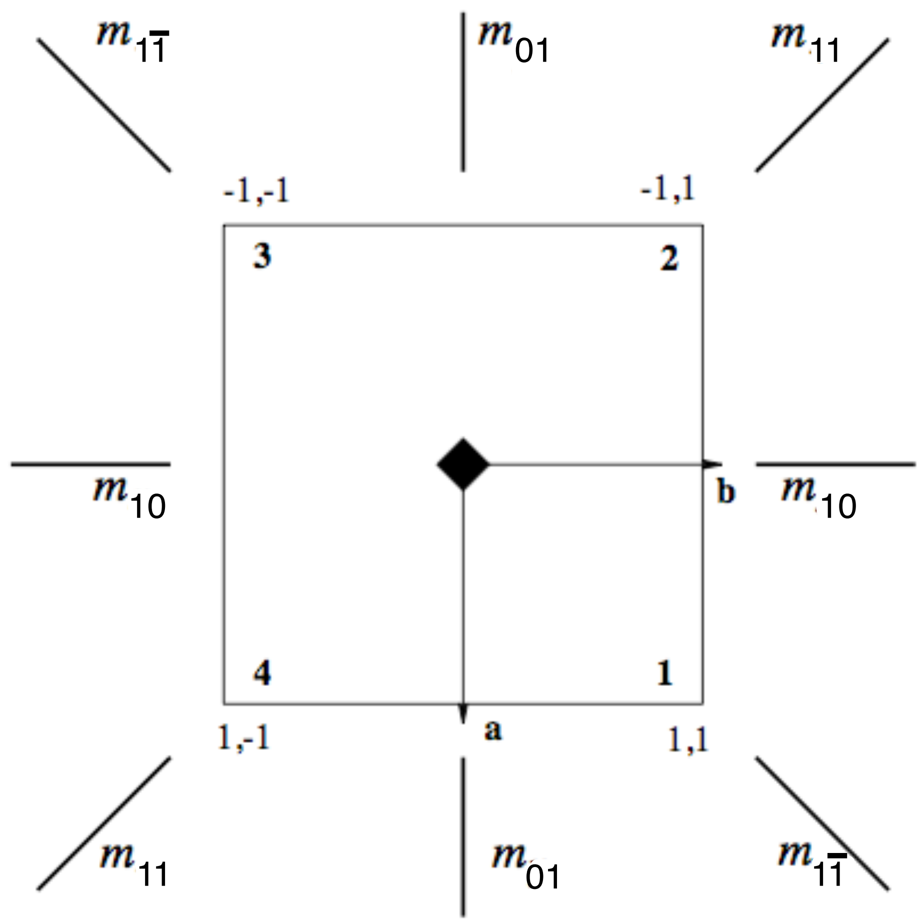
What is the normalizer $N_G(H)$ if $H \lhd G$?

Number of subgroups $H_i < G$ in a conjugate class

$n = [G : N_G(H)]$

Problem 2.10

Consider the group 4*mm* and its subgroups of index 4. Determine their **normalizers** in 4*mm*. Comment on the relation between the distribution of subgroups into conjugacy classes and their normalizers.



4*mm*	1	2	4^+	4^-	m_{01}	m_{10}	$m_{1\bar{1}}$	m_{11}
1	1	2	4^+	4^-	m_{01}	m_{10}	$m_{1\bar{1}}$	m_{11}
2	2	1	4^-	4^+	m_{10}	m_{01}	m_{11}	$m_{1\bar{1}}$
4^+	4^+	4^-	2	1	$m_{1\bar{1}}$	m_{11}	m_{10}	m_{01}
4^-	4^-	4^+	1	2	m_{11}	$m_{1\bar{1}}$	m_{01}	m_{10}
m_{01}	m_{01}	m_{10}	m_{11}	$m_{1\bar{1}}$	1	2	4^-	4^+
m_{10}	m_{10}	m_{01}	$m_{1\bar{1}}$	m_{11}	2	1	4^+	4^-
$m_{1\bar{1}}$	$m_{1\bar{1}}$	m_{11}	m_{01}	m_{10}	4^+	4^-	1	2
m_{11}	m_{11}	$m_{1\bar{1}}$	m_{10}	m_{01}	4^-	4^+	2	1

Hint: The stereographic projections could be rather helpful